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Abstract

Dating from the seminal work of Ellison and Glaeser [7] in 1997, a wealth of evidence for the ubiquity of industrial agglomerations has been published. However, most of these results are based on analyses of single (scalar) indices of agglomeration. Hence, it is not surprising that industries deemed to be similar by such indices can often exhibit very different patterns of agglomeration—with respect to the number, size, and spatial extent of individual agglomerations. The purpose of this paper is thus to propose a more detailed spatial analysis of agglomeration in terms of multiple-cluster patterns, where each cluster represents a (roughly) convex set of contiguous regions within which the density of establishments is relatively uniform. The key idea is to develop a simple probability model of multiple clusters, called *cluster schemes*, and then to seek a "best" cluster scheme for each industry by employing a standard model-selection criterion. Our ultimate objective is to provide a richer characterization of spatial agglomeration patterns that will allow more meaningful comparisons of these patterns across industries.

Keywords: Industrial agglomeration, Cluster analysis, Geodesic convexity, Bayesian information criterion

JEL classification: C49, L60, R12, R14

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1 Introduction

Economic agglomeration is the single most dominant feature of industrial location patterns throughout the modern world. In Japan, with a population density more than ten times that of the US, land is generally considered to be extremely scarce. Yet, more than 60% of the total population and more than 80% of total employment are concentrated in less than 3% of total area. Similar observations can be made for any other developed country. The extent of this concentration phenomenon explains why economic agglomeration is now a major topic in urban and regional economics (see, e.g., Henderson and Thisse [9]). Industrial agglomeration has also gained increasing interest in the management literature, dating from the seminal work of Porter [26] on "industrial cluster theory."

In terms of empirical work, a substantial number of studies on industrial agglomeration have been published in the recent decades. Some of them have proposed indices of industrial agglomeration that allow testable comparisons of the degree of agglomeration among industries (Duranton and Overman [6], Brl̈hart and Traeger [4], and Mori et al. [20]). The results of these works suggest that industrial agglomeration is far more ubiquitous than previously believed, and extends well beyond the traditional types of industrial agglomeration (such as information technology industries in Silicon Valley and automobile manufacturing in Detroit). Moreover, the degree of such agglomeration has been shown to vary widely across industries.

But while these studies provide ample evidence for the ubiquity of industrial agglomerations, they tell us very little about the actual *spatial structure* of agglomerations. In particular (to our knowledge), there have been no systematic efforts to determine the number, location and spatial extent of agglomerations within individual industries. Most indices of agglomeration currently in use measure the discrepancy between industry-specific regional distributions of establishments/employment and some hypothetical reference distribution representing "complete dispersion."[1] But even if industries are judged to be

[1] Examples of such reference distributions are the regional distribution of all-industry employment or establishments (e.g., Ellison and Glaeser [7], Duranton and Overman [6]), and that of economic area (e.g., Mori et al. [20]).

similar with respect to these indices, their spatial patterns of agglomeration may appear to be quite different. The reason for this is that such patterns are basically *multidimensional* in nature, and are not easily compared by any single index.

This can be illustrated by a sample of our results for Japanese manufacturing industries (developed in more detail in Section 5 below, and in our companion paper, Mori and Smith [24]). Here we consider two industries that are virtually indistinguishable in terms of their overall degree of spatial concentration (as measured by the Kulback-Leibler measure of concentration sketched in Section 5). But the actual *patterns* of agglomeration for these two industries are quite different. The agglomeration pattern of the first industry, classified as "plastic compounds and reclaimed plastics,"is seen in Figure 13(b). (For now, the area marked in gray can be considered as industrial agglomerations.) The concentration of this industry lies mainly along the inland Industrial Belt extending westward from Tokyo to Hiroshima. Moreover, the individual clusters of establishments within this belt are seen to be densely packed from end to end. Our second industry, classified as "soft drinks and carbonated water,"exhibits a very different pattern of agglomeration. As seen in Figure 14(b), this industry is spread throughout the nation, but exhibits a large number of local agglomerations. A closer inspection of these industries reveals the nature of these differences. On the one hand, plastic components constitute essential inputs to a variety of manufactured goods, from automobiles to TV sets. Hence the concentration of this industry along the industrial belt forms a series of intermediate markets for other manufacturing industries using these components. On the other hand, soft drinks are more directly oriented to final markets serving consumers. So while there are still sufficient scale economies to warrant industrial agglomerations, these agglomerations are widely scattered and essentially follow patterns of population density.

Thus while summary measures of spatial concentration (or dispersion) are unquestionably useful for a wide range of global comparisons, the above illustration suggests that more detailed representations of spatial agglomeration patterns can in principle allow much richer types of comparisons. With this in mind, our central objective is to propose a methodology for representing and identifying such agglomeration patterns.

Before doing so, it is important to note that there have been other attempts to develop statistical measures that are more multidimensional in nature. Most notably, the K-density approach of Duranton and Overman [6] utilizes pairwise distances between individual establishments, and is capable of indicating the spatial extent of an agglomeration. In a similar vein, Mori et al. [20] proposed a spatially decomposable index of regional localization that yields some information about the most relevant geographic scales of agglomeration within individual industries. However, neither of these approaches is designed to identify specific (map) locations of industrial agglomerations, from which spatial patterns of agglomerations can be characterized.

Methodologically, our approach is closely related to cluster-identification methods proposed by Besag and Newell [3], Kulldorff and Nagarwalla [19], and Kulldorff [18] that have been used for the detection of disease clusters in epidemiology.[2] As with the agglomeration indices mentioned above, these methods start by postulating a null hypothesis of "no clustering" (in terms of a uniform distribution of industrial locations across regions), and then seek to test this hypothesis by finding a single "most significant" cluster of regions with respect to this hypothesis. Candidate clusters are typically defined to be approximately circular areas containing all regions with centroids within some specified distance from a reference point (e.g., the centroid of a "central" region). While this approach is in principle extendable to multiple clusters by recursion (i.e., by removing the cluster found, and repeating the procedure) such extensions are piecemeal at best.[3]

Hence our strategy is essentially to generalize their approach by finding the single most significant "cluster scheme" rather than "cluster." We do so by formalizing these schemes as probability models to which appropriate statistical model-selection criteria can be applied for finding a "best cluster scheme." Here a *cluster scheme* is simply a partition

[2] We shall use "clusters" and "agglomerations" interchangeably throughout the analysis to follow. However, one possible distinction between these terms is suggested in Section 5.3 below.

[3] The recursive application of such procedures gives rise to the notorius "multiple testing" problem that these procedures were originally designed to overcome. In essence, multiple applications of this procedure tend to identify too many clusters as being significant. For a further discussion of this "false discovery"problem, see Castro and Singer [5] together with the references cited therein.

of space in which it is postulated that firms are more likely to locate in "cluster" partitions than elsewhere.[4] Our probability model then amounts to a multinomial sampling model on this partition. These candidate cluster schemes can in principle be compared by means of standard model-selection criteria, including *Akaike's* [1] *Information Criterion*, Schwarz's [27] *Bayesian Information Criterion* (*BIC*), and the *Normalized Maximum Likelihood* of Konkatnen and Myllymäki [15].

To find a best model (cluster scheme) with respect to such criteria, it would of course be ideal to compare all possible cluster schemes constructible from the given system of regions. But even for modest numbers of regions this is a practical impossibility. Hence a second major objective of this paper is to develop a reasonable algorithm for searching the space of possible cluster schemes. Our approach can be considered as an elaboration of the basic ideas proposed by Besag and Newell [3] in which one starts with an individual region and then adds contiguous regions within a given distance from this initial region to identify the single most significant cluster. In particular, we generalize the Besag-Newell concept of clusters by imposing only *convexity* rather than circularity. While searching over possible convex sets of regions is computationally impractical when the number of regions is large, the procedure reduces to be reasonably simple if the (continuous) location space is approximated by a (discrete) regional network. Accordingly, we develop the notion of *convex solid*, representing the convexity in the regional network.

In this context, cluster schemes are grown by (*i*) adding new disjoint clusters, or by (*ii*) either expanding or combining existing clusters until no further improvement in the given model-selection criterion is possible. The final result is thus a "locally best cluster scheme" with respect to this criterion. While the criteria listed above are conceptually different, it turns out that the cluster schemes found are in high agreement across different criteria. Thus, in this paper, we will focus on BIC, which turns out to be the most parsimonious

[4] An alternative approach might be to characterize spatial distributions of establishments by smooth surfaces, utilizing density estimation methods (e.g., Silverman [28]). However, our present discrete characterization of agglomerations in terms of spatially disjoint clusters was motivated by the fact that the industrial concentrations in reality typically take place in a small set of municipalities. In our study of Japanese three-digit manufacturing industries in §5, for instance, the average percent of all 3207 municipalities having any establishments of a given industry was found to be only 22.6%.

criterion in terms of the number of clusters found (see Mori and Smith [22, §3]).

The paper is organized as follows. We begin in Section 2 by defining a probabilistic location model for an establishment, where location probabilities are assumed to be industry-specific, and independent for each establishment within a given industry as well as across industries. Our criterion for model selection in terms of BIC is also developed. In Section 3, we introduce the notion of convex solids, and then in Section 4, present a practical procedure for cluster detection which searches for the best cluster scheme consisting of a set of distinct "convex" clusters. The results of this procedure are then illustrated in Section 5 in terms of the selected pair of Japanese industries discussed above. Here we also sketch a classification scheme for agglomeration patterns in terms of "global extent" and "local density" that can be employed to quantify the spatial scale of industrial agglomeration and dispersion. Finally in Section 6, we briefly discuss a number of directions for further research.

2 A Probability Model of Agglomeration Patterns

To motivate our approach to cluster detection, we begin by observing that recent theoretical results on equilibrium location patterns in continuous space (e.g., Hsu [10], Ikeda et al. [12]) suggest that there is remarkable commonality among possible equilibrium patterns of agglomeration within each industry. In particular, the number, size and spacing of agglomerations are shown to be well preserved under a variety of stable equilibria. From this perspective, our objective is to identify these common features. To do so, we treat such equilibria as *stationary states*, and develop a probabilistic model of location behaviour within such stationary states. In particular, while individual location decisions may be based on the prevailing steady-state distribution, they can nonetheless be treated as statisitically *independent* events, i.e, as random samples from this distribution. This simplification of course precludes any questions about the process of cluster formation, or even the economic rationale for clustering. Rather, our goal here is to provide a simple statistical framework within which the most salient features of these equilibrium cluster patterns can be identified.

To this end, we start by assuming that the location behavior of individual establishments in a given industry can be treated as independent random samples from an unknown industry-specific *locational probability distribution*, P, over a continuous *location space*, Ω (e.g., a national location space). Hence for any (measurable) subregion, $S \subseteq \Omega$, the probability that a randomly sampled establishment locates in S is denoted by $P(S)$. In this context, the class of all possible location models corresponds to the set of probability measures on Ω.

However, observable location data is here assumed to be only in terms of establishment counts for each of a set of disjoint *basic regions* (e.g., municipalities), $\Omega_r \subseteq \Omega$, indexed by $R = \{1, ..., k_R\}$. These regions are assumed to partition Ω, so that $\cup_{r \in R} \Omega_r = \Omega$. Hence the only relevant features of the location probability distribution, P, for our purposes are the location probabilities for each basic region:

$$P = [P(r) \equiv P(\Omega_r) : r \in R] \ . \tag{1}$$

We now consider an approximation of P by probability models, $P_{\mathbf{C}}$, that postulate areas of relatively intense locational activity. Each model is characterized by a "cluster scheme," $\mathbf{C}$, consisting of disjoint *clusters* of basic regions, $C_j \subset R$, $j = 1, ..., k_{\mathbf{C}}$, within which establishments are more densely located. For the present, such clusters are left unspecified. A more detailed model of individual clusters is developed in Section 3 below.

If the full extent of cluster C_j in Ω is denoted by $\Omega_{C_j} = \cup_{r \in C_j} \Omega_r, \ j = 1, ..., k_{\mathbf{C}}$, then the corresponding location probabilities, $p_{\mathbf{C}}(j) \equiv P_{\mathbf{C}}\left(\Omega_{C_j}\right)$, are implicitly taken to define areas of concentration.[5] To complete these probability models, let the set of *residual regions* be denoted by $R_0 (\equiv C_0) = R \setminus \cup_{j=1}^{k_{\mathbf{C}}} C_j$, and let $\Omega_{R_0} = \Omega \setminus \cup_{j=1}^{k_{\mathbf{C}}} \Omega_{C_j}$, with corresponding location probability, $p_{\mathbf{C}}(0) = P_{\mathbf{C}}(\Omega_{R_0}) = 1 - \sum_{j=1}^{k_{\mathbf{C}}} p_{\mathbf{C}}(j)$.

Each *cluster scheme*, $\mathbf{C} = (R_0, C_1, ..., C_{k_{\mathbf{C}}})$, then constitutes a partition of the regional index set, R, and the location probabilities $[p_{\mathbf{C}}(j) : j = 0, 1, ..., k_{\mathbf{C}}]$ yield a probability

[5] An implicit assumption here is that the regions $\{\Omega_r : r \in C_j\}$ in each cluster are contiguous. This assumption is not crucial at present, but will play a central role in the construction of clusters below.

distribution on $\mathbf{C}$.[6] Finally, to specify location probabilities for basic regions, it is assumed that within each cluster, C_j, the location behavior of individual establishments is *completely random*.[7] To define "complete randomness" in the present setting, it is important to focus on those locations within each basic region where establishments could potentially locate (excluding, e.g., bodies of water). Such locations are here designated as the *economic area* of each region.[8] Hence, if for each basic region $r \in R$, we let a_r denote the (economic) *area* of Ω_r, so that the *total area* of cluster C_j is given by

$$a_{C_j} = \sum\nolimits_{r \in C_j} a_r \ , \tag{2}$$

then for each establishment locating in C_j, it is postulated that the conditional probability of locating in basic region, $r \in C_j$, is proportional to the area of region r, i.e., that

$$P_{\mathbf{C}}(\Omega_r | \Omega_{C_j}) = a_r / a_{C_j} \ , \ r \in C_j \ , \quad j = 0, 1, ..., k_{\mathbf{C}} \ . \tag{3}$$

But since $\Omega_r \subseteq \Omega_{C_j}$ implies that $P_{\mathbf{C}}(\Omega_r | \Omega_{C_j}) = P_{\mathbf{C}}(\Omega_r) / P_{\mathbf{C}}(\Omega_{C_j})$, if we let $P_{\mathbf{C}}(r) \equiv P_{\mathbf{C}}(\Omega_r)$, it then follows that for all $r \in R$

$$P_{\mathbf{C}}(r) = p_{\mathbf{C}}(j) \frac{a_r}{a_{C_j}} \quad , \quad r \in C_j \ . \tag{4}$$

Hence for each cluster scheme, $\mathbf{C}$, expression (4) yields a well-defined *cluster probability model*, $P_{\mathbf{C}} = [P_{\mathbf{C}}(r) : r \in R]$, which is comparable with the unknown true model (1). Note moreover that since all area values are known, it follows that for each given cluster scheme, $\mathbf{C} = (R_0, C_1, ..., C_{k_C})$, the only unknown parameters are given by the $k_{\mathbf{C}}$-dimensional vector of *cluster probabilities*, $p_{\mathbf{C}} = [p_{\mathbf{C}}(j) : j = 1, ..., k_{\mathbf{C}}]$.[9]

Within this modeling framework, we now consider a sequence of n independent location

[6] A formal definition of cluster schemes is given in Definition 4.1 below.

[7] This implicitly assumes that the regions within a given cluster not only have high densities of establishments but also that these densities are similar.

[8] As pointed out by a referee, "economic area" is at best a crude approximation to actual usable area for firms. But without more detailed information, we believe that it provides the best approximation currently available.

[9] Note that $p_{\mathbf{C}}(0)$ is constructable from $p_{\mathbf{C}}$ as shown above.

decisions by individual establishments. For each establishment, $i = 1, ..., n$, let its location choice be modeled by a random (indicator) vector, $X^{(i)} = \left(X_r^{(i)} : r \in R\right)$, with $X_r^{(i)} = 1$ if establishment i locates in region r, and $X_r^{(i)} = 0$, otherwise. This set of location decisions is then representable by a random matrix of indicators, $X = (X^{(i)} : i = 1, ..., n)$, with the following finite set of possible realizations (*location patterns*):

$$\triangle_R(n) = \left\{x = (x_r^{(i)} : r \in R, i = 1, ..., n) \in \{0,1\}^{n \times k_R} : \sum\nolimits_{r \in R} x_r^{(i)} = 1,\ i = 1, ..., n\right\}\ . \tag{5}$$

By independence, the probability distribution of X under the unknown true distribution in (1) is given for each location pattern, $x \in \triangle_R(n)$, by

$$P(x) = \prod\nolimits_{i=1}^{n} \prod\nolimits_{r \in R} P(r)^{x_r^{(i)}} = \prod\nolimits_{r \in R} P(r)^{n_r} \tag{6}$$

where the total number of estabishments locating in region r is denoted by

$$n_r = \sum\nolimits_{i=1}^{n} x_r^{(i)} \tag{7}$$

[see expression (5)]. Similarly, for each cluster probability model, $P_{\mathbf{C}}$, the postulated distribution of X is given for each pattern, $x \in \triangle_R(n)$, by:

$$P_{\mathbf{C}}(x|p_{\mathbf{C}}) = \prod\nolimits_{r \in R} P_{\mathbf{C}}(r)^{n_r} = \prod\nolimits_{j=0}^{k_C} \prod\nolimits_{r \in C_j} \left(p_{\mathbf{C}}(j) \frac{a_r}{a_{C_j}}\right)^{n_r} \tag{8}$$

where the relevant parameter vector, $p_{\mathbf{C}}$, for each such model has been made explicit. In most contexts, it will turn out that the locational frequencies $n_j(x) = \sum_{r \in C_j} n_r$, $j = 0, 1, ..., k_{\mathbf{C}}$, are sufficient statistics, since by definition

$$P_{\mathbf{C}}(x|p_{\mathbf{C}}) = \prod\nolimits_{j=0}^{k_{\mathbf{C}}} \left[p_{\mathbf{C}}(j)^{\sum_{r \in C_j} n_r} \prod\nolimits_{r \in C_j} \left(\frac{a_r}{a_{C_j}}\right)^{n_r}\right] = a_{\mathbf{C}}(x) \prod\nolimits_{j=0}^{k_{\mathbf{C}}} p_{\mathbf{C}}(j)^{n_j(x)} \tag{9}$$

where the factor, $a_{\mathbf{C}}(x) = \prod_{j=0}^{k_{\mathbf{C}}} \prod_{r \in C_j} (a_r / a_{C_j})^{n_r}$, is independent of parameter vector, $p_{\mathbf{C}}$.

This likelihood function will form the central element in our comparisons among candidate cluster schemes. As mentioned in the introduction, the specific model selection criterion to be used here is the BIC of Schwarz [27]. As with a number of other criteria, BIC is essentially a "penalized likelihood" measure. To state this criterion precisely, we first recall from expression (9) above, that for any given cluster scheme, $\mathbf{C}$, the *log likelihood* of parameter vector, $p_{\mathbf{C}}$, given an observed location pattern, x, is of the form

$$L(p_{\mathbf{C}}|x) = \sum\nolimits_{j=0}^{k_{\mathbf{C}}} n_j(x) \ln p_{\mathbf{C}}(j) + \ln a_{\mathbf{C}}(x) \ . \tag{10}$$

But since the second term is independent of $p_{\mathbf{C}}$, it follows at once (by differentiation) that the *maximum-likelihood estimate*, $\widehat{p}_{\mathbf{C}} = [\widehat{p}_{\mathbf{C}}(j) : j = 1,..,k_{\mathbf{C}}]$, of $p_{\mathbf{C}}$ is given for each $j = 1,...,k_{\mathbf{C}}$ simply by the fraction of establishments in C_j, i.e.,

$$\widehat{p}_{\mathbf{C}}(j) = n_j(x)/n \ . \tag{11}$$

By substituting (11) into (10) we obtain a corresponding estimate of the *maximum log-likelihood value* for model $P_{\mathbf{C}}$,

$$L_{\mathbf{C}}(x) = L(\widehat{p}_{\mathbf{C}}|x) = \sum\nolimits_{j=0}^{k_{\mathbf{C}}} n_j(x) \ln [n_j(x)/n] \ + \ln a_{\mathbf{C}}(x) \ . \tag{12}$$

But since likelihood values are non-decreasing in the number of parameters estimated, it follows in particular that values of $L_{\mathbf{C}}(x)$ will almost always increase as more clusters are introduced. Hence the "best" cluster scheme with respect to model fit alone is the completely disaggregated scheme in which every basic region constitutes its own cluster. To avoid this obvious "over fitting" problem, BIC penalizes those cluster schemes with larger numbers of clusters, $k_{\mathbf{C}}$, and for any given sample size, n, is of the form,

$$BIC_{\mathbf{C}}(x) = L_{\mathbf{C}}(x) - \frac{k_{\mathbf{C}}}{2} \ln(n) \ . \tag{13}$$

In the actual computations involved in cluster detection (to be described in Section 4), it turned out to be convenient to evaluate the cluster scheme, $P_{\mathbf{C}}$, relative to *the uniform* *probability distribution model* as a benchmark in which individual establishment location follows uniform probability density over economic area. If the BIC value for the uniform probability distribution model is denoted by $BIC_0 = \sum_{j=0}^{k_{\mathbf{C}}} n_j \ln(a_{\mathbf{C}_j}/a)$ $(\equiv L_0)$, where $a \equiv \sum_{r \in R} a_r$ represents the total area, then we may reformulate this measure in terms of *BIC-differences* from this benchmark model as

$$\triangle_{\mathbf{C}} = BIC_{\mathbf{C}}(x) - BIC_0 \equiv T_{\mathbf{C}}(x) - \frac{k_{\mathbf{C}}}{2} \ln(n) \ , \tag{14}$$

where $T_{\mathbf{C}}(x)$ is the log likelihood ratio between the cluster and benchmark models:

$$T_{\mathbf{C}}(x) \equiv L_{\mathbf{C}}(x) - L_0 = \sum_{j=0}^{k_{\mathbf{C}}} n_j(x) \ln \left[\frac{n_j(x)}{n} \Big/ \frac{a_{\mathbf{C}_j}}{a} \right] \ . \tag{15}$$

Since the sample size (number of establishments) for each industry is fixed, it plays no direct role in model selection for that industry. But when comparing cluster patterns for different industries, this penalty term will be more severe in industries with larger numbers of establishments. So, all else being equal, BIC tends to yield more parsimonious cluster schemes for larger industries. Moreover, it tends to yield more parsimonious cluster schemes for *all* industries than the other model selection criteria mentioned above. It is for this reason that we choose to focus on BIC in the present application.

3 A Model of Clusters as Convex Solids

Given the set of basic regions, R, it might seem desirable to treat cluster schemes, $\mathbf{C}$, as arbitrary partitions of R, and then to identify the *best cluster scheme* from this class, i.e.,

$$\mathbf{C}^* = \arg\max_{\mathbf{C}} \triangle_{\mathbf{C}} \ . \tag{16}$$

But from a practical viewpoint, the number of possible partitions can be enormous for even modest numbers of basic regions.[10] Moreover, without further restrictions, the

[10] For instance, the numbers of counties in the US and municipalities in Japan are both over 3000.

components of such partitions can be bizarre, and difficult to interpret as "clusters." This has long been recognized by cluster analysts, who have typically proposed that clusters be roughly circular in shape (as in Besag and Newell [3], Kulldorff and Nagarwalla [19], and Kulldorff [18]). Here, we propose a more flexible class of clusters that preserve spatial compactness by requiring only that they be "approximately convex". We further simplify the identification of convex clusters by representing the location space in terms of a discrete regional network, since from a practical viewpoint, searching over candidate convex clusters is much simpler on networks than in Euclidian space (especially when the space is large). This network-based (as opposed to Euclidian space-based) approach is particularly useful when economically meaningful distances are adopted (such as travel distance and time), rather than simplistic straight-line distances between regions. Before developing the details of this approach, it is useful to begin with a brief overview.

To define clusters of basic regions, we first require that they be *convex sets* with respect to the underlying network. This means simply that clusters must include all regions on shortest paths between their members (in the same way planar convex sets include all lines between their points). But unlike straight-line planar paths, shortest paths on discrete networks can sometimes exclude regions that are obviously interior to the desired clusters, thus leaving "holes" (as shown in Figures 5 and 6 below).[11] It is thus appropriate to "fill" these holes by requiring that regional clusters be *convex solid sets* with respect to the underlying network. The formal procedures for developing these convex solid sets will in fact be utilized in the cluster detection algorithm itself, as detailed in Section 4.2 below.

3.1 A Discrete Network Representation of the Regional System

Recall in Section 2 that the relevant location space, Ω, is partitioned into a set of basic regions, $\Omega_r \subseteq \Omega$, indexed by $R = \{1, ..., k_R\}$. For our present purposes it is convenient to consider a larger *world region*, W, in which Ω resides, so that $W \backslash \Omega$ denotes the "rest of the world," as shown schematically in Figure 1 below. As in Section 2 we identify Ω with

[11] In Section 3.2 it is shown that such holes persist for even straight-line approximations to travel networks.

the set of regional labels for R. In this framework, the *boundary* of the given location space consists of the subset of basic regions, $\overline{R}$, that share boundary points (i.e., the edges of a basic region cell) with $W\backslash\Omega$. This distinguished set of boundary regions (shown in gray) will play an important role in Section 3.3 below.

[Figure 1]

Within this basic continuous geographical framework, we next develop a discrete network representation of the regional system that contains all the relevant information needed for our cluster model. The nodes of this network are represented by the set R of basic regions, and the links are taken to represent pairs of regional "neighbors" in terms of the underlying road network. Here it is assumed that data is available on minimal *travel distances*, $t(r,s)$, between each pair of regions, $r,s \in R$, say between their designated administrative centers. These neighbors should of course include regional pairs (r,s) for which the shortest route from r to s passes through no regions other than r and s. But for computational convenience, we choose to approximate this relation by the standard "contiguity" relation that takes each pair of basic regions sharing some common boundary to be neighbors. While this approximation is reasonable in most cases, there are exceptions. Consider for example the coastal regions, r and s, joined by a bridge, as shown in Figure 2 below. Here it is clear that the shortest route (path) between regions r and s passes through no other regions, even though r and s share no common boundary. Hence to maintain a reasonable notion of "closeness" among neighbors, it is appropriate to include such regional pairs as neighbors. Finally, it is mathematically convenient to include r as a neighbor of itself (since r is always "closer" to itself than to any other region).

[Figure 2]

If this set of *neighbors* for region $r \in R$ is denoted by $N(r)$, then for the region r shown in the schematic regional system of Figure 1, $N(r)$ is seen to consist of eight neighbors other than r itself. Our only formal requirement is that neighbors be symmetric, i.e., that $r \in N(s)$ if and only if $s \in N(r)$. If we now denote the full set of neighbor pairs by

$L = \cup_{r \in R} \cup_{s \in N(r)} (r,s) \;\subseteq R^2$, then this defines the relevant set of *links* for our discrete network representation, (R, L), of the regional system. A simple example of such a regional network, (R, L), is shown in Figure 3 below. Here R consists of twenty five square regions shown on the left. These regions are connected by the road network shown by dotted lines on the left, with travel distances on each of the forty links (to be discussed later) displayed on the right. Hence L in this case consists of the forty distinct regional pairs associated with each of these links, together with the twenty five identity pairs (r, r).

[Figure 3]

Next we employ travel distances between neighbors to approximate the entire road network by a shortest-path metric on network (R, L). To do so, let each sequence, $\rho = (r_1, r_2, ..., r_n)$, of linked neighbors [i.e., with $(r_i, r_{i+1}) \in L$ for $i = 1, ..., n-1$] be designated as a *path* in (R, L), and let the set of all paths in (R, L) be denoted by $\mathcal{P} = \{\rho = (r_1, ..., r_n) : n > 1,\; (r_i, r_{i+1}) \in L,\; i = 1, ..., n-1\}$. If for each pair of regions, $r, s \in R$, we denote the subset of all paths from r to s in $\mathcal{P}$ by $\mathcal{P}(r,s) = \{\rho = (r_1, ..., r_n) \in \mathcal{P} : r_1 = r, r_n = s\}$, then to ensure that shortest paths between all pairs of regions are meaningful, we henceforth assume that that $\mathcal{P}(r,s) \neq \varnothing$ for all $r, s \in R$, i.e., that the given regional network (R, L) is *connected.*[12] In this context, if the *length*, $l(\rho)$, of path, $\rho = (r_1, r_2, ..., r_n)$, is now taken to be the sum of travel distances on each of its links, i.e., $l(\rho) = \sum_{i=1}^{n-1} t(r_i, r_{i+1})$, then for any pair of regions, $r, s \in R$, the *shortest-path distance*, $d(r, s)$, from r to s is taken to be the length of the (possibly nonunique) shortest path from r to s:

$$d(r,s) = \min\{l(\rho) : \rho \in \mathcal{P}(r,s)\} \tag{17}$$

The set of all shortest paths in $\mathcal{P}(r,s)$ is then denoted by $\mathcal{P}_d(r,s) = \{\rho \in \mathcal{P}(r,s) : l(\rho) = d(r,s)\}$. The shortest-path distances in (17) are easily seen to define a *metric* on R, i.e., to satisfy *(i)* $d(r,r) = 0$, *(ii)* $d(r,s) = d(s,r)$, and *(iii)* $d(r,s) \leq d(r,v) + d(v,s)$ for all $r, s, v \in R$. Moreover, these distances always agree with travel distances between

[12] See Mori and Smith [24, S 4.2.1] for the treatment of major off-shore islands.

neighbors [i.e., $d(r,s) = t(r,s)$ for all $(r,s) \in L$]. But for non-neighbors, $(r,s) \notin L$, it will generally be true that $d(r,s) > t(r,s)$ (since the shortest route from r to s on the actual road network may not pass through any intermediate regional centers). Hence these shortest-path distances are only an approximation to shortest-route distances.[13] The advantage of this approximation for our present purposes is that for any r and s, the number of paths in $\mathcal{P}(r,s)$ is generally much smaller than the number of routes from r to s on the road network, so that shortest paths in $\mathcal{P}_d(r,s)$ are more easily identified.

3.2 Convexity in Networks

Within this network framework we now return to the question of defining candidate clusters as spatially coherent groups of basic regions. As mentioned in the Introduction, the standard approach to this problem is to require that clusters be as close to "circular" as possible. To broaden this class, we begin by observing that a key property of circular sets in the plane is their convexity. More generally, a set, S, in the plane is *convex* if and only if for every pair of points, $s, v \in S$, the set S also contains the line segment joining s and v. But since lines are shortest paths with respect to Euclidean distance, an equivalent definition of convexity would be to say that S contains all shortest paths between points in S. Since shortest paths are equally well defined for the network model above, it then follows that we can identify convex sets in the same way.

In particular, a set of basic regions, S, is now said to be *d-convex* if and only if for every pair of regions r and s in S, the set of regions on every shortest path from r to s is also in S.[14] More formally, if for any path, $\rho = (r_1, ..., r_n) \in \mathcal{P}$, we now denote the *set* of distinct points in ρ by $\langle\rho\rangle = \{r_1, ..., r_n\} \subseteq R$, and if the family of all nonempty subsets of R is denoted by $\mathcal{R} = \{S \subseteq R : S \neq \varnothing\}$, then

[13] This approximation appears to be good for the municipality network in Japan considered in §5. For the ratios of short-path over shortest-route distances (d/t) across all 4,491,991 relevant pairs of municipalities, the mean and the 99.5 percentile point are 1.14 and 1.28, respectively.

[14] Our present notion of d-convexity is an instance of the more general notion of geodesic convexity applied to graphs, and appears to have first been introduced by Soltan [29].

Definition 3.1 (d-Convexity) *(i) A subset of basic regions, $S \subseteq R$, is said to be d-*convex *iff for all $s, r \in S$, $\rho \in \mathcal{P}_d(r, s) \Rightarrow \langle \rho \rangle \subseteq S$. (ii) The family of all d-convex sets in $\mathcal{R}$ is denoted by $\mathcal{R}_d$.*

For example, suppose that in the schematic regional system of Figure 4 below it is assumed that regional squares sharing boundary points (faces or corners) are always neighbors, and that travel distance, t, between neighbors is simply the Euclidean distance between their centers. Then with respect to the induced shortest-path distance, d, it is clear that the set, S, on the left consisting of four black squares is not d-convex, since the gray squares in the middle figure belong to shortest paths between the black squares. But even if these gray squares are added to S, the resulting set is still not d-convex, since the four white squares remaining in the middle belong to shortest paths between the gray squares. However, if these four squares are added, then the resulting set on the right is seen to be d-convex since all squares on every shortest path between squares in the set are included.

[Figure 4]

This process of adding shortest paths actually yields a well-defined constructive procedure for "convexifying" a given set, which can be formalized as follows. Let

$$I(r, s) = \bigcup\nolimits_{\rho \in \mathcal{P}_d(r,s)} \langle \rho \rangle \tag{18}$$

denote the (r, s)-*interval* of all points on shortest paths from r to s, and let the mapping, $I : \mathcal{R} \to \mathcal{R}$, defined for all $S \in \mathcal{R}$ by

$$I(S) = \bigcup\nolimits_{r,s \in S} I(r, s) \tag{19}$$

be designated as the *interval function* generated by d. For notational convenience, we set $I^0(S) = S$, $I^1(S) = I(S)$, and construct the m^{th}*-iterate* of I recursively by $I^m(S) = I(I^{m-1}(S))$ for all $m > 1$ and $S \in \mathcal{R}$. Since $\{r, s\} \subseteq I(r, s)$ for all $r, s \in R$, it follows from

(19) that for each set, $S \in \mathcal{R}$,

$$S \subseteq I(S) \ . \tag{20}$$

By the same argument, it follows that for any $S \in \mathcal{R}$ and $r \in I^m(S)$ with $m > 0$, we must have $r \in I[I^m(S)] = I^{m+1}(S)$. Hence these interval iterates satisfy the following nesting property for all $S \in \mathcal{R}$,

$$I^m(S) \subseteq I^{m+1}(S), \quad m \geq 0 \tag{21}$$

and thus constitute a *monotone nondecreasing* sequence of sets. It then follows that for any subset, $S \subseteq R$, of nodes in the *finite* network, (R, L), there must be an integer, m $(\leq |R \backslash S|)$,[15] such that $I^m(S) = I^{m+1}(S)$.[16] The smallest such integer:

$$m(S) = \min\{m : I^m(S) = I^{m+1}(S)\} \tag{22}$$

is called the *geodesic iteration number of set, S*.[17] With these definitions, it is well known that the unique smallest d-convex set containing a given set $S \in \mathcal{R}$ is given by the *d-convex hull* (see Proposition A.2 in the Appendix for a proof of this assertion),

$$c_d(S) = I^{m(S)}(S) \ . \tag{23}$$

The mapping, $c_d : \mathcal{R} \to \mathcal{R}$, defined by (23) is designated as the *d-convexification function.* With this definition, it is shown in Proposition A.3 of the Appendix that d-convex sets are equivalently characterized as the *fixed points* of this mapping, i.e, a set $S \in \mathcal{R}$ is d-convex if and only if $c_d(S) = S$. So the family of all d-convex sets can be equivalently defined as

$$\mathcal{R}_d = \{S \in \mathcal{R} : c_d(S) = S\} \ . \tag{24}$$

However, for purposes of constructing d-convex sets, it is more useful to note that they

[15] Throughout this paper we denote *cardinality* of a set A by $|A|$.

[16] Since $I^m(S) \neq I^{m+1}(S)$ implies from (21) that $|I^{m+1}(S) \backslash I^m(S)| \geq 1$, and since $I^m(S) \subseteq R$ for all m, it follows that this expansion process can involve at most $|R \backslash S|$ steps.

[17] In our present application, this iteration number is typically small.

are equivalently characterized as the fixed points of the *interval function*, $I : \mathcal{R} \to \mathcal{R}$ (as shown in the Corollary to Proposition A.3). Hence $\mathcal{R}_d$ can also be written as

$$\mathcal{R}_d = \{S \in \mathcal{R} : I(S) = S\} \ . \tag{25}$$

This in turn implies that a simple constructive algorithm for obtaining $c_d(S)$ is to iterate I until the iteration number, $m(S)$, is found. This procedure is in fact illustrated by Figure 4 above, where $m(S) = 2$.

But while this particular set, $I^2(S)$, does indeed look reasonably compact (and close to circular), this is not always the case. One simple counterexample is shown in Figure 5 below. Given the regional network, (R, L), in Figure 3 above, suppose that S consists of the four regions shown in black on the left in Figure 5. These regions are assumed to be connected by major highways as shown by the heavy lines on the right in Figure 3, with travel distances, $t = 1$, on each link. All other road links are assumed to be circuitous secondary roads, as represented by a travel distance of $t = 3$ on each link. Here it is clear that the d-convexification, $c_d(S)$, of S is obtained by adding all other regions connected by the ring of major highways (as shown in gray on the right in Figure 5), since shortest paths between such regions are always on these highways. But since the central region shown in white is not on any of these paths, we see that $c_d(S)$ is a d-convex set with a "hole" in the middle.

[Figure 5]

This is very different from convex sets in the plane, which are always "solid." But in more general metric spaces this need not be true. Indeed, for the present case of a network (or graph) structure, the notion of a "hole" itself is not even meaningful. For example, if the central node in Figure 5 were pulled "outside" the coastal regions (leaving all links in tact) then the *network*, (R, L), would remain the same. So it is clear that the above notion of a "hole" depends on additional spatial structure, including the *positions* of regions relative to one another. In particular, since the present notion of d-convexity is intended to approximate convexity in the original location space, it is appropriate to fill these holes.

Finally, it is of interest to note that even with simpler approximations to travel distances, such holes can still exist. For example, if shortest paths between adjacent regions are approximated by straight-line paths between their geometric centroids, then this same convexification procedure can still yield holes. This is illustrated by the simple four-region example in Figure 6, where the three exterior regions are seen to form a convex set containing all shortest paths between them. Hence the central region is not part of this convex set, and constitutes an obvious hole.

[Figure 6]

3.3 Convex Solids in Networks

These observations motivate the spatial structure that we now impose in order to characterize "solid" subsets of R in (R, L). The key idea here is to recall from Figure 1 that relative to the rest of the world, there is a distinguished collection of *boundary regions*, $\overline{R}$, that are essentially "external" to all subsets of R. If for any subset, $S \subseteq R$, and boundary region, $\overline{r} \in \overline{R}$, it is true that $\overline{r} \notin S$, then it is reasonable to assert that $\overline{r}$ is *outside* of S.[18] This set of boundary regions, $\overline{R}$, thus defines a natural reference set for distinguishing regions in complement, $R \backslash S$, of S that are "inside" or "outside" of S. In particular, we now say that a complementary region, $r \in R \backslash S$, is *inside* S if and only if every path joining r to a boundary region in $\overline{R}$ must pass through at least one region of S. For example, given the set, S, of black squares in Figure 7, the complementary region r is seen to be inside of S since every path to the boundary, $\overline{R}$, must intersect S. Similarly, the complementary region s is not inside S, since there is a path from s to $\overline{R}$ that does not intersect S. To formalize this concept, we now let the set of all paths from any region, $r \in R$, to $\overline{R}$ be denoted by $\mathcal{P}(r, \overline{R}) = \cup_{\overline{r} \in \overline{R}} \mathcal{P}(r, \overline{r})$. Then for any nonempty set, $S \in \mathcal{R}$,

[18] Even if $\overline{r}$ is an element of S, it must always be part of the boundary of S. Hence it is still reasonable to assert that $\overline{r}$ is "on the outside" of S.

the set of all complementary regions *inside* S is given by,

$$S_0 = \{r \in R \backslash S : \rho \in \mathcal{P}(r, \overline{R}) \Rightarrow \langle \rho \rangle \cap S \neq \varnothing\} \tag{26}$$

and is designated as the *interior complement* of S.

[Figure 7]

With this concept, we now say that a set, $S \in \mathcal{R}$, is *solid* if and only if its interior complement is empty. In addition, we can now *solidify* a set S by simply adjoining its interior complement. More formally, we now say that:

Definition 3.2 (Solidity) *For any nonempty subset,* $S \in \mathcal{R}$, *(i)* S *is said to be* solid *iff* $S_0 = \varnothing$. *(ii) The set formed by adding* S_0 *to* S,

$$\sigma(S) = S \cup S_0 \tag{27}$$

is designated as the solidification *of* S. *(iii) The family of all solid sets in* $\mathcal{R}$ *is denoted by* $\mathcal{R}_\sigma$.

The justification for the terminology in (*ii*) is given by Lemma A.1 in the Appendix, where it is shown that for any set, $S \in \mathcal{R}$, the set, $\sigma(S)$, is solid in the sense of (*i*) above. The mapping, $\sigma : \mathcal{R} \to \mathcal{R}$, induced by (27) is designated as the *solidification function.* As with the d-convexification function above, it also follows that solid sets are precisely the fixed points of the solidification function (see Lemma A.2 in the Appendix).

With these definitions, the two properties of d-convexity and solidity are taken to constitute our desired model of clusters in R. Hence we now combine them as follows:

Definition 3.3 (d-Convex Solids) *For any nonempty subset,* $S \in \mathcal{R}$, *(i) if* S *is both d-convex and solid, then* S *is designated as a d-convex solid in* $\mathcal{R}$. *(ii) The composite image set,*

$$\sigma c_d(S) = \sigma[c_d(S)] \tag{28}$$

is designated as the d-convex solidification of S.

If we now let $\mathcal{R}_{\sigma d}$ denote the family of all d-convex solids in $\mathcal{R}$, then it follows at once from Definitions 3.1 through 3.3 that

$$\mathcal{R}_{\sigma d} = \mathcal{R}_{\sigma} \cap \mathcal{R}_{d} \tag{29}$$

3.4 Convex Solidification of Sets

As with (26) and (27) above, expression (28) induces a composite mapping, $\sigma c_d : \mathcal{R} \to \mathcal{R}$, designated as the *d-convex solidification function.* We now examine this function in more detail. To do so, it is instructive to begin by observing that the *order* in which these two maps are composed is critical. In particular it is *not* true that the d-convexification of a solid set is necessarily a d-convex solid. This can be illustrated by the example in Figures 3 and 5 above. If the exterior squares are taken to define the relevant boundary set, $\overline{R}$, in Figure 3, then it is clear that the original set, S, of four black squares is solid, since there are paths from every complementary region to $\overline{R}$ that do not intersect S.[19] But, the d-convexification, $c_d(S)$, of S is precisely the *non-solid* set that was used to motivate solidification. So in this case, the composite image, $c_d[\sigma(S)] = c_d(S)$ is not solid (and hence not a d-convex solid).

With this in mind, the key result of this section, established in Theorem A.1 of the Appendix, is to show that the terminology in Definition 3.3 is justified, i.e., that:

Property 3.4 (d-Convex Solidification) *For any set, $S \in \mathcal{R}$, the image set, $\sigma c_d(S)$, is a d-convex solid.*

Hence if one is enlarging a given cluster, C, by adding a set, S, of new regions to construct a new cluster containing $C \cup S$, one need only d-convexify this set by the algorithm

$$C \cup S \to I(C \cup S) \to I^2(C \cup S) \;\cdots\; \to c_d(C \cup S) \tag{30}$$

[19] Note also from this example that the notion of "solidity" by itself is rather weak. However, when applied to d-convex sets, this turns out to be exaclty what is needed for "filling holes."

and then solidify the resulting set by identifying all regions in the interior complement $[c_d(C \cup S)]_0$ of $c_d(C \cup S)$ and forming

$$\sigma c_d(C \cup S) = c_d(C \cup S) \cup [c_d(C \cup S)]_0 \ . \tag{31}$$

This algorithm has already been illustrated by the simple case in Figure 4, where no solidification was required. A somewhat more detailed illustration is given in Figures 8 and 9 below. Figure 8 exhibits a subsystem of nineteen (hexagonal) basic regions in R, along with the major road network (solid and dashed lines) connecting the centers of these regions. As in Figure 4, it is assumed that there are primary roads (freeways) and secondary roads. Some regions lie along freeway corridors, as denoted by solid network links with travel distance (or time) values of $t = 1$. Other regions are connected by secondary roads denoted by dashed network links with higher values of $t = 3$.

[Figure 8]

A possible sequence of steps in the formation of a composite cluster in this subsystem is depicted in Figure 9. Stage 1 begins at the point where it has been determined that an existing cluster (d-convex solid), C_1, of three regions (shown in black) should be expanded to include a secondary set, S_1, of two regions (also shown in black). Given the shortest-path distances, d, generated by the t-values in Figure 8, it is clear that the d-convexification, $c_d(C_1 \cup S_1)$, of this composite set, $C_1 \cup S_1$, is given by adding the gray regions shown in Stage 2. This larger ring of regions lies entirely on freeway corridors, and thus includes all shortest paths joining its members (in a manner similar to the ring of regions in Figure 5). Hence the two regions in the center of this ring lie in the internal complement of $c_d(C_1 \cup S_1)$, and are thus added in Stage 3 to form an new cluster (d-convex solid), $C_2 = \sigma c_d(C_1 \cup S_1)$, containing $C_1 \cup S_1$. In Stage 4 it is determined that one additional singleton set, S_2, should also be added to the existing cluster, C_2. Again, Stage 5 shows that all regions on the freeway corridors from S_2 to C_2 should be added in a new d-convexification, $c_d(C_2 \cup S_2)$. Finally, this d-convex set is again seen to have two regions in its interior complement, which are thus added to achieve the final d-convex solid cluster, $C_3 = \sigma c_d(C_2 \cup S_2)$.

[Figure 9]

Before proceeding, it is appropriate to note several additional features of this d-convex solidification procedure that parallel the basic procedure of d-convexification itself. First, as a parallel to d-convex hulls in (23), it is shown in Theorem A.3 of the Appendix that for any given set of regions, S, the d-convex solidification, $\sigma c_d(S)$, yields a "best d-convex solid approximation" to S in the sense that:

Property 3.5 (Minimality of d-Convex Solidifications) *For any set, $S \in \mathcal{R}$, the d-convex solidification, $\sigma c_d(S)$, of S is the smallest d-convex solid containing S.*

Hence this process of cluster formation can be regarded as a *smoothing procedure* that approximates each candidate set of high-density regions by a more spatially coherent covexified version of this set.

Recall that our network representation of space is mainly for the computational efficiency, and the d-convexity aims for approximating convexity in the original location space. Property 3.5 indicates that d-convex solid in the network corresponds to the convex hull in Euclidian space. Thus, as desired, it is conceptually consistent to adopt d-convex solid as convex approximation of the spatial coverage of a given cluster.

Next, as a parallel to the fixed-point property of d-convexifications, it is shown in Theorem A.4 of the Appendix that the procedure in (30) and (31) always yields a fixed point of the composite mapping, $\sigma c_d : \mathcal{R} \to \mathcal{R}$:

Property 3.6 (d-Convex Solid Fixed Points) *A set, $S \in \mathcal{R}$, is a d-convex solid iff $\sigma c_d(S) = S$.*

Hence the family, $\mathcal{R}_{\sigma d}$, of all d-convex solids in (29) can equivalently be written as $\mathcal{R}_{\sigma d} = \{S \in \mathcal{R} : \sigma c_d(S) = S\}$. In this form, each new cluster is seen to be a natural "stopping point" of the combined d-convexification and solidification procedure above.

4 A Cluster-Detection Procedure

Given the cluster model developed above, the set of relevant cluster schemes for regional network (R, L) can now be formalized as follows:

Definition 4.1 (Cluster Schemes) *A finite partition,* $\mathbf{C} = (R_0, C_1, ..., C_{k_{\mathbf{C}}})$*, of* R *is designated as a cluster scheme for* (R, L) *iff* (i)*[d-convex solidity]* $C_i \in \mathcal{R}_{\sigma d}$ *for all* $i = 1, ..., k_{\mathbf{C}}$*, and* (ii) *[disjointness]* $C_i \cap C_j = \varnothing$ *for all* i, j *with* $1 \leq i < j$*. Let* $\mathcal{C}(R, L)$ *denote the class of admissible cluster schemes for* (R, L)*.*

Below, we develop our search procedure to identify the best cluster scheme. Before developing the details of this procedure, however, it is useful to begin with an overview.

For any given industry, we start with the single best cluster consisting of a single basic region. Then at each subsequent step, we decide whether we should (i) stay with the current cluster scheme; (ii) expand one of the existing clusters; or (iii) start a new cluster. In alternative (ii), we compare potential expansions of all the existing clusters. Such expansions involve annexations of nearby regions (or clusters) which are then further enlarged to maintain d-convex solidity. A new cluster in alternative (iii) consists of the best basic region in the current set of residual regions, R_0. At each step, the best option among these three is selected, and the system of clusters continues growing until option (i) is evaluated as the best among the three. Before completing the description of this procedure (in Section 4.2), we specify the details of option (ii) above in the next section.

4.1 Operational Rules for Cluster Expansion

At each step of the search procedure outlined above, option (ii) involves the expansion of an existing cluster by first annexing certain nearby regions and then further enlarging this set to maintain "spatial cohesiveness." In view of the above definition of a cluster scheme, this requires that such annexations be enlarged so as to maintain both d-convex solidity and disjointness with respect to other existing clusters. This procedure can sometimes require the annexation of other existing clusters, as illustrated by Figure 10 below. Given the subsystem of a regional network shown in Figure 8 above, suppose that the current cluster scheme includes the clusters C_1 and C_2 shown in Stage 1 of Figure 10. Suppose also that it has been determined that the next step of the search procedure should be an expansion of cluster C_1 to include the set Q shown in Stage 1. The composite cluster, $\sigma c_d(C_1 \cup Q)$, resulting from d-convex solidification of $C_1 \cup Q$, includes $C_1 \cup Q$ together with the gray region shown in Stage 2. But since cluster C_2 is seen to overlap this composite cluster, it is clear that disjointness between clusters can only be maintained by annexing cluster C_2 as well. This results in the larger composite cluster, $\sigma c_d[\sigma c_d(C_1 \cup Q) \cup C_2]$, shown by the combined black and gray region of Stage 3 in Figure 10.

[Figure 10]

More generally, if some current cluster, $C_j \in \mathbf{C} = (R_0, C_1, ..., C_{k_\mathbf{C}})$, is to be expanded by annexing a set $Q \subseteq R_0$, then the d-convex solidification, $\sigma_{C_d}(C_j \cup Q)$, must be further enlarged to include all clusters, $C_i \in \mathbf{C}$, intersecting $\sigma_{C_d}(C_j \cup Q)$. For any given current cluster scheme $\mathbf{C} = (R_0, C_1, ..., C_{k_\mathbf{C}})$, this procedure can be formalized in terms of the following operator, $U_\mathbf{C} : R \to R$, defined for all $S \in \mathcal{R}$ by

$$U_\mathbf{C}(S) = \sigma c_d(S) \cup \{C_i \in \mathbf{C} : C_i \cap \sigma c_d(S) \neq \varnothing\} \tag{32}$$

where the relevant sets, S, of interest will be of the form, $S = C_j \cup Q$, with $C_j \in \mathbf{C}$ and $Q \subseteq R_0$. Observe next that this single operation is not sufficient, since the resulting image sets, $U_\mathbf{C}(S)$, may fail to be d-convex solids. Moreover, the d-convex solidification, $\sigma c_d[U_\mathbf{C}(S)]$, may again fail to be disjoint from other existing clusters in $\mathbf{C}$. So it should be clear that what is needed here is an iteration of this operator until both conditions are met. To formalize such iterations, we proceed as in Section 3.2 above by letting the iterates of $U_\mathbf{C}$ be defined for each $S \in R$ by $U^0_\mathbf{C}(S) = S$, $U^1_\mathbf{C}(S) = U_\mathbf{C}(S)$, and $U^m_\mathbf{C}(S) = U_\mathbf{C}[U^{m-1}_\mathbf{C}(S)]$ for all $m > 1$. Since it is clear by definition that $U^m_\mathbf{C}(S) \subseteq U^{m+1}_\mathbf{C}(S)$ for all $m \geq 0$, this yields a monotone nondecreasing sequence of sets in R. Hence by the same arguments leading to (22) above, it again follows that there must be an integer, m ($\leq |R \backslash S|$), such that $U_{\mathbf{C}}^{m}(S) = U_{\mathbf{C}}^{m+1}(S)$. As a parallel to (22) we may thus designate the smallest integer, $m(S|\mathbf{C}) = \min\{m : U_{\mathbf{C}}^{m}(S) = U_{\mathbf{C}}^{m+1}(S)\}$, satisfying this condition as the *expansion iteration number* of S given $\mathbf{C}$. Finally, if (as a parallel to d-convex hulls) we now designate the resulting fixed point of $U_{\mathbf{C}}$,

$$u_{\mathbf{C}}(S) = U_{\mathbf{C}}^{m(S|\mathbf{C})}(S) \tag{33}$$

as the $\mathbf{C}$-*compatible expansion* of S, then it is this set that satisfies the expansion properties we need. First observe that the fixed point property, $U_{\mathbf{C}}[u_{\mathbf{C}}(S)] = u_{\mathbf{C}}(S)$, of this expanded set implies at once from (32) that for all clusters $C_i \in \mathbf{C}$ with $C_i \cap u_{\mathbf{C}}(S) \neq \varnothing$ we must have $C_i \subseteq u_{\mathbf{C}}(S)$. Thus $u_{\mathbf{C}}(S)$ is always disjoint from any clusters, $C_i \in \mathbf{C}$, that have not already been absorbed into $u_{\mathbf{C}}(S)$. Moreover, this in turn implies from (32) that $u_{\mathbf{C}}(S) = \sigma c_d[u_{\mathbf{C}}(S)]$, and hence that $u_{\mathbf{C}}(S)$ must be a d-convex solid.

4.2 Cluster-Detection Procedure

In terms of Definition 4.1, the objective of this procedure, which we now designate as the *cluster-detection procedure*, is to find a cluster scheme, $\mathbf{C}^* \in \mathcal{C}(R, L)$, satisfying,

$$\mathbf{C}^* = \arg \max_{\mathbf{C} \in \mathcal{C}(R,L)} \triangle_{\mathbf{C}} \ . \tag{34}$$

From a practical viewpoint, it should be stressed that the following search procedure will only guarantee that the cluster scheme found is a “local maximum” of (34) with respect to the class of admissible “perturbations” in $\mathcal{C}(R, L)$ defined by the procedure itself.

To specify these perturbations in more detail, we begin with the following notational conventions. At each stage, $t = 0, 1, 2, ...$, of this procedure, let $\mathbf{C}_t = (R_{t,0}, C_{t,1}, ..., C_{t,k_{\mathbf{C}_t}})$, denote the current cluster scheme in $\mathcal{C}(R, L)$. The procedure then starts at stage $t = 0$ with the *null cluster scheme*, $\mathbf{C}_0 = \{R_{0,0}\} = \{R\}$, containing no clusters. By expressions (14) and (15), it follows that the corresponding initial value of the objective function in (34) must be 0. Given data, $[\mathbf{C}_t, \triangle_{\mathbf{C}_t}]$, at stage t, we then seek the modification (perturbation),

$\mathbf{C}_{t+1}$, of $\mathbf{C}_t$ in $\mathcal{C}(R,L)$ which yields the highest value of $\triangle_{\mathbf{C}_{t+1}}$. As outlined above, these modifications are of two types: (i) the formation of a new cluster in scheme $\mathbf{C}_t$, or (ii) the expansion of an existing cluster in scheme $\mathbf{C}_t$. We now develop each of these steps in turn.

4.2.1 New Cluster Formation

Given the current cluster scheme, $\mathbf{C}_t = (R_{t,0}, C_{t,1}, ..., C_{t,k_{\mathbf{C}_t}})$, at stage t, one can start a new cluster, $\{r\}$, by choosing some residual region, $r \in R_{t,0}$, which is disjoint with all existing clusters. Hence the set of feasible choices for r is given by $R_0(\mathbf{C}_t) = R_{t,0}$. For each $r \in R_0(\mathbf{C}_t)$, the corresponding expanded cluster scheme is then given by $\mathbf{C}_t^0(r) = \big(R_{t,0}^0(r), C_{t,1}^0(r), C_{t,2}^0\,, ..., C_{t,k_{\mathbf{C}_t^0(r)}}^0\big)$, where $R_{t,0}^0(r) = R_{t,0}\backslash\{r\}$, $k_{\mathbf{C}_t^0(r)} = k_{\mathbf{C}_t}{+}1$, $C_{t,1}^0(r) = \{r\}$, and $C_{t,i}^0 = C_{t,i-1}$ for $i = 2, ..., k_{\mathbf{C}_t^0(r)}$. The superscript "0" in cluster scheme, $\mathbf{C}_t^0(r)$, indicates that a change is made to the residual region, $R_{t,0}$, rather than to one of the clusters in $\mathbf{C}_t$. Note that since $\{r\}$ is automatically a d-convex solid, and since $r \in R_0(\mathbf{C}_t)$ guarantees that disjointness of all clusters is maintained, it follows that $\mathbf{C}_t^0(r) \in \mathcal{C}(R,L)$, and hence that $\mathbf{C}_t^0(r)$ is an admissible modification of $\mathbf{C}_t$.

The best candidate for new cluster formation is of course the region, $r_0^* \in R_0(\mathbf{C}_t)$, that yields the highest value of the objective function, i.e., for which $r_0^* = \arg\max_{r\in R_0(\mathbf{C}_t)} \triangle_{\mathbf{C}_t^0(r)}$. For purposes of comparison with other possible modifications of $\mathbf{C}_t$, we now set

$$\mathbf{C}_t^0 \equiv \mathbf{C}_t^0(r_0^*)\ . \tag{35}$$

4.2.2 Expansion of an Existing Cluster

Next, we consider a potential expansion of each cluster, $C_{t,j} \in \mathbf{C}_t$, by annexing a set Q of nearby regions in R. While the basic mechanics of this expansion procedure were developed in Section 4.1 above, the specific choice of Q was not. Recall that such annexations can potentially result in large expansions of $C_{t,j}$, given the need to preserve both d-convex solidity and disjointness. Hence to maintain reasonably "small increments" in our search process, it is appropriate to restrict initial annexations to single regions whenever possible.

Of course, when such regions are already part of another cluster, it will be necessary to annex the whole cluster to preserve disjointness. But to motivate our basic approach, it is convenient to start by considering the annexation of a single region not in any other cluster, i.e., to set $Q = \{r\}$ for some $r \in R_{t,0}$. Here it would seem natural to consider only regions in the immediate neighborhood of $C_{t,j}$. However, this often turns out to be too restrictive, since there may exist much better choices that are not direct neighbors of $C_{t,j}$.

In fact, it might seem more reasonable to consider all possible regions in $R \backslash C_{t,j}$, and simply let our model-selection criterion determine the best choice. But if one allows choices of r "far away" from $C_{t,j}$, then our d-convex solidity and disjointness criteria can lead to the formation of very large clusters that violate any notion of spatial cohesiveness.[20] So it is convenient at this point to introduce a new set of neighborhoods which strike a compromise between these two extremes. To do so, we first extend *shortest-path distances*, d, between points to corresponding distances between points and sets by letting

$$d(r, Q) = \min \{d(r, s) : s \in Q\} \tag{36}$$

for $r \in R$ and $Q \in \mathcal{R}$. Since d is a metric on R, it is well known that for each set, $Q \in \mathcal{R}$, (36) yields a well-defined distance function that preserves the usual continuity properties of d on R (e.g., Berge [2, Ch.5]). Hence one can define well-behaved neighborhoods of Q in terms of this distance function as follows. For each $Q \in \mathcal{R}$, the *δ-neighborhood* of Q in R is defined to be $\delta(Q) = \{r \in R : d(r, Q) < \delta\}$. Hence the appropriate choices for expansions of $C_{t,j}$ are taken to be regions in $\delta(C_{t,j})$ for some pre-specified choice of parameter δ.[21]

As mentioned above, there are two cases that need to be distinguished here. First suppose that for some given cluster $C_{t,j}$ we consider the annexation of a region not in any

[20] The inclusion of large undeveloped regions (e.g., mountains and inland sea) of the nation can lead to an exaggerated depiction of agglomeration involving areas that are mostly devoid of establishments. It should be noted that this is in part due to our use of economic area (rather than total area), which effectively ignores such undeveloped land when expanding clusters.

[21] In our application in §5, the value used is $\delta = 36.0$km, which was chosen so that any single expansion of a cluster cannot include a large section without economic area (e.g., inland sea and lakes). This δ value covers about 90% of the shortest-path distances between neighboring basic regions (municipalities) in our application. It is also worth noting from a practical viewpoint that this use of uniform δ-neighborhoods has the added advantage of controlling (at least in part) for size differences among basic regions.

other cluster, i.e., a region $r \in R_{t,0} \cap \delta(C_{t,j})$. Then follows from expression (33) that the corresponding $\mathbf{C}_t$-compatible expansion of $C_{t,j} \cup \{r\}$ is given by

$$C^j_{t,1}(r) = u_{\mathbf{C}_t}(C_{t,j} \cup \{r\}) \ . \tag{37}$$

Thus the cluster scheme, $\mathbf{C}^j_t(r)$, resulting from this expansion has the form

$$\mathbf{C}^j_t(r) = \left(R^j_{t,0}(r), C^j_{t,1}(r), C^j_{t,2}(r) \ , ..., C^j_{t,k_{\mathbf{C}^j_t(r)}}(r) \right) \tag{38}$$

where, by expression (32), the set of all other clusters in $\mathbf{C}^j_t(r)$ is given by

$$\left\{ C^j_{t,2}(r), ..., C^j_{t,k_{\mathbf{C}^j_t(r)}}(r) \right\} = \left\{ C_{t,i} \in \mathbf{C}_t : C_{t,i} \cap C^j_{t,1}(r) = \varnothing \right\} \tag{39}$$

and where the corresponding residual region has the form:

$$R^j_{t,0}(r) = R - \bigcup\nolimits_{i=1}^{k_{\mathbf{C}^j_t(r)}} C^j_{t,i}(r) \ . \tag{40}$$

As above, if r^*_j now denotes the region in $R_{t,0} \cap \delta(C_{t,j})$ that yields the highest value of the objective function, i.e., for which $r^*_j = \arg\max_{r \in R_{t,0} \cap \delta(C_{t,j})} \triangle_{\mathbf{C}^j_t(r)}$, then the best cluster expansion for $C_{t,j}$ in $\mathbf{C}_t$ starting with regions in $R_{t,0} \cap \delta(C_{t,j})$ is given by $\mathbf{C}^j_t(r^*_j)$.

Next recall that it is possible that another cluster, $C_{t,i}$ in $\mathbf{C}_t$, intersects $\delta(C_{t,j})$ so that the annexation of $C_{t,i}$ is a possible expansion of $C_{t,j}$. For this case it is necessary to annex the entire cluster $C_{t,i}$ in order to preserve disjointness. So if we now define the index set, $I_j(\mathbf{C}_t) = \{i \neq j : C_{t,i} \cap \delta(C_{t,j}) \neq \varnothing\}$ [not to be confused with interval sets $I(\cdot)$ in Section 3.2 above], and for each $i \in I_j(\mathbf{C}_j)$ replace (37) with the $\mathbf{C}_t$-compatible expansion $C^j_{t,1}(i) = u_{\mathbf{C}_t}(C_{t,j} \cup C_{t,i})$, then as a parallel to (38) through (40), the cluster scheme, $\mathbf{C}^j_t(i)$, resulting from this expansion now has the form

$$\mathbf{C}^j_t(i) = \left(R^j_{t,0}(i), C^j_{t,1}(i), C^j_{t,2}(i) \ , ..., C^j_{t,k_{\mathbf{C}^j_t(i)}}(i) \right) \tag{41}$$

with the set of all other clusters in $\mathbf{C}_t^j(i)$ given by

$$\left\{C_{t,2}^j(i), ..., C_{t,k_{\mathbf{C}_t^j(i)}}^j(i)\right\} = \{C_{t,i} \in \mathbf{C}_t : C_{t,i} \cap C_{t,1}^j(i) = \varnothing\} \tag{42}$$

and with corresponding residual region:

$$R_{t,0}^j(i) = R - \bigcup\nolimits_{k=1}^{k_{\mathbf{C}_t^j(i)}} C_{t,k}^j(i) \ . \tag{43}$$

If i_j^* denotes the cluster in $I_j(\mathbf{C}_t)$ that yields the highest value of the objective function for which $i_j^* = \arg\max_{i \in I_j(\mathbf{C}_t)} \triangle_{\mathbf{C}_t^j(i)}$, then the best cluster expansion for $C_{t,j}$ in $\mathbf{C}_t$ is given by $\mathbf{C}_t^j(i_j^*)$. Hence the best cluster expansion, $\mathbf{C}_t^j$, of $\mathbf{C}_t$ starting with cluster $C_{t,j}$ is given by

$$\mathbf{C}_t^j \equiv \arg \max_{\mathbf{C} \in \{\mathbf{C}_t^j(r_j^*), \mathbf{C}_t^j(i_j^*)\}} \triangle_{\mathbf{C}} \quad , \quad j = 1, ..., k_{\mathbf{C}_t} \tag{44}$$

4.2.3 Revision of the Cluster Scheme

Finally, given these candidate modifications, $\mathbf{C}_t^0, \mathbf{C}_t^1, ..., \mathbf{C}_t^{k_{\mathbf{C}_t}}$, of $\mathbf{C}_t$ in $\mathcal{C}(R, L)$ [as defined by (35) together with (44)], let $\mathbf{C}_t^*$ be the best candidate, as defined by

$$\mathbf{C}_t^* = \arg\max\nolimits_{\mathbf{C} \in \{\mathbf{C}_t^j : j=0,1,...,k_{\mathbf{C}_t}\}} \triangle_{\mathbf{C}} \ . \tag{45}$$

There are then two possibilities left to consider: If $\triangle_{\mathbf{C}_t^*} > \triangle_{\mathbf{C}_t}$, then set $[\mathbf{C}_{t+1}, \triangle_{\mathbf{C}_{t+1}}] = [\mathbf{C}_t^*, \triangle_{\mathbf{C}_t^*}]$, and proceed to stage $t + 1$. On the other hand, if $\triangle_{\mathbf{C}_t^*} \leq \triangle_{\mathbf{C}_t}$, then no (local) improvement can be made, and the cluster-detection procedure terminates with the (locally) *optimal cluster scheme*, $\mathbf{C}^* = \mathbf{C}_t$.

Finally, it is of interest to note that this cluster-detection procedure is roughly analogous to "mixed forward search" procedure in stepwise regression, where in the present case we add new clusters or merge existing ones until some locally optimal stopping point is found. With this analogy in mind, it is in principle possible to consider "mixed backward search" procedures as well. For example, one could start with a maximal number of singleton clusters, and proceed by either eliminating or merging clusters until a stopping point is reached. Some experiments with this approach produced results similar to the present search procedure, but proved to be far more computationally demanding.

4.3 A Test of Spurious Clustering

While the cluster-detection procedure developed above will always find a (locally) best cluster scheme, $\mathbf{C}^*$, with respect to BIC used, there is still the statistical question of whether such clustering could simply have occurred by chance. Hence one can ask how the optimal criterion value, $\triangle_{\mathbf{C}^*}$, obtained compares with typical values obtainable by applying the same cluster-detection procedure to randomly generated spatial data. This can be formalized in terms of the hypothesis of *complete spatial randomness*, which in this present context asserts that the probability, p_r, that any given establishment will locate in region, $r \in R$, is proportional to the areal size, a_r, of that region, i.e., that

$$p_r = a_r \,/a \quad . \tag{46}$$

While the sampling distribution of $\triangle_{\mathbf{C}}$ under this hypothesis is complex, it can easily be estimated by Monte Carlo simulation. More precisely, for any given industrial location pattern of n establishments, one can use (46) to generate, say, 1000 random location patterns of n establishments, and apply the cluster-detection procedure to each pattern. This will yield 1000 values of $\triangle_{\mathbf{C}}$, say $\triangle_1, ..., \triangle_{1000}$. If the value for the actual cluster scheme, $\triangle_0 = \triangle_{\mathbf{C}^*}$, is say bigger than all but five of these in the ordering of values, $\{\triangle_1, ..., \triangle_{1000}\}$, then the chance, p, of getting a value as large as this (under the hypothesis that $\triangle_0$ is coming from the same population of random patterns) is, $p = (5{+}1)/(1000{+}1) \sim 0.005$. This would indicate very "significant clustering." On the other hand, if $\triangle_0$ were only bigger than say 800 of these values, then the p-value, $p = (200 + 1)/(1000 + 1) \sim 0.20$, would suggest that the observed cluster scheme, $\mathbf{C}^*$, is not sufficiently significant to warrant further investigation. This procedure was used in the following illustrative application (as well as in the more extensive application in Mori and Smith [24]).

4.4 Core Clusters

The identified clusters, $C \in \mathbf{C}^*$, vary in terms of their contribution to the value of $\triangle_{\mathbf{C}^*}$. While the clusters with larger contributions are often insensitive to small perturbations of the original regional distribution of establishments, those with smaller contributions may be sensitive. Thus, depending on the application, it may be useful to focus on the *core clusters* which account for a large share in the value of $\triangle_{\mathbf{C}^*}$ in order to obtain more robust results.

To formalize this idea, we start by assuming that an optimal cluster scheme, $\mathbf{C} = \mathbf{C}^*$, has been found for the industry. To identify the core clusters in $\mathbf{C}$, we proceed recursively by successively adding those clusters in $\mathbf{C}$ with maximum incremental contributions to $\triangle_{\mathbf{C}}$.[22] This recursion starts with the "empty" cluster scheme represented by $\mathbf{C}_0 \equiv \{R_{0,0}\}$ where $R_{0,0}$ denotes the full set of regions, R. If the set of (non-residual) *clusters* in $\mathbf{C}$ is denoted by $\mathbf{C}^+ \equiv \mathbf{C} \backslash \{R_0\}$, then we next consider each possible "one-cluster" scheme created by choosing a cluster, $C \in \mathbf{C}^+$, and forming $\mathbf{C}_0(C) = \{R_{0,0}(C), C\}$, with $R_{0,0}(C) = R_{0,0} \backslash C$. The "most significant" of these, denoted by $\mathbf{C}_1 = \{R_{1,0}(C), C_{1,1}\}$, is then taken to be the cluster scheme with the *maximum BIC value* (defined below). If this is called *stage* $t = 1$, and if the *core cluster scheme* found at each stage $t \geq 1$ is denoted by $\mathbf{C}_t \equiv \{R_{t,0}, C_{t,1}, ..., C_{t,t}\}$, then the recursive construction of these schemes can be defined more precisely as follows.

For each $t \geq 1$ let $\mathbf{C}_{t-1}^+$ denote the (non-residual) clusters in $\mathbf{C}_{t-1}$ (so that for $t = 1$ we have $\mathbf{C}_{t-1}^+ = \mathbf{C}_0^+ = \varnothing$), and for each cluster not yet included in $\mathbf{C}_{t-1}$, i.e., each $C \in \mathbf{C}^+ \backslash \mathbf{C}_{t-1}^+$, let $\mathbf{C}_{t-1}(C)$ be defined by, $\mathbf{C}_{t-1}(C) = (R_{t-1,0}(C), C_{t-1,1}, ..., C_{t-1,t-1}, C)$, where $R_{t-1,0}(C) = R_{t-1,0} \backslash C$. Then the *additional core cluster*, $C_t (\equiv C_{t,t})$ $(\in \mathbf{C}^+ \backslash \mathbf{C}_{t-1}^+)$, at stage $t \geq 1$ is defined by

$$C_t \equiv \arg\max_{C \in \mathbf{C}^+ \backslash \mathbf{C}_{t-1}^+} T_{\mathbf{C}_{t-1}(C)} \ , \tag{47}$$

[22] The procedure for identifying core clusters in $\mathbf{C}$ is different from the one used to indentify $\mathbf{C}$ in §4.2. Here, candidate clusters considered are only those in $\mathbf{C}$ itself.

where $T_{\mathbf{C}_{t-1}(C)}$ is the *estimated maximum log-likelihood ratio* for model $p_{\mathbf{C}_{t-1}(C)}$ given [in a manner paralleling expression (15) above] by

$$T_{\mathbf{C}_{t-1}(C)} = \sum\nolimits_{C' \in \mathbf{C}_{t-1}(C)} n_{C'} \ln\left(\frac{n_{C'}}{n} \Big/ \frac{a_{C'}}{a} \right) \ , \tag{48}$$

where $n_{C'} \equiv \sum_{r \in C'} n_r$ and $n \equiv \sum_{r \in R} n_r$. Thus, at each stage $t \geq 1$ the likelihood-maximizing cluster, C_t, is removed from the residual region, $R_{t-1,0}$, and added to the set of core clusters in $\mathbf{C}_{t-1}$. The resulting $\triangle_{\mathbf{C}}$ value at each stage t is then given by

$$\triangle_{\mathbf{C}_t} = T_{\mathbf{C}_t} - \frac{t}{2}\ln(n) \tag{49}$$

with

$$T_{\mathbf{C}_t} = \sum\nolimits_{C \in \mathbf{C}_t} n_C \ln\left(\frac{n_C}{n} \Big/ \frac{a_C}{a} \right) \ . \tag{50}$$

Finally, the *incremental contribution* of each new cluster, C_t, to BIC within $\mathbf{C}$ is given by the increment for its associated cluster scheme, $\mathbf{C}_t$, as follows:

$$\triangle_t(\mathbf{C}) \equiv \triangle_{\mathbf{C}_t} - \triangle_{\mathbf{C}_{t-1}} \tag{51}$$

To identify the relevant set of the core clusters in $\mathbf{C}$, one simple criterion would be to require that each has a BIC contribution at least some specified fraction, μ, of $\triangle_1(\mathbf{C})$. In terms of this criterion, the procedure would stop at the first stage, t^e, where additional increments fail to satisfy this condition, i.e., where $\triangle_{t^e+1} < \mu\triangle_1$. Refer to Mori and Smith [24, S 3] for an application of these core clusters.

5 An Illustrative Application

In this section we illustrate the above procedure in terms of the two Japanese industries discussed in the Introduction, which for convenience we refer to here as simply "plastics" and "soft drinks,"respectively. These two industries are part of the larger study in Mori and Smith [24] that applies the present methodology to 163 manufacturing industries in Japan. As discussed in Section 4.2 of that paper, the test of spurious clustering above identified 9 industries with spurious clustering, so that only 154 industries were used in the final analysis. The appropriate notion of a "basic region,"r, for purposes of this study was taken to be the municipality category equivalent to a city-ward-town-village in Japan. The relevant set R was then taken to be the 3207 municipalities geographically connected to the major islands of Japan, as shown in Figure 11 below.

[Figure 11]

5.1 Comparison with a Scalar Measure of Agglomeration

The choice of these two industries is motivated by their similarity in terms of overall degree of agglomeration. This can be illustrated in terms of the *D-index* developed in Mori et al. [20],which for a given industry i is defined as the Kullback-Leibler [17] divergence of its establishment location probability distribution, $P_i \equiv [P_i(r) : r \in R]$, [as in expression (1)] from purely random establishment locations. Here the latter is characterized by the uniform probability distribution, $P_0 \equiv [P_0(r) : r \in R]$, with $P_0(r) = a_r / \sum_{j \in R} a_j$ [as in expression (46)]. By using the sample estimate of P_i, namely, $\widehat{P}_i = [\widehat{P}_i(r) : r \in R]$ with $\widehat{P}_i(r) \equiv n_r/n$ [as in expression (7)], a corresponding estimate of this D-index is given by

$$D(\widehat{P}_i|P_0) = \sum_{r \in R} \widehat{P}_i(r) \ln \left[\widehat{P}_i(r) \,/ P_0(r) \right]. \tag{52}$$

The intuition behind this particular index is that it provides a natural measure of distance between probability distributions. So by taking uniformity to represent the complete absence of clustering, it is reasonable to assume that those distributions "more distant" from the uniform distribution should involve more clustering. Note also that since both D and $\triangle_{\mathbf{C}}$ are based on similar log-likelihood measures of "distance from uniformity", our cluster detection procedure is closer in spirit to this scalar measure than other possible choices such as the index by Ellison and Glaeser [7].[23] Hence D provides a

[23] In fact, Ellison-Glaeser index is highly correlated with D (refer to Mori et al. [20, §D]). So, the

natural candidate for comparing the advantages of this approach over scalar measures in general. The histogram of divergence values, D, for the 154 industries in Japan is shown in Figure 12 below, and is seen to range from $D = 0.47$ up to 5.98. With respect to this overall range, the D values, 1.95 and 2.05, for soft drinks and plastics, respectively, are seen to be virtually identical.

[Figure 12]

But in spite of this overall similarity, the agglomeration patterns obtained for these two industries are substantially different, as seen in Figures 13 and 14 below.

[Figures 13 and 14]

Panel (a) of each figure displays the establishment densities for the corresponding industry, where those basic regions with higher densities are shown as darker. In Panel (b), the individual clusters in the derived cluster scheme, $\mathbf{C}_i^*$, are represented by enclosed gray areas. The portion of each cluster in lighter gray shows those basic regions which contain no establishments (but are included in $\mathbf{C}_i^*$ by the process of convex solidification).

Before examining these patterns in detail, it is of interest to consider the results of the cluster-detection procedure itself. By comparing the establishment densities and cluster schemes in Panels (a) and (b) of each figure, respectively, it is clear that these cluster schemes closely reflect the underlying densities from which they were obtained. Notice also that individual clusters are by no means “circular” in shape. Rather each consists of an easily recognizable set of contiguous basic regions (municipalities) in R that approximates the area of higher establishment density in Panel (a) of the figure. Notice also that certain clusters in each pattern are themselves contiguous. We shall return to this point below.

To compare these two agglomeration patterns in more detail, we begin by observing that while the plastics industry is more than twice as large as soft drinks in terms of the number of establishments (1555 versus 777), its agglomeration pattern contains only 43 clusters versus 55 clusters for soft drinks. This illustrates the relative parsimoniousness of

arguments in this section would remain essentially the same.

our cluster-detection procedure with respect to larger industries, as mentioned following the definition of BIC in expression (13) above. Notice also that clustering is indeed much stronger in the plastics industry than in soft drinks. This can be seen in several ways. First, the share of plastics establishments in clusters is much larger than for soft drinks (93.9% versus 64.6%). Second, the average size of these clusters is greater not only in terms of establishments per cluster (as implied by the statistics above), they are also more than three time larger in terms of average areal extent.

5.2 Global Extent versus Local Density of Agglomerations

Aside from these general comparisons in terms of summary statistics, the level of spatial detail in each of these agglomeration patterns allows a much broader range of comparative measures. While such measures are developed in more detail in Mori and Smith [24], their essential elements are well illustrated in terms of the present pair of industries. As mentioned in the Introduction, the plastics industry is primarily concentrated along the Industrial Belt of Japan as in Figure 13(b). More generally, industries often tend to concentrate within specific subregions of the nation, i.e., are themselves "spatially contained." To make this precise in terms of our present model of cluster schemes, we adopt a two-stage approach. First, we identify the core clusters (as defined in Section 4.4) in the optimal cluster scheme, $\mathbf{C}^*$, for a given industry. We then define the *essential containment* (*e-containment*) for that industry to be the convex solidification of these core clusters, in other words, the smallest convex solid[24] containing all these core clusters for the industry. The e-containment for the plastics industry is indicated by the hatched area in Figure 13(c) which clearly distinguishes the "Industrial Belt" portion of this industry. In contrast, the e-containment for soft drinks shown in Figure 14(c) appears to be much larger, and reflects the wide scattering of essential clusters for this industry.

While these visual summaries of "containment" can be very informative, it is often more useful to quantify such relations for purposes of analysis. One possibility here is to

[24] Recall Property 3.3 of convex solidification above.

define the *global extent* (GE) of an industry to be the fraction of area in its e-containment relative to the nation as a whole.[25] In the present case, the GE values for plastics and soft drinks are 0.298 and 0.589, respectively. So in terms of this measure, it is clear that the clusters of the plastics industry is much more localized than those of soft drinks.

Next observe that while the global extent of the plastics industry is much smaller than that of soft drinks, the average size of its core clusters is actually much larger. As is clear from Figures 13 and 14, these clusters are thus more densely packed inside the e-containment of the plastics industry. To capture this additional dimension of agglomeration patterns, we now designate the fraction of e-containment area represented by these essential clusters as the *local density* (LD) of the industry. Since the LD values for plastics and soft drinks are given respectively by 0.465 and 0.133, it is also clear that the agglomeration pattern for plastics is much more locally dense than that of soft drinks.

5.3 Refinements of Cluster Schemes

Recall that in terms of our basic probability model of cluster schemes, $\mathbf{C}$, individual clusters, C_j, are implicitly assumed to constitute sets of basic regions with similar (and unusually high) establishment density. But the relations between these clusters is left unspecified. In this regard it was observed above that the opimal cluster schemes, $\mathbf{C}^*$, for both plastics and soft drinks contain clusters that are mutually *contiguous*. Here it is natural to ask why such clusters were not "joined" at some stage during the cluster-detection procedure. The reason is that our basic cluster probability model assumes that location probabilities are essentially *uniform* within each cluster [as in expression (3)], so that maximum-likelihood estimates for cluster probabilities, $p_{\mathbf{C}}(j)$, are simply proportional to the number of establishments, n_j, in that cluster. Hence with respect to the BIC measure underlying this procedure, contiguous clusters with very different uniform densities often yield a better fit to establishment data than does their union with its associated uniform density. As one illustration, the contiguous chain of clusters for the

[25] Here, we use the full geographic areas of basic regions rather than economic area, to give a better representation of "extent."See further discussions in Mori and Smith [24, S 3.2].

plastics industry [Figure 13(b)] around Nagoya are shown in the enlargement in Figure 15 below. Here the establishment densities in these contiguous areas are sufficiently different so that by treating each as a different cluster, one obtains a better overall fit in terms of BIC – even though the resulting scheme is penalized for this larger number of clusters.

[Figure 15]

This example illustrates a case in which there are not only very different establishment densities among contiguous clusters, but also a strong "central" cluster: Nagoya in this case. More generally, it suggests that there is often more spatial structure in cluster schemes than is captured by a simple listing of their clusters. In particular, this example suggests that groupings of contiguous clusters might best be treated a single *agglomerations* for an industry. So the grouping in Figure 15 might be designated as the "Nagoya agglomeration" centered around the "Nagoya cluster." More generally, while we have implicitly used the terms "clusters" and "agglomerations" interchangeably in this paper, it would seem that latter term is best reserved for *maximal contiguous sets* of clusters.

5.4 Sensitivity Analysis

Finally, we report on the sensitivity of cluster schemes identified with respect to small perturbations to the search algorithm and to regional divisions. While our objective is to propose the first practical framework for identifying industrial clusters on a map using regional data, and not intended to propose either the most efficient search algorithm for the best cluster schemes, or the procedure which guarantees invariant solutions under different regional divisions, it would nonetheless be informative to quantify the robustness of our cluster detection with respect to perturbations in these aspects.

5.4.1 Alternative Initial Clusters

We first investigate the sensitivity of the result under alternative starting cluster, i.e., by initiating the cluster search by setting a randomly chosen municipality (with a strictly positive number of establishments of the industry in question) as an initial cluster. We have generated ten such samples for each of 154 industries with non-spurious clusters. Among all the 1540 samples obtained, the values of $\triangle_{\mathbf{C}}$ associated with the cluster schemes, $\mathbf{C}$, identified under alternative initial clusters range from less than 0.01% to 106% of that under the original initial clusters.

To compare the coverage of cluster schemes, denote by R_C the set of municipalities which belong to clusters identified under the original initial cluster, and by R'_C that under an alternative initial cluster. Then, the agreement between the cluster schemes under the original and alternative initial clusters can be measured in terms of the average share of overlapping clusters defined by

$$S = \frac{1}{2} \sum_{r \in R_C \cap R'_C} n_r \left[\frac{1}{\sum_{r \in R_C} n_r} + \frac{1}{\sum_{r \in R'_C} n_r} \right] \tag{53}$$

where n_r is the number of establishments (of the industry in question) in region r. The minimum value of S among the 1540 samples is 0.958. Hence, we conclude that the cluster schemes identified are highly robust against the perturbation of initial clusters.

5.4.2 Perturbation of Regional Divisions

Next, we employ simulation methods to determine whether the identified cluster schemes are sensitive to small perturbations of municipality boundaries. To construct each perturbation, we first randomly partition the set of all municipalities in R into mutually exclusive adjacent pairs. In particular, if $\mathbf{N} = \{(r, s) \in R : r \in N(s)\}$ denotes the set of all adjacent municipality pairs, then this partition is given by a randomly selected maximal subset, $\mathbf{N}'$, of mutually exclusive pairs in $\mathbf{N}$ [which by definition satisfies the two conditions, that (i) $\{r, s\} \cap \{r', s'\} = \varnothing$ for all $(r, s), (r', s') \in \mathbf{N}'$, and that (ii) for each $(r, s) \notin \mathbf{N}'$ there is some $(r', s') \in \mathbf{N}'$ with $\{r, s\} \cap \{r', s'\} \neq \varnothing$]. Second, for each pair, $(r, s) \in \mathbf{N}'$, we reallocate 5% of both establishments and economic area from one municipality to the other,[26] where the direction of the reallocation is determined randomly.

[26] The number of establishments to be reallocated is rounded to the nearest integer.

Using this procedure, we again generated ten randomly perturbed samples for each of 154 industries. Within each industry, we focus only on the set of core clusters in the original cluster scheme (using $\mu = 0.05$ as defined in Section 4.4 above). With respect to these clusters, we then compute the *industry share* (in terms of the number of establishments) that continues to appear in clusters identified for the perturbation. In all but three industries, these industry shares exceeded 95% in each of the ten sample perturbations. A common property of these three exceptional industries ("alcoholic beverages," "paving materials,"and "cement and its products"), is that they are relatively ubiquitous. As for paving materials, the original clusters account for only 39.1% of all establishments, which is the smallest among all industries (where the average value is 93.6%). Thus, the majority of establishments of this industry are located outside clusters. As for the other two, while original clusters do account for a substantial percentage of industry establishments (more than 70%), these clusters are spread over more than 40% of the national economic area, as opposed to an average share of 22.7% for all industries. Thus, for extremely ubiquitous industries of this type, such perturbations in the regional allocation of establishments and economic area can in principle produce quite different clustering patterns. But for the vast majority of industries, our cluster-identification procedure does appear to produce robust results.[27]

6 Concluding Remarks

In this paper we have developed a simple *cluster-scheme* model of agglomeration patterns and have constructed an information-based algorithm for identifying such patterns. To the best of our knowledge, this constitutes the first systematic framework for doing so. In addition, this formal framework opens up a number of possible directions for further research. In particular, by utilizing clusters identified, it becomes possible for the first time

[27] It is to be noted that since municipality sizes vary significantly for the case of Japan, where the geographic area of municipalities range from 1.64 to $1408.1km^2$, the 5% reallocations of establishments and economic area are actually not "small" perturbations for relatively large municipalities. Hence, the result here indicates strong robustness of our approach for the case of localized industries.

to directly identify the spatial patterns of industrial agglomerations on a map, and test the hypotheses implied by the recent theoretical developments on economic agglomerations under many-region/continuous location space (e.g., Fujita et al. [8], Tabuchi and Thisse [30], Hsu [10], Ikeda et al. [12]). Below, we touch on two areas where initial investigations are already under way.

6.1 Cluster-Based Choice Cities for Industries

In our previous work (Mori et al. [21]) we reported on an empirical regularity between the (population) size and industrial structure of cities in Japan, designated as the *Number-Average Size* (*NAS*) *rule.* This regularity (also established for the United States by Hsu [10]) asserts a negative log-linear relation between the number and average population size of those cities where a given industry is present. Hence the validity of the NAS rule depends critically on how such "industrial presence" is defined. In its follow-up paper (Mori and Smith [23]) we have employed the present cluster-detection procedure to identify cities where given industries exhibit a "substantial" presence with respect to their agglomeration patterns. In particular, if $\mathcal{U}$ denotes the relevant set of cities in R, and if $\mathbf{C}_i$ is the cluster scheme identified for industry i, then each city $U \in \mathcal{U}$ containing establishments from at least one of the clusters in $\mathbf{C}_i$ is designated as a *cluster-based* (*cb*) *choice city* for industry i. This cluster-based approach to industrial presence yields a sharper version of the NAS rule for the case of Japan. In addition, by identifying those *cb*-choice cities shared by different industries, this also provides one approach to analyzing *spatial coordination* between industries. In ongoing work (Hsu, Mori, and Smith [11]), we are examining the consequences of such industrial coordination for city size distributions, and in particular for the *Rank Size Rule.* In addition, by examining the *spacing* between *cb*-cities for industries, one can also formulate a range of testable propositons about the spatial structure of urban hierarchies.

6.2 Regional Agglomeration Analysis

As emphasized in the Introduction, most analyses of industrial agglomeration have relied on overall indices of agglomeration, and hence have necessarily been aggregate in nature. However the present identification of local cluster patterns for industries allows the possibility for more disaggregate spatial analyses. Of particular interest is the question of *why* industries agglomerate in certain regions and not others. While this question has of course been addressed by a variety of theoretical models, there has been little empirical work done to date. This is in large part due to the conspicuous absence of "local agglomeration" measures. While the present cluster-scheme model is not itself numerical, it nonetheless suggests a number of possibilities for such measures.

The simplest are of course binary variables indicating the "presence" or "absence" of agglomeration. Indeed, the above definition of *cb*-choice cities yields precisely a binary variable of this type on the set of cities, $\mathcal{U}$. Hence, given appropriate socio-economic data for cities, $U \in \mathcal{U}$, one could in principle test for significant predictors of industrial presence in these cities by employing standard logit or probit models.

Alternatively, one may focus directly on the individual clusters for each industry. Here one might characterize the degree of local agglomeration for each industry in terms of the contribution of these clusters to the industry as a whole. Natural candidates include the fraction of industry establishments or employment in each cluster. Given the availability of data at the municipality level, one could in principle aggregate such data to the cluster level, and use this to identify predictors of local agglomeration by more standard types of linear regression models. As one illustration, in Japan, data on education levels (among others) is available at the municipality level. Thus, by employing appropriate summary measures, "education accessability" across cluster municipalities can be defined. Then, by treating "industry" as a categorical variable, one can attempt to compare the relative importance of these local accessibilities in attracting various industries. Regression analyses of this type will be presented in subsequent work (Mori and Smith [25]).

7 APPENDIX. Formal Analysis of d-Convex Solids

To develop formal properties of d-convex solids, we require a few additional definitions. First, for any path, $\rho = (r_1, r_{2,}..., r_{n-1}, r_n) \in \mathcal{P}(r_1, r_n)$, let $\widetilde{\rho} = (r_n, r_{n-1}, .., r_2, r_1) \in \mathcal{P}(r_n, r_1)$ denote the *reverse path* in $\mathcal{P}$. Next, for any two paths, $\rho = (r_1, ..., r_n)$, $\rho' = (r'_1, ..., r'_m) \in \mathcal{P}$, with $r_n = r'_1$, the combined path, $\rho \circ \rho' = (r_1, .., r_n, r'_2, ..., r'_m) \in \mathcal{P}$ is designated as the *concatenation* of ρ and ρ'. It then follows by definition that the length of any concatenated path, $\rho \circ \rho'$, is simply the sum of the lengths of ρ and ρ', i.e., that $l(\rho \circ \rho') = \sum_{i=1}^{n-1} d(r_i, r_{i+1}) + d(r_n, r'_2) + \sum_{i=2}^{m-1} d(r'_i, r'_{i+1}) = \sum_{i=1}^{n-1} d(r_i, r_{i+1}) + \sum_{i=1}^{m-1} d(r'_i, r'_{i+1}) = l(\rho) + l(\rho')$. Using this and (20) through (23), it is convenient to establish the following well-known properties of d-convex sets, as in Definition 3.1 of the text. First, we show that for the *d-convexification function*, $c_d : \mathcal{R} \to \mathcal{R}$, in (23), the naming of this function is justified by the fact that:

Proposition A.1 (**d-Convexification**) *For all $S \in \mathcal{R}$, the image set, $c_d(S)$, is d-convex.*

Proof: For any $r_1, r_2 \in c_d(S)$ and shortest path, $\rho \in \mathcal{P}_d(r_1, r_2)$, it must be shown that $\langle\rho\rangle \subseteq c_d(S)$. But by definition, $r_i \in c_d(S) \Rightarrow r_i \in I^{k_i}(S)$ for some k_i, $i = 1, 2$. Hence by (21) it follows that $\{r_1, r_2\} \subseteq I^{k_1+k_2}(S)$. Thus, $\langle\rho\rangle \subseteq I(I^{k_1+k_2}(S)) = I^{k_1+k_2+1}(S) \subseteq c_d(S)$.■

Next we show that the d-convex hull, $c_d(S)$, can be characterized as the unique smallest d-convex superset of S. More precisely, if $\mathcal{R}_d$ denotes the family of all d-convex sets in $\mathcal{R}$, then we have:

Proposition A.2 (**Minimality of d-Convexifications**) *For all $S \in \mathcal{R}$,*

$$c_d(S) = \cap\{C \in \mathcal{R}_d : S \subseteq C\} \ . \tag{54}$$

Proof: By Proposition A.1, $c_d(S) \in \mathcal{R}_d$, and by (20)

$$S \subseteq I(S) \subseteq c_d(S) \tag{55}$$

Hence it suffices to show that for all sets, C, with $C \in \mathcal{R}_d$ and $S \subseteq C$, we must have

$c_d(S) \subseteq C$. By the definition of $c_d(S)$ this in turn is equivalent to showing that $I^k(S) \subseteq C$ for all $k \geq 1$. But by (19),

$$S \subseteq C \Rightarrow \bigcup\nolimits_{r,s\in S} I(r,s) \subseteq \bigcup\nolimits_{r,s\in C} I(r,s) \Rightarrow I(S) \subseteq I(C) \ . \tag{56}$$

Moreover, by (18) and (19) together with the definition of d-convexity it follows that

$$C \in \mathcal{R}_d \Rightarrow I(C) = \bigcup\nolimits_{r,s\in C} I(r,s) \subseteq C \ . \tag{57}$$

Hence we may conclude from (56) and (57) that $I(S) \subseteq C$. Finally, since the same argument shows that $I^k(S) \subseteq C \in \mathcal{R}_d \Rightarrow I^{k+1}(S) = I[I^k(S)] \subseteq C$, the result follows by induction on k.■

Finally, using these two results, we show that d-convex sets can be equivalently characterized as the *fixed points* of the d-convexification mapping, $c_d : \mathcal{R} \to \mathcal{R}$:

Proposition A.3 (**d-Convex Fixed Points**) *For all $S \in \mathcal{R}$,*

$$S \in \mathcal{R}_d \ \Leftrightarrow \ c_d(S) = S \ . \tag{58}$$

Proof: If $c_d(S) = S$ then $S \in \mathcal{R}_d$ by Proposition A.1. Conversely, if $S \in \mathcal{R}_d$ then $S \subseteq c_d(S)$ by (55), and $c_d(S) \subseteq S$ by Proposition A.2, hence $c_d(S) = S$.■

This in turn implies that the family, $\mathcal{R}_d$, of d-convex sets can be equivalently defined as in expression (24) of the text. But while this definition provides a natural parallel to the case of d-convex solids developed below, the more useful *interval* characterization of $\mathcal{R}_d$ in expression (25) of the text, can easily be obtained from Proposition A.3 as follows:

Corollary (**Interval Fixed Points**) *For all $S \in \mathcal{R}$,*

$$S \in \mathcal{R}_d \ \Leftrightarrow \ I(S) = S \ . \tag{59}$$

Proof: Since $S \in \mathcal{R}_d \Rightarrow I(S) \subseteq S$ by (57) [with $C = S$], and since $S \subseteq I(S)$ holds for all S [by (20)], it follows on the one hand that $S \in \mathcal{R}_d \Rightarrow I(S) = S$. Conversely, since $I(S) = S \Rightarrow I^k(S) = S$ for all $k \geq 1$[by recursion on k], it follows from (23) and Proposition A.3 that $I(S) = S \Rightarrow c_d(S) = S \Rightarrow S \in \mathcal{R}_d$. ■

Given these properties of d-convex sets, one objective of this Appendix is to show that each of these properties is inherited by d-convex solids. To do so, we begin with an analysis of *solid* sets as in Definition 3.2 of the text. First, in a manner paralleling Proposition A.1 above, we show for the *solidification function*, $\sigma : \mathcal{R} \to \mathcal{R}$, defined by (27), the naming of this function is justified by the fact that:

Lemma A.1 (**Solidification**) *For all* $S \in \mathcal{R}$, *the image set*, $\sigma(S)$, *is solid.*

Proof: If $V = \sigma(S) = S \cup S_0$, then it must be shown that for all $r \in R - V$ there is some path, $\rho \in \mathcal{P}(r, \overline{R})$ with $\langle\rho\rangle \cap V = \varnothing$. But for any $r \in R - V = R - (S \cup S_0)$, it follows that $r \in R \backslash S$ and $r \notin S_0$, so that by the definition of S_0 in (26) it must be true that there is some boundary region, $\overline{r} \in \overline{R}$, and path, $\rho \in \mathcal{P}(r, \overline{r})$ with $\langle\rho\rangle \cap S = \varnothing$. Next we show that $\langle\rho\rangle \cap S_0 = \varnothing$ as well. To do so, suppose to the contrary that $\langle\rho\rangle \cap S_0 \neq \varnothing$, so that for some $r_0 \in S_0$, $\rho = (r, .., r_0, .., \overline{r}) = \rho_1 \circ \rho_2$ with $\rho_1 \in \mathcal{P}(r, r_0)$ and $\rho_2 \in \mathcal{P}(r_0, \overline{r})$. Then again by the definition of S_0 it must be true that $\langle\rho_2\rangle \cap S \neq \varnothing$, which contracts the fact that $\langle\rho_2\rangle \subseteq \langle\rho\rangle$ and $\langle\rho\rangle \cap S = \varnothing$. Hence $\varnothing = (\langle\rho\rangle \cap S) \cup (\langle\rho\rangle \cap S_0) = \rho \cap (S \cup S_0) = \langle\rho\rangle \cap V$, and the result is established.■

If the family of all solid sets in $\mathcal{R}$ is denoted by $\mathcal{R}_\sigma = \{S \in \mathcal{R} : S_0 = \varnothing\}$, then we next show that these sets are precisely the fixed points of the solidification function:

Lemma A.2 (**Solid Fixed Points**) *For all* $S \in \mathcal{R}$,

$$S \in \mathcal{R}_\sigma \;\Leftrightarrow\; \sigma(S) = S\ . \tag{60}$$

Proof: If $S \in \mathcal{R}_\sigma$ then $S_0 = \varnothing$, so that $\sigma(S) = S$ by (27). Conversely, if $\sigma(S) = S$, then by Lemma A.1, $S \in \mathcal{R}_\sigma$.■

As a parallel to (59), this in turn implies that the family of solid sets in $\mathcal{R}$ can be equivalently defined as follows:

$$\mathcal{R}_\sigma = \{S \in \mathcal{R} : \sigma(S) = S\} \ . \tag{61}$$

Finally, solid sets also exhibit the following nesting property:

Lemma A.3 (**Solid Nesting**) *For all* $S, V \in \mathcal{R}$,

$$S \subseteq V \ \Rightarrow \ \sigma(S) \subseteq \sigma(V) \ . \tag{62}$$

Proof: Since $S \subseteq V \subseteq V \cup V_0 = \sigma(V)$, it suffices to show that $S_0 \subseteq \sigma(V)$. Hence consider any $r \in S_0$, and observe from the above that $r \in V \Rightarrow r \in \sigma(V)$. Hence it remains to consider $r \in S_0 - V$. Here we show that r must be in V_0. To do so, observe first that $r \notin V \Rightarrow r \in R - V$. Moreover, $r \in S_0$ implies that for any path, $\rho \in \mathcal{P}(r, \overline{R})$ we must have $\langle\rho\rangle \cap S \neq \varnothing$. But $S \subseteq V$ then implies $\langle\rho\rangle \cap V \neq \varnothing$. Hence $r \in V_0 \subseteq \sigma(V)$, and the result is established.■

With these properties of solid sets, we are ready to analyze d-convex solids in $\mathcal{R}$. As asserted in the text, our key result is to show that d-convexity is preserved under solidifications:

Theorem A.1 (**Solidification Invariance of *d*-Convexity**) *For all d-convex sets,* $S \in \mathcal{R}$, *the image set,* $\sigma(S)$, *is also d-convex.*

Proof: Suppose to the contrary that for some d-convex set, S, the image set $\sigma(S)$ is not d-convex. Then there must exist some pair of elements, $r_1, r_2 \in \sigma(S) = S \cup S_0$, and some shortest path, $\rho \in \mathcal{P}_d(r_1, r_2)$, with $\langle\rho\rangle \cap [R - \sigma(S)] \neq \varnothing$. But if $\{r_1, r_2\} \subseteq S$ then by the d-convexity of S we would have $\langle\rho\rangle \subseteq S \subseteq \sigma(S)$. So at least one of these elements must be in S_0. Without loss of generality, we may suppose that $r_1 \in S_0$ and that r is some element of $\langle\rho\rangle \cap [R - \sigma(S)]$, so that $\rho = (r_1, .., r, .., r_2) = \rho_1 \circ \rho_2$ with $\rho_1 \in \mathcal{P}(r_1, r)$ and $\rho_2 \in \mathcal{P}(r, r_2)$. But then we must have $S \cap \langle\rho_1\rangle \neq \varnothing$. For if not then we obtain a contradiction as follows. Since $r \notin \sigma(S) \Rightarrow [r \in R \backslash S$ and $r \notin S_0]$, there must be some path, $\rho_3 \in \mathcal{P}(r, \overline{R})$ with $\langle\rho_3\rangle \cap S = \varnothing$. Hence the combined path, $\rho_1 \circ \rho_3 \in \mathcal{P}(r_1, \overline{R})$, then satisfies $\langle \rho_1 \circ \rho_3 \rangle \cap S = \varnothing$, which contradicts the hypothesis that $r_1 \in S_0$. Thus we may assume that there is some $s_1 \in S \cap \langle \rho_1 \rangle$, and consider the following two cases:

(i) Suppose first that r_2 is also an element of S_0. We then show that this contradicts the hypothesized shortest-path property of ρ as follows. Observe first that if $\widetilde{\rho}_2 \in \mathcal{P}(r_2, r)$ denotes the reverse path for $\rho_2 \in \mathcal{P}(r, r_2)$ above, then the same argument used for $\rho_1 \in \mathcal{P}(r_1, r)$ above now shows that there must be some $s_2 \in S \cap \langle \widetilde{\rho}_2 \rangle = S \cap \langle \rho_2 \rangle$, so that $\rho = (r_1, .., s_1, .., r, .., s_2, .., r_2) = \rho_1' \circ \rho_2' \circ \rho_3' \circ\ \rho_4'$ with $\rho_1' \in \mathcal{P}(r_1, s_1)$, $\rho_2' \in \mathcal{P}(s_1, r)$, $\rho_3' \in \mathcal{P}(r, s_2)$,and $\rho_4' \in \mathcal{P}(s_2, r_2)$. These paths are shown in Figure 16 below.

[Figure 16]

But if we choose any shortest path, $\rho_5' \in \mathcal{P}_d(s_1, s_2)$ [as in Figure 16], then it follows from the d-convexity of S, together with $s_1, s_2 \in S$ and $r \notin S$ that $l(\rho_5') < l(\rho_2' \circ \rho_3')$ [since every shortest path in $\mathcal{P}_d(s_1, s_2)$ lies in S, and $\langle \rho_2' \circ \rho_3' \rangle \nsubseteq S$]. Hence for the path, $\rho' = \rho_1' \circ \rho_5' \circ \rho_4' \in \mathcal{P}(r_1, r_2)$, we must have $l(\rho') = l(\rho_1') + l(\rho_5') + l(\rho_4') < l(\rho_1') + [l(\rho_2') + l(\rho_3')] + l(\rho_4') = l(\rho_1' \circ \rho_2' \circ \rho_3' \circ \rho_4') = l(\rho)$ which contradicts the shortest-path property of ρ.

(ii) Finally, suppose that $r_2 \in S$, and for the point $s_1 \in S \cap \langle \rho_1 \rangle$ above, consider the representation of ρ as $\rho = (r_1, .., s_1, .., r, .., r_2) = \rho_1' \circ \rho_2' \circ \rho_2$ with $\rho_1' \in \mathcal{P}(r_1, s_1)$, $\rho_2' \in \mathcal{P}(s_1, r)$, and $\rho_2 \in \mathcal{P}(r, r_2)$, as shown in Figure 17 below.

[Figure 17]

Then we again show that this contradicts the shortest-path property of ρ as follows. For any shortest path, $\rho_6' \in \mathcal{P}_d(s_1, r_2)$ [as in Figure 17], the d-convexity of S, together with $s_1, r_2 \in S$ and $r \notin S$, now implies that $l(\rho_6') < l(\rho_2' \circ \rho_2)$. Thus for the path, $\rho'' = \rho_1' \circ \rho_6' \in \mathcal{P}(r_1, r_2)$, we must have $l(\rho'') = l(\rho_1') + l(\rho_6') < l(\rho_1') + [l(\rho_2') + l(\rho_2)] = l(\rho_1' \circ \rho_2' \circ \rho_2) = l(\rho)$ which again contradicts the shortest-path property of ρ. Hence for each pair of elements, $r_1, r_2 \in \sigma(S) = S \cup S_0$, there can be no shortest path, $\rho \in \mathcal{P}_d(r_1, r_2)$, with $\langle \rho \rangle \cap [R - \sigma(S)] \neq \varnothing$, so that $\sigma(S)$ is d-convex.■

With this result, we can now establish parallels to Propositions A.1, A.2, and A.3 above for d-convex solids, as in Definition 3.3. First, we show that for the *d-convex solidification function*, $\sigma c_d : \mathcal{R} \to \mathcal{R}$, in (28), the naming of this function is justified by the fact that:

Theorem A.2 (**d-Convex Solidification**) *For each set, $S \in \mathcal{R}$, the image set, $\sigma c_d(S)$, is a d-convex solid.*

Proof: First observe from Definition 3.3 that we may use expressions (59) and (60) to define the family of all d-convex solids in equivalent terms as

$$\mathcal{R}_{\sigma d} = \mathcal{R}_\sigma \cap \mathcal{R}_d \ . \tag{63}$$

Hence it suffices to show that $\sigma c_d(S) \in \mathcal{R}_d \cap \mathcal{R}_\sigma$. But by Proposition A.1, it follows that $c_d(S) \in \mathcal{R}_d$, and hence as a direct consequence of Theorem A.1 that $\sigma c_d(S) = \sigma[c_d(S)] \in \mathcal{R}_d$. Moreover, since $c_d(S) \in \mathcal{R}$ also implies from Lemma A.1 that $\sigma[c_d(S)] \in \mathcal{R}_\sigma$, it then follows that $\sigma c_d(S) \in \mathcal{R}_{\sigma d}$.■

Next, as a parallel to Proposition A.2 we now have:

Theorem A.3 (**Minimality of d-Convex Solidifications**) *For each set, $S \in \mathcal{R}$,*

$$\sigma c_d(S) = \cap\{C \in \mathcal{R}_{\sigma d} : S \subseteq C\} \ . \tag{64}$$

Proof: First observe from Theorem A.2 that $\sigma c_d(S) \in \mathcal{R}_{\sigma d}$ and from expression (55) that $S \subseteq c_d(S) \subseteq \sigma[c_d(S)] = \sigma c_d(S)$ [since by definition, $V \in \sigma(V)$ for all V]. Hence, it suffices to show that $\sigma c_d(S) \subseteq C$ whenever $S \subseteq C \in \mathcal{R}_{\sigma d}$. But by Proposition A.2, $C \in \mathcal{R}_{\sigma d} \subseteq \mathcal{R}_d$ and $S \subseteq C$ imply that $c_d(S) \subseteq C$. Moreover, since $C \in \mathcal{R}_{\sigma d} \subseteq \mathcal{R}_\sigma$, we obtain the following conclusion from Lemma A.3 together with Lemma A.2, and the result is established.

$$c_d(S) \subseteq C \Rightarrow \sigma[c_d(S)] \subseteq \sigma(C) = C \Rightarrow \sigma c_d(S) \subseteq C \qquad \blacksquare \tag{65}$$

Finally, we may use these results to show that d-convex sets are equivalently characterized as *fixed points* of the d-convex solidification function, $c_{\sigma d} : \mathcal{R} \to \mathcal{R}$:

Theorem A.4 (*d*-**Convex Solid Fixed Points**) *For all* $S \in \mathcal{R}$,

$$S \in \mathcal{R}_{\sigma d} \ \Leftrightarrow \ c_{\sigma d}(S) = S \ . \tag{66}$$

Proof: If $c_{\sigma d}(S) = S$ then by Theorem A.2, $S \in \mathcal{R}_{\sigma d}$. Conversely, if $S \in \mathcal{R}_{\sigma d}$ then since $S \in \mathcal{R}_{\sigma d} \subseteq \mathcal{R}_d$ implies from Proposition A.3 that $c_d(S) = S$, we may conclude from Lemma A.2 that $c_{\sigma d}(S) = \sigma[c_d(S)] = \sigma(S) = S$, and the result is established.■

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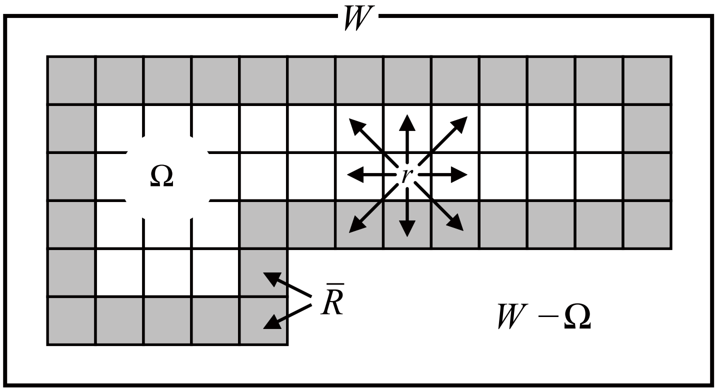


Figure 1: Geographical framework

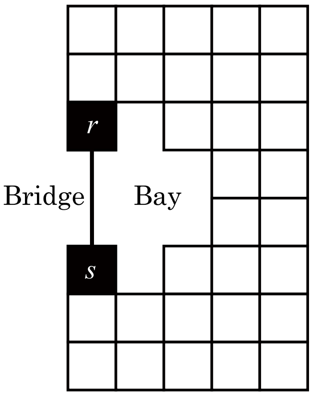


Figure 2: Bridge example

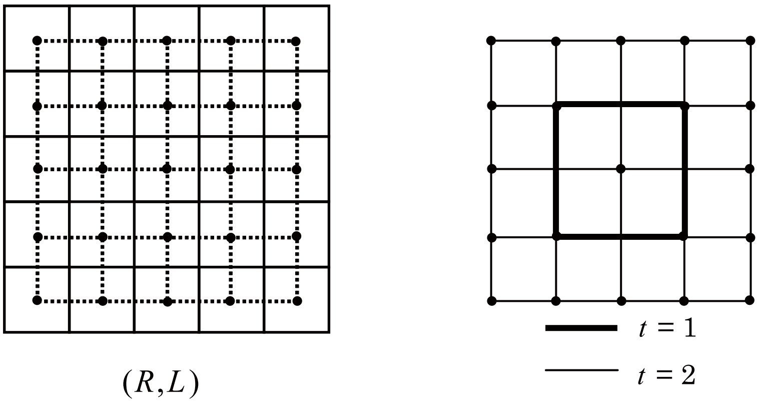


Figure 3: Regional network example

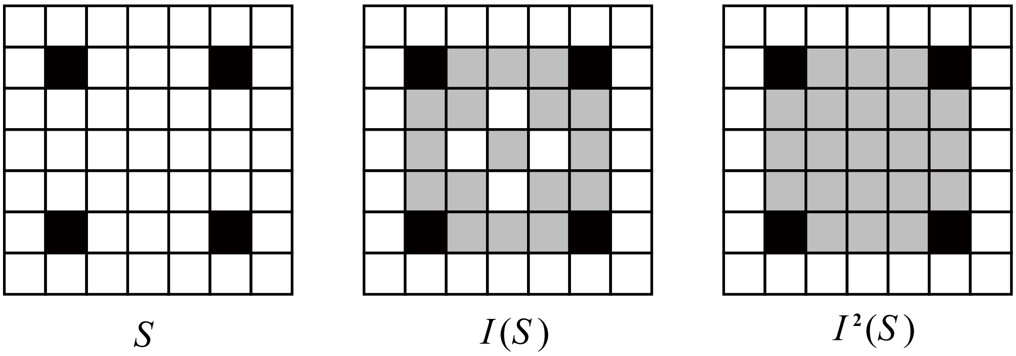


Figure 4: d-convexification of sets

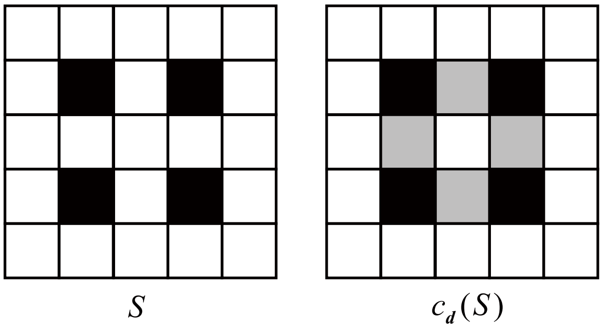


Figure 5: d-convex set with a hole

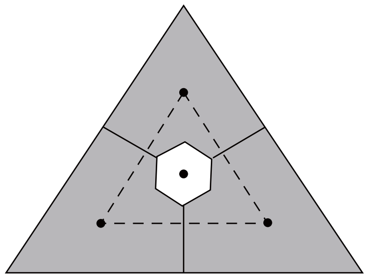


Figure 6: Non-solid d-convex set

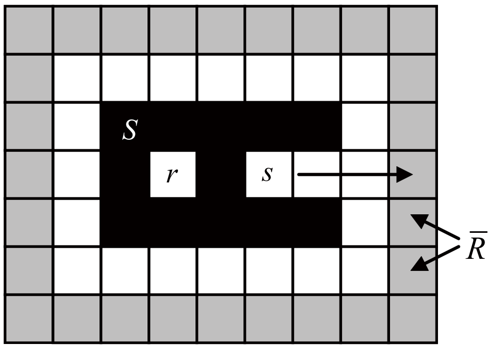


Figure 7: Inside versus outside

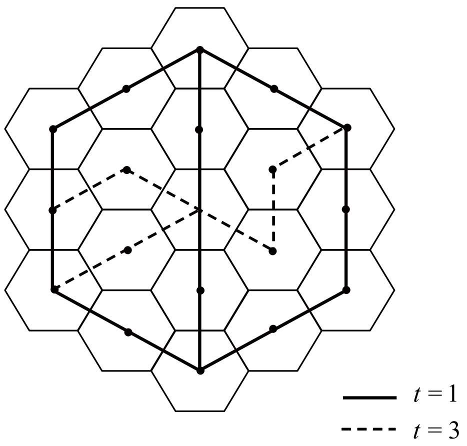


Figure 8: Regional subsystem

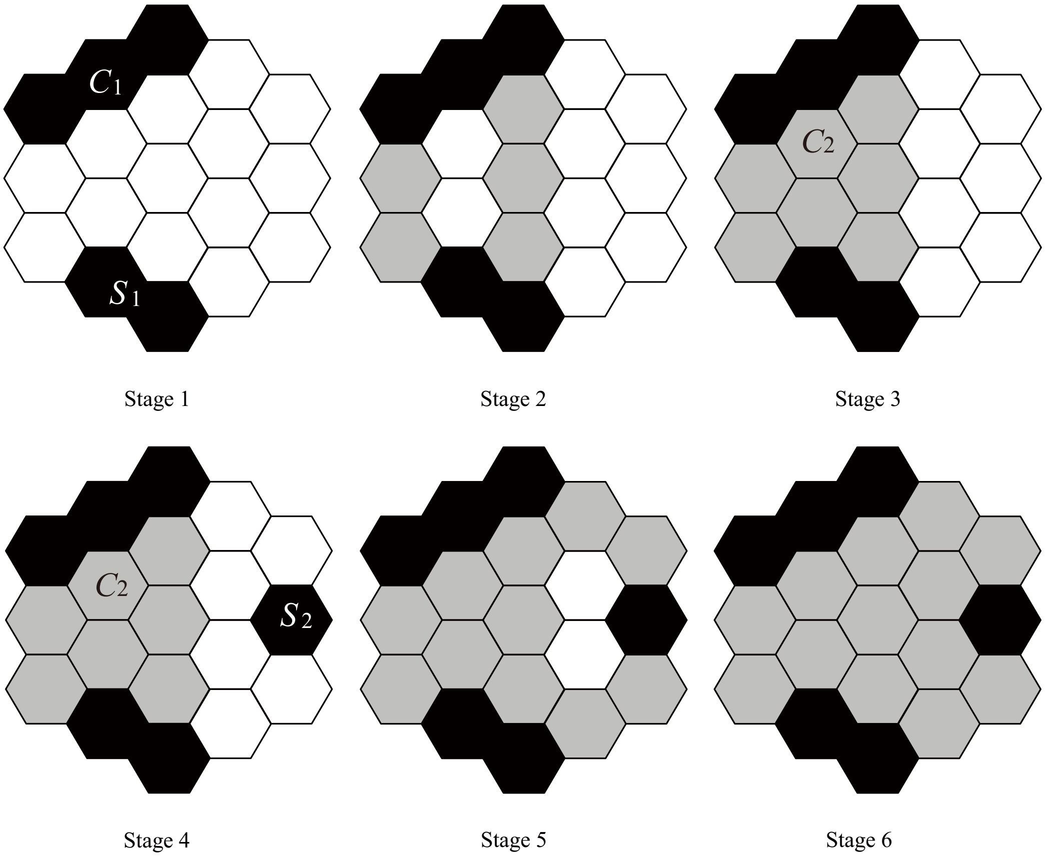


Figure 9: Formation of composite clusters

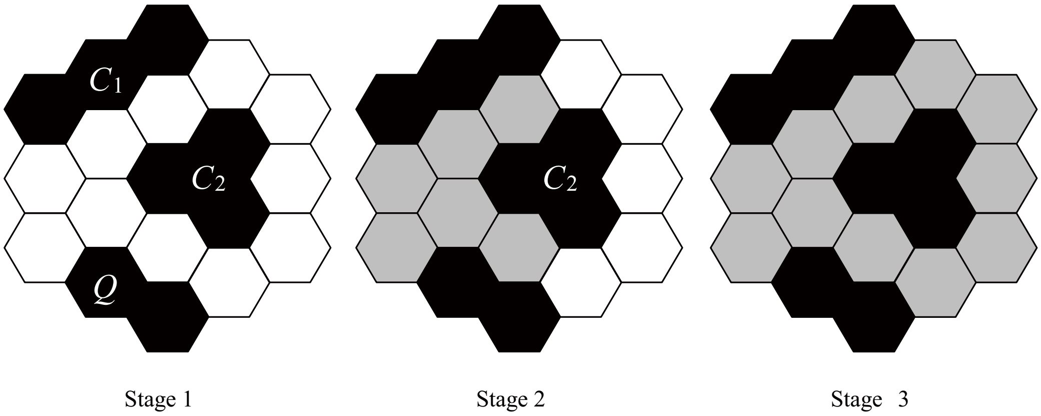


Figure 10: Formation of composite clusters

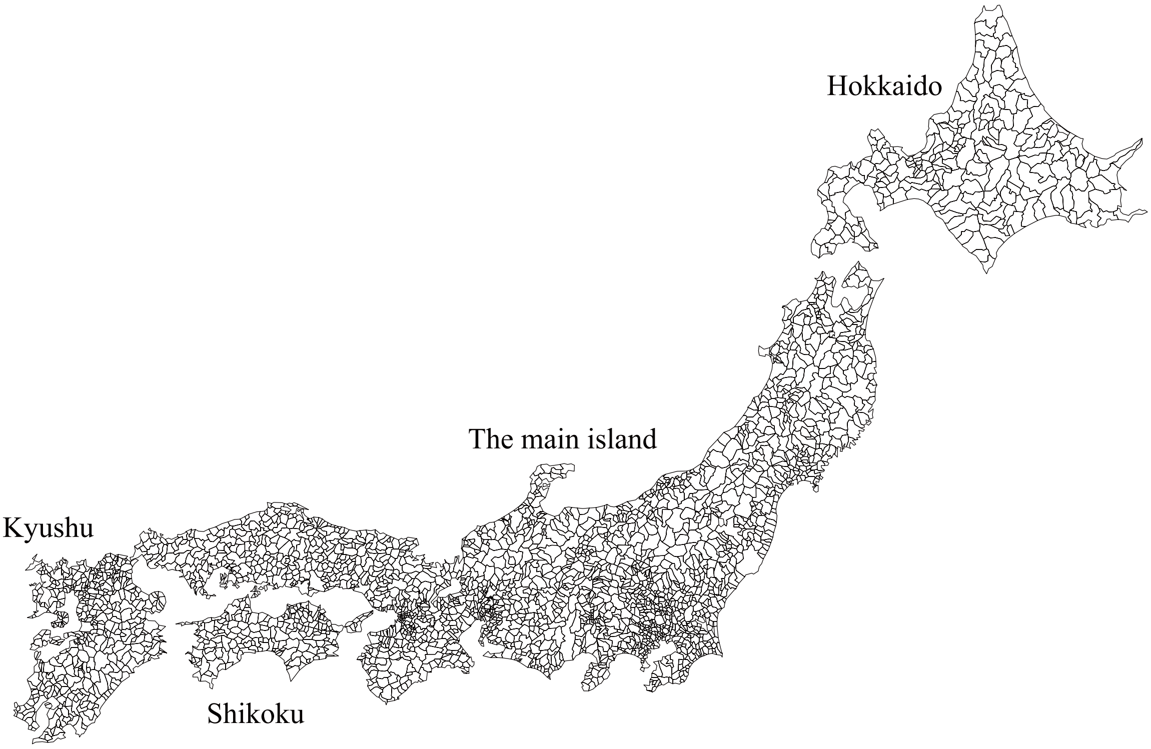


Figure 11: Basic regions (shi-ku-cho-son) of Japan

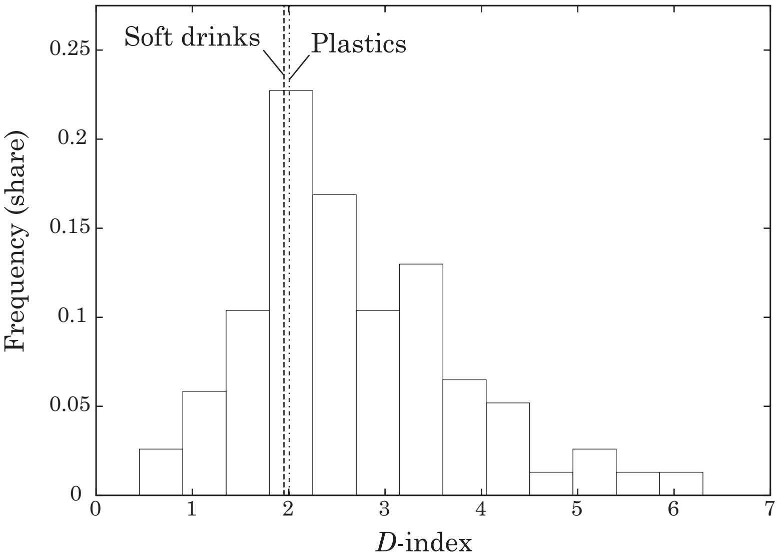
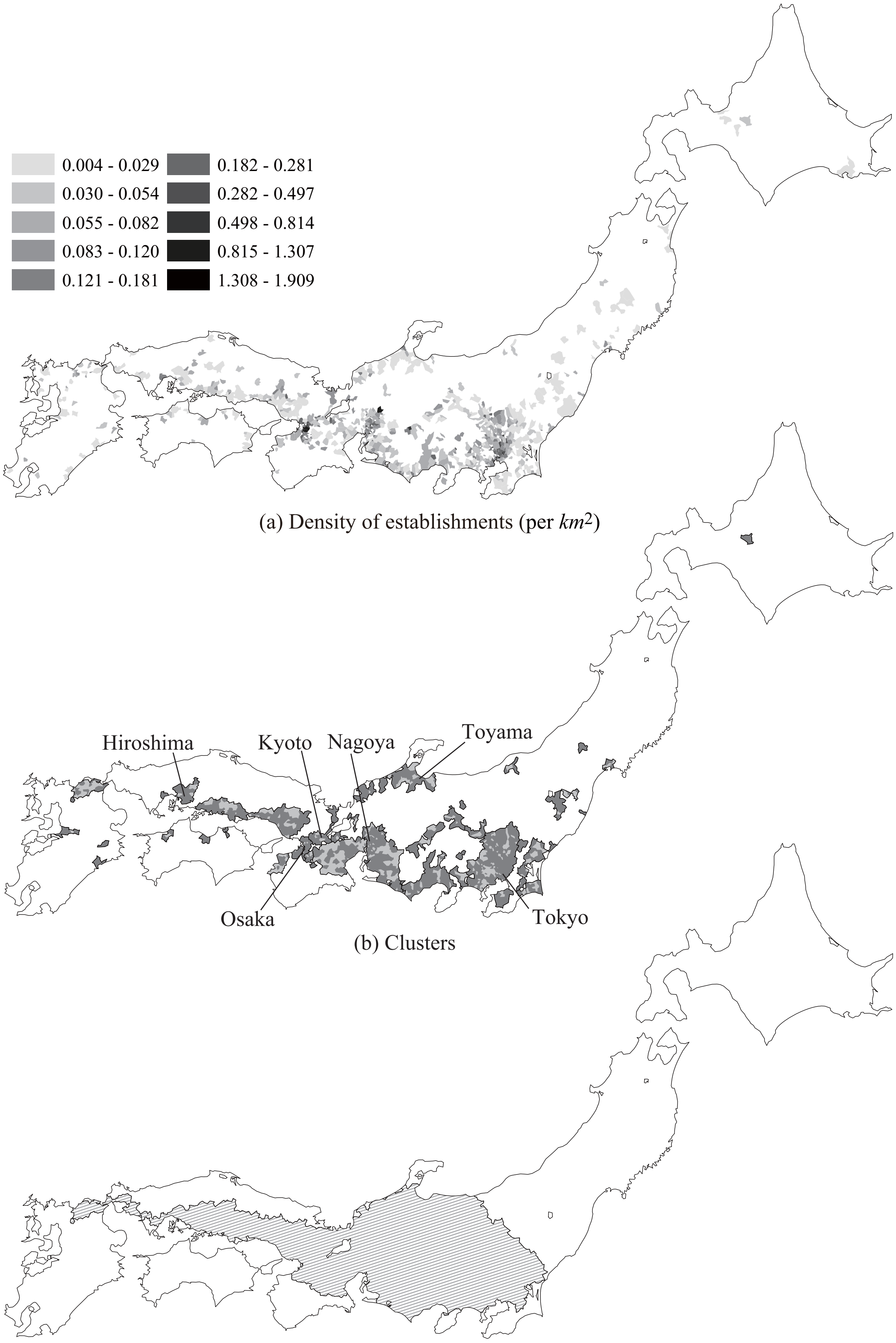


Figure 12: Frequency distribution of D-values of Japanese manufacturing industries

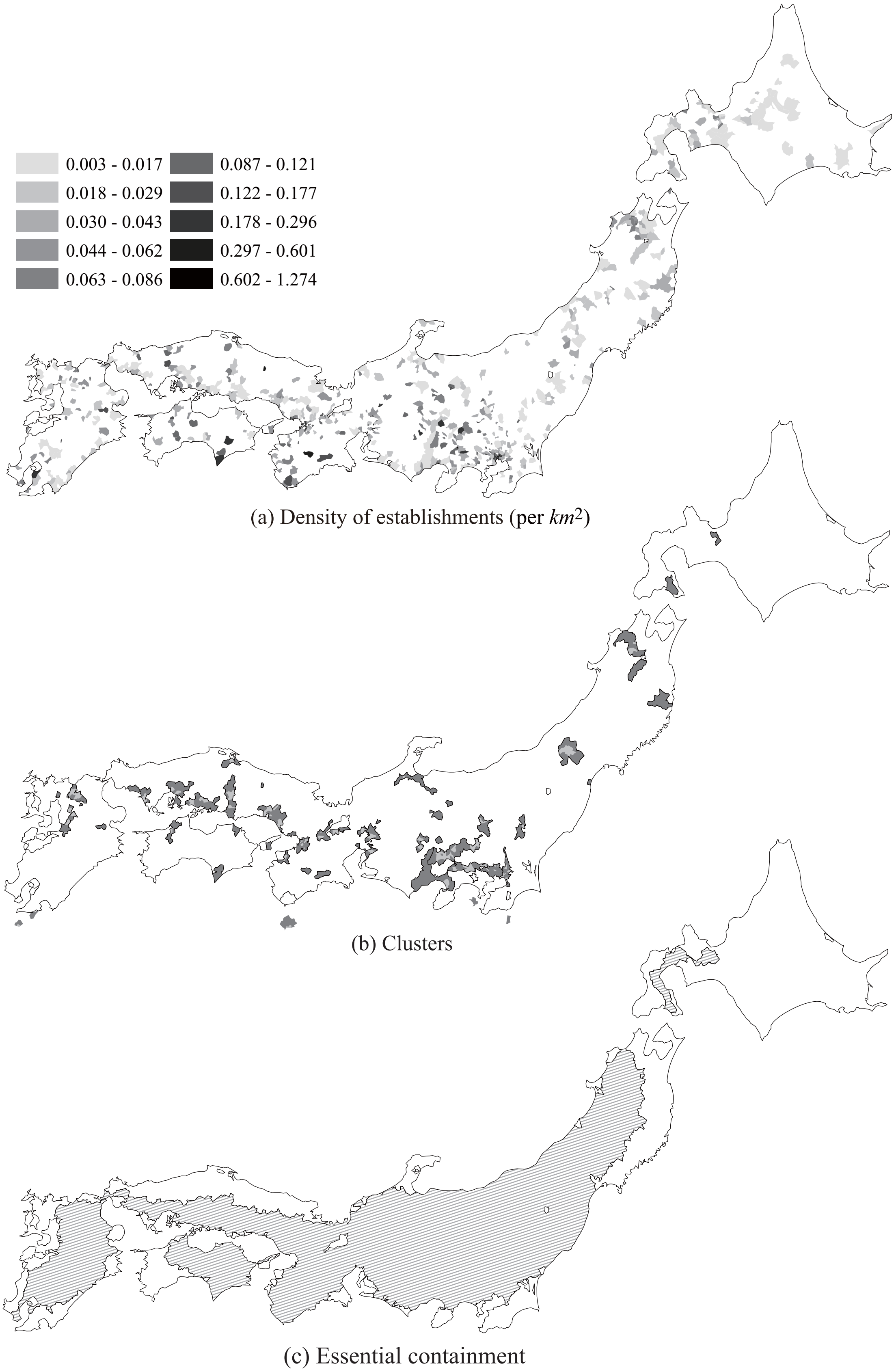


(a) Density of establishments (per km^2)

(b) Clusters

(c) Essential containment

Figure 13: Spatial distributions of establishments and clusters : compounding plastic materials, including reclaimed plastics



(a) Density of establishments (per km^2)

(b) Clusters

(c) Essential containment

Figure 14: Spatial distributions of establishments and clusters : soft drinks and carbonated water

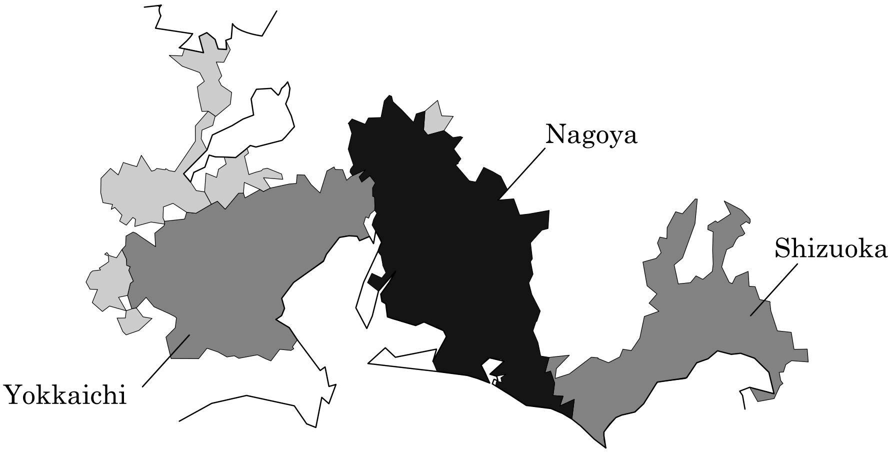


Figure 15: Spatial distributions of establishments and clusters : soft drinks and carbonated water

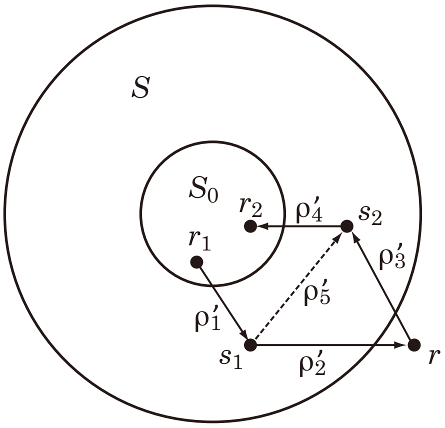


Figure 16: Example (i)

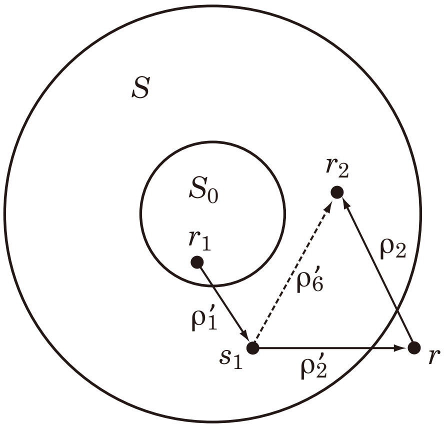


Figure 17: Example (ii)