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Article *in* International Journal of Geographical Information Science · April 2015

DOI: 10.1080/13658816.2015.1031671

Kamyoung Kim
Kyungpook National University

Denis Joseph Dean
University of Texas at Dallas

Hyun Kim
University of Tennessee

International Journal of Geographical Information Science, 2016
Vol. 30, No. 3, 451–473, http://dx.doi.org/10.1080/13658816.2015.1031671

Spatial optimization for regionalization problems with spatial interaction: a heuristic approach

Kamyoung Kim[a], Denis J. Dean[b], Hyun Kim[c] and Yongwan Chun[b]*

[a]*Department of Geography Education, Kyungpook National University, Buk-gu, Daegu, Korea;* [b]*School of Economic, Political and Policy Sciences, The University of Texas at Dallas, Richardson, TX, USA;* [c]*Department of Geography, University of Tennessee at Knoxville, Knoxville, TN, USA*

(*Received 12 August 2014; final version received 9 March 2015*)

Spatial optimization techniques are commonly used for regionalization problems, often represented as *p*-regions problems. Although various spatial optimization approaches have been proposed for finding exact solutions to *p*-regions problems, these approaches are not practical when applied to large-size problems. Alternatively, various heuristics provide effective ways to find near-optimal solutions for *p*-regions problem. However, most heuristic approaches are specifically designed for particular geographic settings. This paper proposes a new heuristic approach named Automated Zoning Procedure-Center Interchange (AZP-CI) to solve the *p*-functional regions problem (PFRP), which constructs regions by combining small areas that share common characteristics with predefined functional centers and have tight connections among themselves through spatial interaction. The AZP-CI consists of two subprocesses. First, the dissolving/splitting process enhances diversification and thereby produces an extensive exploration of the solution space. Second, the standard AZP locally improves the objective value. The AZP-CI was tested using randomly simulated datasets and two empirical datasets with different sizes. These evaluations indicate that AZP-CI outperforms two established heuristic algorithms: the AZP and simulated annealing, in terms of both solution quality and consistency of producing reliable solutions regardless of initial conditions. It is also noted that AZP-CI, as a general heuristic method, can be easily extended to other regionalization problems. Furthermore, the AZP-CI could be a more scalable algorithm to solve computational intensive spatial optimization problems when it is combined with cyberinfrastructure.

Keywords: regionalization; *p*-functional regions problem; hybrid heuristic; automated zoning procedure-center interchange (AZP-CI); spanning tree

1. Introduction

Functional regions often serve as a guide for defining geographical limits and structures. For example, they often play important roles in regional planning and policymaking. Consequently, the delineation of functional regions is an important topic in various fields, including geography and regional science (e.g., Duque *et al.* 2007, Coombes 2013). Generally, a functional region consists of small areal units, which exhibit more interaction with other units within the region than areal units outside the region (Brown and Holmes 1971). In an economic context, it is usually assumed that the level of services and job opportunities provided by one area to another diminishes with distance, and thus a

*Corresponding author. Email: ywchun@utdallas.edu

functional region is usually assumed to be a geographic entity that provides a high level of services and job opportunities to its component areas (Masser and Brown 1975, Kim *et al.* 2013). Often, a functional region represents an influential area of economic activity, where people travel from a hinterland to one or more centers within the region. Hence, frequent interactions are observed between the areal units representing the hinterland and those representing the region's center(s). This relationship between a functional center and its hinterland is often discussed as a hierarchical regional structure (e.g., Goodchild and Kwan 1978, Fusco and Caglioni 2011) and, more specifically, as central place theory (Berry and Garrison 1958).

A critical challenge in regionalization problems is embedding a set of spatial contiguity constraints into the solution approach (Shirabe 2009, Duque *et al.* 2011, Salazar-Aguilar *et al.* 2011, Kim *et al.* 2013). In most models, spatial contiguity constraints are expressed as mathematical formulations. Although several approaches for incorporating this form of spatial contiguity constraints have been proposed, their models become computationally intractable to even small-size problems due to the complexity of the models caused by the additional constraints (see Duque *et al.* 2012). As a result, applications of these models to large-size problems remain challenging, although cyberinfrastructure can provide a viable solution for complex large-scale problems. As a recent example, Kim *et al.* (2013) proposed a model for the *p*-functional regions problem (PFRP), which delineates functional regions using geographical flows and determines functional centers and their vicinities. The PFRP involves two simultaneous optimization processes: (1) determining functional centers and (2) delimiting the hinterland of each center. The model employs spatial contiguity conditions so that a region can be clustered without fragmentation. However, the main difference compared to previous work is that the PFRP formulates decision variables that indicate both the membership of a region and the functional center of a region, thereby reducing the overall number of variables. Although the PFRP can provide an elegant model for the regionalization problem and produce an exact solution, this approach is inherently unsuitable for solving a very large problem due to current limitations of computing capabilities.

This research is motivated by the practical need to solve large instances of the PFRP. Previously, the Automated Zoning Procedure (AZP) was proposed as a heuristic suitable for solving large instances of the PFRP (e.g., Openshaw and Rao 1995). The AZP is a greedy-type algorithm that provides a flexible environment within which any meta-heuristic approach can be incorporated. Along with the AZP, generic meta-heuristic methods including simulated annealing (SA) and tabu search have been highlighted to improve the quality of solutions for a large instance of districting problems and regionalization problems (e.g., Openshaw and Rao 1995, D'Amico *et al.* 2002, Blais *et al.* 2003, Bozkaya *et al.* 2003, 2011, Wei and Chai 2004, Ricca and Simeone 2008, Duque *et al.* 2012). The main idea of these methods is the diversification strategy, which is designed to avoid entrapment within local optima to find the optimal solution effectively. The algorithm focuses on how to effectively expand the set of search points in solution space using the treatment called 'moves' in order not to miss a best solution. This rule is identified as the aspiration criterion or as a continuous diversification process (Pham and Karaboga 2000). It should be noted that any single generic heuristic method has both advantages and limitations and its performance is sensitive to the change of characteristics of a problem at hand.

This paper proposes a hybrid heuristic approach named the AZP-Center Interchange (AZP-CI), which contains a center interchange process in addition to the standard AZP. The center interchange occurs between a center in an intermediate solution and a new potential center. This interchanging method is similar to the Teitz and Bart (1968) interchange algorithm applied for the *p*-median problem. The term 'hybrid' connotes that two different approaches are combined in the method in order to produce more effective and higher-quality solutions than found by a single greedy or meta-heuristic framework. The AZP-CI is based on the AZP but implements a different interchange method. In this paper, the performance of the AZP-CI is compared with those of two popular alternative methods: the original AZP algorithm and SA, a pure meta-heuristic algorithm for the AZP (AZP-SA). These comparisons are conducted with several indicators of solution quality and computational performance, using simulated random datasets and two empirical datasets suitable for regionalization problems.

2. Background

The general principle in delineating *p*-regions is to construct higher-level areal units by identifying clusters of smaller units while optimizing some criteria. This problem has been applied in various fields including political districting (Hess *et al.* 1965, Morrill 1976, Williams 1995), the delimitation of functional regions based on spatial interaction (Brown and Holmes 1971, Mitchell and Watts 2010, Kim *et al.* 2013), natural resource management (Snyder and ReVelle 1996, Murray 1999), market area districting (Zoltners and Sinha 1983, Salazar-Aguilar *et al.* 2011), school districting (Yeates 1963, Armstrong *et al.* 1993), and public service area districting (Malczewski and Ogryczak 1988, Church 1990, Blais *et al.* 2003, Oliveira and Bevan 2006). Most delineation problems require spatial contiguity, which requires that each constructed region must be composed of contiguous smaller areal units.

One of the most challenging issues in districting problems is to find solution strategies capable of handling large-size problems. Any exhaustive search approach based on complete enumeration can only address very small instances of the problem since this method becomes intractable very quickly due to the enormous number of combinations (Browdy 1990, Duque *et al.* 2012). Mixed integer programming (hereafter MIP) is commonly utilized to find exact solutions, and many mathematical formulations have been proposed. One common issue among them is how to explicitly incorporate spatial contiguity as constraints (e.g., Zoltners and Sinha 1983, Duque 2004). Shirabe (2005) showed that MIP can produce an optimal solution but only for small instances because the constraint sets for spatial contiguity inherently increase combinatorial complexity as the scale of a model grows (Shirabe 2009, Duque *et al.* 2011, 2012). For this reason, various non-exact solution methodologies have been developed to efficiently and effectively find near-optimal solutions for large-size problems that an empirical data analysis generally encounters. Openshaw (1973) proposed a *k*-clustering method that begins with random seeds and expands the clusters until all areal units are assigned to clusters while maintaining spatial contiguity. Following Openshaw's pioneering method, similar clustering methods have been proposed in the context of districting problems (e.g., Masser and Scheurwater 1980, Openshaw and Wymer 1995). However, their performance is inconsistent in producing solutions because the quality of the final solution is heavily dependent on the initial solutions (Duque *et al.* 2007).

Alternatively heuristic methods have been often used for large-size problems and widely adapted to a variety of regionalization problems. Classical studies employed simple greedy algorithms or hill-climbing techniques (Nagel 1965, Liittschwager 1973, Moshman and Kokiko 1973). The greedy algorithms, including the AZP proposed by Openshaw (1977), are capable of quickly generating 'good' results with possible applicability for a large empirical delineating problem. Morrill (1976), for another example, used a center-based heuristic to solve a districting problem.

Generic meta-heuristic approaches have been frequently employed in conjunction with the AZP in contemporary regionalization models (e.g., Openshaw and Rao 1995, Duque *et al.* 2012). Meta-heuristics methods provide a framework that prevents a model from being trapped in local optima and thereby increases the chances of finding a global or near-optimal solution. Two primary strategies of meta-heuristic methods are intensification and diversification. Intensification is an accumulation process for improving solutions based on previous experience and elite solutions, while diversification is a search process to explore unvisited solution space to generate different solutions (Blum and Roli 2003). For example, tabu search uses a set of *tabu* lists, which is designed to prevent cycling, and the list changes as units are moved. An addition and removal of entries from the tabu list is not predicated on the objective function value. The tabu list is defined by one or more *moves,* which were used to produce a current solution but are forbidden from being reused until the objective function reaches a certain level (see Glover 1989, 1990 in detail). The tabu heuristic is commonly found in the literature for districting problems; for example, see Openshaw and Rao (1995), Blais *et al.* (2003), Bozkaya *et al.* (2003), Wei and Chai (2004), and Ricca and Simeone (2008).

SA has long been recognized as an effective solution technique for most redistricting or regionalization problems that involve a nonlinear structure and multi-objective optimization. SA allows the search process to continue to build from demonstrably inferior solutions to avoid entrapment in local optima (Golden and Skiscim 1986). In particular, this method has been applied to large-size problems that do not necessarily require an exact solution but need near-optimal solutions quickly (Browdy 1990, MacMillan and Pierce 1994, MacMillan 2001, Ricca and Simeone 2008, Li *et al.* 2014a, b). For example, D'Amico *et al.* (2002) applied SA to a police jurisdiction problem in which emergency response should be provided very rapidly with partitioning being as close to optimal as possible.

The hybridization of two heterogeneous search algorithms has recently been proposed as a strategy for addressing regionalization problems. The basic principle of a hybrid search is to exchange important information between the different frameworks. For example, Wei and Chai (2004) combined a tabu search with a scatter search in a multi-objective spatial zoning problem to improve the search process to reflect complex multi-objectives.

Virtually all of these solution techniques require that a potential move of a spatial unit from one region to another should be evaluated in order to ensure that such a move does not violate the condition of spatial contiguity. These contiguity checks can consume a significant portion of the total solution time for generating a solution (Palladini 2004). For example, the matrix operation-based checking procedure proposed by Openshaw and Rao (1995) is considered a promising method for guaranteeing contiguity with little interference over other algorithmic procedures. However, the algorithm may take a long time to obtain a solution if the contiguity-checking procedure entails significant matrix operations. MacMillan and Pierce (1994) and MacMillan (2001) proposed a similar but enhanced contiguity-checking operation based on the topology of the spatial unit to be moved. This method employs a connectivity matrix, for which the bookkeeping of adjacent units and contiguity should be checked whenever new moves are proposed to improve the objective function. However, this method requires the preprocessing of topological information for adjacent spatial units, assignment, and adjacent regions, resulting in a complex formulation.

3. Designing a hybrid heuristic algorithm for the PFRP

3.1. The PFRP

In this paper, the performance of AZP-CI is compared with other previous methods for the PFRP. The PFRP is a subset of regionalization problems that involve geographical flows (i.e., spatial interaction) among spatial units. This model is formulated to find p functional centers and their corresponding functional regions simultaneously by maximizing the geographical flows between centers and their respective regions, thereby satisfying contiguity requirement. Similar to the model proposed by Shirabe (2009), the PFRP can be characterized as a location-allocation model in that any spatial unit should be exhaustively allocated to a selected location. However, the PFRP is distinguished from the existing location-allocation models in two aspects. First, while it is true that the result will represent geographical or geometric centers of regions if the functional centers are determined based on geographic distance, the PFRP does not require geographic distance to be used as a determining factor in region identification. More commonly, functional centers are found where spatial interactions with their neighboring areas are strong. In other words, the concept of centrality in a functional region problem is different from geographic centrality. Second, the PFRP considers 'internal' flows within a unit as well as external flows between units. Generally, when spatial interaction flows are organized in an origin/destination (OD) matrix form, the resulting matrix has nonzero values in its diagonal elements. This poses a problem, because previous distance-based regionalization models cannot identify the functional centers with high internal flows. Further, previous heuristic approaches that can be applied to the PFRPs do not pay much attention to the identification of center locations as they assume center locations are defined *a priori*. As a result, spatial interaction has not been incorporated in the process of locating functional centers. Hence, a new heuristic method needs to solve the PFRP, a more demanding problem than previous regionalization problems.

The MIP version of the PFRP is formulated as follows (see Kim *et al.* 2013 for details):

$$Maximize \sum_i \sum_k a_{ik} y_{ik} \tag{1}$$

Subject to

$$\sum_k y_{ik} = 1, \ \forall i \tag{2}$$

$$w_{ik} \le y_{ik}, \ \forall i, k \tag{3}$$

$$\sum_i w_{ik} \le 1, \ \forall k \tag{4}$$

$$\sum_k \sum_i w_{ik} = p \tag{5}$$

$$f_{ijk} \le y_{ik}(n - p), \ \forall i, \ j \in N_i, k \tag{6}$$

$$f_{ijk} \le y_{jk}(n - p), \ \forall i, \ j \in N_i, k \tag{7}$$

$$\sum_{j \in N_i} f_{ijk} - \sum_{j \in N_i} f_{jik} \geq y_{ik} - (n-p)w_{ik}, \ \forall i, k \tag{8}$$

$$y_{ik} = \{0, 1\}, \ \forall i, k \tag{9}$$

$$w_{ik} = \{0, 1\}, \ \forall i, k \tag{10}$$

$$f_{ijk} \geq 0, \ \forall i, j \in N_i, k \tag{11}$$

where

$i =$ index of the basic spatial units, $i = 1, \ldots, n$
$k =$ index of the spatial units selected as the function centers of the region, $k = 1, \ldots, n$
$p =$ the number of regions to be regionalized
$c_{ij} = \begin{cases} 1, & \text{if spatial units } i \text{ and } j \text{ are adjacent} \\ 0, & \text{otherwise} \end{cases}$
$N_i = \{j | c_{ij} = 1\}$, a set of spatial units that are adjacent to i
$a_{ik} =$ the amount of spatial interaction (i.e., journey-to-work flows) from spatial units i to regional center k

The decision variables are as follows:

$y_{ik} = \begin{cases} 1, & \text{if spatial unit } i \text{ is included in region } k \\ 0, & \text{otherwise} \end{cases}$
$w_{ik} = \begin{cases} 1, & \text{if spatial unit } i \text{ is chosen as a sink (i.e., the functional center) of region } k \\ 0, & \text{otherwise} \end{cases}$
$f_{ijk} =$ the amount of unit flow from i to j in region k ($f_{ijk} \geq 0$)

The objective function (1) maximizes the spatial interactions (a_{ik}) from the assigned areal units to the centers within each region. The values of the decision variables (y_{ik}) indicate the ideal pattern of geographic flow among the spatial units as well as the influential areas of the functional centers. Constraint (2) ensures that each spatial unit i should be assigned to only one center k, where k represents the index of the spatial unit that is selected as the functional center (i.e., the sink) of the region. Constraint (3) enforces the logic that spatial unit i can be a sink in region k only if i is assigned to k. Constraint (4) requires that each region contains only one sink. Constraint (5) requires that p functional centers are created. Constraints (6) and (7), similar to the logic of flow-based constraints by Shirabe (2009), are structured to ensure spatial contiguity by establishing a flow-based tree in each region. In detail, flows between spatial units i and j are only possibly made only if both units are adjacent and assigned to the same region k. Constraint (8) enforces unit flows between the areal units assigned to the same region. Constraints (9) and (10) impose integer restrictions on the location and allocation decision variables, and constraint (11) ensures that f_{ijk} is nonnegative. This MIP model can be tractable for modest-sized PFRP problems, but it is unlikely to be workable in large-size instances due to the intrinsic complexity of the mathematical programming approach.

3.2. Developing the hybrid algorithm (AZP-CI)

As is well-known in the literature, the original AZP (Openshaw 1977) provides a flexible environment within which any meta-heuristic approach can be incorporated into the algorithm. The implementation of a heuristic algorithm for districting problems generally requires a rule to govern the *moves* of spatial unit(s) to a neighboring region or to switch the assignments of spatial units between one region and a neighboring region (Nagel 1965, Liittschwager 1973, Moshman and Kokiko 1973, Openshaw 1977, Horn 1995). The original AZP has a computationally intensive procedure to optimize the zoning areas because it iteratively recombines a large set of geographic areas into a smaller set of zones to improve the objective function. The AZP step examines all feasible neighboring spatial units that are adjacent to a randomly selected region from an initial solution. Neighboring spatial units could be moved into a selected region while the contiguity of the region is maintained. The algorithm swaps a neighboring unit in the selected region with one unit in the original region until the objective function improves, and then it terminates if the improvement reaches prespecified parameter constraints.

As the first step in developing the AZP-CI for the PFRP, we construct a standard AZP (AZP-ST) algorithm for the PFRP. The AZP-ST serves as a basis for comparison with the AZP-CI and the AZP-SA, which is the meta-heuristic algorithm developed for the PFRP. Considering the contexts of the PFRP, the AZP-ST modifies the original AZP framework and is implemented as follows:

- Step 1: Randomly generate an initial set of p-regions from n spatial units ($p < n$).
- Step 2: For each region, determine its regional center based on the objective function that maximizes the spatial interactions with the hinterland. Then, calculate the objective value (f^{current}) of the initial system of functional regions.
- Step 3: Randomly select a region (R_{sel}), and make a list of the edge spatial units (E_{list}) of the region that share a common boundary with the adjacent regions (R_{adj}).
- Step 4: Select an edge spatial unit (e_{sel}) from the E_{list} of R_{sel}.
- Step 5: Examine whether or not e_{sel} can be assigned to adjacent region(s) without violating the contiguity requirement.
  - Step 5-1: If e_{sel} is movable, then move it to one adjacent region and identify the new centers of R_{adj} and R_{sel}. Then, recalculate the objective value (f^{new}) of the new system of regions under the assumption that e_{sel} is moved.
  - Step 5-2: Otherwise, go back to Step 4 to select the next e_{sel}.
- Step 6: Accept the move if there is an improvement in the objective value ($f^{\text{current}} \leftarrow f^{\text{new}}$).
- Step 7: Update the E_{list} by removing e_{sel} and adding new edge spatial units and return to Step 4 until all spatial units in the E_{list} have been examined.
- Step 8: Repeat Steps 3–7 until there is no improvement in the objective value.

Notice that the key principle of the AZP uses a simple structure of a *move* by which a spatial unit from an original region is handed over to one of the neighboring regions randomly and repetitively. Despite its simple structure, it is known to be susceptible to entrapment in local optima, which is a similar limitation as other greedy-type heuristics have in searching for optimal solutions. Additionally, the quality of the solutions varies significantly depending on the number of regions to be delineated, the initial solution, and the random *moves*.

The second model, denoted here by AZP-SA, is developed from the AZP-ST as a representative meta-heuristic for comparison. The AZP-SA follows the general procedure that is suggested in previous works on districting problems (Browdy 1990, D'Amico *et al.* 2002, Duque *et al.* 2012). Specifically, the AZP-SA starts from a random initial feasible solution, permits the *moves* of spatial units that produce worse objective values, and accepts the *moves* that improve the objective values. The *move* resulting in a deteriorated solution is allowed based on a probability, $p = e^{-\Delta H/T}$, where ΔH is the change in objective value and T is the current temperature. The temperature diminishes gradually based on a predefined cooling rate (α) through iterations (αT), and the algorithm terminates when the temperature reaches either a predefined tolerance (ε) or a maximum number of iterations without improvement. This meta-frame of the SA is applied in Step 5-2. The AZP-SA differs from the AZP-ST in that it allows *moves* that produce deteriorated solutions with a certain probability for diversification. This strategy enables the AZP-SA to expand the initial search points, thereby obtaining a further improvement in the objective function value. The quality of the AZP-SA results depends highly on the parameter settings, such as the initial temperature and cooling rate. Therefore, a significant number of trial and errors are often required to identify the best good parameter setting (Pham and Karaboga 2000).

The third model, the AZP with Center Interchange (AZP-CI), is a hybrid method that is designed to intensify and diversify a solution space. This hybrid search combines two different but complementary search algorithms. Most heuristics within the SA framework tend to be limited from diversifying search space because the main strategy of the SA is based on the local search process, that is, the *move* of a spatial unit between two neighboring regions is similar to the AZP-ST. In contrast, the key principle of the AZP-CI is to embed a new rule called the 'dissolve/split procedure' to facilitate a wider exploration of solution space, which considers the *interchange* among the centers of regions as well as the *moves* of a spatial unit between adjacent regions. The AZP-CI is partially similar to the interchange method of Teitz and Bart (1968) in that a facility in a current solution is interchanged with a potential facility that is not in the current solution set, maintaining the contiguity requirement while the centers are interchanged. The AZP-CI procedure is as follows:

- Step 1: Generate a random initial feasible solution and calculate the objective value (f^{current}) of the initial solution.
- Step 2: Randomly select a region (R_{selected}) and its center (C_{selected}) to be interchanged with a new center.
- Step 3: Make a list of the potential center units ($L_{\text{potential}}$) that satisfy a set of criteria. For a more intense search, all of the spatial units that are not selected as a center in the current solution can be members of the list.
- Step 4: Randomly select a new center (C_{new}) from $L_{\text{potential}}$.
- Step 5: Interchange C_{selected} with C_{new} through the *dissolve/split procedure.*
  - Step 5-1: *Dissolve* by randomly assigning all spatial units in $R_{selected}$ to neighboring regions (p-1 regions).
  - Step 5-2: *Split* a new region with C_{new} while preserving spatial contiguity from an existing region. If the split does not violate spatial contiguity, then the new region consists of only one unit C_{new}. Otherwise, the new region consists of all spatial units in subregion(s) where C_{selected} is not contained as well as C_{new} (p-regions).

- Step 6: Perform AZP-ST.
  - If the dissolve/split procedure and the subsequent AZP-ST improve the objective value (f^{new}), then accept the interchange, update the current solution ($f^{\text{current}} \leftarrow f^{\text{new}}$), and go to Step 2.
  - Otherwise, go to Step 4.
- Step 7: Repeat Steps 2–6 until there is no improvement in the objective value.

The dissolve/split procedure in the AZP-CI can be described better with comparison to two common methods by Sammons (1978) and Horn (1995). First, Sammons's method is known as the 'merging/splitting procedure' in a hill-climbing heuristic. This procedure splits regions with a large population into two subregions and simultaneously merges two neighboring regions with significantly lower populations into one region, maintaining spatial contiguity. The main problem of this procedure is observed when a low-population region is surrounded by large-population regions, which often makes the algorithm recursive and consequently the solution is not improved. Horn (1995) proposed a different method, called 'move/splitting procedure', which was applied for political districting problems. The procedure allows *moves* between two adjacent regions while merging two adjacent regions and splitting a spatial unit from an existing region. However, the algorithm needs an additional process of re-merging unnecessarily expanded regions as the procedure generates an increased fragmentation of the existing regions, which is greater than *p*. The post-merging process ultimately increases the solution time, which is relatively excessive for the algorithmic complexity of a given instance size.

In contrast, the AZP-CI performs two procedures, dissolving existing regions (rather than merge regions) and splitting a new region from an existing region, in a single step, which achieves better diversification and intensification in finding the optimal solution. In terms of spatial contiguity, the AZP-CI employs spanning tree to explicitly maintain spatial contiguity with tractable complexity during the dissolve/split procedure. This spanning tree method enables the AZP-CI to outperform both existing heuristic methods that limit *move* only for a set of individual areas in a region to an adjacent region due to the difficulty in handling spatial contiguity requirement, which may result in a limited quality of solutions.

3.3. *Handling spatial contiguity using spanning tree in the AZP-CI*

As mentioned, contiguity is a critical concern not only in the development of heuristic algorithms but also in the formulation of mathematical models (Openshaw and Rao 1995, Shirabe 2009, Duque *et al.* 2011, Salazar-Aguilar *et al.* 2011). Without an efficient contiguity-checking algorithm or a mathematical structure, a heuristic algorithm is potentially limited by the high degree of complexity encountered in solving the problem (MacMillan 2001). Two issues for the validation of contiguity arise when implementing the AZP-CI. The first issue concerns how contiguity is checked when a spatial unit moves from an original region to an adjacent region (i.e., Step 5 in the AZP-ST), while the second issue involves the maintenance of contiguity when an existing center and region are replaced by a potential center and region (i.e., Step 5 in the AZP-CI).

To address this problem, Openshaw and Rao (1995) proposed a method using the property of connectivity matrix multiplication. The method utilizes a sub-matrix for the connectivity of each region. To establish the full connectivity of a region, it powers a regional sub-matrix up to (r – 1) times (r is the number of spatial units in the region). The logic is that if all of the cells of the resultant matrix are nonzero values, the region is contiguous. If some elements remain zero even in the (r – 1)th powered matrix, then the constructed region is not contiguous. This approach is mathematically sound but computationally inefficient so that its application is limited to small problems. Alternatively, MacMillan and Pierce (1994) and MacMillan (2001) introduced a new method called the *switching point method* for checking contiguity. This method focuses on changing the boundary type for a candidate spatial unit that is to be moved to neighboring regions. Two boundary types are interiorly shared with spatial units in the same region and exteriorly shared with spatial units in different regions. Using this property, contiguity is checked algebraically by counting the number of switching points where the boundary type is changed by removing a spatial unit (MacMillan and Pierce 1994). Because this method considers only one spatial unit to be moved instead of all units assigned to the region, this may be more computationally efficient than matrix-based contiguity-checking methods.

A more straightforward procedure for checking contiguity is proposed in this paper using the property of spanning tree. The procedure is applied when the spatial unit of a region is moved to adjacent regions. In Figure 1a, suppose that spatial unit 1 of a region will be moved to an adjacent region to improve the objective function. A spanning tree is constructed for the remaining spatial units (2, 3, 4, 5, 6, and 7) in the region using the strategy of breadth-first search. If the spanning tree is successfully created for all units except unit 1, the move of unit 1 is allowed because the move does not violate the contiguity requirement of the current structure. In this step, the root of the spanning tree can be randomly selected. In contrast, as shown in Figure 1b, if spatial unit 3 is to move to an adjacent region, then the constructed spanning tree indicates that the move violates the contiguity requirement because the spanning tree fails to cover the remaining elements. Therefore, spatial unit 3 is not a candidate for a *move*. The spanning tree method for checking contiguity is simple but more efficient than other contiguity methods because this spanning tree procedure is directly adapted from the original mathematical formulation of the contiguity constraints of the PFRP, where the continuity of a region is validated based on the tree generation for a given p center condition. An advantage of this method can be recognized from the perspective of complexity theory. That is, it is computationally efficient since the complexity for the breadth-first search to construct spanning tree only requires $O(|m|+|n|)$ for given n spatial units and m edges in adjacency to connect n units (Cormen *et al.* 2001). Consequently, the complexity for contiguity check is reliable and predictable regardless of the size and shape of instances. As a result, the AZP-CI produces better solvability and little variability in terms of computation time, compared to other contiguity-checking methods.

Another challenging situation shown in previous methods is how effectively the spatial contiguity is preserved when existing regions are merged and a potential center

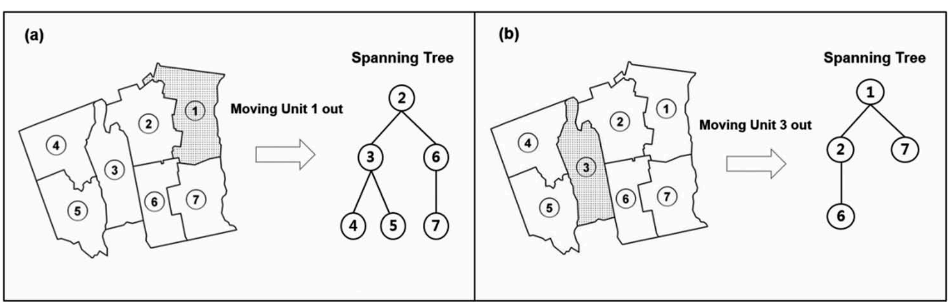

Figure 1. Constructing a spanning tree for checking contiguity.

and region split from an existing region. To address this situation, the AZP-CI sets two rules: (1) the adjacent spatial units are first assigned to neighboring regions when dissolving the existing regions, and (2) a new potential center splits from an existing region when the existing region is fragmented into two subregions. The contiguity-checking procedure examines whether or not the split of a spatial unit as a center forming a new region violates the contiguity requirement. If the violation of the contiguity requirement due to the interchange process is identified, the algorithm assigns spatial units, which are detached from the center of the existing region to the potential center. In this case, the new region consists of more than two units.

Figure 2 illustrates the violation of the contiguity requirement based on the interchange process and the solution to this problem. The numbers are the identifiers of the spatial units and the regional centers are denoted by a circled number, and the alphabet letters correspond to the regions. In Figure 2a and b, if center 25 in region E is replaced by spatial unit 7 as a potential center, this center interchange does not violate the contiguity

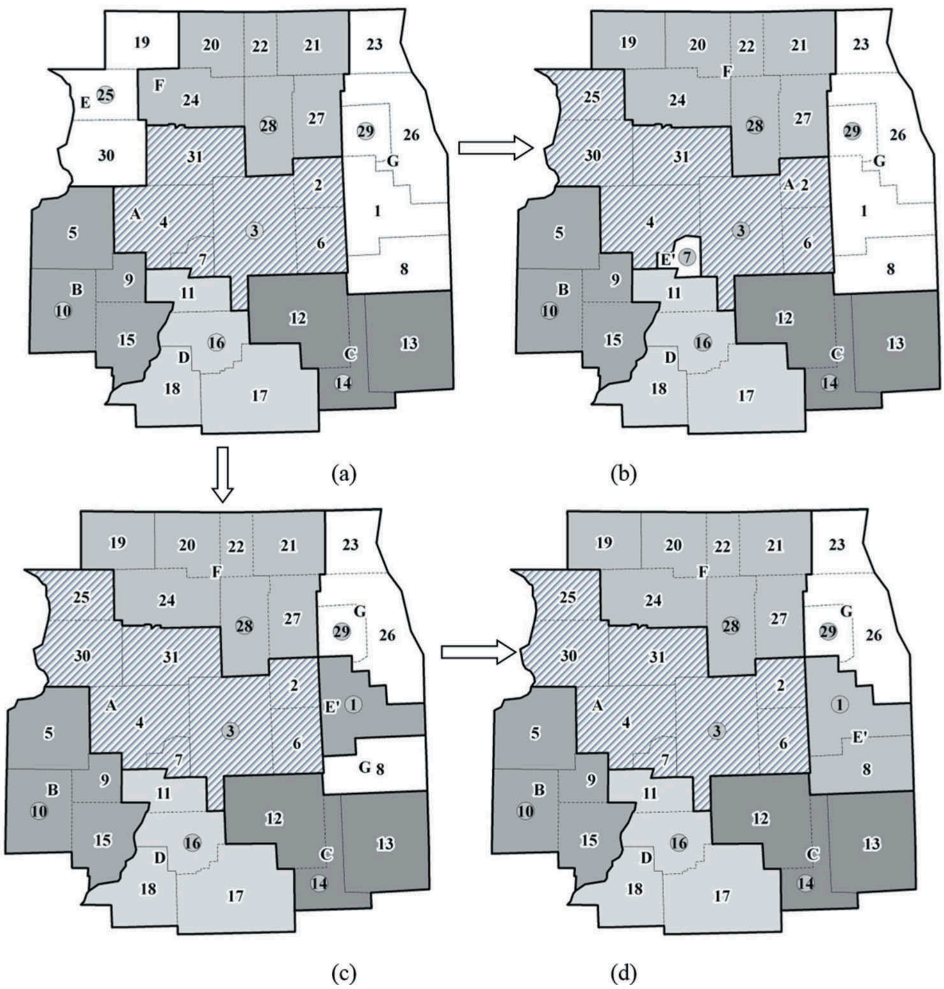

Figure 2. Maintaining contiguity in center interchange.

requirement. In this case, region E is dissolved by assigning its spatial units to adjacent regions, as spatial unit 7 becomes a potential center of a new region (E′). However, suppose that center 25 in region E is replaced by spatial unit 1 in region G as a potential center; this interchange separates region G into two subregions and violates the contiguity requirement (Figure 2c). In this case, the new potential region (E′) includes the separated spatial unit 8 and thus consists of spatial units 1 (center) and 8 (Figure 2d).

3.4. Design of simulations to benchmark performance

One of the most persistent issues in regionalization problems is to what extent the heuristic can maintain its tractability regarding a problem size. Another issue is the algorithm's stability to produce reliable solutions regardless of the initial solution as well as datasets. Here, the computational results of the AZP-CI are compared with those of the original AZP-ST and AZP-SA to evaluate the performance of these methods with respect to quality, efficiency, and consistency in producing solutions using a set of indicators (i.e., gap to the optimal or best known solution, solution times, improvement rate, and hitting rate). This evaluation is performed with an experiment using simulated random datasets. The main objective of this experiment is to test how the algorithms maintain its performance to various settings of realizations of the data. Notice that the performance of the existing algorithms is highly dependent upon how well the algorithm is designed to reflect the geographic characteristics of input data (e.g., spatial configurations of basic spatial units and spatial interaction among them).

Random spatial interaction datasets were generated with random tessellations and random flows. Random tessellations were created by constructing Thiessen polygons with 20 randomly located points in a 100 × 100 square unit. Random flows among these 20 polygons were drawn from a truncated normal distribution to avoid negative flow values. Furthermore, intra- and interregion flows were separately generated with different means and standard deviations, because intra-region flows are considerably larger than interregion flows in most empirical interaction flow datasets (e.g., Chun *et al.* 2012). In this experiment, the parameters of the truncated normal distribution were set with the descriptive statistics (i.e., mean and standard deviation) of the 2000 Census journey-to-work flows among the counties in South Carolina. One notable point is that distance-decay effect is not likely to exist in the random datasets. In total, 50 random spatial interaction datasets were generated and used to evaluate the proposed method.

The performances of these methods are further compared with two empirical datasets. The first dataset is the 2000 Census journey-to-work flows among the counties in South Carolina (n = 46) whose optimal solutions were determined by Kim *et al.* (2013). The second dataset is the 2000 Census journey-to-work flows among all counties in the conterminous US (n = 3111), which is one of the largest empirical spatial interaction datasets currently available in the national scale.

The main goal of the first experiment is to test how solidly the AZP-CI can perform to the various random datasets compared to the traditional heuristic methods in regionalization problems. The two empirical datasets cover a reasonable range of problem sizes since, to the best of our knowledge, maximum problem sizes in the current literature are n = 46 for the exact MIP solution approach (Kim *et al.* 2013), and n = 2926 for an AZP approach (Openshaw and Rao 1995), or n = 3085 for meta-heuristic approaches (Duque *et al.* 2012). The three algorithms are implemented in a GIS environment using Visual Basic and tested using a machine with an Intel Core2 Duo 3.0 GHz processor and 2 GB RAM on Windows XP.

4. Computational results and comparison

Table 1 summarizes the computational results for the 50 random spatial interaction datasets (n = 20) with 1000 randomly generated initial solutions for each of the datasets. These initial solutions are constructed through two steps. First, p centers are completely randomly selected, and the spatial units are assigned to the nearest centers maintaining spatial contiguity. The exact solutions for the 50 random datasets are identified using an MIP solution approach. The objective values in Table 1 are averaged across the total 50,000 cases (i.e., the 50 datasets with 1000 initial solutions). Two indicators, the *average gap* (*AvgG*) and *average hitting ratio (AvgHR*), are used for the performance comparison. The *AvgG* indicates the average value of the difference (gap) in the objective value between the exact solutions and the three heuristic approaches. As shown in the first two columns, the MIP approach requires the solution times from 2.51 to up to 3.67 hours on average to identify the exact solutions for p = 2–5. In terms of the solution quality, the AZP-CI found the exact solutions to be more than 84% (*AvgHR*) with very small gaps (≤0.05) for the 50,000 events, followed by the AZP-SA with 50–77% of *AvgHR* and small gaps (≤0.15). The AZP-ST iterates its procedures up to 197.6 within a fixed time due to its simple algorithmic structure. However, its performance is worse than those of the other two algorithms. The parameters for the AZP-SA were found using an experiment. The sets of parameters that produce the finest result are: 1000 for initial temperature (T), 0.005(α) for the temperature cooling-down rate, and 0.01(ε) for terminating temperature. Furthermore, the procedure was terminated after 100 consecutive iterations without improvement. All three algorithms are allowed one second as a solution time for each event, which is experimentally determined by solving the three algorithms by increasing the solution time from 0.1 to 1.5 by 0.1. After one second, increasing the solution time marginally improved the solution quality with respect to both average gap and average hitting ratio. The AZP-ST and AZP-SA were solved repetitively in the given time with the same initial solution and the best results are summarized (in Table 1, ItCnt indicates the number of iterations). In contrast, the AZP-CI repeats the *dissolve/split procedure* within the given time without restarting the algorithm.

Figure 3a displays boxplots for the gap of the three algorithms when p = 5. Clearly, the AZP-CI has a very small and narrow range of solution gap with only several outliers compared with the AZP-ST and AZP-SA. For the most of the 50 random datasets, the hits of the AZP-CI are in the range 900–1000, which is clearly different from those of the other algorithms (Figure 3b). Two findings are worth noting. First, the AZP-CI overall produces better solutions than the other two algorithms in a very short time (1 second). Second, the AZP-CI has little variability in solution quality for the randomly generated 50 datasets and even 1000 different initial solutions per set. Given that performance of the existing algorithms is sensitive to the change of geographic setting and initial solutions (e.g., spatial interactions, geographic distribution of demand and supply, and transportation systems), the results clearly confirm that the performance of the AZP-CI is not affected by these factors and hence the AZP-CI can be applied to other applications with little efforts such as calibrating parameters to improve the solution quality.

Figure 4 demonstrates why the AZP-CI outperforms the other algorithms. Figures 4a, b, and c, respectively, are the most frequently found solutions by the three heuristics. The AZP-ST, AZP-SA, and AZP-CI reached the solutions in Figure 4, respectively, 251, 397, and 872 times for the 1000 simulations. The solution by the AZP-CI is the global optimum identified by the MIP solution. Although the three algorithms found the same centers in the end, the allocations of spatial units are different from each other. The

Table 1. Computational results for random datasets (n = 20).

	MIP		AZP-ST				AZP-SA				AZP-CI		
p	Obj.(average)	Time (sec)	Obj.	*AvgG* (%)	*AvgHR* (%)	ItCnt*	Obj.(average)	*AvgG* (%)	*AvgHR* (%)	ItCnt	Obj.(average)	*AvgG* (%)	*AvgHR* (%)
2	22,559	10,223	22,298	1.16	22.8	92.2	22,536	0.10	77.2	2.0	22,552	0.03	85.4
3	30,439	13,225	30,018	1.38	19.9	136.7	30,395	0.15	68.5	2.9	30,423	0.05	84.2
4	37,341	10,905	36,877	1.25	14.3	184.4	37,294	0.13	56.1	3.6	37,331	0.03	85.8
5	43,563	9,039	43,126	1.02	13.0	197.6	43,510	0.13	51.8	4.1	43,551	0.03	84.9

Note: *ItCnt = the iteration number of each heuristic procedure for a fixed time.

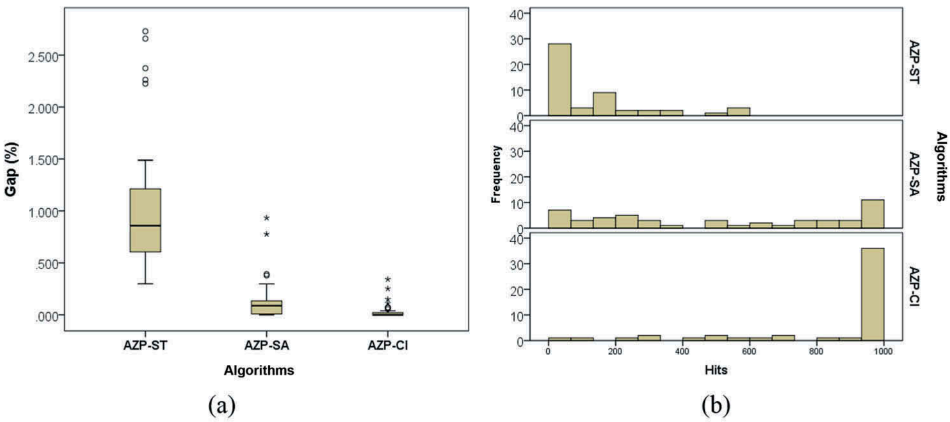

Figure 3. A graphical summary of solution quality for 50 random datasets (m = 5).

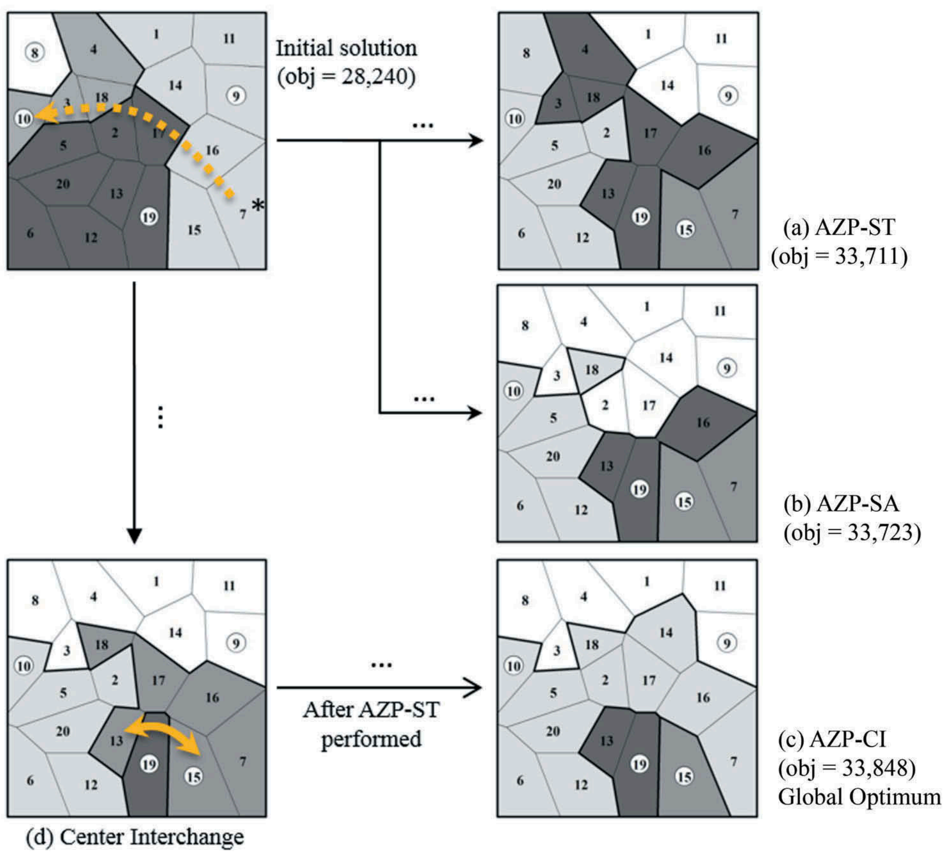

Figure 4. Spatial solutions of the three heuristic algorithms for a random dataset (m = 4).

Note: *Unit 7 is assigned to center 10 in the MIP solution, which is the global optimum result, because of large interaction from unit 7 to center 10.

challenge is to make the spatial unit 7 to be allocated to center 10, given that the spatial units 16 and 17 have larger interactions with centers 19 and 9, respectively. In the AZP-ST (Figure 4a), all spatial units are assigned to centers based on the maximum interaction among the adjacent regions and the procedure terminates its search at a local optimum solution (the AZP-ST hits the global optima only 12 times). Although spatial unit 16 or 17 can be allocated to center 10 by allowing a deteriorated move in the AZP-SA, they are more likely to assign to other centers shortly. As a result, the AZP-SA is more likely to be trapped into a local optimum than reach the global optimum (the AZP-SA found the global optimum 154 times among the 1000 simulations). In contrast, the center interchange in the AZP-CI, particularly its dissolving procedure, provides a high possibility of assigning multiple spatial units to a center simultaneously. Figure 4d demonstrates a center interchange between the existing center 15 and the new center 13 and subsequent assignments of spatial units. As the region with center 15 dissolves, the spatial units 7, 16, and 17 can be assigned to the region with center 10, which is randomly selected among adjacent neighboring regions at a time. The following procedures by the AZP-ST determine the final centers and allocate spatial units to the centers in order to ensure the entire procedure can reach the global optimum solution as a consequence.

Table 2 summarizes the computational results of three heuristic algorithms as well as the exact solutions for the case of South Carolina. The journey-to-work flows among the counties in South Carolina present a prominent distance-decay effect, which is a typical pattern of empirical geographic flows. The exact solutions were excerpted directly from Kim *et al.* (2013). The solutions of three algorithms were found in a different computing environment from the other three algorithms. However, it should not be an issue for a comparison purpose since the three heuristic approaches dramatically reduced the computation time to less than one second, which is sufficient for the AZP-CI to reduce the optimality gap for all problem instances completely. To compute the best solutions, the AZP-ST and AZP-SA algorithms were allowed to iterate the entire procedure for full one second to achieve an improved solution as much as they can get. The maximum number of non-improving moves for the AZP-SA is set to 200 under the best identified parameter settings of initial temperature T = 1000, cooling rate α = 0.03, and tolerance ε = 0.10. These parameter values are experimentally driven. The results of the heuristic algorithms with 1000 random initial solutions are reported with the objective values, gaps, and hitting rates of these solutions, which are averaged in Table 2. All three heuristic algorithms effectively solved the PFRP with the exact solutions, although the optimality of the heuristics was not necessarily guaranteed among the 1000 trials. The AZP-ST solved instances at a relatively small gap (0.53–3.56%) in the objective values, but the *AvgHR* varies significantly from 14.6 to 97.2% with p values. In contrast, the AZP-SA clearly shows much reduced gaps (<1% for most p values) in the objective values with improved hitting ratios (57.0–100%) compared with the AZP-ST. However, the AZP-CI outperformed the AZP-SA in terms of both indicators since it found the exact solutions for all 1000 instances regardless of p values.

Finally, as shown in Table 3, in the case of a regionalization of the US counties (n = 3111), which would be the largest empirical dataset in the current literature, the performances of the three heuristics are more readily comparable. To track performance, the test was conducted from p = 100 to 500 with special criteria of p = 179 (the number of BEA economic areas) and p = 363 (the number of MSAs as of 2000). Each heuristic algorithm is applied using 10 random initial solutions and the results are averaged. Due to the large size of the problem, it is impossible to verify the global optimum for those p values using the MIP approach. Therefore, the performance is compared with the best-

Table 2. Computational results of exact and heuristics solutions for South Carolina (n = 46).

p	MIP*		AZP-ST				AZP-SA				AZP-CI		
	Obj. (A)	Time (sec)	Obj. (B)	*AvgG* (%)	*AvgHR* (%)	ItCnt	Obj. (C)	*AvgG* (%)	*AvgHR* (%)	ItCnt	Obj. (D)	*AvgG* (%)	*AvgHR* (%)
3	590.4	15,532	587.2	0.53	97.2	11.8	590.3	0.00	100.0	2.0	590.4	0.00	100.0
4	683.6	7285	673.4	1.48	62.2	17.2	679.6	0.58	73.7	2.7	683.6	0.00	100.0
5	770.6	10,623	743.1	3.56	26.2	23.7	757.4	1.71	58.8	2.9	770.6	0.00	100.0
6	827.9	19,747	803.8	2.91	16.5	30.9	825.2	0.32	77.2	3.5	827.9	0.00	100.0
7	883.6	26,466	861.0	2.55	14.6	33.0	880.4	0.36	57.0	4.0	883.6	0.00	100.0
8	936.8	28,946	914.0	2.42	15.7	38.1	932.9	0.41	63.8	4.8	936.8	0.00	100.0
9	984.0	38,444	960.9	2.35	31.5	51.9	981.1	0.29	62.3	5.4	984.0	0.00	100.0
10	1024.0	15,373	1002.0	2.15	31.9	61.6	1023.8	0.02	93.4	6.9	1024.0	0.00	100.0

Note: *MIP solutions obtained using CPLEX 12.1 with Intel's Xeon Quad Core 3.2GHz/3GB RAM based on the Windows 7 operating system (Kim *et al.* 2013).

Table 3. Computational results for US counties (n = 3111).

			AZP-ST			AZP-SA			AZP-CI		
P	Initial Obj.	Best-known Obj.	Obj. (Average)	IMR (%)	Gap (%)	Obj. (Average)	IMR (%)	Gap (%)	Obj. (Average)	IMR (%)	Gap (%)
100	34,487	49,965	39,933	15.79	20.08	41,433	20.14	17.08	49,902	44.70	0.13
179	41,614	60,762	49,690	19.41	18.22	50,838	22.17	16.33	60,565	45.54	0.32
200	42,884	62,734	51,217	19.43	18.36	52,774	23.06	15.88	62,632	46.05	0.16
300	48,755	69,703	57,831	18.61	17.03	59,286	21.60	14.95	69,588	42.73	0.17
363	51,120	72,579	61,610	20.52	15.11	63,151	23.54	12.99	72,521	41.87	0.08
400	52,668	74,184	63,593	20.74	14.28	64,771	22.98	12.69	74,087	40.67	0.13
500	54,823	77,585	67,287	22.74	13.27	68,802	25.50	11.32	77,391	41.17	0.25

known objectives for each p. All best known objectives are found by the AZP-CI. Given the size of the instance, the three algorithms were allowed to run for 500 seconds, which is the average computation time of the AZP-CI procedure for $p = 500$, to compare the computational results. For the best results, the parameters of the AZP-SA were set as follows: temperature $T = 1000$, cooling rate $\alpha = 0.001$, tolerance $\varepsilon = 0.05$, and the maximum number of non-improving moves 1000. For the given computation time, the AZP-ST and AZP-SA iterated, respectively, 30.2 and 2.6 times on average for each p value. Two indicators, (1) IMR (%), the improvement rate in the objective of heuristic approach compared to the initial objective, and (2) Gap (%), the relative difference of the averaged objectives of the algorithm from the best known objective, are used for comparison. The IMR indicates how much the performance of the algorithm is enhanced from the initial solution. The Gap represents the performance of the consistency in generating the best quality of the objective values. From the results, two noticeable points are identified. First, the AZP-CI is the most promising approach in terms of IMR. For example, the best improvement in the objective values achieved using the AZP-ST was 22.74% and using the AZP-SA was 25.5% at best, while the AZP-CI always resulted in an improvement over 40% for all p. Second, the Gap displays that the AZP-CI produces solutions consistently compared with the other algorithms. The AZP-CI solutions only vary less than 0.32% to find the best known solutions regardless of the initial solutions and p. These observations clearly demonstrate that the AZP-CI is superior to the other two heuristic approaches for the PFRP.

5. Conclusions and discussions

The main goal of this paper is to propose an effective and reliable heuristic algorithm for the PFRP. The AZP-CI is developed for the functional regionalization problem, which requires simultaneously identifying multiple functional centers as well as delineating their influential areas. As the results demonstrated, the AZP-CI is a promising method that outperforms the previous methods with consistency in terms of solution quality, efficiency, and reliability in producing solutions regardless of initial solutions. Noticeably, the experimental results with randomly simulated dataset indicate that the AZP-CI can be extended to other general regionalization problems with benefits from its two unique and innovative aspects. The AZP-CI increases diversification by interchanging centers directly coupled with the dissolve/split procedure, which prevents the search from getting trapped into local optima. Notice that existing heuristic methods allow *move* only for a set of individual areas in a region to an adjacent region due to difficulty in maintaining spatial contiguity. Accordingly, an exploration for a better solution is inherently limited only at the edge of a region, causing an inefficiency of current methods for regionalization problems. Second, the proposed contiguity-checking procedure using a spanning tree prevents the model from resulting in infeasible solutions. This method can be applied to other heuristic approaches concerning the consistency of the solution time because the structure of the spanning only needs polynomial time in complexity regardless of the size of instance.

With these characteristics, the AZP-CI can be directly applied to various functional region delineation based on spatial interaction, especially for large-size problems, such as housing market areas (Brown and Hincks 2008, Royuela and Vargas 2009), local labor market areas or commuting areas (Coombes *et al.* 1986, Van der Laan and Schalke 2001, Landré 2012), daily urban systems (Coombes *et al.* 1979, Schwanen *et al.* 2003), or city regions (Parr 2005, Davoudi 2008, Coombes 2013). Beyond the PFRP, if a regionalization problem uses two-level determination in optimization, for example, location-allocation framework (e.g., political districting or school districting problems), the key components of the AZP-CI can be utilized since the structure is inherently designed for two-level optimization problems where both delineating areas and determining their centrality are of interest. Furthermore, the AZP-CI could be a more scalable algorithm to solve computational intensive spatial optimization problems when it is combined with cyberinfrastructure.

However, some potential limitations still exist in the current structure of the AZP-CI. Specifically, two aspects are reserved as future research. First, the AZP-CI may need a modification based on the context of a regionalization problem. The cases include more complex regionalization problems where the number of functional centers is endogenously determined or multicenter areas need to be delineated with nonexclusive influential areas such as metropolitan areas (Bode 2008). The current AZP-CI assumes a general regional system in which regions are exclusively dichotomized with centers and surrounding areas. The applicability of the AZP-CI can be further extended considering compactness (e.g., Li *et al.* 2013). Second, the performance of the AZP-CI needs to be assessed with other greedy-based algorithms and meta-heuristics (e.g., TABU) since a better hybrid-type algorithm can be developed by combining the advantages of more than two heuristics.

Acknowledgements

This work was supported by the National Research Foundation of Korea Grant, funded by the Korean Government (NRF-2011-327-B00856).

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