2007-11-30

Clustering Methods for Delineating Regions of Spatial Stationarity

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CLUSTERING METHODS FOR DELINEATING REGIONS OF
SPATIAL STATIONARITY

by

Jared M. Collings

A thesis submitted to the faculty of
Brigham Young University
in partial fulfillment of the requirements for the degree of

Master of Science

Department of Statistics
Brigham Young University

December 2007
BRIGHAM YOUNG UNIVERSITY

GRADUATE COMMITTEE APPROVAL

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ABSTRACT

CLUSTERING METHODS FOR DELINEATING REGIONS OF SPATIAL STATIONARITY

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Master of Science

The purpose of this paper is to examine and develop methods that can be used to delineate regions of stationarity. One of the major assumptions used in spatial estimation is that the data field is homogeneous with respect to the mean and the covariance function. As such, any spatial estimation presupposes that these criteria are met. With respect to analyses that may be considered new or experimental, however, there is no evidence that these assumptions will hold.

This paper seeks to further investigate data extracted by the use of Functional Magnetic Resonance Imaging (FMRI) as it is applied to brain tissue and how it measures blood flow to certain areas of the brain following the application of a stimulus. As a precursor to detailed spatial analysis of this kind of data, this paper develops methods of grouping data based on the necessary conditions for spatial statistical analysis.
ACKNOWLEDGEMENTS

The completion of this paper would not have been possible without the support and encouragement of many. It has been a long road to completion. I would like to thank my wife for pushing me as needed (and appropriate) and encouraging me that finishing was actually possible.

Additionally, I am very appreciative of the support from my parents who are able to remind me that I was not done, support me in finishing, and even provide technical assistance as necessary.

Lastly, I would like to extend appreciation to Dr. Christensen for introducing me to this area of study, for providing a great foundation of knowledge, and for allowing me to jump back into things after an extended break. Thanks to all for helping me finish.
CONTENTS

CHAPTER

1 Introduction ........................................................................................................................................... 1

2 Literature Review ............................................................................................................................... 3

  2.1 Brain Imaging Data (FMRI) ........................................................................................................ 3

  2.2 Spatial Statistics ......................................................................................................................... 5

    2.2.1 Estimation of the variogram ............................................................................................. 9

  2.3 Hierarchical Cluster Analysis .................................................................................................... 10

    2.3.1 Clustering Methods ......................................................................................................... 10

    2.3.2 Clustering Outcomes ................................................................................................. 12

  2.4 Methods of Clustering Spatial Data: History ........................................................................ 12

    2.4.1 Clustering ..................................................................................................................... 12

    2.4.2 Methods to Evaluate Clustering Techniques .................................................................. 16

3 Methods of Clustering Observations in a Non-Stationary Field ..................................................... 20

  3.1 Methods: Data Structure ........................................................................................................... 20

  3.2 Proposed Methods ...................................................................................................................... 23

    3.2.1 Basic Window Method .................................................................................................... 28

    3.2.2 Adjacent Constrained Method ...................................................................................... 31

    3.2.3 Two-Part Method ........................................................................................................... 36

4 Results ................................................................................................................................................... 41
B.5 Two Part Method........................................................................................................ 122
B.6 Simulated Data Examples ........................................................................................ 126
B.7 SFMRI Brain Data Analysis ..................................................................................... 137
5.1 SFMRI Brain Data (Image Plot) .................................................................................. 51
5.2 Graphical Clustering Results (Adjacent Constraint - a = 0.75) ............................ 54
5.3 Clustering Results for SFMRI Brain Data ................................................................. 55
1. INTRODUCTION

In considering the human brain, one area of interest is the relationship between location and function. It is well known that the brain controls all functions of the body and that parts of the brain are specialized to certain tasks. One area of interest, however, is to determine whether or not parts of the brain associated with these certain tasks may be identified by analyzing blood flow to a given region after some sort of stimulus is applied.

In Silent Functional Magnetic Resonance Imaging (SFMRI), a series of audio impulses are given to a patient and blood flow in the brain is measured. The blood flow is measured in the “on” state, where the brain is subject to the stimulus, and in the “off” state, where the brain returns to a normal or resting state. Each area of measurement is a three-dimensional cube wherein the blood flow is measured, and these areas of measurement are referred to as voxels. A voxel is called “active” when there exists a significant difference between the “on” and “off” states.

Given the nature of blood flow, it is unreasonable to assume that the voxels are independent of each other. Thus, before estimating the level of activation for each voxel, the spatial dependence structure of the voxel measurements is estimated. Once such estimates of the spatial dependence are obtained, voxel activation maps exhibiting spatial smoothness can be created. However, in order to carry out spatial estimation of the voxel activation levels for the measured regions, it is necessary to subdivide the brain into regions that exhibit local stationarity. Stationarity is the condition where all the
observations in the region are distributed with the same mean and variance covariance structures.
2. LITERATURE REVIEW

The first section of this chapter is devoted to explaining the nature of the FMRI data. In order to clarify the spatial nature of such data, a brief overview of spatial statistics will be given in Section 2.2. Section 2.3 outlines the process of hierarchical clustering, which will be employed to delineate regions of stationarity. A discussion of prior research and methodologies can be found in Section 2.4.

2.1 Brain Imaging Data (FMRI)

The idea that neuronal activity is connected to changes in brain metabolism and blood flow was suggested by Roy and Sherrington (1890) when they conducted highly invasive experiments with dogs, cats, and rabbits.

One method of measuring changes in brain blood flow is the high speed functional magnetic resonance imaging (FMRI), which makes use of the paramagnetic and diamagnetic properties of deoxyhemoglobin and oxyhemoglobin and the local, tissue-specific changes in blood volume, blood flow, and blood oxygenation in response to some controlled stimuli (Belliveau et al. 1991; Kwong et al. 1992; Ogawa et al., 1992). As applied to analyses of brain activity, FMRI serves to map neurological function to neuroanatomy, making it possible to connect function to location. One benefit of FMRI is that it becomes possible to obtain, in a few seconds, hundreds of noninvasive “moving pictures” of the brain as it processes stimuli.
Lange and Zeger (1997) gave a highly simplified explanation of the process of FMRI. In blood, there exists iron (hemoglobin) and iron is paramagnetic—the property of being weakly attracted to an external field. Deoxygenated blood, or “blue blood,” is more paramagnetic than oxygenated blood, or “red blood.” So, when brain activity increases, the flow and volume of red blood will also increase at the capillary level, causing an increase in the relative oxygen content. This increase in red blood volume results in a difference in the magnetic susceptibility of red blood with respect to blue blood. This difference can be used to produce a detectable local signal. Signals such as this can then be used to create contrast in a digital image.

Such digital images as produced by FMRI can be broken up into pixels (picture elements) in the two-dimensional case and into voxels (volume elements) in the three-dimensional case. Each two-dimensional image, or slice, consists of a 64 x 64 grid measuring the response to the stimulus. The physical size of the voxels are typically 3.125 mm x 3.125 mm x 5 mm. Lange and Zeger (1997) studied the visual cortex, where each voxel contained roughly 2 million neurons.

For this study, audio impulses are used as the stimuli. Instead of traditional FMRI measurements, silent functional magnetic resonance imaging (SFMRI) is used. SFMRI differs from FMRI in that only one measurement is taken during each recurrence of the stimulus state and the rest state. Measurements are taken alternately in an “on” state where an impulse is set upon the subject, denoted by (x), and an “off” state when the subject returns to a resting or non-stimulated state, denoted by (y). This process is repeated many times and the “activation” state of a voxel is assessed using some function of \( x \) and \( y \), like \( x - y \).
The voxels of the brain that specialize in interpreting audio impulses are expected to have higher blood flow. These active voxels are expected to cluster together in contiguous groups with similar function, such as in the audio cortex. These hypothesized groups within the brain may possess mean, variance, or spatial structures that are vastly different from the structure of other sections. Traditionally, voxel activation is assessed via t-tests. For a discussion of traditional approaches, see Genovese (2000). One problem with this method lies in the fact that the data are noisy and, therefore, the activation maps created from individual t-tests are unrealistically noisy or rough. Additionally, there may be an insufficient number of observations to adequately test for significant activation.

In order to apply spatial prediction methods to create voxel activation maps, the usual approach is to assume stationarity for the region of interest to be mapped; however, in this case (brain activation), the stationarity assumption is violated. The voxels in different regions should not necessarily have the same means, nor should they necessarily have the same variances or spatial dependence structures. Moreover, the highly irregular manner in which brain tissue folds back on itself yields the potential for neighboring voxels to have dramatically different behavior. Hence, the voxel observations can be dramatically non-stationary.

2.2 Spatial Statistics

In this section, a short description of the general spatial model is given. In general, the variable of interest $Z$ is given as a function of its location $s$, where $s \in \mathbb{R}^d$ is
a point in d-dimensional Euclidean space. Because $s$ is allowed to vary over the fixed 
index set $D \subset \mathbb{R}^d$ the following random field is generated:

$$\{Z(s) : s \in D\}.$$ 

In this paper, $Z(s)$ is modeled in terms of mean structure, or large-scale variation, 
and in terms of the variogram, which models the dependent nature of the data. Let $Z(s) = 
\mu(s) + \delta(s)$, $s \in D$, where $\mu(s)$ denotes the deterministic mean structure, or large-scale 
variation; that is, $\mu(s)$ is equal to $E(Z(s))$ and $\delta(s)$ denotes a zero-mean intrinsically 
stationary stochastic process with variogram $2\gamma(h)$.

The assumption of stationarity is upheld when the characteristics of the data 
elements do not vary across the region $D$. In other words, the probability of a given 
fluctuation from the mean level (measured by $\delta(s)$) is assumed to be the same for each 
point $Z(s)$ within the region. The variogram, $2\gamma(h)$, from above is defined as $2\gamma(s_1 - s_2) 
\equiv \text{var}(Z(s_1) - Z(s_2))$. (Note: $\gamma(s)$ has been referred to as the semivariogram. See Figure 
2.1 for a graphical presentation of the semivariogram.)

The isotropic variogram and the semivariogram are solely functions of distance. 
That is, when $2\gamma(s_1 - s_2)$ is a function solely of $\|s_1 - s_2\|$, $2\gamma(\cdot)$ is said to be isotropic. In this 
case, $\gamma(h)$ can be redefined using $\gamma(\|h\|)$ where $\|\cdot\|$ is the $L_2$ norm. Clearly $\gamma(h) = \gamma(-h)$, 
where $h$ is the distance between points and $\gamma(0) = 0$. However, where $\gamma(h) \rightarrow c_0 > 0$ 
as $h \rightarrow 0$, $c_0$ is referred to as the nugget effect by Matheron (1962). This so-called nugget 
effect represents microscale variation that causes this discontinuity at the origin, and is 
comprised of two parts. The nugget effect, $c_0$, is due in part to measurement error, $c_{ME}$, 
and a white noise process that is assumed to occur on the very small scale, $c_{MS}$. Thus, 

$$c_0 = c_{MS} + c_{ME}.$$
The sill is equal to twice the variance of $\mathbf{Z}(\mathbf{s})$. Notationally, $2\sigma^2 = \lim_{|\mathbf{h}| \to \infty} 2\gamma(\mathbf{h})$.

Additionally, the sill, $2\sigma^2$, is equal to $2\gamma(\|\mathbf{s}_1 - \mathbf{s}_2\|)$ when $\mathbf{s}_1$ and $\mathbf{s}_2$ are far enough apart to be considered independent.
Figure 2.1 Semivariogram. The above diagram shows the behavior of the semivariogram. The value of the semivariogram approaches $c_0$ (the nugget effect) as the distance approaches zero. As the distance increases, the value of the semivariogram approaches its upper limit (the sill).
As is implied by the above definition for \( \delta(s) \), the variogram, \( 2\gamma(h) \), can be estimated only when the process is stationary. The proposed approach for modeling non-stationary processes is to first discriminate, or delineate, areas of stationarity, after which it should be possible to proceed with spatial analysis within each neighborhood of stationarity.

2.2.1 Estimation of the variogram

Based on method-of-moments, Matheron (1962) suggested the following method as a way of estimating the variogram. This method is often referred to as the classical estimator of the variogram. Let

\[
2\hat{\gamma}(h) \equiv \frac{1}{N(h)} \sum_{N(h)} (Z(s_i) - Z(s_j))^2, \quad h \in \mathbb{R}^d
\]  

where

\[
N(h) = \{(s_i, s_j) : s_i - s_j = h; i, j = 1, \ldots, n\}
\]  

(2.2.1)

and \( |N(h)| \) is the number of distinct pairs in \( N(h)\).

Similarly, robust estimators of the variogram were introduced by Cressie and Hawkins (1980). They set

\[
2\tilde{\gamma}(h) = \left\{ \frac{1}{|N(h)|} \sum_{N(h)} |Z(s_i) - Z(s_j)|^{1/2} \right\}^4
\]

\[
\left( 0.457 + \frac{0.494}{|N(h)|} \right)
\]

(2.2.3)

and

\[
2\tilde{\gamma}(h) = \left[ \text{med} \left\{ |Z(s_i) - Z(s_j)|^{1/2} : (s_i, s_j) \in N(h) \right\} \right]^4
\]

\[
\left( 0.457 + \frac{0.494}{|N(h)|} \right)
\]

(2.2.4)
Cressie and Hawkins also show through simulation that $2\tilde{\gamma}(\cdot)$ is generally preferred over $2\tilde{\gamma'}(\cdot)$.

2.3 Hierarchical Cluster Analysis

2.3.1 Clustering Methods

Cluster analysis is used to group observations, usually multivariate, into clusters—groups containing observations that are “close” in terms of Euclidean distance. The basic idea is to find an optimal grouping where the observations are similar within each cluster, and the clusters themselves are different from each other. One common approach to clustering is hierarchical clustering. This approach begins with $n$ clusters, one for each observation, and ends with all $n$ observations in the same cluster. In other words, the observations begin in separate clusters, then the two “closest” observations are combined into one new cluster. This process of combining the two closest clusters into a new single cluster continues until all the observations have been combined into a single cluster.

Euclidean distance is a common measure of similarity, or dissimilarity, among observations. For two vectors $x = (x_1, x_2, \ldots, x_p)'$ and $y = (y_1, y_2, \ldots, y_p)'$ the Euclidean distance between $x$ and $y$ is defined by

$$d(x, y) = \sqrt{(x - y)'(x - y)} = \sqrt{\sum_{j=1}^{p} (x_j - y_j)^2}.$$  

Another method of measuring distance is using the statistical difference defined by

$$D(x, y) = \sqrt{(x - y)' \Sigma^{-1} (x - y)}.$$
This measure adjusts for differing variances and covariances among the differing groups. However, since there are assumed to be different groups within the data set, there is no obvious way to choose $\Sigma$.

Attention should also be given to the scale of measurements used in computing the Euclidean distance. Depending on the scale of measurements, the relative distances can change. To counter this, many authors recommend the usual standardizing of the variables—subtracting the mean and dividing by the standard deviation.

While the Euclidean distance between two points is clearly defined above, the distance between two clusters can be defined in several ways. The following are some of the most common methods for determining the distance between clusters (Fisher and Van Ness 1971; Van Ness 1973).

In the single linkage (or nearest neighbor) method, the distance between two clusters $A$ and $B$ is defined as the minimum distance from a point in $A$ to a point in $B$. Thus,

$$D(A,B) = \min \{d(y_i, y_j), \text{ for } y_i \text{ in } A \text{ and } y_j \text{ in } B\}.$$  

In the complete linkage (or farthest neighbor) method, the distance between two clusters $A$ and $B$ is defined as the maximum distance from a point in $A$ to a point in $B$. Thus,

$$D(A,B) = \max \{d(y_i, y_j), \text{ for } y_i \text{ in } A \text{ and } y_j \text{ in } B\}.$$  

In the average linkage method, the distance between two clusters $A$ and $B$ is defined as the average of the $n_A \times n_B$ distances from each of the $n_A$ points in $A$ to each of the $n_B$ points in $B$. That is,

$$D(A, B) = \frac{1}{n_A n_B} \sum_{i=1}^{n_A} \sum_{j=1}^{n_B} d(y_i, y_j).$$
2.3.2 Clustering Outcomes

The agglomerative hierarchical method of clustering begins with each point in the set as its own cluster. Then, the two closest clusters are grouped together, where closeness is determined by the linkage method being used. This process is repeated until all the observations are grouped into a single cluster. The results are often displayed graphically in a tree diagram, which shows the development of the clusters. The method of determining the number of clusters ultimately used in analysis depends largely upon the judgment of the analyst and may vary according to the specific situation.

Generally, the use of single linkage differs from complete and average linkage in that it will create long string-like clusters. This phenomenon, known as chaining, generally yields undesirable clustering results. The results from complete and average linkage generally agree with each other. For additional information on displaying the results of hierarchical clustering, see Gordon (1987).

2.4 Methods of Clustering Spatial Data: History

2.4.1 Clustering

In the case of spatially dependent data, the results of normal clustering techniques do not always make sense given the nature of the data. With spatial data, one of the assumptions is that each observation is dependent on other nearby observations. In the case where similar observations exist but are separated by large distances it is often unreasonable to group them together.

This idea is supported by Legendre (1987), who found that imposing constraints on spatial data results in answers that are meaningful in context. He describes various forms of constrained clustering and then examines whether constrained clustering is
needed to get meaningful results and how to determine if the groups found by constrained clustering are real. Legendre answers the first question through a simulated data set, where he found that constrained clustering recovered more information than unconstrained clustering.

Legendre’s studies led to the conclusion that constrained clustering should always be used when the data are assumed to be spatially (or temporally) correlated. Legendre also states, in answer to the second question, that it is possible to discern whether the groups found by constrained clustering are real. Legendre found that the spatially correlated data sets generally have larger differences between groups. Additionally, Legendre found that with constrained clustering techniques, the different linkage methods result in more similar groupings as compared to unconstrained clustering.

Wartenberg (in an unpublished manuscript cited by Legendre 1987) gives an example of what happens in situations of unconstrained clustering and constrained clustering through a study from the health sciences. Lung ailments may come from many different causes: occupational (such as coal mining), ambient (such as living near industrial areas), or personal habits (such as tobacco consumption), all of which can lead to differing severity of lung conditions. The unconstrained clustering tended to group the samples by severity of cases while the spatially constrained clustering was more likely to group observations with similar types of causes.

Another method of constrained clustering was also used by Huel, Petiot, and Lazar (1986) as they developed an algorithm for analyzing contiguous zones in a geographical epidemiology study. They developed an algorithm that groups the
continuous geographical units that are similar with respect to the variables of interest. First, a distance measure between the zones is defined. This measure is defined in such a way as to prevent two or more of the distances measured from resulting in equal magnitudes; in other words, all distances calculated are unique and can be ranked from smallest to largest. Next, a distance threshold is chosen beyond which two zones cannot be grouped (i.e. if the distance between zones is less than the threshold, the zones are considered to be adjacent). Then, the two zones that have the smallest distance, subject to the constraint that the zones are adjacent, are grouped together. This process is continued until all the groups have been combined. Huel, Petiot, and Lazar then use this algorithm to group geographical zones in Normandy, France, where measurements of suicide rates were taken. In this study, the probability level from Cochran’s test was defined as the distance for the algorithm. (Note that Cochran’s test is useful for measuring samples on a categorical scale and measures whether or not different samples have the same number of successes and failures.)

One problem that arises in analysis of spatial data is that of non-stationarity. If, for example, the data are assumed to be spatial in nature and are assumed to have separate intrinsic groups, then estimating the variogram for the entire data set will violate the stationarity assumption. This problem is addressed by Haas (1990), in which the ecological effects of sulfuric and nitric acid (found in rainfall) on the environment in the United States were studied. This process of statistical estimation was complicated because of a strong spatial trend (mean non-stationarity) and an apparent spatial covariance structure dependent on location (covariance non-stationarity). Haas evaluated four statistical methods of estimating confidence intervals for the precipitation chemistry
at the locations of measurement. Of interest is a method of estimation where the sample variogram is estimated using only data within a circular neighborhood immediately surrounding the estimate location—this method is called a window. This window moves along with the estimate location, where a new variogram estimate is calculated. This allows for the variance covariance structure to be a function of location and allows the model to account for more of the spatial trends.

However, the implementation of this moving window brings about the conflicting goals of having the window as small as possible while still allowing for a covariance model to be fitted using only the window’s data. The smaller the window, the better the approximation of stationarity, while the larger the window, the more accurate the semi-variogram estimates. Haas (1990) suggests that the semi-variogram estimates at shorter lags have lower variance than estimates at longer lags given the same number of distance pairs; thus, fewer pairs are needed at shorter lag distances.

Another problem in the analysis of spatially correlated data is that of scale. Spatial resolution is associated with the smallest area for which data can be obtained. High resolution comes from small geographical units, which allow for an increase in the ability to differentiate nearby objects. However, small geographical areas, which usually have small populations, tend to have large variability.

Carvalho, Cruz and Nobre (1996) developed an algorithm to combine small, homogeneous areas in order to achieve minimum sample size requirements. As applied to census data, the algorithm begins with a specified census tract for which a search is performed among all adjacent tracts with the same risk profiles. In each census tract, a centroid is defined as an average of all the data collected in the tract. Using Euclidean
distances between these centroids, a measurement is available to compare how close
different tracts are to each other. The neighboring tract that is closest to the specified
tract is subsequently combined with the specified tract to create a new tract. Then, if the
desired sample size is achieved, the algorithm will move on to the next specified tract;
otherwise, it will compare the new tract with its neighboring tracts, repeating the process
until all census tracts have been specified by the algorithm. If, however, a census tract
exists without neighboring tracts exhibiting similar risk profiles, it is defined as isolated.

The results of this agglomerative algorithm include (1) complete—the desired
sample size is reached, (2) incomplete—the desired sample size is not reached, but there
are no additional neighboring tracts of the same class, and (3) isolated—no neighboring
tracts existed to be combined.

For additional studies in clustering see Anderson and Titterington (1997), Cuzick

2.4.2 Methods of Evaluating Clustering Techniques

Two methods of assessing the efficiency of clustering models were recommended
by Milligan (1983)—the Jaccard index and the Rand index. For a situation with n
observations where the true groups are known, two half matrices (triangular n × n) are
computed—one is computed according to the true groups and another is computed
according to the classification method, or estimated groups. The $ij$ position of these
matrices contains a 1 when the $i$ observation and the $j$ observation are members of the
same group, and a 0 otherwise. Then a summary two-way table is set up using the counts
of 1s and 0s for each observation. The Jaccard index and the Rand index are calculated
using such two-way tables (as in Figure 2.4.1) and are defined as
Figure 2.2 General Two Way Table. The two way tables summarizes the comparison counts, represented here by a, b, c, and d. The Rand and Jaccard indeces both, then, reference these counts.

\[
\text{Jaccard} = \frac{a}{a + b + c},
\]

\[
\text{Rand} = \frac{a + d}{a + b + c + d}.
\]

For example, in the simple situation where there are two groups, as given in Figure 2.4.2, and there are three estimated groups, as given in Figure 2.4.3, the indices would be computed by first constructing:

Figure 2.3 True Grouping

Figure 2.4 Estimated Grouping
To begin with, the two half matrices are computed for the true and estimated groups—
given in Figure 2.4.4. Each cell in the data field is compared to each other cell. A value
of 1 is assigned to the half matrix position if both cells are in the same group, otherwise
the value assigned to the half matrix position is a 0. For the true groupings, the first cell
(top left) is compared to the second cell (top right) and a value of 1 is assigned to the half
matrix. The same is true for the third and fourth cells (middle left and right). A value of 0
is assigned for cells five and six (bottom left and right) because they are in different
groups. The same process is continued for other columns of the half matrices.
Figure 2.5 Index Calculation Example. The half matrices are shown above. The matrix for the true groups is on the left and the matrix for the estimated groups is on the right. Below the matrices is the two-way table along with the calculations for both the Jaccard and Rand indices.

\[
\text{Jaccard Index} = \frac{1}{1 + 6 + 2} = \frac{1}{9}
\]

\[
\text{Rand Index} = \frac{1 + 6}{1 + 6 + 2 + 6} = \frac{7}{15}
\]
3. METHODS OF CLUSTERING OBSERVATIONS IN A NON-STATIONARY RANDOM FIELD

3.1 Data Structure

The previous approaches attempt to create contiguous clusters that have similar mean structures. In addition to having the same mean structure, however, the clusters should group observations that have similar variances and similar spatial structures. In other words, the non-stationary random field is to be broken down into contiguous regions (clusters) that exhibit spatial stationarity.

In order to attain localized estimates of the spatial variogram, the moving window approach introduced by Haas (1990) was used. In the moving window approach, a window, or neighborhood, around each point is used to estimate the variance structure at that point. In terms of this approach, the smaller the region, the better the approximation of stationarity. On the other hand, with larger windows, more data points are available for use in estimation.

In attempting to separate the observations into stationary regions, hierarchical clustering can be performed. If the data to be analyzed exhibits spatial characteristics, a location index should be included to encourage the creation of clusters that contain spatially contiguous observations.

For each data point, a data vector was obtained with the form

\[ \mathbf{v}(\mathbf{s}) = (v_1(\mathbf{s}), v_2(\mathbf{s}), v_3(\mathbf{s}), v_4(\mathbf{s}), v_5(\mathbf{s}), v_6(\mathbf{s}), v_7(\mathbf{s})) \],

where \( \mathbf{v}(\mathbf{s}) \) represents the (possibly vector-valued) responses to be used in the clustering. In the case of SFMRI, \( v_1(\mathbf{s}) \) represents the observed level of activation for a specific
location \( s \), defined using the difference between stimulated measurements and the average blood flow for the non-stimulated measurements, \( \tilde{x}(s) - \tilde{y}(s) \); \( v_2(s) \) represents the row (or x-coordinate) index; \( v_3(s) \) represents the column (or y-coordinate) index; \( v_4(s) \) is \( 2 \bar{\gamma}_s(1) \), referred to as the lag 1 estimate of the variogram; \( v_5(s) \) is \( 2 \bar{\gamma}_s(2) \), the lag 2 estimate; \( v_6(s) \) is \( 2 \bar{\gamma}_s(3) \), the lag 3 estimate; \( v_7(s) \) is the estimated 90th percentile of the measurements \( 2 \bar{\gamma}_s(1) \), \( 2 \bar{\gamma}_s(2) \), \( 2 \bar{\gamma}_s(3) \), \( 2 \bar{\gamma}_s(4) \), \( 2 \bar{\gamma}_s(5) \), \( 2 \bar{\gamma}_s(6) \), and \( 2 \bar{\gamma}_s(7) \). The quantity \( v_7(s) \) represents an approximation of the sill, which is equivalent to \( 2\sigma^2(s) \), the variance at location \( s \).

To estimate the variogram, we recommend the use of the robust variogram estimator \( 2\bar{\gamma}(\cdot) \) as discussed by Cressie and Hawkins (see Section 2.2.1). For data points close to the natural boundary of a group, the estimates of the variogram are generally clustered into two different and distinct “clouds” (see Figure 3.1). The more robust (median-based) estimators generally provide variogram estimates that lie closer to the actual variogram cloud as compared to the non-robust (mean-based) estimators. This is particularly true for data points along a natural border between groups. The existence of multiple groups causes the distinct variogram clouds shown in Figure 3.1.
Figure 3.1 Robust vs. Non-Robust Estimators of the Variogram. The Δ’s represent data points from one group and the ○’s represent data points from a second group.
3.2 Proposed Methods

In this paper we will develop three methods of clustering data (as described later in this chapter). To compare and evaluate these methods, simulated data sets on a $20 \times 20$ grid are used. The grid is separated into three different regions—one in the upper left, one in the center and one in the lower right. Figure 3.2 provides two plots for each simulated data set. In the top plot of each pair, darker shades of purple represent low simulated values; the white squares represent intermediate simulated values; and darker shades of blue represent high simulated values. The bottom plot of each pair provides a three-dimensional view of the data set. In the first data set, the three different regions have different mean structures. This allows each region to be identified with relative ease. In the second data set, the three different regions have the same mean structure, but different variance structures; thus, the smoothness of the plotted points is very different across the regions and these regions are more difficult to identify.

The complete linkage clustering method, which clusters based solely on the distance between $Z(s)$, is demonstrated on the two sample data sets and results in the clusters shown in Figures 3.3 and 3.4. As might be expected, this technique does a relatively good job at identifying the groups in Simulated Data Set 1 (Figure 3.3). However, as the number of groups increases, the clustered groupings become more and more fragmented. As might be expected, the complete linkage method is ineffective at identifying the groups in Simulated Data Set 2 (Figure 3.4). This technique is not able to identify any of the true groups. The same problems exist as with Data Set 1, in that the groups become increasingly fragmented as the number of groups increases.
In general, complete linkage is able to identify the three main regions for Simulated Data Set 1, but is not able to identify any of the regions in Simulated Data Set 2. In applying the complete linkage method to \( z(s) \) only the different mean structures are identified, whereas no information is identified with regard to the variance structures. Additionally, this method can produce non-contiguous groupings that cannot be used for spatial analysis; as the number of clusters increases so does the fragmented quality of the clusters. The three methods proposed in this chapter seek to address the limitations of complete linkage methods as applied to spatial analysis.
**Figure 3.2** Simulated Data Sets. Each data set has three distinct regions: one in the top left, one in the center, and one in the bottom right. In the first data set the three regions have different mean structures. In the second data set the three regions have the same mean structure, but different variance structures. The shades of purple represent low simulated values; the white values represent intermediate simulated values; and the blue values represent high simulated values.
Figure 3.3 Complete Clustering Results for Simulated Data Set 1. The upper left plot shows the original three groups in the data set. The remaining plots represent the clustering produced by the Complete Linkage Method for 2 through 9 groups. The Jaccard and Rand indices are provided for each plot.
Figure 3.4 Complete clustering results for Simulated Data Set 2. The upper left plot shows the original three groups in the data set. The remaining plots represent the clustering produced by the Complete Linkage Method for 2 through 9 groups. The Jaccard and Rand indices are provided for each plot.
3.2.1 Basic Window Method

In order to obtain estimates of $v_4(s)$, $v_5(s)$, $v_6(s)$, and $v_7(s)$ that are valid at the specific location $s$, the moving window described by Haas (1987) is used. For each position in the data field (usually a grid), the variogram is estimated at distances of 1 through 7. For $2\gamma_s(1)$, or lag 1, the window consists of all the data points within a window of ±1 row or column of the specified position. For $2\gamma_s(2)$, or lag 2, all points within a window of ±2 are used. The window size continues to grow in this manner until $2\gamma_s(7)$, or lag 7, is estimated. For positions along the edges or in the corners, portions of the window will be outside of the data grid. In this case, only the positions that are aligned within the window and the grid are used for estimating the appropriate lags.

Finally, the 90 percentile among $2\gamma_s(1)$, $2\gamma_s(2)$, $2\gamma_s(3)$, $2\gamma_s(4)$, $2\gamma_s(5)$, $2\gamma_s(6)$, and $2\gamma_s(7)$ is found at each specified location. After the data vector $v(s)$ is constructed, the measurements in $v(s)$ are centered and scaled.

Weights are applied to the data vector depending upon the composition of the data field. A weighting of $(3, 1, 1)$ is applied to the mean structure and a weighting of $(2, 1, 1, 0, 1)$ is applied to the spatial structure. The weights are chosen to be similar in their total effect on the data vector $v(s)$. The weights are then adjusted by multiplying the mean structure weighting by $a$ and the spatial structure weighting by $1-a$, for increasing values of $a$. These weighted data vectors are then clustered using the hierarchical clustering method described above. Because both the Jaccard and the Rand indices evaluate clustering processes in basically the same way, only the Jaccard index is shown.

Using the Jaccard index as the criterion for analysis of the Basic Window Method, Figures 3.5 and 3.6 provide a summary of how well this method identifies the groups.
within Data Examples 1 and 2, respectively. (Additional images of the hierarchical
clusters produced by application of the Basic Window Method to Simulated Data Sets 1
and 2 can be found in Appendix A.)

Generally, as the number of groups increases, the value of the Jaccard index
decreases. Recall that Simulated Data Set 1 contains differing mean structures and
similar spatial structures (see Figure 3.2). The Basic Window Method performs best with
equal weighting between mean structure and spatial structure (that is, when $a = 0.50$) for
Simulated Data Set 1. Recall that Simulated Data Set 2 has a similar mean structure
throughout the region (see Figure 3.3). The Basic Window Method using only spatial
information ($a = 0.0$) is at least as good as the subsequent iterations that include the mean
structure data (i.e. $a > 0$).

In summary, the Basic Window Method includes additional information in the
clustering process and thus provides an improvement over traditional clustering
techniques. However, in order to perform spatial analysis on a data structure, the data
within each cluster must be contiguous. The Basic Window Method fails to adequately
address this issue.
**Figure 3.5** Basic Window Clustering for Simulated Data Set 1. The vertical axis shows the Jaccard Index as a function of the number of groups with various weights being given to the mean spatial structure and the spatial structure. The relative weight given to the mean structure is represented by $a$, with relative weight $1-a$ given to the spatial structure.

**Figure 3.6** Basic Window Clustering for Simulated Data Set 2. The vertical axis shows the Jaccard Index as a function of the number of groups with various weights being given to the mean spatial structure and the spatial structure. The relative weight given to the mean structure is represented by $a$, with relative weight $1-a$ given to the spatial structure.
3.2.2 Adjacent Constraint Method

As mentioned in the previous section, one of the difficulties with the Basic Window Method lies in the fact that it will often produce groups that fail to be spatially contiguous. The solution to this seems to be easy; one could simply increase the weights applied to the location index of $v(s) - v_2(s)$ and $v_3(s)$. However, in order to achieve spatially contiguous groups, the location indices begin to have a greater effect than the other elements of the data vector. This results in groups that tend to reflect the four quadrants of the grid rather than producing groups of similar data points.

Instead of including the location indices of the data vector, the next proposed method—the Adjacent Constraint Method—utilizes the addition of an adjacency constraint. In order for two observations or groups to be clustered together, they must meet the requirement of being adjacent to each other. The data vectors for each position are constructed according to the method described in section 3.1.

The imposition of this constraint on the clustering method allow for the results to make sense in terms of the problem. Because the desired result of these clustering methods is to separate regions for the application of spatial analysis, the delineated regions must meet the required assumptions implicit in such analysis—one such assumption is that of contiguous regions. Legendre gives examples of constraints in ecological theory where the clusters are constrained to be contiguous; he then shows that constrained clustering methods always recover a larger fraction of the information when compared with the unconstrained methods (Legendre 1987).

After constructing $v(s)$ for all $s$ in the random field, the Adjacent Constraint Method compares the data vectors for all adjacent observations and then groups the two
observations that are closest together. In this case, adjacency is determined by how far apart the two observations are located within the grid. Locations are considered to be adjacent when the Euclidean distance between the two observations is less than 1.5. For data sets that are set up in two-dimensional grids, this is equivalent to the eight nearest neighbors. The process continues combining data in the same manner until all the observations are combined into groups. Note that for an observation to be adjacent to a group of observations, the observation only needs to be adjacent to one of the observations in the group. Similarly, for two groups to be adjacent, at least one observation from the first group must be adjacent to at least one observation from the second group. This algorithm is similar to the one used by Huel, Petiot, and Lazar (1986).

In addition to the imposition of this adjacency constraint, the weights applied to the data vector, $\mathbf{v}(s)$, are also adjusted. Weights are applied to the data vector in two ways. Recall that the data vector may be split into two different sections—a section containing mean structure data points and a section containing spatial structure data points. Weights are first applied to these structures—a weight on the mean structure, represented by $a$, and a weight on the spatial structure, represented by $1-a$. Where $a$ is constrained to be between 0 and 1.

The second way that weights are applied to the data vector is in determining the relative importance of data elements within the mean structure and spatial structure. These weights are not limited, but should be equal in total magnitude. Some care should be taken to determine these weights, as they have a large impact on the results. Recall from Chapter 2 that the data vector is of the form
\[ \mathbf{v}(\mathbf{s}) = (v_1(\mathbf{s}), v_2(\mathbf{s}), v_3(\mathbf{s}), v_4(\mathbf{s}), v_5(\mathbf{s}), v_6(\mathbf{s}), v_7(\mathbf{s})). \]

The mean structure is reflected in the values \((v_1(\mathbf{s}), v_2(\mathbf{s}), v_3(\mathbf{s}))\) and the spatial structure is reflected in the remaining elements, \((v_4(\mathbf{s}), v_5(\mathbf{s}), v_6(\mathbf{s}), v_7(\mathbf{s}))\). The weights applied to the mean structure are 5, 0, and 0, respectively. Note that weights of zero are applied to the \(x\) and \(y\) coordinates, which effectively removes their effect on clustering. These effects are removed because the Adjacent Constraint Method of clustering forces groups to be contiguous, thereby removing the need to include location elements in the data vector.

The weights applied to the variance structure are 2, 1, 1, and 1. This weight structure seeks to reflect the relative importance of each lag estimate on clustering. Essentially, the weights indicate that the most important data element for clustering based on a spatial perspective is the estimate of lag 1, followed by the estimate of the sill (using the 90th percentile of the lags as the estimate), then the estimates for lags 2 and 3.

As in the previous section, the effectiveness of the Adjacent Constraint Method may be evaluated by examining the Jaccard indexes at differing values of \(a\) and differing numbers of separated groups. The Jaccard index will generally decrease as the number of groups increase. With the Adjacent Constraint Method, however, the summary of Jaccard indices show a general increase up to a certain number of groups, and then the customary decrease (see Figures 3.7 and 3.8). This is especially evident for Simulated Data Set 1 in the case where \(a = 0.25\), and can be seen for Simulated Data Set 2 with \(a = 0.0\). As each Simulated Data Set contains only three “true” groups, this seems a little counterintuitive.

The Jaccard indices reach a maximum at around 15 to 17 groups. Upon further examination, there appear to be many small groups of elements that are clustered along the borders of the natural groups. This phenomenon is examined in more detail in the
following section. The hierarchical clustering produced by application of the Adjacent Constraint Method to Simulated Data Sets 1 and 2 can be found in Appendix A.
Figure 3.7 Adjacent Constraint Clustering Results for Simulated Data Set 1. The vertical axis shows the value of the Jaccard Index as a function of groups using the Adjacent Constraint Method. The relative weight given to the mean structure is $a$ and the relative weight given to the spatial structure is $1-a$.

Figure 3.8 Adjacent Constraint Clustering Results for Simulated Data Set 2. The vertical axis shows the value of the Jaccard Index as a function of groups using the Adjacent Constraint Method. The relative weight given to the mean structure is $a$ and the relative weight given to the spatial structure is $1-a$. 

3.2.3 Two-Part Method

While using the two methods described above on the simulated data, the non-stationarity is clearly evident at the border of two different regions. This leads to estimated clusters that will be referred to as border clusters. When points reside along the natural borders between regions, the estimation of the variance and spatial dependence structure is highly affected by non-stationarity, or the vast difference between the natural regions. When near such regional borders, the window used in the previous methods (described in sections 3.2.1 and 3.2.2) spans the two regions and points from both regions are included in the estimation process. This leads to the artificial creation of small, often chain-like groups along the diagonal division between the three true groups. See Figure 3.9 for an illustration of such border clusters. The creation of border clusters is particularly evident when bordering regions have dramatically different mean levels for $Z(s)$, yielding exaggerated values of $v_7(s)$ or $2\sigma^2(s)$. See, for example, the clusters formed where the known regional boundaries are located in Figure 3.7.

In order to account for the potential non-stationarity of the analyzed regions and in an attempt to prevent the creation of border clusters, the clustering process was split into two steps. The first step is to perform a cluster analysis only on $v_1(s)$—that is $Z(s)$. As before, $v_2(s)$ and $v_3(s)$ (the row and column indices) are not included as the clustering is already subject to the data elements being adjacent. Since this initial clustering is an attempt to get better estimates of spatial structure, a stricter criterion of adjacent is used. To prevent the chaining of data elements (where a sequence of data elements only border each other diagonally), the physical distance must equal 1.0—only elements directly above, below, or to either side will be considered for clustering.
Figure 3.9  Border Clusters. This plot illustrates the artificial creation of groups on or near the borders of the natural group divisions.
This initial clustering is considered to be finished when each estimate of $v_4(s)$—lag 1—is close enough in relation to all other estimates of $v_4(s)$ within a specific region. The estimates are considered close enough if they fall within the central 99.9% of the range of a chi-squared distribution with a mean equal to the average estimate of $v_4(s)$ within the region. In essence, this method prevents the estimation of extreme values for $v_4(s)$ that result from differing mean structures between groups (as exhibited by border clusters), not from natural variation within a group. For this initial clustering, the less robust classical estimator of the variogram is used. Choosing a less robust estimator will allow for more extreme values of $v_4(s)$ where different underlying groups fall within a specific region, which this method seeks to identify.

Within these previously determined regions of significantly different mean structures, $Z(s)$, the data elements are clustered by variance and spatial dependence structure using the Adjacent Constraint Method as described in Section 3.2.2. This method will have the greatest impact on data regions where there is significant fluctuation in the mean structure (as with Simulated Data Set 1). For regions where the mean structure is fairly constant, this method is expected to perform approximately the same as the Adjacent Constraint Method—in other words, all estimates of $v_4(s)$ may be assumed to fall within the chi-squared distribution with the required cutoff. These conclusions are supported by Figures 3.10 and 3.11. Figure 3.11 shows the Jaccard Index values for varying numbers of groups using the Two-Part Method on Simulated Data Set 1. The problem created by the border clusters is mitigated somewhat, but there is still evidence of such regions (for example, when $a = 0.25$). Figure 3.12 shows the Jaccard Index values for varying numbers of groups using the Two-Part Method on Simulated
Data Set 2. As expected, the results for Simulated Data Set 2 appear to be generally the same as those obtained with the Adjacent Constraint Method.

The hierarchical cluster results produced by application of the Two-Part Method to Simulated Data Set s 1 and 2 may be found in Aappendix A.
Figure 3.10 Two-Part Clustering Results for Simulated Data Set 1. The vertical axis shows the value of the Jaccard Index as a function of groups using the Two-Part Method. The relative weight given to the mean structure is $a$ and the relative weight given to the spatial structure is $1-a$.

Figure 3.11 Two-Part Clustering Results for Simulated Data Set 2. The vertical axis shows the value of the Jaccard Index as a function of groups using the Two-Part Method. The relative weight given to the mean structure is $a$ and the relative weight given to the spatial structure is $1-a$.  

40
4. RESULTS

4.1 Simulated Examples

Each of the three previously described methods is used to cluster a series of simulated data sets. Four separate data sets were simulated with differing mean and covariance structures (as shown in Figures 4.1 and 4.2). Each data set has three different regions. The left side of the grid is one data region, the center is the second data region, and the right side is the third data region. The regions vary by mean and variance structure. Lower variance and higher range regions appear to be more smooth. The following provides a short description of each simulated data set’s characteristics.

Data Set 1:
Region 1 exhibits high mean, moderate variance, and moderate range
Region 2 exhibits low mean, moderate variance, and moderate range
Region 3 exhibits moderate mean, moderate variance, and moderate range

Data Set 2:
Region 1 exhibits moderate mean, moderate variance, and moderate range
Region 2 exhibits moderate mean, small variance, and moderate range
Region 3 exhibits moderate mean, large variance, and moderate range

Data Set 3:
Region 1 exhibits moderate mean, moderate variance, and small range
Region 2 exhibits moderate mean, moderate variance, and large range
Region 3 exhibits moderate mean, moderate variance, and moderate range

Data Set 4:
Region 1 exhibits high mean, moderate variance, and small range
Region 2 exhibits low mean, small variance, and large range
Region 3 exhibits moderate mean, large variance, and moderate range
Figure 4.1 Sample Data Sets (Perspective Plot). Each data set has three different regions. The left side of the grid is one data region, the center is the second data region, and the right side is the third data region. The regions vary by mean and variance structure. Lower variance and higher range regions appear to be more smooth.
Figure 4.2 Sample Data Sets (Image View). This figure provides an alternate view of each of the data sets. Each data set has three different regions. The upper left portion of the grid is one data region, the center is the second, and the lower right portion is the third. The regions vary by mean and variance structure. Darker shades of purple represent low simulated values, the white values represent intermediate simulated values, and the darker shades of blue represent high simulated values.
The reasons for comparing and contrasting these three methods are as follows: 1) to determine how well the methods correctly identify the true groupings within each data sets—measured according to the Jaccard index value, and 2) to determine how useful the results will be in the view of performing spatial analysis on the resulting clusters.

4.2 Evaluation of Performance

The Jaccard index values resulting from the clustering methods proposed in this paper are shown in tables and charts in Appendix A (chapter 4 tables). Figure 4.3 presents a portion of these results for the case where $a = 0.50$. Different values of $a$ were used for clustering the sample data sets. In most instances, however, $a$ produced the highest values of the Jaccard index when set to 0.50.

An analysis of these results indicates that the Adjacent Constraint Method and the Two-Part Method perform at least as well as the Basic Window Method and the value of the Jaccard index is generally higher for these two methods. This result is consistent with the findings of Legendre (see Section 2.4) in that through imposing constraints on the clustering criteria more of the information is retained. It is evident that when delineating regions of spatial stationarity it is important to impose constraints upon the clustering criteria. These constraints will not only allow the clustering methods to retain more information, and thus perform better, but they provide the added benefit of resulting in clusters where the data points are spatially contiguous, as required for subsequent spatial analysis.

In general, the first groups that are identified through the proposed clustering techniques do not reflect the true groups. Initially, the regions that stand out represent
small artificial groups found along the natural borders of the true groups. The Two-Part Method

**Figure 4.3** Sample Data Sets (Graphical Clustering Results $a = 0.50$). Graphical summary of the clustering results (based on the Jaccard Index) for the four simulated data sets using the Basic Window method, the Adjacent Constraint Method and the Two-Part Method. The vertical axis gives the Jaccard Index value as a function of the number of groups.
Data Set 2 Summary Statistics

<table>
<thead>
<tr>
<th></th>
<th>Group 1</th>
<th></th>
<th>Group 2</th>
<th></th>
<th>Group 3</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean</td>
<td>Standard</td>
<td>Mean</td>
<td>Standard</td>
<td>Mean</td>
<td>Standard</td>
</tr>
<tr>
<td>Activation Level — $v_1(s)$</td>
<td>4.3</td>
<td>1.1</td>
<td>4.2</td>
<td>1.2</td>
<td>4.9</td>
<td>1.9</td>
</tr>
<tr>
<td>Lag 1 Estimate — $v_4(s)$</td>
<td>1.3</td>
<td>1.3</td>
<td>0.4</td>
<td>0.4</td>
<td>2.4</td>
<td>2.3</td>
</tr>
<tr>
<td>Lag 2 Estimate — $v_5(s)$</td>
<td>1.6</td>
<td>1.5</td>
<td>0.7</td>
<td>0.7</td>
<td>3.1</td>
<td>2.9</td>
</tr>
<tr>
<td>Lag 3 Estimate — $v_6(s)$</td>
<td>1.7</td>
<td>1.9</td>
<td>0.8</td>
<td>0.8</td>
<td>3.7</td>
<td>4.2</td>
</tr>
<tr>
<td>Estimate of 90th Percentile — $v_{7}(s)$</td>
<td>2.6</td>
<td>2.1</td>
<td>1.9</td>
<td>1.6</td>
<td>5.4</td>
<td>5.8</td>
</tr>
</tbody>
</table>

**Figure 4.4** Summary statistics for Data Set 2. The relatively high standard deviations for the estimates of the spatial structure (with comparison to the average estimate values) make it difficult to accurately delineate the simulated regions within this data set.

mitigates this problem somewhat, but does not completely remove it. Figure 4.4 illustrates this for Data Set 4. Notice that the Two-Part Method does not completely solve the problem of the creation of small groups generally found along the natural borders. In fact, it is not until there are 10 groups that we see the division of all three true groups.

Because of this initial artificial border grouping issue, the Jaccard index starts off relatively low and then may exhibit large increases. Similarly, the final results generally indicate the presence of more groups than there actually are. In the simulated case, there are three actual groups, but Figures 4.3 and 4.4 indicate the presence of anywhere from five to ten groups.

The proposed clustering techniques perform better with regard to Data Sets 1 and 4. By construction, Data Sets 1 and 4 have differing mean structures across groups, whereas Data Sets 2 and 3 have the same mean structure with differing spatial structures. This suggests that the estimates of the variogram are inadequately reflecting differences in the spatial structure. (See Figure 4.4 for the summary statistics of Data Set 2). Recall
that these methods employ a moving window approach. As a result, there are relatively few data points available for the estimates for each lag. For future studies, it would be worthwhile to investigate methods to improve these estimates, or to increase the number of data points used in estimation.

One possible way to improve the variogram estimation would be to calculate the variogram for the specified location using the methods proposed in this paper. Then, as a second step, calculate the variogram for each data point adjacent to the specified location (again using the methods proposed in this paper). Lastly, take the average of all the estimated variograms as the estimate of the variogram at the specified location. This method of estimation might also mitigate the impact of the border clusters by smoothing some of the extreme estimates of the variogram that are found along natural borders.
For 2 Groups, the indexes are:
Jaccard = 0.696  Rand = 0.843

For 3 Groups, the indexes are:
Jaccard = 0.688  Rand = 0.839

For 4 Groups, the indexes are:
Jaccard = 0.663  Rand = 0.824

For 5 Groups, the indexes are:
Jaccard = 0.659  Rand = 0.821

For 6 Groups, the indexes are:
Jaccard = 0.652  Rand = 0.819

For 7 Groups, the indexes are:
Jaccard = 0.656  Rand = 0.825

For 8 Groups, the indexes are:
Jaccard = 0.649  Rand = 0.821

For 9 Groups, the indexes are:
Jaccard = 0.645  Rand = 0.819

For 10 Groups, the indexes are:
Jaccard = 0.608  Rand = 0.923

For 11 Groups, the indexes are:
Jaccard = 0.795  Rand = 0.916

For 12 Groups, the indexes are:
Jaccard = 0.789  Rand = 0.908

For 13 Groups, the indexes are:
Jaccard = 0.778  Rand = 0.911

For 14 Groups, the indexes are:
Jaccard = 0.777  Rand = 0.911

For 15 Groups, the indexes are:
Jaccard = 0.769  Rand = 0.908

For 16 Groups, the indexes are:
Jaccard = 0.765  Rand = 0.906

For 17 Groups, the indexes are:
Jaccard = 0.753  Rand = 0.901

For 18 Groups, the indexes are:
Jaccard = 0.752  Rand = 0.901

Figure 4.5 Graphical Clustering Results (Data Set 4). Graphical clustering results for Data Set 4 (with $a = 0.50$) for $n$ groups where $n = 2, 3, \ldots, 18$. The upper left plot shows the true groups.
From a practical standpoint and as described in previous sections, the Two-Part and the Adjacent Constraint Methods are superior to the Basic Window Method when the aim is to perform spatial analyses. To perform spatial statistical procedures on a data region, all of the data points within the region must be contiguous, as will be the case with the Two-Part Method and the Adjacent Constraint Method. This is not to say that the clustered groups produced using the Two-Part Method and the Adjacent Constraint Methods are necessarily ideal for spatial analysis. These two methods may produce groupings that include many groups with a small number of data points (border clusters). This necessitates careful judgment before performing spatial analysis; groups with small numbers of data points may need to be manually combined with neighboring groups.
5. SFMRI DATA ANALYSIS

5.1 Clustering of SFMRI Data

This section details the results of applying the proposed clustering techniques to SFMRI data. The data represent measurements of blood flow to areas of the brain (as described in chapter 2). Recall that measurements within the voxels are taken in the “on” (stimulated) and the “off” (non-stimulated) positions. Figure 5.1 shows the average blood flow for these two conditions within the defined voxels.

5.2 Evaluation of Clustering

Upon inspection of the SFMRI data set (see Figure 5.1), there is evidence of differences in blood flow across the various regions of the brain. These changes in mean structure indicate that increasing the weights applied to the mean structure might be appropriate. Because of this, clustering results for \( a = 0.75 \) are chosen as representative of the underlying groups (even though the clustering was done for all five values of \( a \)).

When evaluating the clusters produced as a result of applying the clustering techniques, it becomes apparent that each additional group does not necessarily add information to the clustering (See Figure 5.2). Note the groups added that appear to be mere border clusters. For example, groups 4 through 8 do not add any real value to the identification of the underlying regions. As more groups are split out, some contain very few data points.
Figure 5.1 SFMRI Brain Data (Image Plot). This figure represents the average blood flow between the “on” and “off” conditions to the defined voxels of the brain. The highlighted area is the area to which the clustering techniques are applied. Darker shades of purple represent lower measurements of blood flow, the white values represent intermediate measurements of blood flow, and darker blue shades represent higher measurements of blood flow.
Also, as the larger groups emerge within the target region, these smaller groups are seen to be along the edges of, or between the larger groups—evidence that they are likely not true groups, but merely manifestations of the border cluster issue. Moreover, these groups also increase the number of groups that must be separated before all the underlying true groups show up in the cluster analysis.

It is also useful to compare results from both the Adjacent Constraint Method and Two-Part Methods. A representative sample of this information is presented in Figure 5.3, giving the image plots for all three clustering methods with $a = 0.75$ and 12 groups. Overall, there tends to be agreement in the location of the larger groups. In identifying the general underlying differences across regions of the brain, the small groups that are inconsistent across methods may be attributed to the border cluster issue. Also, the voxels outside the outline of the brain clearly do not reflect blood flow measures, and any clusters that show up there may be ignored, as is the case with the Basic Window Method where some groups are identified outside the measurement area. As was shown in Chapter 4, both of the proposed methods perform similarly in terms of accuracy. Thus, they may be used as a cross-check to determine which groups reflect underlying structure and which groups are likely to be border clusters.

These techniques as applied to the SFMRI data set enable the delineation of the different regions within the brain. However, it is insufficient to take the resulting groups straight into an analytic application. Care and judgment must be applied to ensure that the resulting groups are appropriate and reflective of underlying information. Any groups that are artificially split out should be rejoined to an adjacent group. As indicated, these groups may be identified through analysis of the cluster images as well as cross
validation between clustering methods. The subsequent application of spatial statistical
methods on the delineated regions should provide increased understanding of the
structure within these distinct regions of the brain.
Figure 5.2 Graphical Clustering Results (Adjacent Constraint Method $a = 0.75$).
Clustering results for the Adjacent Constraint Method with $a = 0.75$, for $n$ groups with $n = 2, 3, \ldots, 18$. The upper left plot shows the original data.
Figure 5.3 Clustering Results for the SFMRI Brain Data. Comparison of the three clustering techniques as applied to the SFMRI data with $a = 0.75$ and 12 groups.
6. CONCLUSIONS AND DIRECTIONS FOR FURTHER RESEARCH

6.1 Conclusions

In general, the application of constraints greatly improved the usefulness of the clustering methods. The clustering of contiguous regions allows for further spatial analysis to take place. However, these methods still have difficulty in grouping all of the data elements into regions of sufficient size to perform this type of analysis. As with all clustering methods, the results of these methods are unable to produce definite results as to the correct number and placement of the true groups. Some judgment is required for the application of the clustering results.

Of the three methods presented, the Two-Part Method appears to be best equipped for delineating regions of spatial stationarity. This method is able to anticipate and account for potential problems due to non-stationarity of the mean structure, while still preserving the benefits gained from forcing grouped data elements to be adjacent to each other.

The last item of note is in regard to the weights applied to the data structure. Since the results must be viewed as indications of grouping rather than concrete evidence, it is useful to use various values of $a$. The weights must also be reasonable with regard to the data to be analyzed. If it can be assumed that the data field has similar mean structure, selection of a value of $a$ that up-weights the variance components would be appropriate, whereas up-weighting the mean structure would not make as much sense.
6.2 Directions for Further Research

Further research options in this field exist primarily in two distinct areas: 1) how to improve the clustering of groups and analysis of how data regions are delineated, and 2) what to do with the data after the groups have been delineated.

With regards to clustering of the groups and the analysis of how the data regions are delineated, it would be useful to examine the extreme estimates of the variance structure more closely. In this paper, it was noted that one of the problems was the clustering and grouping of the border regions. If a method could be developed that could more accurately identify where border regions exist, one could divide a region based on where the most likely place for a border exists. Instead of trying to group data elements within a region, one could attempt to divide a region into homogenous groups.

One difficulty that exists with these methods is that they tend to produce various small clusters within the entire data region. A method to prevent or limit these small clusters would be very useful. Alternatively, one could examine how to recombine these small clusters with others in order to produce regions of sufficient size to perform additional spatial analysis.

Improvements to the clustering methods may also be realized through improved estimates of the variogram. As discussed in Chapter 4, there are various ways to increase the amount of data used to estimate the variogram for each location.

Another question of interest would be how to better identify regions with differing spatial structures. The approach of combining data points with the closest covariance structures seems to favor clustering results that produce many groups with very similar
spatial structures rather than producing fewer groups with more variability in spatial structure between groups.

After data regions have been delineated, spatial statistical methods may be used for estimation within the region or space. With regards to the SFMRI data, these methods may be used to identify specifically which areas of the brain are associated with specific types of impulses and ultimately allow researchers to predict the physiological effects of such specified impulses or stimuli


A. HIERARCHICAL CLUSTER IMAGES

A.1 Graphical Examples

The following images provide a selection of clustering resulting from applying the three proposed methods to the two data examples from Chapter 3. Each chart indicates the method used as well as the weight used for \( a \).
Basic Window Method—Simulated Data Set 1

Simulated Data Set 1 Basic Window Method \((a = 0.50)\)

For 2 Groups, the indexes are:
- Jaccard = 0.366
- Rand = 0.374

For 3 Groups, the indexes are:
- Jaccard = 0.692
- Rand = 0.842

For 4 Groups, the indexes are:
- Jaccard = 0.658
- Rand = 0.826

For 5 Groups, the indexes are:
- Jaccard = 0.658
- Rand = 0.826

For 6 Groups, the indexes are:
- Jaccard = 0.63
- Rand = 0.818

For 7 Groups, the indexes are:
- Jaccard = 0.592
- Rand = 0.808

For 8 Groups, the indexes are:
- Jaccard = 0.586
- Rand = 0.81

For 9 Groups, the indexes are:
- Jaccard = 0.586
- Rand = 0.81

For 10 Groups, the indexes are:
- Jaccard = 0.586
- Rand = 0.81

For 11 Groups, the indexes are:
- Jaccard = 0.586
- Rand = 0.809

For 12 Groups, the indexes are:
- Jaccard = 0.586
- Rand = 0.81

For 13 Groups, the indexes are:
- Jaccard = 0.543
- Rand = 0.816

For 14 Groups, the indexes are:
- Jaccard = 0.543
- Rand = 0.816

For 15 Groups, the indexes are:
- Jaccard = 0.543
- Rand = 0.816

For 16 Groups, the indexes are:
- Jaccard = 0.421
- Rand = 0.77

For 17 Groups, the indexes are:
- Jaccard = 0.421
- Rand = 0.77

For 18 Groups, the indexes are:
- Jaccard = 0.355
- Rand = 0.746
Simulated Data Set 1 Basic Window Method ($a = 0.75$)

For 2 Groups, the indexes are: 
Jaccard = 0.679  Rand = 0.833

For 3 Groups, the indexes are: 
Jaccard = 0.658  Rand = 0.824

For 4 Groups, the indexes are: 
Jaccard = 0.523  Rand = 0.761

For 5 Groups, the indexes are: 
Jaccard = 0.406  Rand = 0.741

For 6 Groups, the indexes are: 
Jaccard = 0.414  Rand = 0.754

For 7 Groups, the indexes are: 
Jaccard = 0.409  Rand = 0.752

For 8 Groups, the indexes are: 
Jaccard = 0.389  Rand = 0.754

For 9 Groups, the indexes are: 
Jaccard = 0.357  Rand = 0.741

For 10 Groups, the indexes are: 
Jaccard = 0.356  Rand = 0.741

For 11 Groups, the indexes are: 
Jaccard = 0.292  Rand = 0.721

For 12 Groups, the indexes are: 
Jaccard = 0.29  Rand = 0.721

For 13 Groups, the indexes are: 
Jaccard = 0.29  Rand = 0.728

For 14 Groups, the indexes are: 
Jaccard = 0.227  Rand = 0.704

For 15 Groups, the indexes are: 
Jaccard = 0.227  Rand = 0.704

For 16 Groups, the indexes are: 
Jaccard = 0.224  Rand = 0.703

For 17 Groups, the indexes are: 
Jaccard = 0.203  Rand = 0.695

For 18 Groups, the indexes are: 
Jaccard = 0.207  Rand = 0.701
Basic Window Method— Simulated Data Set 2

Simulated Data Set 2 Basic Window Method ($a = 0.25$)

For 2 Groups, the indexes are:
Jaccard = 0.363  Rand = 0.392

For 3 Groups, the indexes are:
Jaccard = 0.361  Rand = 0.403

For 4 Groups, the indexes are:
Jaccard = 0.361  Rand = 0.403

For 5 Groups, the indexes are:
Jaccard = 0.341  Rand = 0.465

For 6 Groups, the indexes are:
Jaccard = 0.341  Rand = 0.465

For 7 Groups, the indexes are:
Jaccard = 0.337  Rand = 0.495

For 8 Groups, the indexes are:
Jaccard = 0.335  Rand = 0.494

For 9 Groups, the indexes are:
Jaccard = 0.237  Rand = 0.569

For 10 Groups, the indexes are:
Jaccard = 0.236  Rand = 0.569

For 11 Groups, the indexes are:
Jaccard = 0.233  Rand = 0.569

For 12 Groups, the indexes are:
Jaccard = 0.233  Rand = 0.569

For 13 Groups, the indexes are:
Jaccard = 0.233  Rand = 0.569

For 14 Groups, the indexes are:
Jaccard = 0.212  Rand = 0.588

For 15 Groups, the indexes are:
Jaccard = 0.212  Rand = 0.588

For 16 Groups, the indexes are:
Jaccard = 0.212  Rand = 0.588

For 17 Groups, the indexes are:
Jaccard = 0.212  Rand = 0.588

For 18 Groups, the indexes are:
Jaccard = 0.211  Rand = 0.588
Simulated Data Set 2 Basic Window Method ($a = 0.50$)

For 2 Groups, the indexes are:
- Jaccard = 0.345
- Rand = 0.459

For 3 Groups, the indexes are:
- Jaccard = 0.336
- Rand = 0.488

For 4 Groups, the indexes are:
- Jaccard = 0.295
- Rand = 0.563

For 5 Groups, the indexes are:
- Jaccard = 0.294
- Rand = 0.563

For 6 Groups, the indexes are:
- Jaccard = 0.294
- Rand = 0.563

For 7 Groups, the indexes are:
- Jaccard = 0.294
- Rand = 0.563

For 8 Groups, the indexes are:
- Jaccard = 0.283
- Rand = 0.59

For 9 Groups, the indexes are:
- Jaccard = 0.282
- Rand = 0.592

For 10 Groups, the indexes are:
- Jaccard = 0.282
- Rand = 0.593

For 11 Groups, the indexes are:
- Jaccard = 0.279
- Rand = 0.593

For 12 Groups, the indexes are:
- Jaccard = 0.279
- Rand = 0.593

For 13 Groups, the indexes are:
- Jaccard = 0.278
- Rand = 0.593

For 14 Groups, the indexes are:
- Jaccard = 0.278
- Rand = 0.593

For 15 Groups, the indexes are:
- Jaccard = 0.278
- Rand = 0.593

For 16 Groups, the indexes are:
- Jaccard = 0.191
- Rand = 0.603

For 17 Groups, the indexes are:
- Jaccard = 0.189
- Rand = 0.602

For 18 Groups, the indexes are:
- Jaccard = 0.186
- Rand = 0.605
Adjacent Constraint Method—Simulated Data Set 1

Simulated Data Set 1 Adjacent Constraint Method ($a = 0.50$)

For 2 Groups, the indexes are:
Jaccard = 0.367  Rand = 0.369

For 3 Groups, the indexes are:
Jaccard = 0.713  Rand = 0.853

For 4 Groups, the indexes are:
Jaccard = 0.709  Rand = 0.851

For 5 Groups, the indexes are:
Jaccard = 0.717  Rand = 0.858

For 6 Groups, the indexes are:
Jaccard = 0.698  Rand = 0.850

For 7 Groups, the indexes are:
Jaccard = 0.652  Rand = 0.827

For 8 Groups, the indexes are:
Jaccard = 0.643  Rand = 0.824

For 9 Groups, the indexes are:
Jaccard = 0.639  Rand = 0.822

For 10 Groups, the indexes are:
Jaccard = 0.615  Rand = 0.843

For 11 Groups, the indexes are:
Jaccard = 0.540  Rand = 0.812

For 12 Groups, the indexes are:
Jaccard = 0.536  Rand = 0.811

For 13 Groups, the indexes are:
Jaccard = 0.489  Rand = 0.791

For 14 Groups, the indexes are:
Jaccard = 0.486  Rand = 0.790

For 15 Groups, the indexes are:
Jaccard = 0.350  Rand = 0.735

For 16 Groups, the indexes are:
Jaccard = 0.361  Rand = 0.761

For 17 Groups, the indexes are:
Jaccard = 0.322  Rand = 0.746

For 18 Groups, the indexes are:
Jaccard = 0.315  Rand = 0.743
Simulated Data Set 1 Adjacent Constraint Method ($a = 0.50$) (continued)

For 19 Groups, the indexes are:
- Jaccard = 0.315
- Rand = 0.743

For 20 Groups, the indexes are:
- Jaccard = 0.315
- Rand = 0.743

For 21 Groups, the indexes are:
- Jaccard = 0.314
- Rand = 0.743

For 22 Groups, the indexes are:
- Jaccard = 0.314
- Rand = 0.743

For 23 Groups, the indexes are:
- Jaccard = 0.311
- Rand = 0.742

For 24 Groups, the indexes are:
- Jaccard = 0.309
- Rand = 0.741

For 25 Groups, the indexes are:
- Jaccard = 0.289
- Rand = 0.734

For 26 Groups, the indexes are:
- Jaccard = 0.267
- Rand = 0.725

For 27 Groups, the indexes are:
- Jaccard = 0.266
- Rand = 0.725

Simulated Data Set 1 Adjacent Constraint Method ($a = 0.75$)

For 2 Groups, the indexes are:
- Jaccard = 0.716
- Rand = 0.854

For 3 Groups, the indexes are:
- Jaccard = 0.941
- Rand = 0.977

For 4 Groups, the indexes are:
- Jaccard = 0.798
- Rand = 0.923

For 5 Groups, the indexes are:
- Jaccard = 0.794
- Rand = 0.922

For 6 Groups, the indexes are:
- Jaccard = 0.586
- Rand = 0.842

For 7 Groups, the indexes are:
- Jaccard = 0.484
- Rand = 0.805

For 8 Groups, the indexes are:
- Jaccard = 0.481
- Rand = 0.804

For 9 Groups, the indexes are:
- Jaccard = 0.461
- Rand = 0.797
Simulated Data Set 1 Adjacent Constraint Method ($\alpha = 0.75$) (continued)

For 10 Groups, the indexes are:
Jaccard = 0.457  Rand = 0.795

For 11 Groups, the indexes are:
Jaccard = 0.426  Rand = 0.784

For 12 Groups, the indexes are:
Jaccard = 0.4  Rand = 0.774

For 13 Groups, the indexes are:
Jaccard = 0.391  Rand = 0.771

For 14 Groups, the indexes are:
Jaccard = 0.37  Rand = 0.763

For 15 Groups, the indexes are:
Jaccard = 0.343  Rand = 0.753

For 16 Groups, the indexes are:
Jaccard = 0.34  Rand = 0.752

For 17 Groups, the indexes are:
Jaccard = 0.337  Rand = 0.751

For 18 Groups, the indexes are:
Jaccard = 0.335  Rand = 0.75

For 19 Groups, the indexes are:
Jaccard = 0.332  Rand = 0.749

For 20 Groups, the indexes are:
Jaccard = 0.33  Rand = 0.749

For 21 Groups, the indexes are:
Jaccard = 0.323  Rand = 0.746

For 22 Groups, the indexes are:
Jaccard = 0.3  Rand = 0.737

For 23 Groups, the indexes are:
Jaccard = 0.297  Rand = 0.736

For 24 Groups, the indexes are:
Jaccard = 0.297  Rand = 0.736

For 25 Groups, the indexes are:
Jaccard = 0.289  Rand = 0.733

For 26 Groups, the indexes are:
Jaccard = 0.287  Rand = 0.732

For 27 Groups, the indexes are:
Jaccard = 0.283  Rand = 0.731
Adjacent Constraint Method—Simulated Data Set 2

Simulated Data Set 2 Adjacent Constraint Method ($a = 0.25$)

For 2 Groups, the indexes are:
- Jaccard = 0.369
- Rand = 0.371

For 3 Groups, the indexes are:
- Jaccard = 0.365
- Rand = 0.391

For 4 Groups, the indexes are:
- Jaccard = 0.365
- Rand = 0.391

For 5 Groups, the indexes are:
- Jaccard = 0.366
- Rand = 0.394

For 6 Groups, the indexes are:
- Jaccard = 0.366
- Rand = 0.394

For 7 Groups, the indexes are:
- Jaccard = 0.366
- Rand = 0.397

For 8 Groups, the indexes are:
- Jaccard = 0.366
- Rand = 0.397

For 9 Groups, the indexes are:
- Jaccard = 0.365
- Rand = 0.398

For 10 Groups, the indexes are:
- Jaccard = 0.364
- Rand = 0.399

For 11 Groups, the indexes are:
- Jaccard = 0.363
- Rand = 0.4

For 12 Groups, the indexes are:
- Jaccard = 0.376
- Rand = 0.447

For 13 Groups, the indexes are:
- Jaccard = 0.377
- Rand = 0.451

For 14 Groups, the indexes are:
- Jaccard = 0.371
- Rand = 0.456

For 15 Groups, the indexes are:
- Jaccard = 0.32
- Rand = 0.523

For 16 Groups, the indexes are:
- Jaccard = 0.293
- Rand = 0.537

For 17 Groups, the indexes are:
- Jaccard = 0.281
- Rand = 0.539

For 18 Groups, the indexes are:
- Jaccard = 0.276
- Rand = 0.54
Simulated Data Set 2 Adjacent Constraint Method ($a = 0.25$) (continued)

For 19 Groups, the indexes are:
Jaccard = 0.276  Rand = 0.54

For 20 Groups, the indexes are:
Jaccard = 0.273  Rand = 0.541

For 21 Groups, the indexes are:
Jaccard = 0.273  Rand = 0.541

For 22 Groups, the indexes are:
Jaccard = 0.262  Rand = 0.612

For 23 Groups, the indexes are:
Jaccard = 0.232  Rand = 0.692

For 24 Groups, the indexes are:
Jaccard = 0.231  Rand = 0.652

For 25 Groups, the indexes are:
Jaccard = 0.232  Rand = 0.654

For 26 Groups, the indexes are:
Jaccard = 0.231  Rand = 0.654

For 27 Groups, the indexes are:
Jaccard = 0.23  Rand = 0.654

Simulated Data Set 2 Adjacent Constraint Method ($a = 0.50$)

For 2 Groups, the indexes are:
Jaccard = 0.369  Rand = 0.371

For 3 Groups, the indexes are:
Jaccard = 0.363  Rand = 0.515

For 4 Groups, the indexes are:
Jaccard = 0.326  Rand = 0.586

For 5 Groups, the indexes are:
Jaccard = 0.321  Rand = 0.584

For 6 Groups, the indexes are:
Jaccard = 0.271  Rand = 0.654

For 7 Groups, the indexes are:
Jaccard = 0.27  Rand = 0.654

For 8 Groups, the indexes are:
Jaccard = 0.27  Rand = 0.654

For 9 Groups, the indexes are:
Jaccard = 0.246  Rand = 0.622
Simulated Data Set 2 Adjacent Constraint Method ($a = 0.50$) (continued)

For 10 Groups, the indexes are:
Jaccard = 0.232  Rand = 0.621

For 11 Groups, the indexes are:
Jaccard = 0.232  Rand = 0.621

For 12 Groups, the indexes are:
Jaccard = 0.233  Rand = 0.625

For 13 Groups, the indexes are:
Jaccard = 0.238  Rand = 0.64

For 14 Groups, the indexes are:
Jaccard = 0.238  Rand = 0.64

For 15 Groups, the indexes are:
Jaccard = 0.237  Rand = 0.641

For 16 Groups, the indexes are:
Jaccard = 0.236  Rand = 0.642

For 17 Groups, the indexes are:
Jaccard = 0.236  Rand = 0.642

For 18 Groups, the indexes are:
Jaccard = 0.236  Rand = 0.642

For 19 Groups, the indexes are:
Jaccard = 0.233  Rand = 0.641

For 20 Groups, the indexes are:
Jaccard = 0.233  Rand = 0.642

For 21 Groups, the indexes are:
Jaccard = 0.236  Rand = 0.685

For 22 Groups, the indexes are:
Jaccard = 0.238  Rand = 0.691

For 23 Groups, the indexes are:
Jaccard = 0.23  Rand = 0.688

For 24 Groups, the indexes are:
Jaccard = 0.229  Rand = 0.688

For 25 Groups, the indexes are:
Jaccard = 0.224  Rand = 0.687

For 26 Groups, the indexes are:
Jaccard = 0.224  Rand = 0.687

For 27 Groups, the indexes are:
Jaccard = 0.195  Rand = 0.675
Two-Part Method—Simulated Data Set 1

Simulated Data Set 1 Two-Part Method ($a = 0.50$)

For 2 Groups, the indexes are:
Jaccard = 0.716  Rand = 0.854

For 3 Groups, the indexes are:
Jaccard = 0.708  Rand = 0.851

For 4 Groups, the indexes are:
Jaccard = 0.704  Rand = 0.972

For 5 Groups, the indexes are:
Jaccard = 0.912  Rand = 0.966

For 6 Groups, the indexes are:
Jaccard = 0.902  Rand = 0.961

For 7 Groups, the indexes are:
Jaccard = 0.898  Rand = 0.960

For 8 Groups, the indexes are:
Jaccard = 0.895  Rand = 0.959

For 9 Groups, the indexes are:
Jaccard = 0.881  Rand = 0.958

For 10 Groups, the indexes are:
Jaccard = 0.875  Rand = 0.957

For 11 Groups, the indexes are:
Jaccard = 0.873  Rand = 0.956

For 12 Groups, the indexes are:
Jaccard = 0.859  Rand = 0.946

For 13 Groups, the indexes are:
Jaccard = 0.855  Rand = 0.945

For 14 Groups, the indexes are:
Jaccard = 0.636  Rand = 0.861

For 15 Groups, the indexes are:
Jaccard = 0.631  Rand = 0.860

For 16 Groups, the indexes are:
Jaccard = 0.618  Rand = 0.854

For 17 Groups, the indexes are:
Jaccard = 0.567  Rand = 0.836

For 18 Groups, the indexes are:
Jaccard = 0.567  Rand = 0.835
Simulated Data Set 1 Two-Part Method ($a = 0.50$) (continued)

For 19 Groups, the indexes are:
- Jaccard = 0.472
- Rand = 0.801

For 20 Groups, the indexes are:
- Jaccard = 0.466
- Rand = 0.798

For 21 Groups, the indexes are:
- Jaccard = 0.423
- Rand = 0.782

For 22 Groups, the indexes are:
- Jaccard = 0.413
- Rand = 0.779

For 23 Groups, the indexes are:
- Jaccard = 0.41
- Rand = 0.778

For 24 Groups, the indexes are:
- Jaccard = 0.41
- Rand = 0.778

For 25 Groups, the indexes are:
- Jaccard = 0.409
- Rand = 0.777

For 26 Groups, the indexes are:
- Jaccard = 0.391
- Rand = 0.771

For 27 Groups, the indexes are:
- Jaccard = 0.386
- Rand = 0.768

Simulated Data Set 1 Two-Part Method ($a = 0.75$)

Original Data Set
- $a = 0.75$

For 2 Groups, the indexes are:
- Jaccard = 0.716
- Rand = 0.854

For 3 Groups, the indexes are:
- Jaccard = 0.908
- Rand = 0.964

For 4 Groups, the indexes are:
- Jaccard = 0.894
- Rand = 0.958

For 5 Groups, the indexes are:
- Jaccard = 0.688
- Rand = 0.877

For 6 Groups, the indexes are:
- Jaccard = 0.512
- Rand = 0.815

For 7 Groups, the indexes are:
- Jaccard = 0.433
- Rand = 0.785

For 8 Groups, the indexes are:
- Jaccard = 0.42
- Rand = 0.78

For 9 Groups, the indexes are:
- Jaccard = 0.347
- Rand = 0.753
Simulated Data Set 1 Two-Part Method ($a = 0.75$) (continued)

For 10 Groups, the indexes are:
Jaccard = 0.324  Rand = 0.744

For 11 Groups, the indexes are:
Jaccard = 0.294  Rand = 0.733

For 12 Groups, the indexes are:
Jaccard = 0.292  Rand = 0.732

For 13 Groups, the indexes are:
Jaccard = 0.29  Rand = 0.731

For 14 Groups, the indexes are:
Jaccard = 0.262  Rand = 0.725

For 15 Groups, the indexes are:
Jaccard = 0.259  Rand = 0.724

For 16 Groups, the indexes are:
Jaccard = 0.256  Rand = 0.723

For 17 Groups, the indexes are:
Jaccard = 0.254  Rand = 0.722

For 18 Groups, the indexes are:
Jaccard = 0.252  Rand = 0.721

For 19 Groups, the indexes are:
Jaccard = 0.249  Rand = 0.72

For 20 Groups, the indexes are:
Jaccard = 0.248  Rand = 0.72

For 21 Groups, the indexes are:
Jaccard = 0.24  Rand = 0.717

For 22 Groups, the indexes are:
Jaccard = 0.233  Rand = 0.714

For 23 Groups, the indexes are:
Jaccard = 0.23  Rand = 0.713

For 24 Groups, the indexes are:
Jaccard = 0.228  Rand = 0.712

For 25 Groups, the indexes are:
Jaccard = 0.226  Rand = 0.712

For 26 Groups, the indexes are:
Jaccard = 0.209  Rand = 0.705

For 27 Groups, the indexes are:
Jaccard = 0.201  Rand = 0.702
Two-Part Method—Simulated Data Set 2

Simulated Data Set 2 Two-Part Method ($a = 0.25$)

For 2 Groups, the indexes are:
Jaccard = 0.369  Rand = 0.371

For 3 Groups, the indexes are:
Jaccard = 0.369  Rand = 0.375

For 4 Groups, the indexes are:
Jaccard = 0.369  Rand = 0.376

For 5 Groups, the indexes are:
Jaccard = 0.369  Rand = 0.379

For 6 Groups, the indexes are:
Jaccard = 0.367  Rand = 0.437

For 7 Groups, the indexes are:
Jaccard = 0.368  Rand = 0.440

For 8 Groups, the indexes are:
Jaccard = 0.367  Rand = 0.441

For 9 Groups, the indexes are:
Jaccard = 0.368  Rand = 0.444

For 10 Groups, the indexes are:
Jaccard = 0.369  Rand = 0.447

For 11 Groups, the indexes are:
Jaccard = 0.369  Rand = 0.447

For 12 Groups, the indexes are:
Jaccard = 0.371  Rand = 0.457

For 13 Groups, the indexes are:
Jaccard = 0.372  Rand = 0.460

For 14 Groups, the indexes are:
Jaccard = 0.371  Rand = 0.461

For 15 Groups, the indexes are:
Jaccard = 0.369  Rand = 0.463

For 16 Groups, the indexes are:
Jaccard = 0.369  Rand = 0.462

For 17 Groups, the indexes are:
Jaccard = 0.369  Rand = 0.462

For 18 Groups, the indexes are:
Jaccard = 0.364  Rand = 0.467
Simulated Data Set 2 Two-Part Method ($a = 0.25$) (continued)

For 19 Groups, the indexes are:
Jaccard = 0.358  Rand = 0.473

For 20 Groups, the indexes are:
Jaccard = 0.357  Rand = 0.474

For 21 Groups, the indexes are:
Jaccard = 0.358  Rand = 0.478

For 22 Groups, the indexes are:
Jaccard = 0.359  Rand = 0.481

For 23 Groups, the indexes are:
Jaccard = 0.359  Rand = 0.481

For 24 Groups, the indexes are:
Jaccard = 0.358  Rand = 0.482

For 25 Groups, the indexes are:
Jaccard = 0.358  Rand = 0.481

Simulated Data Set 2 Two-Part Method ($a = 0.50$)

Original Data Set
$a = 0.5$

For 2 Groups, the indexes are:
Jaccard = 0.37  Rand = 0.378

For 3 Groups, the indexes are:
Jaccard = 0.351  Rand = 0.41

For 4 Groups, the indexes are:
Jaccard = 0.36  Rand = 0.559

For 5 Groups, the indexes are:
Jaccard = 0.287  Rand = 0.589

For 6 Groups, the indexes are:
Jaccard = 0.283  Rand = 0.587

For 7 Groups, the indexes are:
Jaccard = 0.283  Rand = 0.587

For 8 Groups, the indexes are:
Jaccard = 0.282  Rand = 0.588

For 9 Groups, the indexes are:
Jaccard = 0.281  Rand = 0.589
Simulated Data Set 2 Two-Part Method ($a = 0.50$) (continued)

For 10 Groups, the indexes are:
Jaccard = 0.27  Rand = 0.663

For 11 Groups, the indexes are:
Jaccard = 0.27  Rand = 0.664

For 12 Groups, the indexes are:
Jaccard = 0.264  Rand = 0.662

For 13 Groups, the indexes are:
Jaccard = 0.259  Rand = 0.666

For 14 Groups, the indexes are:
Jaccard = 0.259  Rand = 0.666

For 15 Groups, the indexes are:
Jaccard = 0.258  Rand = 0.667

For 16 Groups, the indexes are:
Jaccard = 0.257  Rand = 0.667

For 17 Groups, the indexes are:
Jaccard = 0.232  Rand = 0.665

For 18 Groups, the indexes are:
Jaccard = 0.231  Rand = 0.664

For 19 Groups, the indexes are:
Jaccard = 0.217  Rand = 0.670

For 20 Groups, the indexes are:
Jaccard = 0.217  Rand = 0.669

For 21 Groups, the indexes are:
Jaccard = 0.217  Rand = 0.670

For 22 Groups, the indexes are:
Jaccard = 0.216  Rand = 0.667

For 23 Groups, the indexes are:
Jaccard = 0.209  Rand = 0.676

For 24 Groups, the indexes are:
Jaccard = 0.207  Rand = 0.678

For 25 Groups, the indexes are:
Jaccard = 0.204  Rand = 0.677

For 26 Groups, the indexes are:
Jaccard = 0.201  Rand = 0.676

For 27 Groups, the indexes are:
Jaccard = 0.201  Rand = 0.676
A.2 Numerical and Graphical Results

The following Tables and associated charts show the Jaccard indexes resulting from the application of each of the three proposed clustering methods as applied to the four simulated data sets. Select weights of $a$ are used for each of the clustering methods (values of $a$ vary between 0.00, 0.25, 0.50, 0.75 and 1.00).
Data Set 1 ($a = 0.50$)

<table>
<thead>
<tr>
<th>Number of Groups</th>
<th>Basic Window ($a = 0.50$)</th>
<th>Adjacent Constraint ($a = 0.50$)</th>
<th>Two Part ($a = 0.50$)</th>
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</thead>
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</tr>
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Data Set 2 \((a = 0.00)\)

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<th>Two Part ((a = 0.00))</th>
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<tr>
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Data Set 4 ($a = 0.75$)

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<th>Two Part ($a = 0.75$)</th>
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<td>0.615</td>
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Data Set 1 Basic Window Method ($a = 0.50$)

For 10 Groups, the indexes are:
Jaccard = 0.546  Rand = 0.789

For 11 Groups, the indexes are:
Jaccard = 0.44  Rand = 0.742

For 12 Groups, the indexes are:
Jaccard = 0.44  Rand = 0.742

For 13 Groups, the indexes are:
Jaccard = 0.44  Rand = 0.742

For 14 Groups, the indexes are:
Jaccard = 0.44  Rand = 0.743

For 15 Groups, the indexes are:
Jaccard = 0.44  Rand = 0.743

For 16 Groups, the indexes are:
Jaccard = 0.505  Rand = 0.81

For 17 Groups, the indexes are:
Jaccard = 0.493  Rand = 0.806

For 18 Groups, the indexes are:
Jaccard = 0.493  Rand = 0.806

Original Data Set
For 2 Groups, the indexes are:
Jaccard = 0.36  Rand = 0.383

For 3 Groups, the indexes are:
Jaccard = 0.36  Rand = 0.383

For 4 Groups, the indexes are:
Jaccard = 0.617  Rand = 0.8

For 5 Groups, the indexes are:
Jaccard = 0.617  Rand = 0.801

For 6 Groups, the indexes are:
Jaccard = 0.611  Rand = 0.806

For 7 Groups, the indexes are:
Jaccard = 0.564  Rand = 0.79

For 8 Groups, the indexes are:
Jaccard = 0.564  Rand = 0.79

For 9 Groups, the indexes are:
Jaccard = 0.546  Rand = 0.789
Data Set 1 Basic Window Method ($a = 0.50$) (continued)

For 19 Groups, the indexes are:
Jaccard = 0.445  Rand = 0.788

For 20 Groups, the indexes are:
Jaccard = 0.443  Rand = 0.788

For 21 Groups, the indexes are:
Jaccard = 0.384  Rand = 0.766

For 22 Groups, the indexes are:
Jaccard = 0.384  Rand = 0.766

For 23 Groups, the indexes are:
Jaccard = 0.384  Rand = 0.766

For 24 Groups, the indexes are:
Jaccard = 0.381  Rand = 0.765

For 25 Groups, the indexes are:
Jaccard = 0.368  Rand = 0.762

For 26 Groups, the indexes are:
Jaccard = 0.315  Rand = 0.743

For 27 Groups, the indexes are:
Jaccard = 0.315  Rand = 0.743

Data Set 2 Basic Window Method ($a = 0.00$)

For 2 Groups, the indexes are:
Jaccard = 0.365  Rand = 0.375

For 3 Groups, the indexes are:
Jaccard = 0.361  Rand = 0.411

For 4 Groups, the indexes are:
Jaccard = 0.361  Rand = 0.411

For 5 Groups, the indexes are:
Jaccard = 0.347  Rand = 0.434

For 6 Groups, the indexes are:
Jaccard = 0.347  Rand = 0.434

For 7 Groups, the indexes are:
Jaccard = 0.347  Rand = 0.434

For 8 Groups, the indexes are:
Jaccard = 0.311  Rand = 0.553

For 9 Groups, the indexes are:
Jaccard = 0.311  Rand = 0.553
Data Set 2 Basic Window Method ($a = 0.00$) (continued)

For 10 Groups, the indexes are:
Jaccard = 0.311  Rand = 0.553

For 11 Groups, the indexes are:
Jaccard = 0.311  Rand = 0.553

For 12 Groups, the indexes are:
Jaccard = 0.302  Rand = 0.557

For 13 Groups, the indexes are:
Jaccard = 0.302  Rand = 0.557

For 14 Groups, the indexes are:
Jaccard = 0.302  Rand = 0.557

For 15 Groups, the indexes are:
Jaccard = 0.302  Rand = 0.557

For 16 Groups, the indexes are:
Jaccard = 0.286  Rand = 0.583

For 17 Groups, the indexes are:
Jaccard = 0.285  Rand = 0.583

For 18 Groups, the indexes are:
Jaccard = 0.284  Rand = 0.583

For 19 Groups, the indexes are:
Jaccard = 0.284  Rand = 0.583

For 20 Groups, the indexes are:
Jaccard = 0.284  Rand = 0.583

For 21 Groups, the indexes are:
Jaccard = 0.284  Rand = 0.584

For 22 Groups, the indexes are:
Jaccard = 0.283  Rand = 0.584

For 23 Groups, the indexes are:
Jaccard = 0.283  Rand = 0.584

For 24 Groups, the indexes are:
Jaccard = 0.283  Rand = 0.584

For 25 Groups, the indexes are:
Jaccard = 0.283  Rand = 0.584

For 26 Groups, the indexes are:
Jaccard = 0.283  Rand = 0.584

For 27 Groups, the indexes are:
Jaccard = 0.283  Rand = 0.584
Data Set 3 Basic Window Method ($a = 0.25$)

For 2 Groups, the indexes are:
Jaccard = 0.365  Rand = 0.379

For 3 Groups, the indexes are:
Jaccard = 0.362  Rand = 0.389

For 4 Groups, the indexes are:
Jaccard = 0.351  Rand = 0.431

For 5 Groups, the indexes are:
Jaccard = 0.351  Rand = 0.431

For 6 Groups, the indexes are:
Jaccard = 0.35  Rand = 0.431

For 7 Groups, the indexes are:
Jaccard = 0.35  Rand = 0.432

For 8 Groups, the indexes are:
Jaccard = 0.35  Rand = 0.526

For 9 Groups, the indexes are:
Jaccard = 0.35  Rand = 0.526

For 10 Groups, the indexes are:
Jaccard = 0.262  Rand = 0.543

For 11 Groups, the indexes are:
Jaccard = 0.262  Rand = 0.543

For 12 Groups, the indexes are:
Jaccard = 0.262  Rand = 0.543

For 13 Groups, the indexes are:
Jaccard = 0.258  Rand = 0.553

For 14 Groups, the indexes are:
Jaccard = 0.258  Rand = 0.553

For 15 Groups, the indexes are:
Jaccard = 0.21  Rand = 0.584

For 16 Groups, the indexes are:
Jaccard = 0.209  Rand = 0.584

For 17 Groups, the indexes are:
Jaccard = 0.209  Rand = 0.584

For 18 Groups, the indexes are:
Jaccard = 0.208  Rand = 0.585
Data Set 3 Basic Window Method \((a = 0.25)\) (continued)

For 19 Groups, the indexes are:
\[
\text{Jaccard} = 0.208 \quad \text{Rand} = 0.585
\]

For 20 Groups, the indexes are:
\[
\text{Jaccard} = 0.206 \quad \text{Rand} = 0.591
\]

For 21 Groups, the indexes are:
\[
\text{Jaccard} = 0.205 \quad \text{Rand} = 0.591
\]

For 22 Groups, the indexes are:
\[
\text{Jaccard} = 0.205 \quad \text{Rand} = 0.591
\]

For 23 Groups, the indexes are:
\[
\text{Jaccard} = 0.205 \quad \text{Rand} = 0.591
\]

For 24 Groups, the indexes are:
\[
\text{Jaccard} = 0.205 \quad \text{Rand} = 0.591
\]

For 25 Groups, the indexes are:
\[
\text{Jaccard} = 0.202 \quad \text{Rand} = 0.594
\]

For 26 Groups, the indexes are:
\[
\text{Jaccard} = 0.202 \quad \text{Rand} = 0.594
\]

For 27 Groups, the indexes are:
\[
\text{Jaccard} = 0.202 \quad \text{Rand} = 0.594
\]

Data Set 4 Basic Window Method \((a = 0.75)\)

For 2 Groups, the indexes are:
\[
\text{Jaccard} = 0.609 \quad \text{Rand} = 0.784
\]

For 3 Groups, the indexes are:
\[
\text{Jaccard} = 0.76 \quad \text{Rand} = 0.897
\]

For 4 Groups, the indexes are:
\[
\text{Jaccard} = 0.702 \quad \text{Rand} = 0.873
\]

For 5 Groups, the indexes are:
\[
\text{Jaccard} = 0.696 \quad \text{Rand} = 0.871
\]

For 6 Groups, the indexes are:
\[
\text{Jaccard} = 0.695 \quad \text{Rand} = 0.87
\]

For 7 Groups, the indexes are:
\[
\text{Jaccard} = 0.565 \quad \text{Rand} = 0.817
\]

For 8 Groups, the indexes are:
\[
\text{Jaccard} = 0.383 \quad \text{Rand} = 0.753
\]

For 9 Groups, the indexes are:
\[
\text{Jaccard} = 0.377 \quad \text{Rand} = 0.751
\]
Data Set 4 Basic Window Method ($a = 0.75$) (continued)

For 10 Groups, the indexes are:
Jaccard = 0.35  Rand = 0.742

For 11 Groups, the indexes are:
Jaccard = 0.35  Rand = 0.742

For 12 Groups, the indexes are:
Jaccard = 0.349  Rand = 0.741

For 13 Groups, the indexes are:
Jaccard = 0.316  Rand = 0.728

For 14 Groups, the indexes are:
Jaccard = 0.308  Rand = 0.727

For 15 Groups, the indexes are:
Jaccard = 0.245  Rand = 0.707

For 16 Groups, the indexes are:
Jaccard = 0.227  Rand = 0.7

For 17 Groups, the indexes are:
Jaccard = 0.225  Rand = 0.7

For 18 Groups, the indexes are:
Jaccard = 0.221  Rand = 0.699

For 19 Groups, the indexes are:
Jaccard = 0.226  Rand = 0.706

For 20 Groups, the indexes are:
Jaccard = 0.225  Rand = 0.706

For 21 Groups, the indexes are:
Jaccard = 0.226  Rand = 0.709

For 22 Groups, the indexes are:
Jaccard = 0.224  Rand = 0.708

For 23 Groups, the indexes are:
Jaccard = 0.19  Rand = 0.697

For 24 Groups, the indexes are:
Jaccard = 0.19  Rand = 0.697

For 25 Groups, the indexes are:
Jaccard = 0.19  Rand = 0.697

For 26 Groups, the indexes are:
Jaccard = 0.174  Rand = 0.694

For 27 Groups, the indexes are:
Jaccard = 0.174  Rand = 0.694
Data Set 1 Adjacent Constraint Method ($a = 0.50$)

For 2 Groups, the indexes are:
Jaccard = 0.366  Rand = 0.37

For 3 Groups, the indexes are:
Jaccard = 0.64  Rand = 0.805

For 4 Groups, the indexes are:
Jaccard = 0.632  Rand = 0.923

For 5 Groups, the indexes are:
Jaccard = 0.804  Rand = 0.922

For 6 Groups, the indexes are:
Jaccard = 0.802  Rand = 0.922

For 7 Groups, the indexes are:
Jaccard = 0.802  Rand = 0.922

For 8 Groups, the indexes are:
Jaccard = 0.708  Rand = 0.885

For 9 Groups, the indexes are:
Jaccard = 0.698  Rand = 0.881

For 10 Groups, the indexes are:
Jaccard = 0.689  Rand = 0.878

For 11 Groups, the indexes are:
Jaccard = 0.665  Rand = 0.869

For 12 Groups, the indexes are:
Jaccard = 0.665  Rand = 0.868

For 13 Groups, the indexes are:
Jaccard = 0.676  Rand = 0.876

For 14 Groups, the indexes are:
Jaccard = 0.671  Rand = 0.874

For 15 Groups, the indexes are:
Jaccard = 0.653  Rand = 0.867

For 16 Groups, the indexes are:
Jaccard = 0.637  Rand = 0.861

For 17 Groups, the indexes are:
Jaccard = 0.604  Rand = 0.848

For 18 Groups, the indexes are:
Jaccard = 0.588  Rand = 0.843
Data Set 1 Adjacent Constraint Method \((a = 0.50)\) (continued)

For 19 Groups, the indexes are:
- Jaccard = 0.588
- Rand = 0.843

For 20 Groups, the indexes are:
- Jaccard = 0.588
- Rand = 0.843

For 21 Groups, the indexes are:
- Jaccard = 0.587
- Rand = 0.842

For 22 Groups, the indexes are:
- Jaccard = 0.587
- Rand = 0.842

For 23 Groups, the indexes are:
- Jaccard = 0.574
- Rand = 0.837

For 24 Groups, the indexes are:
- Jaccard = 0.556
- Rand = 0.831

For 25 Groups, the indexes are:
- Jaccard = 0.552
- Rand = 0.829

For 26 Groups, the indexes are:
- Jaccard = 0.547
- Rand = 0.827

For 27 Groups, the indexes are:
- Jaccard = 0.547
- Rand = 0.827

Data Set 2 Adjacent Constraint Method \((a = 0.00)\)

Original Data Set
- \(a = 0\)

For 2 Groups, the indexes are:
- Jaccard = 0.369
- Rand = 0.371

For 3 Groups, the indexes are:
- Jaccard = 0.373
- Rand = 0.391

For 4 Groups, the indexes are:
- Jaccard = 0.374
- Rand = 0.399

For 5 Groups, the indexes are:
- Jaccard = 0.375
- Rand = 0.402

For 6 Groups, the indexes are:
- Jaccard = 0.371
- Rand = 0.405

For 7 Groups, the indexes are:
- Jaccard = 0.371
- Rand = 0.409

For 8 Groups, the indexes are:
- Jaccard = 0.371
- Rand = 0.409

For 9 Groups, the indexes are:
- Jaccard = 0.37
- Rand = 0.409
Data Set 2 Adjacent Constraint Method ($a = 0.00$) (continued)

For 10 Groups, the indexes are:
Jaccard = 0.372  Rand = 0.416

For 11 Groups, the indexes are:
Jaccard = 0.371  Rand = 0.417

For 12 Groups, the indexes are:
Jaccard = 0.372  Rand = 0.42

For 13 Groups, the indexes are:
Jaccard = 0.37  Rand = 0.42

For 14 Groups, the indexes are:
Jaccard = 0.37  Rand = 0.422

For 15 Groups, the indexes are:
Jaccard = 0.371  Rand = 0.445

For 16 Groups, the indexes are:
Jaccard = 0.37  Rand = 0.446

For 17 Groups, the indexes are:
Jaccard = 0.37  Rand = 0.446

For 18 Groups, the indexes are:
Jaccard = 0.37  Rand = 0.446

For 19 Groups, the indexes are:
Jaccard = 0.37  Rand = 0.446

For 20 Groups, the indexes are:
Jaccard = 0.368  Rand = 0.447

For 21 Groups, the indexes are:
Jaccard = 0.367  Rand = 0.448

For 22 Groups, the indexes are:
Jaccard = 0.366  Rand = 0.449

For 23 Groups, the indexes are:
Jaccard = 0.365  Rand = 0.574

For 24 Groups, the indexes are:
Jaccard = 0.364  Rand = 0.574

For 25 Groups, the indexes are:
Jaccard = 0.362  Rand = 0.573

For 26 Groups, the indexes are:
Jaccard = 0.362  Rand = 0.573

For 27 Groups, the indexes are:
Jaccard = 0.358  Rand = 0.572
Data Set 3 Adjacent Constraint Method \( (a = 0.25) \)

For 2 Groups, the indexes are:
- Jaccard = 0.367
- Rand = 0.369

For 3 Groups, the indexes are:
- Jaccard = 0.366
- Rand = 0.37

For 4 Groups, the indexes are:
- Jaccard = 0.365
- Rand = 0.375

For 5 Groups, the indexes are:
- Jaccard = 0.362
- Rand = 0.376

For 6 Groups, the indexes are:
- Jaccard = 0.361
- Rand = 0.376

For 7 Groups, the indexes are:
- Jaccard = 0.36
- Rand = 0.377

For 8 Groups, the indexes are:
- Jaccard = 0.356
- Rand = 0.381

For 9 Groups, the indexes are:
- Jaccard = 0.262
- Rand = 0.5

For 10 Groups, the indexes are:
- Jaccard = 0.261
- Rand = 0.501

For 11 Groups, the indexes are:
- Jaccard = 0.26
- Rand = 0.502

For 12 Groups, the indexes are:
- Jaccard = 0.252
- Rand = 0.51

For 13 Groups, the indexes are:
- Jaccard = 0.248
- Rand = 0.513

For 14 Groups, the indexes are:
- Jaccard = 0.247
- Rand = 0.513

For 15 Groups, the indexes are:
- Jaccard = 0.247
- Rand = 0.513

For 16 Groups, the indexes are:
- Jaccard = 0.247
- Rand = 0.513

For 17 Groups, the indexes are:
- Jaccard = 0.246
- Rand = 0.514

For 18 Groups, the indexes are:
- Jaccard = 0.246
- Rand = 0.515
Data Set 3 Adjacent Constraint Method ($a = 0.25$) (continued)

For 19 Groups, the indexes are:
Jaccard = 0.243  Rand = 0.519

For 20 Groups, the indexes are:
Jaccard = 0.243  Rand = 0.519

For 21 Groups, the indexes are:
Jaccard = 0.242  Rand = 0.52

For 22 Groups, the indexes are:
Jaccard = 0.238  Rand = 0.527

For 23 Groups, the indexes are:
Jaccard = 0.237  Rand = 0.529

For 24 Groups, the indexes are:
Jaccard = 0.237  Rand = 0.529

For 25 Groups, the indexes are:
Jaccard = 0.236  Rand = 0.529

For 26 Groups, the indexes are:
Jaccard = 0.231  Rand = 0.542

For 27 Groups, the indexes are:
Jaccard = 0.231  Rand = 0.542

Data Set 4 Adjacent Constraint Method ($a = 0.75$)

Original Data Set
$a = 0.75$

For 2 Groups, the indexes are:
Jaccard = 0.347  Rand = 0.441

For 3 Groups, the indexes are:
Jaccard = 0.342  Rand = 0.468

For 4 Groups, the indexes are:
Jaccard = 0.423  Rand = 0.665

For 5 Groups, the indexes are:
Jaccard = 0.42  Rand = 0.663

For 6 Groups, the indexes are:
Jaccard = 0.546  Rand = 0.805

For 7 Groups, the indexes are:
Jaccard = 0.544  Rand = 0.805

For 8 Groups, the indexes are:
Jaccard = 0.55  Rand = 0.809

For 9 Groups, the indexes are:
Jaccard = 0.52  Rand = 0.799
Data Set 4 Adjacent Constraint Method ($a = 0.75$) (continued)

For 10 Groups, the indexes are:
Jaccard = 0.538  Rand = 0.813

For 11 Groups, the indexes are:
Jaccard = 0.534  Rand = 0.812

For 12 Groups, the indexes are:
Jaccard = 0.531  Rand = 0.81

For 13 Groups, the indexes are:
Jaccard = 0.525  Rand = 0.808

For 14 Groups, the indexes are:
Jaccard = 0.524  Rand = 0.808

For 15 Groups, the indexes are:
Jaccard = 0.519  Rand = 0.806

For 16 Groups, the indexes are:
Jaccard = 0.516  Rand = 0.805

For 17 Groups, the indexes are:
Jaccard = 0.516  Rand = 0.805

For 18 Groups, the indexes are:
Jaccard = 0.408  Rand = 0.764

For 19 Groups, the indexes are:
Jaccard = 0.403  Rand = 0.762

For 20 Groups, the indexes are:
Jaccard = 0.403  Rand = 0.762

For 21 Groups, the indexes are:
Jaccard = 0.389  Rand = 0.757

For 22 Groups, the indexes are:
Jaccard = 0.298  Rand = 0.725

For 23 Groups, the indexes are:
Jaccard = 0.297  Rand = 0.724

For 24 Groups, the indexes are:
Jaccard = 0.213  Rand = 0.701

For 25 Groups, the indexes are:
Jaccard = 0.212  Rand = 0.701

For 26 Groups, the indexes are:
Jaccard = 0.211  Rand = 0.701

For 27 Groups, the indexes are:
Jaccard = 0.207  Rand = 0.699
Data Set 1 Two-Part Method ($a = 0.50$)

Original Data Set $a = 0.5$

For 2 Groups, the indexes are:
Jaccard = 0.696  Rand = 0.843

For 3 Groups, the indexes are:
Jaccard = 0.688  Rand = 0.839

For 4 Groups, the indexes are:
Jaccard = 0.631  Rand = 0.817

For 5 Groups, the indexes are:
Jaccard = 0.631  Rand = 0.818

For 6 Groups, the indexes are:
Jaccard = 0.619  Rand = 0.813

For 7 Groups, the indexes are:
Jaccard = 0.619  Rand = 0.813

For 8 Groups, the indexes are:
Jaccard = 0.615  Rand = 0.811

For 9 Groups, the indexes are:
Jaccard = 0.607  Rand = 0.808

For 10 Groups, the indexes are:
Jaccard = 0.588  Rand = 0.798

For 11 Groups, the indexes are:
Jaccard = 0.444  Rand = 0.732

For 12 Groups, the indexes are:
Jaccard = 0.497  Rand = 0.805

For 13 Groups, the indexes are:
Jaccard = 0.497  Rand = 0.805

For 14 Groups, the indexes are:
Jaccard = 0.495  Rand = 0.804

For 15 Groups, the indexes are:
Jaccard = 0.495  Rand = 0.804

For 16 Groups, the indexes are:
Jaccard = 0.493  Rand = 0.803

For 17 Groups, the indexes are:
Jaccard = 0.492  Rand = 0.803

For 18 Groups, the indexes are:
Jaccard = 0.49  Rand = 0.802
Data Set 1 Two-Part Method \( (a = 0.50) \) (continued)

For 19 Groups, the indexes are:
Jaccard = 0.486  Rand = 0.801

For 20 Groups, the indexes are:
Jaccard = 0.478  Rand = 0.798

For 21 Groups, the indexes are:
Jaccard = 0.475  Rand = 0.797

For 22 Groups, the indexes are:
Jaccard = 0.472  Rand = 0.796

For 23 Groups, the indexes are:
Jaccard = 0.469  Rand = 0.795

For 24 Groups, the indexes are:
Jaccard = 0.468  Rand = 0.794

For 25 Groups, the indexes are:
Jaccard = 0.466  Rand = 0.793

For 26 Groups, the indexes are:
Jaccard = 0.474  Rand = 0.801

For 27 Groups, the indexes are:
Jaccard = 0.472  Rand = 0.8

Data Set 2 Two-Part Method \( (a = 0.00) \)

For 2 Groups, the indexes are:
Jaccard = 0.369  Rand = 0.371

For 3 Groups, the indexes are:
Jaccard = 0.365  Rand = 0.375

For 4 Groups, the indexes are:
Jaccard = 0.364  Rand = 0.376

For 5 Groups, the indexes are:
Jaccard = 0.361  Rand = 0.379

For 6 Groups, the indexes are:
Jaccard = 0.363  Rand = 0.385

For 7 Groups, the indexes are:
Jaccard = 0.362  Rand = 0.386

For 8 Groups, the indexes are:
Jaccard = 0.362  Rand = 0.389

For 9 Groups, the indexes are:
Jaccard = 0.361  Rand = 0.39
Data Set 2 Two-Part Method ($a = 0.00$) (continued)

For 10 Groups, the indexes are:
Jaccard = 0.361  Rand = 0.39

For 11 Groups, the indexes are:
Jaccard = 0.362  Rand = 0.393

For 12 Groups, the indexes are:
Jaccard = 0.361  Rand = 0.394

For 13 Groups, the indexes are:
Jaccard = 0.36  Rand = 0.395

For 14 Groups, the indexes are:
Jaccard = 0.359  Rand = 0.396

For 15 Groups, the indexes are:
Jaccard = 0.358  Rand = 0.397

For 16 Groups, the indexes are:
Jaccard = 0.357  Rand = 0.398

For 17 Groups, the indexes are:
Jaccard = 0.358  Rand = 0.401

For 18 Groups, the indexes are:
Jaccard = 0.359  Rand = 0.407

For 19 Groups, the indexes are:
Jaccard = 0.36  Rand = 0.411

For 20 Groups, the indexes are:
Jaccard = 0.356  Rand = 0.414

For 21 Groups, the indexes are:
Jaccard = 0.343  Rand = 0.436

For 22 Groups, the indexes are:
Jaccard = 0.344  Rand = 0.439

For 23 Groups, the indexes are:
Jaccard = 0.343  Rand = 0.44

For 24 Groups, the indexes are:
Jaccard = 0.342  Rand = 0.443

For 25 Groups, the indexes are:
Jaccard = 0.342  Rand = 0.441

For 26 Groups, the indexes are:
Jaccard = 0.342  Rand = 0.441

For 27 Groups, the indexes are:
Jaccard = 0.341  Rand = 0.444
Data Set 3 Two-Part Method ($a = 0.25$)

For 2 Groups, the indexes are:
Jaccard = 0.364  Rand = 0.372

For 3 Groups, the indexes are:
Jaccard = 0.36  Rand = 0.377

For 4 Groups, the indexes are:
Jaccard = 0.359  Rand = 0.378

For 5 Groups, the indexes are:
Jaccard = 0.358  Rand = 0.379

For 6 Groups, the indexes are:
Jaccard = 0.359  Rand = 0.382

For 7 Groups, the indexes are:
Jaccard = 0.358  Rand = 0.383

For 8 Groups, the indexes are:
Jaccard = 0.357  Rand = 0.384

For 9 Groups, the indexes are:
Jaccard = 0.356  Rand = 0.385

For 10 Groups, the indexes are:
Jaccard = 0.355  Rand = 0.386

For 11 Groups, the indexes are:
Jaccard = 0.354  Rand = 0.387

For 12 Groups, the indexes are:
Jaccard = 0.354  Rand = 0.387

For 13 Groups, the indexes are:
Jaccard = 0.354  Rand = 0.387

For 14 Groups, the indexes are:
Jaccard = 0.351  Rand = 0.392

For 15 Groups, the indexes are:
Jaccard = 0.35  Rand = 0.393

For 16 Groups, the indexes are:
Jaccard = 0.348  Rand = 0.395

For 17 Groups, the indexes are:
Jaccard = 0.338  Rand = 0.417

For 18 Groups, the indexes are:
Jaccard = 0.282  Rand = 0.465
Data Set 3 Two-Part Method ($a = 0.25$) (continued)

For 19 Groups, the indexes are:
Jaccard = 0.282  Rand = 0.465

For 20 Groups, the indexes are:
Jaccard = 0.276  Rand = 0.473

For 21 Groups, the indexes are:
Jaccard = 0.277  Rand = 0.555

For 22 Groups, the indexes are:
Jaccard = 0.271  Rand = 0.553

For 23 Groups, the indexes are:
Jaccard = 0.271  Rand = 0.553

For 24 Groups, the indexes are:
Jaccard = 0.267  Rand = 0.553

For 25 Groups, the indexes are:
Jaccard = 0.267  Rand = 0.552

For 26 Groups, the indexes are:
Jaccard = 0.266  Rand = 0.553

For 27 Groups, the indexes are:
Jaccard = 0.266  Rand = 0.553

Data Set 4 Two-Part Method ($a = 0.75$)

Original Data Set  

For 2 Groups, the indexes are:
Jaccard = 0.705  Rand = 0.848

For 3 Groups, the indexes are:
Jaccard = 0.686  Rand = 0.839

For 4 Groups, the indexes are:
Jaccard = 0.679  Rand = 0.835

For 5 Groups, the indexes are:
Jaccard = 0.885  Rand = 0.955

For 6 Groups, the indexes are:
Jaccard = 0.881  Rand = 0.953

For 7 Groups, the indexes are:
Jaccard = 0.811  Rand = 0.927

For 8 Groups, the indexes are:
Jaccard = 0.736  Rand = 0.898

For 9 Groups, the indexes are:
Jaccard = 0.725  Rand = 0.894
Data Set 4 Two-Part Method ($a = 0.75$) (continued)

For 10 Groups, the indexes are:
Jaccard = 0.715  Rand = 0.89

For 11 Groups, the indexes are:
Jaccard = 0.636  Rand = 0.862

For 12 Groups, the indexes are:
Jaccard = 0.622  Rand = 0.856

For 13 Groups, the indexes are:
Jaccard = 0.617  Rand = 0.855

For 14 Groups, the indexes are:
Jaccard = 0.615  Rand = 0.854

For 15 Groups, the indexes are:
Jaccard = 0.619  Rand = 0.855

For 16 Groups, the indexes are:
Jaccard = 0.617  Rand = 0.855

For 17 Groups, the indexes are:
Jaccard = 0.615  Rand = 0.854

For 18 Groups, the indexes are:
Jaccard = 0.564  Rand = 0.834

For 19 Groups, the indexes are:
Jaccard = 0.349  Rand = 0.756

For 20 Groups, the indexes are:
Jaccard = 0.346  Rand = 0.755

For 21 Groups, the indexes are:
Jaccard = 0.328  Rand = 0.748

For 22 Groups, the indexes are:
Jaccard = 0.326  Rand = 0.748

For 23 Groups, the indexes are:
Jaccard = 0.325  Rand = 0.747

For 24 Groups, the indexes are:
Jaccard = 0.322  Rand = 0.746

For 25 Groups, the indexes are:
Jaccard = 0.32  Rand = 0.745

For 26 Groups, the indexes are:
Jaccard = 0.32  Rand = 0.745

For 27 Groups, the indexes are:
Jaccard = 0.319  Rand = 0.745
A.3 SFMRI Brain Data Graphical Analysis

The following images show the clustering resulting from applying the three proposed methods to the SFMRI data from Chapter 5. A weight of 0.75 was selected for $a$.

SFMRI Brain Data Set Basic Window Method ($a = 0.75$)
SFMRI Brain Data Set Basic Window Method ($a = 0.75$) (continued)

- Data Clustered into 10 Groups.
- Data Clustered into 11 Groups.
- Data Clustered into 12 Groups.

- Data Clustered into 13 Groups.
- Data Clustered into 14 Groups.
- Data Clustered into 15 Groups.

- Data Clustered into 16 Groups.
- Data Clustered into 17 Groups.
- Data Clustered into 18 Groups.

- Data Clustered into 19 Groups.
- Data Clustered into 20 Groups.
- Data Clustered into 21 Groups.

- Data Clustered into 22 Groups.
- Data Clustered into 23 Groups.
- Data Clustered into 24 Groups.

- Data Clustered into 25 Groups.
- Data Clustered into 26 Groups.
- Data Clustered into 27 Groups.
SFMRI Brain Data Set Adjacent Constraint Method ($a = 0.75$)

Original Data Set

Data Clustered into 2 Groups.

Data Clustered into 3 Groups.

Data Clustered into 4 Groups.

Data Clustered into 5 Groups.

Data Clustered into 6 Groups.

Data Clustered into 7 Groups.

Data Clustered into 8 Groups.

Data Clustered into 9 Groups.

Data Clustered into 10 Groups.

Data Clustered into 11 Groups.

Data Clustered into 12 Groups.

Data Clustered into 13 Groups.

Data Clustered into 14 Groups.

Data Clustered into 15 Groups.

Data Clustered into 16 Groups.

Data Clustered into 17 Groups.

Data Clustered into 18 Groups.
SFMRI Brain Data Set Adjacent Constraint Method \((a = 0.75)\) (continued)

Data Clustered into 19 Groups.

Data Clustered into 20 Groups.

Data Clustered into 21 Groups.

Data Clustered into 22 Groups.

Data Clustered into 23 Groups.

Data Clustered into 24 Groups.

Data Clustered into 25 Groups.

Data Clustered into 26 Groups.

Data Clustered into 27 Groups.

SFMRI Brain Data Set Two-Part Method \((a = 0.75)\)

Original Data Set \(a = 0.75\)

Data Clustered into 2 Groups.

Data Clustered into 3 Groups.

Data Clustered into 4 Groups.

Data Clustered into 5 Groups.

Data Clustered into 6 Groups.

Data Clustered into 7 Groups.

Data Clustered into 8 Groups.

Data Clustered into 9 Groups.
SFMRI Brain Data Set Two-Part Method ($a = 0.75$) (continued)
### B. SPLUS CODE

#### B.1 Data Generation

```splus
#for (s in 1:wd)
#
# w[s,j[j<(s-10)^3/100+10]] <- g2[s,j[j<(s-10)^3/100+10]]
# grp[s,j[j<(s-10)^3/100+10]] <- "Grp 2"
# w[s,j[(s-10)^2/2+(j-10)^2/3<9]] <- g3[s,j[(s-10)^2/2+(j-10)^2/3<9]]
# grp[s,j[(s-10)^2/2+(j-10)^2/3<9]] <- "Grp 3"
#
#
###The following sequence of code simulates the following regions###
##
grid <- expand.grid(x=1:wd,y=1:wd)
##
## Test Region 1                   
## 1. Region 1 => high mean, moderate variance, moderate range 
## 1. Region 2 => low mean, moderate variance, moderate range 
## 1. Region 3 => moderate mean, moderate variance, moderate range 
##
testdata.1.1 <- matrix(8+rfsim(grid,covfun=exp.cov,range=3,sill=3,nc=10000),wd,wd)
testdata.1.2 <- matrix(0+rfsim(grid,covfun=exp.cov,range=3,sill=3,nc=10000),wd,wd)
testdata.1.3 <- matrix(4+rfsim(grid,covfun=exp.cov,range=3,sill=3,nc=10000),wd,wd)
testdata.1.grid <- testdata.1.1
testdata.1.grid[grp=="Grp 2"] <- testdata.1.2[grp=="Grp 2"]
testdata.1.grid[grp=="Grp 3"] <- testdata.1.3[grp=="Grp 3"]
##
## Test Region 2                   
## 2. Region 1 => moderate mean, moderate variance, moderate range 
## 2. Region 2 => moderate mean, small variance, moderate range 
## 2. Region 3 => moderate mean, large variance, moderate range 
##
testdata.2.1 <- matrix(4+rfsim(grid,covfun=exp.cov,range=3,sill=3,nc=10000),wd,wd)
testdata.2.2 <- matrix(4+rfsim(grid,covfun=exp.cov,range=3,sill=1,nc=10000),wd,wd)
testdata.2.3 <- matrix(4+rfsim(grid,covfun=exp.cov,range=3,sill=5,nc=10000),wd,wd)
testdata.2.grid <- testdata.2.1
testdata.2.grid[grp=="Grp 2"] <- testdata.2.2[grp=="Grp 2"]
testdata.2.grid[grp=="Grp 3"] <- testdata.2.3[grp=="Grp 3"]
##
## Test Region 3                   
## 3. Region 1 => moderate mean, moderate variance, small range 
## 3. Region 2 => moderate mean, moderate variance, large range 
## 3. Region 3 => moderate mean, moderate variance, moderate range 
##
testdata.3.1 <- matrix(4+rfsim(grid,covfun=exp.cov,range=1,sill=3,nc=10000),wd,wd)
testdata.3.2 <- matrix(4+rfsim(grid,covfun=exp.cov,range=5,sill=3,nc=10000),wd,wd)
testdata.3.3 <- matrix(4+rfsim(grid,covfun=exp.cov,range=3,sill=3,nc=10000),wd,wd)
```
testdata.3.grid <- testdata.3.1
testdata.3.grid[, grp=="Grp 2"] <- testdata.3.2[, grp=="Grp 2"]
testdata.3.grid[, grp=="Grp 3"] <- testdata.3.3[, grp=="Grp 3"]

#-----------------------------
###Test Region 4

###4. Region 1 => high mean, moderate variance, small range
###4. Region 2 => low mean, small variance, large range
###4. Region 3 => moderate mean, large variance, moderate range
#-----------------------------

testdata.4.1 <- matrix(8+rfsim(grid, covfun=exp.cov, range=1, sill=3, nc=10000), wd, wd)
testdata.4.2 <- matrix(0+rfsim(grid, covfun=exp.cov, range=5, sill=1, nc=10000), wd, wd)
testdata.4.3 <- matrix(4+rfsim(grid, covfun=exp.cov, range=3, sill=5, nc=10000), wd, wd)
testdata.4.grid <- testdata.4.1
testdata.4.grid[, grp=="Grp 2"] <- testdata.4.2[, grp=="Grp 2"]
testdata.4.grid[, grp=="Grp 3"] <- testdata.4.3[, grp=="Grp 3"]

#----------------------------------------
###Chart all regions
#----------------------------------------

par(mfrow=c(2,2))
image(testdata.1.grid)
title("Image of Test Data 1")
image(testdata.2.grid)
title("Image of Test Data 2")
image(testdata.3.grid)
title("Image of Test Data 3")
image(testdata.4.grid)
title("Image of Test Data 4")
persp(testdata.1.grid)
title("Image of Test Data 1")
persp(testdata.2.grid)
title("Image of Test Data 2")
persp(testdata.3.grid)
title("Image of Test Data 3")
persp(testdata.4.grid)
title("Image of Test Data 4")
### Defined Functions ###

The following three functions are estimators of the variogram:

- **gamma.classic**: 
  ```r
  gamma.classic <- function(zdat) {
    nh <- length(zdat)
    gval <- .5*(sum(zdat*zdat))/nh
    return (gval)
  }
  ```

- **gamma.bar**: 
  ```r
  gamma.bar <- function(zdat) {
    nh <- length(zdat)
    bh <- 0.457
    gval <- .5*((sum(sqrt(abs(zdat)))/nh)^(4/(bh+.494/nh)))
    return (gval)
  }
  ```

- **gamma.tilda**: 
  ```r
  gamma.tilda <- function(zdat) {
    nh <- length(zdat)
    bh <- 0.457
    gval <- .5*((median(sqrt(abs(zdat)))^4)/(bh+.494/nh))
    return (gval)
  }
  ```

### Function to test if ind < 0 ###

```r
  test.fun <- function (ind) {
    if (ind < 0) return (T)
    return (F)
  }
  ```

### Calculates groups to be similar to S-Plus output ###

```r
  order.fun <- function (t,m,i){
    index.history <- NULL
    index.history <- c(i,index.history)
    column.history <- NULL
    column.history <- c(1,column.history)
    while (length(t) < i+1){
      while (m[index.history[1],column.history[1]] > 0) {
        index.history <- c(m[index.history[1],column.history[1]],index.history)
        column.history <- c(1,column.history)
      }
    t <- c(t,-m[index.history[1],column.history[1]])
    if (column.history[1] == 1) {
      column.history[1] <- 2
    } else {
```
while ((column.history[1] == 2) && (length(column.history >0))) {
    index.history <- index.history[-1]
    column.history <- column.history[-1]
}
column.history[1] <- 2

return(t)

ord.fun <- function (t,m,i) {
    ind1 <- m[i,1]
    if (test.fun(ind1)) t <- c(t,-ind1) else t <- ord.fun(t,m,ind1)
    ind2 <- m[i,2]
    if (test.fun(ind2)) t <- c(t,-ind2) else t <- ord.fun(t,m,ind2)
    return(t)
}

get.index <- function(group.mat, cluster.mat) {
    v.known <- c(group.mat)
    v.clust <- c(cluster.mat)
    nn <- length(v.known)
    mat.known <- matrix(-1,nn,nn)
    mat.clust <- matrix(-1,nn,nn)
    for (i in 1:(nn-1)) {
        mat.known[i,(i+1):nn] <- (v.known[(i+1):nn] == v.known[i])
        mat.clust[i,(i+1):nn] <- (v.clust[(i+1):nn] == v.clust[i])
    }
    count.mat <- mat.known + mat.clust
    a <- length(count.mat[count.mat==2])
    bc.sum <- length(count.mat[count.mat==1])
    d <- length(count.mat[count.mat==0])
    index <- c(Jaccard=a/(a+bc.sum),Rand=(a+d)/(a+bc.sum+d))
    return(index)
}
Constrained Clustering (using complete linkage, or maximum, as distance criteria)

```
ntot <- nr*nc

# general positions for any data matrix
# data.pos represents a matrix with the pairings of each point of the data matrix (i.e. column 1 provides the row number, column 2 the column number)

data.pos <- matrix(c(rep(1:nr, times=nc),rep(1:nc, each=nr)),ncol=2,byrow=F,dimnames=list(NULL,c("row","col")))

temp.dist <- dist(data.vec)

temp.dist.pos <- dist(data.pos)

# lists the observation pairs that correspond to the distances from the S-PLUS dist function

tt.c1 <- tt.c2 <- NULL
for (i in 1:(ntot-1)) {
    temp.seq <- seq(1:(ntot-i))+i
    tt.c2 <- c(tt.c2,temp.seq)
    tt.c1 <- c(tt.c1,numeric(length(temp.seq))+i)
}

#temp.merge, temp.height, and temp.order match the output from the S-PLUS hclust function dist.mat contains the distance between data points, physical locations and the data index for which the distances correspond

tt <- matrix(-c(tt.c1,tt.c2),ncol=2,byrow=F)
dist.mat <- matrix(c(temp.dist,temp.dist.pos,tt),ncol=4,byrow=F,dimnames=list(NULL,c("dist","pos dist","","")))
```

This algorithm clusters based on maximum distance

---

111
for (i in 1:(ntot-1)) {
  if (length(dist.mat) > 4) {

    #---------------------------------------------------------------------------#
    ###records the point number and row and column coordinates of the         ###
    ###observations with the smallest distance.                           ###
    ###Note that the physical locations must be adjacent              ###
    #---------------------------------------------------------------------------#
    min.dist <- min(dist.mat[,2] <
                adjacent.distance & (dist.mat[,1]>0),1)
    temp.pos <- which(dist.mat[,1]==min.dist)[1]
    temp.merge[i,] <- dist.mat[temp.pos,3:4][order(dist.mat[temp.pos,3:4])]

    #---------------------------------------------------------------------------#
    ###records the min distance between points                           ###
    #---------------------------------------------------------------------------#
    temp.height[i] <- min.dist

    #---------------------------------------------------------------------------#
    ###adjust the distance matrix dist.mat by combining the joined groups   ###
    #---------------------------------------------------------------------------#
    dist.mat <-
    dist.mat[!((dist.mat[,3]==temp.merge[i,][1])&dist.mat[,4]==temp.merge[i,][2])|
              (dist.mat[,3]==temp.merge[i,][2])&dist.mat[,4]==temp.merge[i,][1])]

    #---------------------------------------------------------------------------#
    ###change the negative point number to a positive group number        ###
    #---------------------------------------------------------------------------#
    temp.pairs <- temp.merge[i,]

    #---------------------------------------------------------------------------#
    ###recalculate the distances between groups in dist.mat               ###
    #---------------------------------------------------------------------------#
    pos.lst <- which((dist.mat[,3]==i)|(dist.mat[,4]==i))
    delete.row <- NULL
    for (k in 1:length(pos.lst)) {
      temp.pairs <- dist.mat[pos.lst[k],3:4]
      ind.pos <-
      which((dist.mat[pos.lst,3]==temp.pairs[1])&(dist.mat[pos.lst,4]==temp.pairs[2])) |
              (dist.mat[pos.lst,3]==temp.pairs[2])&dist.mat[pos.lst,4]==temp.pairs[1])
      dist.mat[pos.lst[ind.pos],1] <- max(dist.mat[pos.lst[ind.pos],1])
      dist.mat[pos.lst[ind.pos],2] <- min(dist.mat[pos.lst[ind.pos],2])
      delete.row <- c(delete.row,pos.lst[ind.pos[2:length(ind.pos)]]
    )
    dist.mat <- dist.mat[-unique(delete.row),]
  }
  else {
    temp.merge[i,] <- dist.mat[3:4]
    temp.height[i] <- dist.mat[1]
  }
}
###combine data into a list---similar to output of hclust function in S-Plus###

```r
mlen <- length(temp.merge[,1])
temp.order <- NULL
temp.order <- order.fun(temp.order,temp.merge,mlen)
link.adj <- list(temp.merge,temp.height,temp.order)
names(link.adj) <- c("merge","height","order")

return (link.adj)
```

###Constrained Clustering (using average linkage as distance criteria)###

```r
hclust.adj.ave <- function(data.vec,nr,nc,adjacent.distance) {
  ntot <- nr*nc

  # general positions for any data matrix
  # data.pos represents a matrix with the pairings of each point of the
data.pos <- matrix(c(rep(1:nr, times=nc),rep(1:nc, each=nr)),ncol=2,byrow=F,dimnames=list(NULL,c("row","col")))

  # temp.dist contains the distances between each data point of the data
  temp.dist <- dist(data.vec)

  # temp.dist.pos contains the distances between each physical location in
  temp.dist.pos <- dist(data.pos)

  # lists the observation pairs that correspond to the distances from the
  # S-PLUS dist function
  tt.cl <- tt.c2 <- NULL
  for (i in 1:(ntot-1)) {
    temp.seq <- seq(1:(ntot-i))+i
    tt.c2 <- c(tt.c2,temp.seq)
    tt.cl <- c(tt.cl,numeric(length(temp.seq))+i)
  }
  tt <- matrix(-c(tt.cl,tt.c2),ncol=2,byrow=F)

  # temp.merge, temp.height, and temp.order match the output from the
```
S-PLUS hclust function dist.mat contains the distance between data points, physical locations and the data index for which the distances correspond

```
temp.merge <- matrix(0,nrow=ntot-1,ncol=2)
temp.height <- temp.order <- numeric(length = ntot-1)
dist.mat <- matrix(c(temp.dist,temp.dist.pos,tt),ncol=4,byrow=F,dimnames=list(NULL,c("dist","pos dist","","")))
```

This algorithm clusters based on average distance

```
for (i in 1:(ntot-1)) {
  if (length(dist.mat) > 4) { 
    min.dist <- min(dist.mat[(dist.mat[,2] <
adjacent.distance)&(dist.mat[,1]>0),1])
    temp.pos <- which(dist.mat[,1]==min.dist)[1]
    temp.merge[i,] <- dist.mat[temp.pos,3:4][order(dist.mat[temp.pos,3:4])]
    temp.height[i] <- min.dist
    dist.mat <-
    dist.mat[!((dist.mat[,3]==temp.merge[i,][1])&(dist.mat[,4]==temp.merge[i,][2])|((
dist.mat[,3]==temp.merge[i,][2])&(dist.mat[,4]==temp.merge[i,][1]))),]
    temp.pairs <- temp.merge[i,]
    pos.lst <- which((dist.mat[,3]==i)|(dist.mat[,4]==i))
    delete.row <- NULL
    for (k in 1:length(pos.lst)) { 
```

```
temp.pairs <- dist.mat[pos.lst[k],3:4]
ind.pos <-
which(((dist.mat[pos.lst,3]==temp.pairs[1])&(dist.mat[pos.lst,4]==temp.pairs[2]))|((
  dist.mat[pos.lst,3]==temp.pairs[2])&(dist.mat[pos.lst,4]==temp.pairs[1])))
  dist.mat[pos.lst[ind.pos],1] <- mean(dist.mat[pos.lst[ind.pos],1])
  dist.mat[pos.lst[ind.pos],2] <- min(dist.mat[pos.lst[ind.pos],2])
delete.row <- c(delete.row,pos.lst[ind.pos[2:length(ind.pos)]])
}  
dist.mat <- dist.mat[-unique(delete.row),]
}
else {
  temp.merge[i,] <- dist.mat[3:4]
  temp.height[i] <- dist.mat[1]
}
}

#---------------------------------------------------------------#
###combine data into a list---similar to output of hclust function in S-Plus###
#---------------------------------------------------------------#
mlen <- length(temp.merge[,1])
temp.order <- NULL
temp.order <- order.fun(temp.order,temp.merge,mlen)
link.adj <- list(temp.merge,temp.height,temp.order)
names(link.adj) <- c("merge","height","order")

  return (link.adj)
}
B.3 Basic Window (Central) Method Function

```r
Central.Method.Cluster <- function(data.grid, distance.type, estimator.type){
  data.rows <- nrow(data.grid)
  data.columns <- ncol(data.grid)
  sz <- data.rows*data.columns

  zval <- c(data.grid)
  c.row <- diag(c(1:data.rows))
  c.col <- diag(c(1:data.columns))
  iwd.row <- diag(c(1),data.columns)
  iwd.col <- diag(c(1),data.rows)
  yval <- diag(kronecker(c.col,iwd.col))
  xval <- diag(kronecker(iwd.row,c.row))

  for (i in 1:7) {
    for (cc in 1:data.columns) {
      h.max <- min(i,data.columns-cc)
      h.min <- max(1-cc,-i)
      for (rr in 1:data.rows) {
        v.max <- min(i,data.rows-rr)
        v.min <- max(1-rr,-i)
        temp.pos.c <-
        diag(kronecker(diag(c(h.min:h.max)),diag(length(v.min:v.max))))
        temp.pos.r <-
        diag(kronecker(diag(length(h.min:h.max)),diag(c(v.min:v.max))))
        temp.dist <-
        matrix(c(temp.pos.r,temp.pos.c),ncol=2,byrow=F,dimnames=list(NULL,c("row","col")))
        dist.pos <- sqrt(temp.dist[,1]^2+temp.dist[,2]^2)
        temp.window <- temp.dist[(dist.pos > i-.5)&(dist.pos < i+.5),]
        temp.window[,1] <- temp.window[,1]+rr
        temp.window[,2] <- temp.window[,2]+cc
        diff.use <- data.grid[temp.window]-data.grid[rr,cc]
      }
    }
  }
}
```
temp.b <- c(temp.b, gamma.bar(diff.use))
temp.t <- c(temp.t, gamma.tilda(diff.use))
temp.cl <- c(temp.cl, gamma.classic(diff.use))

#---------------------------------------------------------------------------#
###estimates of the variogram at each lag are split into separate arrays   ###
### (1 through 7)                   ###
#---------------------------------------------------------------------------#

if (estimator.type == "gamma bar") {
#Gamma Bar Estimator
  lag.b1 <- temp.b[1:sz]
  lag.b2 <- temp.b[(sz+1):(2*sz)]
  lag.b3 <- temp.b[(2*sz+1):(3*sz)]
  lag.b4 <- temp.b[(3*sz+1):(4*sz)]
  lag.b5 <- temp.b[(4*sz+1):(5*sz)]
  lag.b6 <- temp.b[(5*sz+1):(6*sz)]
  lag.b7 <- temp.b[(6*sz+1):(7*sz)]

  ##90th Lag Percentile
  q90.b <- numeric(sz)
  for (i in 1:sz) {
    q90.b[i] <- quantile(c(lag.b1[i],lag.b2[i],lag.b3[i],lag.b4[i],lag.b5[i],lag.b6[i],lag.b7[i]),.9 ,na.rm=T)
  }

  measure.b <- matrix(c(xval,yval,zval,lag.b1,lag.b2,lag.b3,lag.b4,q90.b),nrow=sz,ncol=8,byrow=F,dmnames=list(NULL,c("xval","yval","zval","lag1","lag2","lag3","lag4","q90")))
  mstand.b <- scale(measure.b,center=T,scale=T)
  return (mstand.b)
}

if (estimator.type == "gamma tilda") {
#Gamma Tilda Estimator
  lag.t1 <- temp.t[1:sz]
  lag.t2 <- temp.t[(sz+1):(2*sz)]
  lag.t3 <- temp.t[(2*sz+1):(3*sz)]
  lag.t4 <- temp.t[(3*sz+1):(4*sz)]
  lag.t5 <- temp.t[(4*sz+1):(5*sz)]
  lag.t6 <- temp.t[(5*sz+1):(6*sz)]
  lag.t7 <- temp.t[(6*sz+1):(7*sz)]

  ##90th Lag Percentile
  q90.t <- numeric(sz)
  for (i in 1:sz) {
    q90.t[i] <- quantile(c(lag.t1[i],lag.t2[i],lag.t3[i],lag.t4[i],lag.t5[i],lag.t6[i],lag.t7[i]),.9 ,na.rm=T)
  }

  measure.t <- matrix(c(xval,yval,zval,lag.t1,lag.t2,lag.t3,lag.t4,q90.t),nrow=sz,ncol=8,byrow=F,dmnames=list(NULL,c("xval","yval","zval","lag1","lag2","lag3","lag4","q90")))
  mstand.t <- scale(measure.t,center=T,scale=T)
  return (mstand.t)
if (estimator.type == "classical") {
    # Classical Estimator
    lag.cl1 <- temp.cl[1:sz]
    lag.cl2 <- temp.cl[(sz+1):2*sz]
    lag.cl3 <- temp.cl[(2*sz+1):3*sz]
    lag.cl4 <- temp.cl[(3*sz+1):4*sz]
    lag.cl5 <- temp.cl[(4*sz+1):5*sz]
    lag.cl6 <- temp.cl[(5*sz+1):6*sz]
    lag.cl7 <- temp.cl[(6*sz+1):7*sz]

    # 90th Lag Percentile
    q90.cl <- numeric(sz)
    for (i in 1:sz) {
        q90.cl[i] <- quantile(c(lag.cl1[i],lag.cl2[i],lag.cl3[i],lag.cl4[i],lag.cl5[i],lag.cl6[i],lag.cl7[i]),.9,na.rm=T)
    }

    measure.cl <- matrix(c(xval,yval,zval,lag.cl1,lag.cl2,lag.cl3,lag.cl4,q90.cl),nrow=sz,ncol=8,by row=F,dimnames=list(NULL,c("xval","yval","zval","lag1","lag2","lag3","lag4","q90")))
    mstand.cl <- scale(measure.cl,center=T,scale=T)

    return (mstand.cl)
}
}
### B.4 Adjacent Constraint Method Function

```r
#--- Beginning of Code for Adjacent Constraint Method Function
#
Adjacent.Constraint.Cluster <- function(data.grid, distance.type, adjacent.distance, maximum.groups, estimator.type){

data.rows <- nrow(data.grid)
data.columns <- ncol(data.grid)
sz <- data.rows*data.columns

#--- defining the measurement value, and the location (row/column number) ---#
#--- denoted by x and y ---#
#---
zval <- c(data.grid)
c.row <- diag(c(1:ncol(grid)))
c.col <- diag(c(1:nrow(grid)))
iwd.row <- diag(c(1),nrow(grid))
iwd.col <- diag(c(1),ncol(grid))
yval <- diag(kronecker(c.col,iwd.col))
xval <- diag(kronecker(iwd.row,c.row))

#--- Step 1 -- Get estimates of the variogram ---#
#---
temp.b <- numeric(0)
temp.t <- numeric(0)
temp.cl <- numeric(0)

#--- Estimates of the variogram are calculated at lags 1 through 7 ---#
#--- For each cell in the data grid, this function determines the other data points to be included in the calculations of the variogram at each lag ---#
#--- (1 through 7) ---#
#---
for (i in 1:7) {
  for (cc in 1:ncol(grid)) {
    h.max <- min(i,ncol(grid)-cc)
    h.min <- max(1-cc,-i)

    for (rr in 1:nrow(grid)) {
      v.max <- min(i,nrow(grid)-rr)
      v.min <- max(1-rr,-i)

      temp.pos.c <-
      diag(kronecker(diag(c(h.min:h.max)),diag(length(v.min:v.max))))
      temp.pos.r <-
      diag(kronecker(diag(length(h.min:h.max)),diag(c(v.min:v.max))))
      temp.dist <-
      matrix(c(temp.pos.r,temp.pos.c),ncol=2,byrow=F,dimnames=list(NULL,c("row","col")))
      dist.pos <- sqrt(temp.dist[,1]^2+temp.dist[,2]^2)

      temp.window <- temp.dist[(dist.pos > i-.5)&(dist.pos < i+.5),]
      temp.window[,1] <- temp.window[,1]+rr
      temp.window[,2] <- temp.window[,2]+cc
      diff.use <- data.grid[temp.window]-data.grid[rr,cc]
    }
  }
}
```

---

119
temp.b <- c(temp.b, gamma.bar(diff.use))
temp.t <- c(temp.t, gamma.tilda(diff.use))
temp.cl <- c(temp.cl, gamma.classic(diff.use))

if (estimator.type == "gamma bar") {
  # Gamma Bar Estimator
  lag.b1 <- temp.b[1:sz]
  lag.b2 <- temp.b[(sz+1):(2*sz)]
  lag.b3 <- temp.b[(2*sz+1):(3*sz)]
  lag.b4 <- temp.b[(3*sz+1):(4*sz)]
  lag.b5 <- temp.b[(4*sz+1):(5*sz)]
  lag.b6 <- temp.b[(5*sz+1):(6*sz)]
  lag.b7 <- temp.b[(6*sz+1):(7*sz)]

  # 90th Lag Percentile
  q90.b <- numeric(sz)
  for (i in 1:sz) {
    q90.b[i] <- quantile(c(lag.b1[i], lag.b2[i], lag.b3[i], lag.b4[i], lag.b5[i], lag.b6[i], lag.b7[i]), .9, na.rm=T)
  }

  measure.b <- matrix(c(xval, yval, zval, lag.b1, lag.b2, lag.b3, lag.b4, q90.b), nrow=sz, ncol=8, byrow=F, dimnames=list(NULL, c("xval", "yval", "zval", "lag1", "lag2", "lag3", "lag4", "q90")))
  mstand.b <- scale(measure.b, center=T, scale=T)
  return (mstand.b)
}

if (estimator.type == "gamma tilda") {
  # Gamma Tilda Estimator
  lag.t1 <- temp.t[1:sz]
  lag.t2 <- temp.t[(sz+1):(2*sz)]
  lag.t3 <- temp.t[(2*sz+1):(3*sz)]
  lag.t4 <- temp.t[(3*sz+1):(4*sz)]
  lag.t5 <- temp.t[(4*sz+1):(5*sz)]
  lag.t6 <- temp.t[(5*sz+1):(6*sz)]
  lag.t7 <- temp.t[(6*sz+1):(7*sz)]

  # 90th Lag Percentile
  q90.t <- numeric(sz)
  for (i in 1:sz) {
    q90.t[i] <- quantile(c(lag.t1[i], lag.t2[i], lag.t3[i], lag.t4[i], lag.t5[i], lag.t6[i], lag.t7[i]), .9, na.rm=T)
  }

  measure.t <- matrix(c(xval, yval, zval, lag.t1, lag.t2, lag.t3, lag.t4, q90.t), nrow=sz, ncol=8, byrow=F, dimnames=list(NULL, c("xval", "yval", "zval", "lag1", "lag2", "lag3", "lag4", "q90")))
  mstand.t <- scale(measure.t, center=T, scale=T)
return (mstand.t)
}

if (estimator.type == "classical") {

# Classical Estimator
lag.cl1 <- temp.cl[1:sz]
lag.cl2 <- temp.cl[(sz+1):(2*sz)]
lag.cl3 <- temp.cl[(2*sz+1):(3*sz)]
lag.cl4 <- temp.cl[(3*sz+1):(4*sz)]
lag.cl5 <- temp.cl[(4*sz+1):(5*sz)]
lag.cl6 <- temp.cl[(5*sz+1):(6*sz)]
lag.cl7 <- temp.cl[(6*sz+1):(7*sz)]

## 90th Lag Percentile
q90.cl <- numeric(sz)
for (i in 1:sz) {
  q90.cl[i] <- quantile(c(lag.cl1[i], lag.cl2[i], lag.cl3[i], lag.cl4[i], lag.cl5[i], lag.cl6[i], lag.cl7[i]), .9, na.rm = T)
}

measure.cl <- matrix(c(xval, yval, zval, lag.cl1, lag.cl2, lag.cl3, lag.cl4, q90.cl), nrow = sz, ncol = 8, byrow = F, dimnames = list(NULL, c("xval", "yval", "zval", "lag1", "lag2", "lag3", "lag4", "q90")))
mstand.cl <- scale(measure.cl, center = T, scale = T)

return (mstand.cl)
}
B.5 Two Part Method Function

```r
#----------------------------------------------------------------------#
###Beginning of Code for Two Part Method Function                  ###
#----------------------------------------------------------------------#
Two.Part.Method.Cluster <- function(data.grid, distance.type, adjacent.distance,
                                      maximum.groups, estimator.type){
  data.rows <- nrow(data.grid)
  data.columns <- ncol(data.grid)
  sz <- data.rows*data.columns

  #----------------------------------------------------------------------#
  ###defining the measurement value, and the location (row/column number)###
  ##denoted by x and y                                                  ##
  #----------------------------------------------------------------------#
  zval <- c(data.grid)
  c.row <- diag(c(1:data.rows))
  c.col <- diag(c(1:data.columns))
  iwd.row <- diag(c(1),data.columns)
  iwd.col <- diag(c(1),data.rows)
  yval <- diag(kronecker(c.col,iwd.col))
  xval <- diag(kronecker(iwd.row,c.row))

  #----------------------------------------------------------------------#
  ###Step 1 -- Cluster Based upon Mean Structure (ignore location, limiting ###
  ###distance to be "1.1")                                           ###
  #----------------------------------------------------------------------#
  measure1 <- matrix(c(xval,yval,zval),ncol=3,byrow=F)
  mstd1 <- scale(measure1, center=T ,scale=T)
  ms.w <- mstd1%*%diag(c(0,0,1))
  if (distance.type == "complete")
    mean.adj.comp <- hclust.adj.com(ms.w,data.rows,data.columns, adjacent.distance)
  if (distance.type == "average")
    mean.adj.comp <- hclust.adj.ave(ms.w,data.rows,data.columns, adjacent.distance)

  #----------------------------------------------------------------------#
  ###Step 2 -- Get "good" estimates of the variogram                 ###
  #----------------------------------------------------------------------#
  done.test <- 0
  loop.number <- 1
  while (done.test == 0) {
    tree.mean.temp <-
      matrix(cutree(mean.adj.comp,k=loop.number),nrow=data.rows,ncol=data.columns,
              byrow=F)
    temp.b <- numeric(0)
    temp.t <- numeric(0)
    temp.cl <- numeric(0)
```
for (i in 1:7)
{
for (cc in 1:data.columns) {
    h.max <- min(i, data.columns - cc)
    h.min <- max(1 - cc, -i)

    for (rr in 1:data.rows) {
        v.max <- min(i, data.rows - rr)
        v.min <- max(1 - rr, -i)

        temp.group <- tree.mean.temp[rr, cc]
        temp.pos.c <-
        diag(kronecker(diag(c(h.min:h.max)), diag(length(v.min:v.max))))
        temp.pos.r <-
        diag(kronecker(diag(length(h.min:h.max)), diag(c(v.min:v.max))))

        temp.dist <-
        matrix(c(temp.pos.r, temp.pos.c), ncol = 2, byrow = F, dimnames = list(NULL, c("row", "col")))

        dist.pos <- sqrt(temp.dist[, 1]^2 + temp.dist[, 2]^2)
        temp.window <- temp.dist[(dist.pos > i - 0.5) & (dist.pos < i + 0.5),]
        temp.window[, 1] <- temp.window[, 1] + rr
        temp.window[, 2] <- temp.window[, 2] + cc

        diff <- data.grid[temp.window] - data.grid[rr, cc]
        diff.use <- diff[which(tree.mean.temp[temp.window] == temp.group)]

        if (length(diff.use) > 0) {
            temp.b <- c(temp.b, gamma.bar(diff.use))
            temp.t <- c(temp.t, gamma.tilda(diff.use))
            temp.cl <- c(temp.cl, gamma.classic(diff.use))
        } else {
            temp.b <- c(temp.b, -1)
            temp.t <- c(temp.t, -1)
            temp.cl <- c(temp.cl, -1)
        }
    }
}

lag.1.b <- temp.b[1:400]
lag.1.t <- temp.t[1:400]
lag.1.cl <- temp.cl[1:400]

if (max(lag.1.b) < qchisq(.999, mean(lag.1.b)))
    done.test <- 1

loop.number = loop.number + 1
## Gamma Bar Estimator

```r
lag.b1 <- temp.b[1:sz]
lag.b2 <- temp.b[(sz+1):(2*sz)]
lag.b3 <- temp.b[(2*sz+1):(3*sz)]
lag.b4 <- temp.b[(3*sz+1):(4*sz)]
lag.b5 <- temp.b[(4*sz+1):(5*sz)]
lag.b6 <- temp.b[(5*sz+1):(6*sz)]
lag.b7 <- temp.b[(6*sz+1):(7*sz)]
```

```r
## lag set to -1 if region is not large enough to calculate.
## in this case, set estimate to value of next lowest lag
lag.b2[lag.b2==-1] <- lag.b1[lag.b2==-1]
lag.b3[lag.b3==-1] <- lag.b2[lag.b3==-1]
lag.b4[lag.b4==-1] <- lag.b3[lag.b4==-1]
lag.b5[lag.b5==-1] <- lag.b4[lag.b5==-1]
lag.b6[lag.b6==-1] <- lag.b5[lag.b6==-1]
lag.b7[lag.b7==-1] <- lag.b6[lag.b7==-1]
```

## 90th Lag Percentile
```r
q90.b <- numeric(sz)
for (i in 1:sz) {
  q90.b[i] <- quantile(c(lag.b1[i],lag.b2[i],lag.b3[i],lag.b4[i],lag.b5[i],lag.b6[i],lag.b7[i]), .9, na.rm=T)
}
```

```r
measure.b <- matrix(c(xval,yval,zval,lag.b1,lag.b2,lag.b3,lag.b4,q90.b), nrow=sz, ncol=8, byrow=F, dimnames=list(NULL, c("xval","yval","zval","lag1","lag2","lag3","lag4","q90")))
mstand.b <- scale(measure.b, center=T, scale=T)
return(mstand.b)
```

```r
if (estimator.type == "gamma tilda") {
# Gamma Tilda Estimator
lag.t1 <- temp.t[1:sz]
lag.t2 <- temp.t[(sz+1):(2*sz)]
lag.t3 <- temp.t[(2*sz+1):(3*sz)]
lag.t4 <- temp.t[(3*sz+1):(4*sz)]
lag.t5 <- temp.t[(4*sz+1):(5*sz)]
lag.t6 <- temp.t[(5*sz+1):(6*sz)]
lag.t7 <- temp.t[(6*sz+1):(7*sz)]
```

```r
## lag set to -1 if region is not large enough to calculate.
## in this case, set estimate to value of next lowest lag
lag.t2[lag.t2==-1] <- lag.t1[lag.t2==-1]
lag.t3[lag.t3==-1] <- lag.t2[lag.t3==-1]
lag.t4[lag.t4==-1] <- lag.t3[lag.t4==-1]
lag.t5[lag.t5==-1] <- lag.t4[lag.t5==-1]
lag.t6[lag.t6==-1] <- lag.t5[lag.t6==-1]
lag.t7[lag.t7==-1] <- lag.t6[lag.t7==-1]
```

## 90th Lag Percentile
```r
q90.t <- numeric(sz)
for (i in 1:sz) {
  q90.t[i] <- quantile(c(lag.t1[i],lag.t2[i],lag.t3[i],lag.t4[i],lag.t5[i],lag.t6[i],lag.t7[i]), .9, na.rm=T)
}
```
measure.t <-
matrix(c(xval,yval,zval,lag.t1,lag.t2,lag.t3,lag.t4,q90.t),nrow=sz,ncol=8,byrow =F,dimnames=list(NULL,c("xval","yval","zval","lag1","lag2","lag3","lag4","q90")))
mstand.t <- scale(measure.t,center=T,scale=T)
return(mstand.t)
}

if (estimator.type == "classical") {
#Classical Estimator
  lag.cl1 <- temp.cl[1:sz]
  lag.cl2 <- temp.cl[(sz+1):(2*sz)]
  lag.cl3 <- temp.cl[(2*sz+1):(3*sz)]
  lag.cl4 <- temp.cl[(3*sz+1):(4*sz)]
  lag.cl5 <- temp.cl[(4*sz+1):(5*sz)]
  lag.cl6 <- temp.cl[(5*sz+1):(6*sz)]
  lag.cl7 <- temp.cl[(6*sz+1):(7*sz)]

  ##lag set to -1 if region is not large enough to calculate.
  ##in this case, set estimate to value of next lowest lag
  lag.cl2[lag.cl2==-1] <- lag.cl1[lag.cl2==-1]
  lag.cl3[lag.cl3==-1] <- lag.cl2[lag.cl3==-1]
  lag.cl4[lag.cl4==-1] <- lag.cl3[lag.cl4==-1]
  lag.cl5[lag.cl5==-1] <- lag.cl4[lag.cl5==-1]
  lag.cl6[lag.cl6==-1] <- lag.cl5[lag.cl6==-1]
  lag.cl7[lag.cl7==-1] <- lag.cl6[lag.cl7==-1]

  ##90th Lag Percentile
  q90.cl <- numeric(sz)
  for (i in 1:sz) {
    q90.cl[i] <- quantile(c(lag.cl1[i],lag.cl2[i],lag.cl3[i],lag.cl4[i],lag.cl5[i],lag.cl6[i],
                           lag.cl7[i]),.9,na.rm=T)
  }

  measure.cl <-
matrix(c(xval,yval,zval,lag.cl1,lag.cl2,lag.cl3,lag.cl4,q90.cl),nrow=sz,ncol=8,byrow=F,dimnames=list(NULL,c("xval","yval","zval","lag1","lag2","lag3","lag4","q90")))
mstand.cl <- scale(measure.cl,center=T,scale=T)
return(mstand.cl)
}
B.6 Simulated Data Examples

```r
# Chapter 3 Examples

chapter.3.1.1 <- matrix(0+rfsim(grid,covfun=exp.cov,range=3,sill=3,nc=10000),wd,wd)
chapter.3.1.2 <- matrix(8+rfsim(grid,covfun=exp.cov,range=3,sill=3,nc=10000),wd,wd)
chapter.3.1.3 <- matrix(4+rfsim(grid,covfun=exp.cov,range=3,sill=3,nc=10000),wd,wd)
Chapter.3.Data.Set.1 <- chapter.3.1.1
Chapter.3.Data.Set.1[grp=="Grp 2"] <- chapter.3.1.2[grp=="Grp 2"]
Chapter.3.Data.Set.1[grp=="Grp 3"] <- chapter.3.1.3[grp=="Grp 3"]

chapter.3.2.1 <- matrix(4+rfsim(grid,covfun=exp.cov,range=5,sill=3,nc=10000),wd,wd)
chapter.3.2.2 <- matrix(4+rfsim(grid,covfun=exp.cov,range=5,sill=1,nc=10000),wd,wd)
chapter.3.2.3 <- matrix(4+rfsim(grid,covfun=exp.cov,range=5,sill=5,nc=10000),wd,wd)
Chapter.3.Data.Set.2 <- chapter.3.2.1
Chapter.3.Data.Set.2[grp=="Grp 2"] <- chapter.3.2.2[grp=="Grp 2"]
Chapter.3.Data.Set.2[grp=="Grp 3"] <- chapter.3.2.3[grp=="Grp 3"]

par(mfrow=c(1,1))
image(Chapter.3.Data.Set.1)
persp(Chapter.3.Data.Set.1)
image(Chapter.3.Data.Set.2)
persp(Chapter.3.Data.Set.2)

example.3.1.cluster <- hclust(dist(c(Chapter.3.Data.Set.1)), method = 'compact')
par(mfrow=c(1,1))
image(Chapter.3.Data.Set.1)
persp(Chapter.3.Data.Set.1)
for (i in 2:9) {
  tree.adj.constraint <-
  matrix(cutree(example.3.1.cluster,k=i),nrow=data.rows,ncol=data.columns,byrow=F)
  index <- get.index(grp.mat,tree.adj.constraint)
  title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ",
                 round(index[1],digits=3), ", Rand = ",round(index[2],digits=3),collapse = "\""))
}

example.3.2.cluster <- hclust(dist(c(Chapter.3.Data.Set.2)), method = 'compact')
par(mfrow=c(1,1))
image(Chapter.3.Data.Set.2)
for (i in 2:9) {
  tree.adj.constraint <-
  matrix(cutree(example.3.2.cluster,k=i),nrow=data.rows,ncol=data.columns,byrow=F)
  index <- get.index(grp.mat,tree.adj.constraint)
  title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ",
                 round(index[1],digits=3), ", Rand = ",round(index[2],digits=3),collapse = "\""))
}

## Chapter 3 Basic Window Method Example

Chapter.3.Data.Set.1.Central <- Central.Method.Cluster(Chapter.3.Data.Set.1,
"complete","gamma bar")
for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(1,1,3),w.spatial*c(2,1,1,0,1)))
}
```

msw <- Chapter.3.Data.Set.1.Central%*%weight.adjcon

msw <- dist(data.matrix(msw))

constraint.cluster.3.1 <- hclust(msw, method = 'compact')

par(mfrow=c(3,3))
image(testdata.1.grid)
title(main=paste("Original Data Set\n a = ", inc*.25))
for (i in 2:18) {
  tree.adj.constraint <-
  matrix(cutree(constraint.cluster.3.1,k=i),nrow=data.rows,ncol=data.columns,
  byrow=F)
  index <- get.index(grp.mat,tree.adj.constraint)
  image(tree.adj.constraint)
title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ",
  round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ""))
}

Chapter.3.Data.Set.2.Central <- Central.Method.Cluster(Chapter.3.Data.Set.2, "complete", "gamma bar")

for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(1,1,3),w.spatial*c(2,1,1,0,1)))
  msw <- Chapter.3.Data.Set.2.Central%*%weight.adjcon
  msw <- dist(data.matrix(msw))

  constraint.cluster.3.2 <- hclust(msw, method = 'compact')

  par(mfrow=c(3,3))
  image(Chapter.3.Data.Set.2)
title(main=paste("Original Data Set\n a = ", inc*.25))
for (i in 2:18) {
  tree.adj.constraint <-
  matrix(cutree(constraint.cluster.3.2,k=i),nrow=data.rows,ncol=data.columns,
  byrow=F)
  index <- get.index(grp.mat,tree.adj.constraint)
  image(tree.adj.constraint)
title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ",
  round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ""))
}

###Chapter 3 Adjacent Contstraint Method Example


for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
  msw <- Chapter.3.Data.Set.1.Adjacent%*%weight.adjcon

  constraint.cluster.3.1 <- hclust.adj.com(msw,data.rows,data.columns,1.5)
  par(mfrow=c(3,3))
}
```r
image(Chapter.3.Data.Set.1)
title(main=paste("Original Data Set\n a = ", inc*.25))
for (i in 2:27) {
  tree.adj.constraint <-
  matrix(cutree(constraint.cluster.3.1,k=i),nrow=data.rows,ncol=data.columns,byrow=F)
  index <- get.index(grp.mat,tree.adj.constraint)
  title(main=paste("For ",i," Groups, the indexes are:
  Jaccard = ", round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ""))
}

Chapter.3.Data.Set.2.Adjacent <- Adjacent.Constraint.Cluster (Chapter.3.Data.Set.2,
"complete", 1.5, 20, "gamma bar")
for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
  msw <- Chapter.3.Data.Set.2.Adjacent%*%weight.adjcon
  constraint.cluster.3.2 <- hclust.adj.com(msw, data.rows, data.columns, 1.5)

  par(mfrow=c(3,3))
  image(Chapter.3.Data.Set.2)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <-
    matrix(cutree(constraint.cluster.3.2,k=i),nrow=data.rows,ncol=data.columns,byrow=F)
    index <- get.index(grp.mat,tree.adj.constraint)
    title(main=paste("For ",i," Groups, the indexes are:
    Jaccard = ", round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ""))
  }
}

###Chapter 3 Two Part Method Example

Chapter.3.Data.Set.1.TwoPart <- Two.Part.Method.Cluster (Chapter.3.Data.Set.1,
"complete", 1.1, 20, "gamma bar")
for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
  msw <- Chapter.3.Data.Set.1.TwoPart%*%weight.adjcon
  constraint.cluster.3.1 <- hclust.adj.com(msw, data.rows, data.columns, 1.1)

  par(mfrow=c(3,3))
  image(Chapter.3.Data.Set.1)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <-
    matrix(cutree(constraint.cluster.3.1,k=i),nrow=data.rows,ncol=data.columns,byrow=F)
    index <- get.index(grp.mat,tree.adj.constraint)
  }
```

for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
  msw <- Chapter.3.Data.Set.2.TwoPart%*%weight.adjcon
  constraint.cluster.3.2 <- hclust.adj.com(msw, data.rows, data.columns, 1.1)
  par(mfrow=c(3,3))
  image(Chapter.3.Data.Set.2)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <-
      matrix(cutree(constraint.cluster.3.2,k=i),nrow=data.rows,ncol=data.columns,
             byrow=F)
    index <- get.index(grp.mat,tree.adj.constraint)
    image(tree.adj.constraint)
    title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ", round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ""))
  }
}

---------------------------------------------------------------------------#
###Analysis of Simulated Data Sets with above functions                   ###
---------------------------------------------------------------------------#
grp.mat <- grp
grp.mat[grp.mat == "Grp 1"] <- 1
grp.mat[grp.mat == "Grp 2"] <- 2
grp.mat[grp.mat == "Grp 3"] <- 3
grp.mat <- matrix(as.numeric(grp.mat),20,20)
---------------------------------------------------------------------------#
###Central Method - Data Set 1                                           ###
---------------------------------------------------------------------------#
                                                  "gamma bar")
for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(1,1,3),w.spatial*c(2,1,1,0,1)))
  msw <- datacluster.1.Central%*%weight.adjcon
  msw <- dist(data.matrix(msw))
  constraint.cluster.1 <- hclust(msw, method = 'compact')
  par(mfrow=c(3,3))
  image(testdata.1.grid)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
tree.adj.constraint <- matrix(cutree(constraint.cluster.1,k=i),nrow=data.rows,ncol=data.columns,byrow=F)
index <- get.index(grp.mat,tree.adj.constraint)
image(tree.adj.constraint)
title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ",round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collaps = ""))
}

###Central Method - Data Set 2

for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(1,1,3),w.spatial*c(2,1,1,0,1)))
  msw <- datacluster.2.Central%*%weight.adjcon
  msw <- dist(data.matrix(msw))
  constraint.cluster.2 <- hclust(msw, method = 'compact')
  par(mfrow=c(3,3))
  image(testdata.2.grid)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <- matrix(cutree(constraint.cluster.2,k=i),nrow=data.rows,ncol=data.columns,byrow=F)
    index <- get.index(grp.mat,tree.adj.constraint)
    image(tree.adj.constraint)
    title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ",round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collaps = ""))
  }
}

###Central Method - Data Set 3

for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(1,1,3),w.spatial*c(2,1,1,0,1)))
  msw <- datacluster.3.Central%*%weight.adjcon
  msw <- dist(data.matrix(msw))
  constraint.cluster.3 <- hclust(msw, method = 'compact')
  par(mfrow=c(3,3))
  image(testdata.3.grid)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <- matrix(cutree(constraint.cluster.3,k=i),nrow=data.rows,ncol=data.columns,byrow=F)
    index <- get.index(grp.mat,tree.adj.constraint)
    image(tree.adj.constraint)
    title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ",round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collaps = ""))
  }
}
tree.adj.constraint <-
matrix(cutree(constraint.cluster.3,k=i),nrow=data.rows,ncol=data.columns
,byrow=F)
index <- get.index(grp.mat,tree.adj.constraint)
image(tree.adj.constraint)
title(main=paste("For ",i," Groups, the indexes are: 
Jaccard = ",
round(index[1],digits=3), " Rand = ",round(index[2],digits=3),
collapse = ""))
}

datacluster.4.Central <- Central.Method.Cluster(testdata.4.grid, "complete", "gamma bar")
for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(1,1,3),w.spatial*c(2,1,1,0,1)))
  msw <- datacluster.4.Central%*%weight.adjcon
  msw <- dist(data.matrix(msw))
  constraint.cluster.4 <- hclust(msw, method = 'compact')
  par(mfrow=c(3,3))
  image(testdata.4.grid)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <-
    matrix(cutree(constraint.cluster.4,k=i),nrow=data.rows,ncol=data.columns,byrow=F)
    index <- get.index(grp.mat,tree.adj.constraint)
    image(tree.adj.constraint)
    title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ",
    round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ""))
  }
}

for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
  msw <- datacluster.1.Adjacent%*%weight.adjcon
  constraint.cluster.1 <- hclust.adj.com(msw, data.rows, data.columns, 1.5)
  par(mfrow=c(3,3))
  image(testdata.1.grid)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <-
    matrix(cutree(constraint.cluster.1,k=i),nrow=data.rows,ncol=data.columns,byrow=F)
    index <- get.index(grp.mat,tree.adj.constraint)
    image(tree.adj.constraint)
    title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ",
    round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ""))
  }
}
### Adjacent Constraint Method -- Data Set 2

```r
datacluster.2.Adjacent <- Adjacent.Constraint.Cluster (testdata.2.grid, "complete", 1.5, 20, "gamma bar")
for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
  msw <- datacluster.2.Adjacent%*%weight.adjcon
  constraint.cluster.2 <- hclust.adj.com(msw, data.rows, data.columns, 1.5)
  par(mfrow=c(3,3))
  image(testdata.2.grid)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <- matrix(cutree(constraint.cluster.2,k=i),nrow=data.rows,ncol=data.columns,
                                 byrow=F)
    index <- get.index(grp.mat,tree.adj.constraint)
    image(tree.adj.constraint)
    title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ",
                     round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ""))
  }
}
```

### Adjacent Constraint Method -- Data Set 3

```r
datacluster.3.Adjacent <- Adjacent.Constraint.Cluster (testdata.3.grid, "complete", 1.5, 20, "gamma bar")
for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
  msw <- datacluster.3.Adjacent%*%weight.adjcon
  constraint.cluster.3 <- hclust.adj.com(msw, data.rows, data.columns, 1.5)
  par(mfrow=c(3,3))
  image(testdata.3.grid)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <- matrix(cutree(constraint.cluster.3,k=i),nrow=data.rows,ncol=data.columns,
                                 byrow=F)
    index <- get.index(grp.mat,tree.adj.constraint)
    image(tree.adj.constraint)
    title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ",
                     round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ""))
  }
}
```
datacluster.4.Adjacent <- Adjacent.Constraint.Cluster (testdata.4.grid, "complete", 1.5, 20, "gamma bar")

for (inc in 0:4) {
    w.mean <- .25*inc
    w.spatial <- 1-w.mean
    weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
    msw <- datacluster.4.Adjacent%*%weight.adjcon

    constraint.cluster.4 <- hclust.adj.com(msw, data.rows, data.columns, 1.5)
    par(mfrow=c(3,3))
    image(testdata.4.grid)
    title(main=paste("Original Data Set\n a = ", inc*.25))
    for (i in 2:27) {
        tree.adj.constraint <- matrix(cutree(constraint.cluster.4,k=i),nrow=data.rows,ncol=data.columns, byrow=F)
        index <- get.index(grp.mat,tree.adj.constraint)
        image(tree.adj.constraint)
        title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ", round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ")}
}

datacluster.1.TwoPart <- Two.Part.Method.Cluster (testdata.1.grid, "complete", 1.1, 20, "gamma bar")

for (inc in 0:4) {
    w.mean <- .25*inc
    w.spatial <- 1-w.mean
    weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
    msw <- datacluster.1.TwoPart%*%weight.adjcon

    constraint.cluster.1 <- hclust.adj.com(msw, data.rows, data.columns, 1.1)
    par(mfrow=c(3,3))
    image(testdata.1.grid)
    title(main=paste("Original Data Set\n a = ", inc*.25))
    for (i in 2:27) {
        tree.adj.constraint <- matrix(cutree(constraint.cluster.1,k=i),nrow=data.rows,ncol=data.columns, byrow=F)
        index <- get.index(grp.mat,tree.adj.constraint)
        image(tree.adj.constraint)
        title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ", round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ")}
index <- get.index(grp.mat,tree.adj.constraint)
image(tree.adj.constraint)
title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ",
round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ""))
}
}

#---------------------------------------------------------------------------#
###Two Part Method -- Data Set 2              ###
#---------------------------------------------------------------------------#
datacluster.2.TwoPart <- Two.Part.Method.Cluster (testdata.2.grid, "complete",
1.1, 20, "gamma bar")
for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
  msw <- datacluster.2.TwoPart%*%weight.adjcon
  constraint.cluster.2 <- hclust.adj.com(msw, data.rows, data.columns, 1.1)
  par(mfrow=c(3,3))
  image(testdata.2.grid)
title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <-
    matrix(cutree(constraint.cluster.2,k=i),nrow=data.rows,ncol=data.columns,
    byrow=F)
    index <- get.index(grp.mat,tree.adj.constraint)
    image(tree.adj.constraint)
title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ",
round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ""))
  }
  }
}

#---------------------------------------------------------------------------#
###Two Part Method -- Data Set 3              ###
#---------------------------------------------------------------------------#
datacluster.3.TwoPart <- Two.Part.Method.Cluster (testdata.3.grid, "complete",
1.1, 20, "gamma bar")
for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
  msw <- datacluster.3.TwoPart%*%weight.adjcon
  constraint.cluster.3 <- hclust.adj.com(msw, data.rows, data.columns, 1.1)
  par(mfrow=c(3,3))
  image(testdata.3.grid)
title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <-
    matrix(cutree(constraint.cluster.3,k=i),nrow=data.rows,ncol=data.columns,
    byrow=F)
    index <- get.index(grp.mat,tree.adj.constraint)
    image(tree.adj.constraint)
title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ",
round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ""))
  }
  }
for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
  msw <- datacluster.4.TwoPart%*%weight.adjcon

  constraint.cluster.4 <- hclust.adj.com(msw, data.rows, data.columns, 1.1)

  par(mfrow=c(3,3))
  image(testdata.4.grid)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <- matrix(cutree(constraint.cluster.4,k=i),nrow=data.rows,ncol=data.columns, byrow=F)
    index <- get.index(grp.mat,tree.adj.constraint)
    image(tree.adj.constraint)
    title(main=paste("For ",i," Groups, the indexes are: \n Jaccard = ", round(index[1],digits=3), " Rand = ",round(index[2],digits=3),collapse = ""))
  }
}
B.7 SFMRI Brain Data Analysis

###Brain Data

```r
a6s10.sort <- a6s10
a6s10.sort[,2] <- 65 - a6s10.sort[,2]
a6s10.sort <- a6s10.sort[order(a6s10.sort[,2], a6s10.sort[,1]), ]
a6s10.mean.0 <- matrix(apply(a6s10.sort[,4:39], 1, mean), nrow = 64, ncol = 64, byrow = F)

###equivalent method to plot the data
a6s10.mean.1 <- interp(a6s10[, 1], 65-a6s10[, 2], apply(a6s10[,4:39], 1, mean), xo = c(1:64), yo = c(1:64))

on.array.sort <- c(a6s10.sort[, 4], a6s10.sort[, 6], a6s10.sort[, 8], a6s10.sort[, 10], a6s10.sort[, 12], a6s10.sort[, 14], a6s10.sort[, 16], a6s10.sort[, 18], a6s10.sort[, 20], a6s10.sort[, 22], a6s10.sort[, 24], a6s10.sort[, 26], a6s10.sort[, 28], a6s10.sort[, 30], a6s10.sort[, 32], a6s10.sort[, 34], a6s10.sort[, 36], a6s10.sort[, 38])
a6s10.on <- matrix(on.array.sort, nrow = 4096, ncol = 18, byrow = F)
a6s10.on.mean <- apply(a6s10.on, 1, mean)

off.array.sort <- c(a6s10.sort[, 5], a6s10.sort[, 7], a6s10.sort[, 9], a6s10.sort[, 11], a6s10.sort[, 13], a6s10.sort[, 15], a6s10.sort[, 17], a6s10.sort[, 19], a6s10.sort[, 21], a6s10.sort[, 23], a6s10.sort[, 25], a6s10.sort[, 27], a6s10.sort[, 29], a6s10.sort[, 31], a6s10.sort[, 33], a6s10.sort[, 35], a6s10.sort[, 37], a6s10.sort[, 39])
a6s10.off <- matrix(off.array.sort, nrow = 4096, ncol = 18, byrow = F)
a6s10.off.mean <- apply(a6s10.off, 1, mean)
a6s10.mean.diff.0 <- matrix(a6s10.on.mean - a6s10.off.mean, nrow = 64, ncol = 64, byrow = F)

###Captures all meaningful brain data
a6s10.mean <- a6s10.mean.0[13:52, 6:48]
a6s10.mean.diff <- a6s10.mean.diff.0[13:52, 6:48]

###Captures portion for computing (physical computing restraints)
a6s10.mean <- a6s10.mean.0[14:34, 15:48]
a6s10.mean.diff <- a6s10.mean.diff.0[14:34, 15:48]
```

```r
par(mfrow=c(2,2))
image(a6s10.mean.0)
persp(a6s10.mean.0)
image(a6s10.mean)
persp(a6s10.mean)
image(a6s10.mean.diff)
persp(a6s10.mean.diff)
```
###increase the following to help with the dynamic memory problems
options(memory = 14336*1024^2)

#----------------------------------#
###Central Method - Brain Data      ###
#----------------------------------#

braincluster.1.Central <- Central.Method.Cluster(a6s10.mean, "complete", "gamma bar")

braindata.rows <- nrow(a6s10.mean)
braindata.columns <- ncol(a6s10.mean)

for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(1,1,3),w.spatial*c(2,1,1,0,1)))
  msw <- braincluster.1.Central%*%weight.adjcon
  msw <- dist(data.matrix(msw))
  constraint.cluster.1 <- hclust(msw, method = 'compact')

  par(mfrow=c(3,3))
  image(a6s10.mean)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <-
    matrix(cutree(constraint.cluster.1,k=i),nrow=braindata.rows,ncol=braindata.columns,byrow=F)
    image(tree.adj.constraint)
    title(main=paste("Data Clustered into ",i," Groups."))
  }
}

braincluster.2.Central <- Central.Method.Cluster(a6s10.mean.diff, "complete", "gamma bar")

braindata.rows <- nrow(a6s10.mean.diff)
braindata.columns <- ncol(a6s10.mean.diff)

for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(1,1,3),w.spatial*c(2,1,1,0,1)))
  msw <- braincluster.2.Central%*%weight.adjcon
  msw <- dist(data.matrix(msw))
  constraint.cluster.2 <- hclust(msw, method = 'compact')

  par(mfrow=c(3,3))
  image(a6s10.mean.diff)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <-
    matrix(cutree(constraint.cluster.2,k=i),nrow=braindata.rows,ncol=braindata.columns,byrow=F)
    image(tree.adj.constraint)
    title(main=paste("Data Clustered into ",i," Groups."))
  }
}
braincluster.1.Adjacent <- Adjacent.Constraint.Cluster(a6s10.mean, "complete", 1.5, "gamma bar")

braindata.rows <- nrow(a6s10.mean)
braindata.columns <- ncol(a6s10.mean)

for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
  msw <- braincluster.1.Adjacent%*%weight.adjcon

  constraint.cluster.1 <- hclust.adj.com(msw, braindata.rows, braindata.columns, 1.5)

  par(mfrow=c(3,3))
  image(a6s10.mean)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <- matrix(cutree(constraint.cluster.1,k=i),nrow=braindata.rows,ncol=braindata.columns,byrow=F)
    image(tree.adj.constraint)
    title(main=paste("Data Clustered into ",i," Groups.\n"))
  }
}

braincluster.2.Adjacent <- Adjacent.Constraint.Cluster(a6s10.mean.diff, "complete", 1.5, "gamma bar")

braindata.rows <- nrow(a6s10.mean.diff)
braindata.columns <- ncol(a6s10.mean.diff)

for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
  msw <- braincluster.2.Adjacent%*%weight.adjcon

  constraint.cluster.2 <- hclust.adj.com(msw, braindata.rows, braindata.columns, 1.5)

  par(mfrow=c(3,3))
  image(a6s10.mean.diff)
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <- matrix(cutree(constraint.cluster.2,k=i),nrow=braindata.rows,ncol=braindata.columns,byrow=F)
    image(tree.adj.constraint)
    title(main=paste("Data Clustered into ",i," Groups.\n"))
  }
}
braincluster.1.TwoPart <- Two.Part.Method.Cluster (a6s10.mean, "complete", 1.1, "gamma bar")

braindata.rows <- nrow(a6s10.mean)
braindata.columns <- ncol(a6s10.mean)

for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
  msw <- braincluster.1.TwoPart%*%weight.adjcon

  constraint.cluster.1 <- hclust.adj.com(msw, braindata.rows, braindata.columns, 1.1)

  par(mfrow=c(3,3))
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <- matrix(cutree(constraint.cluster.1,k=i),nrow=braindata.rows,ncol=braindata.columns,byrow=F)
    image(tree.adj.constraint)
    title(main=paste("Data Clustered into ",i," Groups."))
  }
}

braincluster.2.TwoPart <- Two.Part.Method.Cluster (a6s10.mean.diff, "complete", 1.1, "gamma bar")

braindata.rows <- nrow(a6s10.mean.diff)
braindata.columns <- ncol(a6s10.mean.diff)

for (inc in 0:4) {
  w.mean <- .25*inc
  w.spatial <- 1-w.mean
  weight.adjcon <- diag(c(w.mean*c(0,0,5),w.spatial*c(2,1,1,0,1)))
  msw <- braincluster.2.TwoPart%*%weight.adjcon

  constraint.cluster.2 <- hclust.adj.com(msw, braindata.rows, braindata.columns, 1.1)

  par(mfrow=c(3,3))
  title(main=paste("Original Data Set\n a = ", inc*.25))
  for (i in 2:27) {
    tree.adj.constraint <- matrix(cutree(constraint.cluster.2,k=i),nrow=braindata.rows,ncol=braindata.columns,byrow=F)
    image(tree.adj.constraint)
    title(main=paste("Data Clustered into ",i," Groups."))
  }
}