Centre for Health Research School of Medicine University of Western Sydney

# A MULTI-OBJECTIVE MAXIMUM FLOW SET PARTITIONING PROBLEM WITH CUSTOMIZABLE CONSTRAINTS TO THE DEFINITION OF RATIONAL PRIMARY CARE CATCHMENT AREAS

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Ludovico Pinzari : A Multi-objective Maximum Flow Set Covering Problem with Customizable constraints to the definition of rational Primary Care catchment areas., A Mathematical Programming approach to a Graph Partitioning problem, © August 2015 In this work a new formulation to the definition of rational Primary Care catchment areas is proposed.

The framework enables the user to select the minimum and maximum number of zones as well as the number of the basic spatial units inside the single zones. Moreover, an important feature is undoubtedly to capture the maximum patient-flow in the study area. For this purpose, a population index has been defined. According to the definition of the index, several maximum and minimum threshold values can be selected to identify a set of equal populated zones. Albeit one of the objective to maximise is the number of people served in a specific zone, an important property is Homogeneity. Henceforth a paramount of attention is given to serve as many people as possible, keeping low the attributes variance inside the single zones. These two opposing goals are essential to the study of geographic variations.

In order to find out a reasonable trade-off solution to the problem, rather than using heuristic parametric functions often based on spatial variables, an innovative mathematical programming approach is applied.

The model is scalable and customizable to the specific domain application regardless the spatial dimension.

Furthermore, the design modularity makes the constraints totally transparent and independent in order to provide a flexible and maintainable tool for any decision maker's needs.

Thus, given the pre-determined criteria and the relevant data, the proposed model serves as a basis for any partitioning engine.

Finally the integration of the zoning scheme output with a GIS through a graphical user interface provides a framework suitable for general purposes applications. There are some guidelines concerning the notation I have used in this work. In general, calligraphic and Greek capitals denotes sets (or some combinatorial objects), latin capitals denote matrices and small latin or greek letters denote elements of sets, variables, functions, parameters or indices. Matrices and vector are written in bold types and their elements in italic type. By default vectors are column vectors. Superscript indicate entities (such as particular vectors), subscripts indicate components of a vector or matrix. Due to a limited supply of alphabetical symbols, I may reuse some for several purposes. Their usage should be clear from the context, nevertheless I apologize for any confusion that may arise. The following list summarizes the most commonly used symbols.

Symbol	Description
Ν	The number of basic spatial units inside the study area.
Ω	The set of all the basic spatial units in the study area, aka Universal set. e.g if $N = 2$ then $\Omega = \{\omega_1, \omega_2\}$ and $ \Omega  = 2$ .
$\mathcal{P}(\Omega)$	The Power set of the Universal set. e.g if N = 2 then $ \mathcal{P}(\Omega)  = 2^{ \Omega } = 4$ . Thus $\mathcal{P}(\Omega) = \{\{\emptyset\}, \{\omega_1\}, \{\omega_2\}, \{\omega_1, \omega_2\}\}.$
$\mathcal{P}(\Omega^+)$	$\mathfrak{P}(\Omega^+) = \mathfrak{P}(\Omega) \setminus \{\emptyset\}.$
$\mathfrak{F}^k_{\mathcal{P}(\Omega^+)}$	The Family of $\mathbb{P}(\Omega)$ subsets such that $ \mathbb{F}^k_{\mathbb{P}(\Omega)} =k,$ $k\leqslant 2^{ \Omega }-1.$
$\mathfrak{F}^{k,i}_{\mathfrak{P}(\Omega^+)}$	A Family of $\mathcal{P}(\Omega)$ subsets such that $\mathcal{F}_{\mathcal{P}(\Omega^+)}^{k,i} \in \mathcal{F}_{\mathcal{P}(\Omega^+)}^k$ and $i \leqslant k$ . e.g if $\mathcal{P}(\Omega^+) = \{\{\omega_1\}, \{\omega_2\}, \{\omega_1, \omega_2\}\}$ , a possible choice is $\mathcal{F}_{\mathcal{P}(\Omega^+)}^{2,i} = \{\{\omega_2\}, \{\omega_1, \omega_2\}\}$ . Obviously iff $k = 2^{ \Omega }$ then $\mathcal{F}_{\mathcal{P}(\Omega^+)}^{k,1} = \mathcal{P}(\Omega^+)$ .
$\Pi_{\Omega}$	Feasible partition set of an integer set partitioning optimization problem.
Π <sub>υ</sub>	Unfeasible partition set of an integer set covering optimization problem.
Π	Partition set of an integer set covering optimization problem. i.e $\Pi = \Pi_{\chi} \bigcup \Pi_{\upsilon}$ .
Π	Overlapping set of an integer set covering optimiza- tion problem (i.e all the unfeasible solutions that do not satisfy the partitioning constraints).
Υ	Unfeasible set of an integer set Covering optimization problem. i.e $\Upsilon = \overline{\Pi} \bigcup \Pi_{\upsilon}$ .
x	The solution space of an integer set covering optimization problem. i.e $\mathcal{X} = \Pi_{\chi} \bigcup \Upsilon$ .
$\sigma_n^k$	Stirling number of the second kind (or Stirling par- tion number). i.e the number of ways to partition a set of n objects into k non empty subsets.
B <sub>n</sub>	Bell number. i.e the number of ways to partition a set of n objects.
$\Pi(\sigma_n^k)$	The partition set composed by k sets. In other words all the possible partition with k subsets of $\Omega$ .

$\Pi_{\sigma_{n,i}^k}$	A partition solution composed by k sets such that $i \leqslant \sigma_n^k$ . i.e $\Pi_{\sigma_{n,i}^k} \varepsilon \Pi_(\sigma_{n,i}^k) = \{\Pi_{\sigma_{n,i}^k}, \dots, \Pi_{\sigma_{n,\sigma_n^k}^k}\}$
$\pi_{\sigma_{n_i}^k}$	The real value solution associated to $\Pi_{\sigma_{n,i}^k}$ .
$\binom{n}{k}$	The number of k-subset possible out of a set of n distinct items. aka Binomial Coefficient
x <sup>i</sup>	A vector decision variable. If it's clear from the con- text we do not use the superscript.
xji	The j-th scalar component of vector i. e.g $x^i=\{x_1^i,x_2^i,\ldots,x_j^i,\ldots,x_n^i\}.$
f	A vector of objective functions. i.e $\mathbf{f} = (f_1, f_2, \dots, f_n)$
g	A vector of constraints functions. i.e $\mathbf{g} = (g_1, g_2, \dots, g_p)$
Ι	The identity matrix, i.e its elements are zeros except those on the main diagonal that are ones.
$\mathbf{Diag}(\mathbf{z})$	The diagonal matrix which diagonal elements are the elements of the $z$ vector.
$\mathbf{z}^{'}$	The transpose of vector <b>z</b> .
$\mathbf{Z}'$	The transpose of the matrix <b>Z</b> .
0	The column vector of length N which components are $\boldsymbol{0}.$
1	The column vector of length N which components are 1.
1 <sub>A</sub>	the column vector of length $2^N - 1$ which components are 0 except the component corresponding to $A \subseteq \Omega$ which value is 1.

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Part I

# THE PROBLEM STATEMENT

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### INTRODUCTION

In this section we provide a new formulation to use survey data to establish catchment areas of primary care or Primary Care Service Areas.

The model is based on an origin-destination matrix that has patient postcodes on the rows and provider postcodes on the columns. Each cell carries information about the strength of the flow of patients from a patient postcode to a provider postcode. Primary Care Service Areas (PCSAs) are expected to represent natural travel behavior of patients and it is possible for people with chronic illness who make more than the average number of visits to a GP to bias the geography. To minimise this bias, each patient is assigned one 'vote' which is spent in proportion to the number of visits made by the patient to a postal code. The final product is thus a spatial interaction matrix or origin-destination matrix of total votes flowing between patient and provider postcodes. Each cell in the matrix represents the total number of votes moving from a patient postcode to a provider postcode.

Each patient Postal Code Area (POA) is assigned to the provider POA that receives the maximum percentage of votes from the POA. The geographical aggregate of assigned patient POA together with the provider POA form a Primary Care Service Area.

At the heart of the assignment procedure lies the notion of the Localization of Utilization, which I personally call the Preference Index. This key performance indicator is the proportion of summed preference fractions for the population residing in a PCSA that occurs in provider POA within the same PCSA.

Ideally the population inside a PCSA (zone) obtains all of its primary care from clinicians within the area and recognizing that there will always be some patients who seek care in other areas, an important criteria is to maximise this index in order to capture the maximum patient-flow in the study area.

In the first part we prove that the maximisation of the index can be formulated as a sort of Quadratic Set Partitioning problem. Specifically for a fixed number of zones (say k) we have a linear combination of (k)Quadratic forms.

However, one of the most serious difficulties in zone design is the approach adopted to maintain zone contiguities, as well as to check the partitioning and covering constraints. These methods should be as simple as possible avoiding complicated structures. That may lead to an exponential increase of processing time, during the iterative zone design procedure.

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Therefore, we first discuss the computational effort of some existing procedure and then propose a plant location model where the constraints can be formulated as integer inequalities. The goal of our study is to examine the zone design problem using a more general approach. This flexibility is achieved by treating the problem of zone design as a problem of partitioning a mathematical graph to meet a set of generalised objectives. In particular, a simple contiguity method is implemented to overcome the computational issue.

Another essential property is zonal homogeneity in social economic characteristic (i.e age, social class, etc). As a matter of fact the result of a specific partition is a stratified sampling. It may possible to divide a heterogeneous population in the sub populations, each of which is internally homogeneous. This is suggested by the name strata, with its implication of a division into layers. If each stratum is homogeneous, in that the measurement vary little from one unit to another, a precise estimate of any stratum mean can be obtained from a small sample in that stratum.

Moreover, these estimates can be than combined into a precise estimate for the whole population. In fact in aggregating adjacent basic areal units to form a larger zone, the original individual attribute values of the basic units are replace by a single value. The uniqueness of each areal unit and the variation for the whole area is often lost. Depending on the aggregation scale and the spatial configuration, the construction of new zones can yield different representations of the same data set. Any analytical or statistical result, derived from the data may vary depending on the particular zoning system chose. The significance of this so-called Modifiable Areal Unit Problem (MAUP) has been long recognised(Openshaw 1984).

The existence of scale and aggregation effects are seen as a fundamental characteristics of spatial data. They cannot be removed without doing possibly irreversible damage to the data and thus any subsequent geographical interpretation. The only alternative to the modelling approach is to try to control the scale and aggregation characteristics of spatially aggregated data in some way.

Therefore, in order to produce homogeneous zones consisting of areal units with similar values for the selected variable, a possible solution is based on the minimisation of distances between the mean of zones and their areal units.

Although the above three characteristics of this zone design system (objective function (maximisation of the Preference Index and minimisation of the Homogeneity function), contiguity and set partitioning check algorithm) are structurally important, additional criteria perform special tasks expanding the capabilities of zone design systems. Such criteria could be for example the construction of compact or balanced zones in terms of shape formation and equal populated zones respectively. Moreover, sometimes a good accessibility is required, for

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examples by means of public transportation or highways within areal units inside the zone as well as another characteristic are physical barrier such as non traversable obstacle like rivers or mountain ranges. Evidently, each criterion applied to zone design performs a constraint to the output optimum solution with an additional increase of processing time and may also make the problem unfeasible.

Therefore extensive use of criteria should be avoided if the study does not require such constraints, while through organisation of the zone design methodology is essential before aggregation process.

The purpose of this first part is to provide a mathematical framework. Then (in the second part) some strategies will be presented in order to provide a geographic solution to the problem.

#### 1.1 PROBLEMS IN SPATIAL MODELLING

The conventional approach to spatial analysis involves the application of a model to a study area which has been partitioned into zones. The definition of these zonal boundaries involves the selection of the scale of the study and the aggregation of the data to match the choice of scale. In nearly all cases, there are an incredibly large number of alternative scales and aggregations which could be used. It follows, therefore, that spatial data and the patterns and processes they describe are the product of a particular set of zonal boundaries, and that qualitative or quantitative studies of spatial data are not invariant with the choice of these boundaries.

**Scale** is an abstract concept which cannot be easily measured except in relative terms. The best surrogates are probably the **size** and the **number of zones** used to partition a study area.

- The Scale Problem arises because of uncertainty about the number of zones needed for a particular study.
- **The Aggregation Problem** arises because of uncertainty about how the data is to be aggregated to form a given number of zones.

The effects of these problems are known to researchers as *the scale effect* and *the zoning effect*.

- The scale effect is the variation in results that can be obtained when data for one set of areal units are progressively aggregated into fewer and lager units.
- **The zoning effect** is the variation in numerical results arising from the grouping of small areas into larger units to form a given number of zones.

For example, when census enumeration districts are aggregated into wards or other administrative units the results change with increasing scale and when an aggregation of enumeration districts into an

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aggregated level equivalent to wards occurs then it is possible to create a variety of output zones at the same level.

These problems always occur in the design of zones for the study of spatial data; and the two together represent one of the greatest unsolved problems facing spatial study today.

Current zone design procedures are typically haphazard, basically using rule-of-thumb guidelines (Like the n-steps Float Catchment Areas). Zones are thus mainly based on considerations of convenience and the existence of readily available data, but on occasions may be selected at a certain scale in order to isolate a particular spatial pattern. However, in many cases current knowledge of spatial phenomena is insufficient to define with any precision the scale and the aggregation needed. In other studies zone design is not regarded as being very important, and the relationship between the choice of zones and the results is seldom investigated, even when the data is sufficient for such a study.

As Wong and Amrhein (1996) mentioned "*researchers have to deal with the scale effect more frequently then the zoning effect* "because most of them usually work with specific aggregated levels and the use administrative areas that have been already specified. However, dealing only with one side of the problem is not the appropriate approach and it is important that zoning effect analysis takes place for suitable results.

In the following section we will focus on aspects that are shared by most of the zone design models. They cover the essential aspects of any zone design problem and can be applied to most of the applications.

Focusing on basic modelling aspects might be considered as a disadvantage, since a user may find that some of his requirments are not reflected in such a model. However, there exist several reasons why general purpose models for zone design are worth studying:

- 1. Often such a model provides a sufficient approximation for the practical application.
- 2. The model provide "good "solutions, which can in turn serve as a starting point for manual improvements or local search heuristics, which are able to take more complex criteria into account.
- 3. There exists a broad range of practical problems to which the models can be applied.
- 4. General purpose models can serve as a starting point for more complex models that take additional planning criteria into account, depending on the real-world situation.

Our objective is to provide algorithms that run in a general purpose geographical information system (GIS). Therefore we do not know the exact problem that a potential user has. Modelling only the most common and basic aspects of the zone design problem allows a wide applicability of the provided algorithms.

In the following we present "**building blocks** "for basic models in zone design.

#### 1.2 THE ZONE DESIGN PROBLEM

A first important distinction is made between **basic spatial units** (**b.s.u**) and **zones**.

- **b.s.u**: The smallest spatial unit for which data are available (e.g Postal Code Areas, Statistical Local Area, etc).
- zone: A geographic Area containing one or more **b.s.u**.

Thus a **catchment area** is nothing more than a zone and the identification of catchment areas is essentially a **feasible partition**.

- Feasible partition: A disjoint set of zones which completely covers a study area so that each b.s.u is allocated to only one zone and <u>all the members</u> of any zone are **spatially contiguous**.
- Unfeasible partition: A disjoint set of zones which completely covers a study area so that each b.s.u is allocated to only one zone and <u>not all the members</u> of any zone are **spatially contiguous**.

The notion of contiguity is quite general and must be defined in the specific context and topology. It is possible to define it as a geographical concept or any other criteria such as time-travel distance. In this work we define contiguity in a simple way.

• Contiguous zone: A set of b.s.u who shares the same boundary.

In this way a zone is called contiguous if it is possible to travel between the b.s.u of the zone without having to leave the zone. This consideration actually introduce another important criterion of a zone: **compactness**. In most applications, compact zones usually have geographically concentrated activity, therefore less travel, more service times. In other words, the term compactness express the desire for zones with minimal total travel times. Unfortunately, a rigid and concise mathematical definition of compactness is often difficult and strongly depends on the available data. A possible solution to model compactness is to minimize the total weighted distance (Euclidean, squared Euclidian..) from zone center to their b.s.u, in such a way is essentially a constraint with a sort of threshold value. However this definition is still vague and we would like to apply a more rigourous

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definition. Therefore, in this work we face the problem using a geometric approach measure based on convex hulls in order to achieve compact zones. At the moment a general definition of compactness may be the following.

• **Compact zone**: a round-shaped, "undistorted set "of b.s.u without holes.

Finally another criteria is **Balance**. Usually zones which are balanced relative to one or more attributes (called activity measures) are sought for. This criterion expresses a relation of zones among each other and is motivated by the desire of an even distribution of people in the study area. Apart from the desire for balanced zones, sometimes strict upper or lower bounds for the size of zones are given. For example on maximal travel times or minimal number of people within the zone. In vision of this qualitative description of the problem we can have a broad idea of the goal:

• Catchment Areas Identification: is the problem of grouping small geographical areas, called basic spatial units, into larger geographic clusters, called zones (catchment areas), in a way that the latter are acceptable according to relevant planning criteria.

These criteria are essential to analyse the structural properties of the problem and to explore the solution space. Although all the mentioned zone properties are relevant, in the next section we present a first formulation with only connectivity constraints. Also some notation is introduced that is summarized in the 1 table.

### 1.3 THE AUTOMATIC ZONE DESIGN PROBLEM

- N The number of basic spatial units inside the study area.
- Ω The set of all the basic spatial units in the study area, aka Universal set. e.g if N = 2 then Ω = {ω<sub>1</sub>, ω<sub>2</sub>} and |Ω| = 2.
- $\Pi_{\Omega}$  Feasible partition set.
- $\Pi_{\Upsilon}$  Unfeasible partition set.
- $\Pi$  Partition set i.e  $\Pi = \Pi_{\chi} \bigcup \Pi_{\upsilon}$ .
- T All the unfeasible solutions that do not satisfy the partitioning constraints).
- $\Upsilon$  Unfeasible set i.e  $\Upsilon = \overline{\Pi} \bigcup \Pi_{\upsilon}$ .
- $\mathfrak{X}$  The solution space of the problem. i.e  $\mathfrak{X} = \Pi_{\chi} \bigcup \Upsilon$ .

Let m represent the number of attributes related to a b.s.u. Then let be:

$$\mathbf{d}(\boldsymbol{\omega}_{i}) = \mathbf{d}^{i} = \begin{bmatrix} d_{1}^{i} \\ d_{2}^{i} \\ \vdots \\ d_{m}^{i} \end{bmatrix} \forall i = 1, \dots, N$$

The vector representing the b.s.u data. Thus we can collect all these data in a matrix **D**.

$$\mathbf{D} = \begin{bmatrix} \mathbf{d}^{\mathbf{1}'}, \mathbf{d}^{\mathbf{2}'}, \dots, \mathbf{d}^{\mathbf{N}'} \end{bmatrix}$$
$$\mathbf{D} = \begin{bmatrix} d_1^1 & d_2^1 & \dots & d_m^1 \\ d_1^2 & d_2^2 & \dots & d_m^2 \\ \vdots & & \vdots \\ d_1^N & d_2^N & \dots & d_m^N \end{bmatrix}$$

It is worth noting that part of the data in this matrix are in the Origin-Destination matrix. In fact for every b.s.u we have 2N - 1 attribute. I remind that each row represents the geographic area of where patient live and each column the geographic areas of where health care services are accessed. Thus for each b.s.u we have the patient in-flow and out-flow. However it seems we have (2N - 1) \* N data but some of them are redundant. For each couple of row we have two numbers in common, then the total number of attributes are  $N * N = (2N - 1) * N - {n \choose 2}$ . This is natural as the Origin Destination matrix is a N by N matrix.

In order to analyse the *spatial variation* over the study area, it is crucial to give a clear definition of this matrix. Technically, these flows between places represent spatial interactions which can be measured in a variety of ways using different *zonal systems* and *observation intervals*:

- the *zonal system* refers to the way in which the geographic area is disaggregated into geographic units- the number of the zones and the shape into which the space is divided; and
- the *observational interval* refers to the time period over which the interactions are measured. In practice, these aspects of the flow matrix:

- the type of data, the zonal system and the observation intervalhave significant implications for the result obtained from any analysis. Let's define more rigorously this matrix **O**. The first step in the construction of this matrix is to assign one "vote "to each patient living in a specific postal code (b.s.u) on the basis of the number of visits made by the patient to a postal code (b.s.u). At the end of this operation we have a spatial interaction matrix **V** of total votes flowing between patient and provider postcodes (b.s.u).

$$\mathbf{V} = \begin{bmatrix} v_{11} & v_{12} & \dots & v_{1j} & \dots & v_{1N} \\ v_{21} & v_{22} & \dots & \cdots & v_{2j} & \dots & v_{2N} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{v_{i1}} & \mathbf{v_{i2}} & \dots & \ddots & \mathbf{v_{ij}} & \dots & v_{iN} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ v_{N1} & v_{N2} & \dots & \mathbf{v_{Nj}} & \dots & v_{NN} \end{bmatrix}$$

Each cell in the matrix represents the total number of votes moving from a patient postcode to a provider postcode. The principal diagonal of the matrix can represent just the number of people moving within the same area, or it may include non-movers as well (e.g the same health provider within the unit), depending on the data available and how the table is constructed. Knowing the number of non-movers is important because it enables calculation of the total population in each origin at the start of the interval, which is needed for several of the measures computed below. By convention, however, and to maintain consistency, the *same population base* is used to calculate different indicators. Following this simple assumption, we can exclude subscripts representing time.

We can now perform some basic analyses:

- v<sub>jj</sub>: the total number of patients (movers and non-movers) living in postal code j that accessed the services provided by the health care area of the same unit.
- 2.  $H_j$ : summing down column j gives the number of patients living in the study area that accessed the services provided by the health care area of postal code j.  $H_j = \phi^I(j) = \sum_{i=1}^N v_{ij}$
- 3.  $M_j^I$ : summing down column j excluding the principal diagonal element gives the total number of *migrant-patients* (i.e patients that leave their postal code area to receive care in a different health care postal code area) to the health care area of postal code j. These are the *migration-patients inflows*.  $M_i^I = H_i v_{ij}$ .
- 4. P<sub>j</sub>: summing across row j gives the number of patients living in postal code area j. P<sub>j</sub> =  $\phi^{O}(j) = \sum_{j=1}^{N} v_{ij}$

V	1	2	3	4	Pj
1	5	15	0	5	25
2	15	10	5	5	35
3	2	4	20	4	30
4	3	0	2	5	10
Hj	25	29	27	19	100

Table 2: **Origin-Destination instance** $|\Omega| = 4$ 

POA	Inflows	Outflows	NetGain/Loss	$\mathbf{Gross}-\mathbf{flows}$	Population
j	$M_j^{I}$	$M_j^O$	$M_j^{I} - M_j^{O}$	$M^{\mathrm{I}}_{j} + M^{\mathrm{O}}_{j}$	Pj
1	20	20	0	40	25
2	19	25	-6	44	35
3	7	10	-3	17	30
4	14	5	9	19	10
Total ∑	60	60	0	120	100

- M<sup>O</sup><sub>j</sub>: summing across row j excluding the principal diagonal element gives the total number of *migrant-patients* leaving their place of origin j. These are the *migration-patients outflows*.
   M<sup>O</sup><sub>j</sub> = P<sub>j</sub> ν<sub>jj</sub>
- 6. P: Therefore the total number of votes gives the population size in the study area.  $P = \sum_{j=1}^{N} P_j = \sum_{j=1}^{N} H_j = \sum_{i=1}^{N} \sum_{j=1}^{N} v_{ij}.$

In order to give a summary of these measures, we make a simple numeric example. Suppose we have the following Votes matrix:

$$\mathbf{V} = \begin{bmatrix} 5 & 15 & 0 & 5 \\ 15 & 10 & 5 & 5 \\ 2 & 4 & 20 & 4 \\ 3 & 0 & 2 & 5 \end{bmatrix}$$

The table 2 gives an overview of the Votes matrix.

In order to control for population size, migration flows need to be expressed as rates or probabilities. Therefore a first operation is to normalize the matrix  $\mathbf{V}$ .

$$\mathbf{O} = \frac{1}{P} \dot{\mathbf{V}}$$

There are essentially two reasons to normalize our data:

0	1	2	3	4	pj
1	.05	.15	•	.5	.25
2	.15	.1	.05	.05	.35
3	.02	.04	.2	.04	.3
4	.03		.02	.05	.1
hj	.25	.29	.27	.19	1

Table 3: **Origin-Destination-O instance** $|\Omega| = 4$ 

- 1. The analysis should be independent from the particular instance.
- 2. As the problem is unit independent we can study some important **statistical measures** of the problem as well as possible **Lower and Upper bounds** to the optimisation solution.

	011	012	•••	•••	<b>0</b> 1j	•••	01N
	021	022	•••	•••	0 <sub>2j</sub>	•••	0 <sub>2N</sub>
	:	÷	·	÷	÷	÷	÷
0 =	0 <sub>i1</sub>	<b>0</b> <sub>i2</sub>	•••	·	o <sub>ij</sub>	•••	0 <sub>iN</sub>
	÷	÷	÷	÷	۰.	÷	÷
	÷	÷	÷	÷	÷	•	:
	0 <sub>N1</sub>	0 <sub>N2</sub>	•••	•••	o <sub>Nj</sub>	•••	0 <sub>NN</sub>

Turning our attention back to the instance 2 we can compute the matrix **O**:

	.05	.15		.05
0 –	.15	.1	.05	.05
0 -	.02	.04	.02	.04
	.03		.02	.05

In order to save space we represent 0 as a dot (0 = .) and proportion as a dot followed by the decimal part .15 = 0.15. Now we can compute the inward, outward and net flows in terms of proportion.

Now, moving beyond simple calculations of inward, outward and net flows, it is possible to identify four distinct perspectives on internal migration, each associated with a set of statistical measures that draw different insights from an inter-regional flow matrix. Originally developed to provide a framework for cross-national comparisons (Bell et at., 2002), these four perspectives focus on:

POA	Inflows	Outflows	NetGain/Loss	$\mathbf{Gross}-\mathbf{flows}$	Population
j	$\mathfrak{m}_j^{\mathrm{I}}$	$\mathfrak{m}_j^O$	$\mathfrak{m}_j^{\mathrm{I}} - \mathfrak{m}_j^{\mathrm{O}}$	$\mathfrak{m}_j^{\mathrm{I}} + \mathfrak{m}_j^{\mathrm{O}}$	pj
1	.2	.2	•	.4	.25
2	.19	.25	06	.44	.35
3	.07	.1	03	.17	.3
4	.14	.05	.09	.19	.1
Total ∑	.6	.6		1.2	1

Table 4: **network-parameter instance** $|\Omega| = 4$ 

- *migration intensity* the overall level or incidence of population mobility between zones within the system;
- *migration impact* the extent to which migration transforms the pattern of human settlement;
- *migration distance-* the way in which the friction of distance operates to diminish the intensity of movement to more distant locations; and
- *migration connectivity-* the way in which migration flows serve to make stronger links between some zones than between others.

Drawing on a previously literature, Bell et al.(2002) evaluated a battery of 15 statistical indicators designed to capture these four dimensions of mobility. Here we confine our attention to a selection of the 15 indicators and illustrate their application in the optimisation model using matrices of migration flows between Postal Code Areas.

### **Migration Intensity**:

Crude Migration Intensity for Outflow

 $\mathbf{CMIO}_{j} = 100 * m_{j}^{O}$ 

Crude Migration Intensity for Inflow

 $CMII_{i} = 100 * m_{i}^{I}$ 

### **Migration Impact:**

Net Migration Probability

$$\mathbf{NMP}_{j} = 100 * (\mathfrak{m}_{j}^{I} - \mathfrak{m}_{j}^{O})$$

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A system-wide measure of migration impact, the aggregate net migration probability (ANMP) can also be calculated to indicate the overall extent of population redistribution between zones through migration. In this case the equation simply sums the total of the absolute values of net migration across zones(some of which will be positive and some negative), divides by two to avoid double counting, and divides by the population of the study area.

Aggregate Net Migration Probability

**ANMP** = 
$$100 * \frac{0.5 * \sum_{j=1}^{N} N_j}{\sum_{j=1}^{N} P_j}$$

Another way to measure the impact of migration is by comparing inflows with outflows. The migration effectiveness ratio (MER) effectively quantifies the asymmetry or imbalance in migration flows to and from a zone. The index can be calculated in terms of total inwards and outwards flows:

Migration Effectiveness Ratio

$$\textbf{MER}_{j} = 100*\frac{\textbf{M}_{j}^{I}-\textbf{M}_{j}^{O}}{\textbf{M}_{j}^{I}+\textbf{M}_{j}^{O}}$$

or in its simplest form, confined to the two-way flows between a pair of zones:

$$\mathbf{MER}_{j} = 100 * \frac{v_{jk} - v_{kj}}{v_{jk} + v_{kj}}$$

The MER can assume values between +100 and -100, with the sign denoting whether there was a net gain or net loss to the zone in question.

Migration Effectiveness Index

$$\mathbf{MEI} = \frac{\sum \sum_{j=1}^{N} |\mathbf{N}_j|}{\mathbf{M}_j^{\mathrm{I}} + \mathbf{M}_j^{\mathrm{O}}}$$

The Migration Effectiveness Index is a system-wide equivalent to the MER. Because the MEI is calculated using absolute values, the index can only be positive, but otherwise interpretation is the same as for the MER: high values indicate a large degree of asymmetry or imbalance in flows, leading to high migration efficiency, or substantial distribution for the given volume of movement. In contrast, low values indicate that the migration system is more closely balanced with little net distribution, irrespective of the intensity of the flows.

#### Migration Connectivity:

In any system of inter-regional migration the magnitude of the flows between different pairs of origins and destinations varies widely. These variations are partly a product of differences in population size and the effect of distance decay, but they also reflect the strength of the functional linkages between regions.

A variety of indicators have been proposed to measure these linkages (Bell et al.,2002). Here we confine our attention to just two measures:

- the *index of migration inequality* which compares the observed flow matrix with a hypothetical distribution;and
- the *coefficient of variation* which indicates the extent of dispersion of the flows around the mean.

Index of migration inequality:

$$\mathbf{I}_{MI} = 0.5 * \sum_{i \neq j}^{N} \sum_{j \neq i}^{N} |\mathbf{o}_{ij} - \hat{\mathbf{o}}_{ij}|$$

This index  $(I_{MI})$  is obtained as the difference between the observed distribution of inter-POAS flows  $o_{ij}$  and the expected distribution  $\hat{o}_{ij}$ . The latter might simply assume that all inter-regional flows are identical.

Coefficient of Variations:

$$\mathbf{CV} = \frac{\sqrt{\sigma}}{\overline{\mathbf{M}}} \qquad \sigma = \frac{\sum_{i=1}^{N} \sum_{j=1}^{N} (v_{ij} - \overline{\mathbf{M}})^2}{N(N-1)}, i \neq j$$

The coefficient of variation is calculated as the standard deviation divided by the mean of the inter-zonal flows.

The next step is the definition of the Connectivity matrix.

At this stage it is worth noting that there are two different types of zonal arrangement. Most geographical studies have employed spatial aggregations based on contiguous arrangements of zones, sometimes referred to as **zoning system**. However, a zoning system is only a special case of a grouping system that incorporates a contiguity constraint. The non-contiguous case is referred to as a **grouping system**. The use of a contiguity constraint restricts the degree of aggregational variability and thus reducing the number of the feasible solutions. However, in order to define the notion of contiguity we introduce another important input to the problem:

### The Connectivity matrix A.

	-						-
	0	a <sub>12</sub>	•••	•••	a <sub>1j</sub>	•••	$a_{1N}$
	a <sub>21</sub>	0	•••	•••	a <sub>2j</sub>	•••	$a_{2N}$
	:	÷	·	÷	÷	÷	÷
$\mathbf{A} =$	a <sub>i1</sub>	a <sub>i2</sub>	•••	·	a <sub>ij</sub>		$a_{iN}$
	:	÷	÷	÷	·•.	÷	÷
	:	÷	÷	÷	÷	·	÷
	a <sub>N1</sub>	a <sub>N2</sub>	•••		a <sub>Nj</sub>	•••	0

 $a_{ij} = \begin{cases} 1, \forall i \neq j & \text{if postal code i and postal code j have a common border;} \\ 0, & \text{otherwise.} \end{cases}$ 

Clearly the matrix **A** is symmetric (i.e  $a_{ij} = a_{ji}$ ). Moreover another trivial consideration is:

 $\sum_{i=1}^{N} \sum_{j=1}^{N} a_{ij} = \begin{cases} 0, & \text{Totally disconnected. (i.e all postal codes are isolated)} \\ N(N-1), & \text{Totally connected. (i.e unconstrained grouping system)} \end{cases}$ 

Now that we have the main inputs in hand, our first goal is to understand what the solutions look like. A first step is to introduce the main decision variables of the problem.

The aim is to aggregate the N b.s.u in  $\Omega$  to form a partition of a study area into k zones, denoted  $Z^1, \ldots, Z^k$  such that  $1 \le k \le N - 1$ . Thus a **zone** is essentially a non-empty set of b.s.u. In other words is an element of the power set  $\mathcal{P}(\Omega^+)$ .

 $Z^i \in \mathcal{P}(\Omega^+), \qquad i = 1, \dots, 2^{|\Omega|} - 1$ 

Therefore a solution  $\mathcal{Z}$  is a subset of the power set (i.e a set of zones).

$$\mathcal{Z} \subseteq \mathcal{P}(\Omega^+) : \forall \mathcal{Z}_j \in \mathcal{Z}, \exists Z^i \in \mathcal{P}(\Omega^+) \qquad j \in \{1, \dots, k\}.$$

 $Z^{\mathfrak{i}}\in\mathfrak{Z}\Longrightarrow\mathfrak{Z}^{\mathfrak{i}}_{\mathfrak{j}}=Z^{\mathfrak{i}}\qquad\mathfrak{j}\in\{1,\ldots,k\}$ 

Henceforth all the possible subsets of the power set constitutes the solution space X.

$$\mathcal{Z} \in \mathcal{X}:$$
  $|\mathcal{X}| = \sum_{i=1}^{2^{|\Omega|}-1} {2^{|\Omega|}-1 \choose i}$ 

For instance let  $\Omega = \{\omega_1, \omega_2\}$  then:

$$\begin{aligned} \mathcal{P}(\Omega^+) &= \{\{\omega_1\}, \{\omega_2\}, \Omega\} \\ \\ \mathcal{X} &= \{\{\omega_1\}, \{\omega_2\}, \Omega, \{\{\omega_1\}, \{\omega_2\}\}, \{\{\omega_1\}, \Omega\}, \{\{\omega_2\}, \Omega\}, \mathcal{P}(\Omega^+)\} \end{aligned}$$

However it should be noted that we cannot select arbitrary any element of the solution space (some are feasible and other ones are unfeasible). Therefore a first important question is:

What properties must  $\mathcal{Z}$  satisfy in order to be a feasible solution for the non-contiguous case ?

To answer at this question we need to introduce two basic subsets of  $\mathfrak{X}$  first.

$$\Pi \subset \mathfrak{X}: \qquad \mathfrak{Z} \in \Pi \qquad \Longleftrightarrow \qquad \mathfrak{Z}_{\mathfrak{i}}^{\mathfrak{s}} \bigcap \mathfrak{Z}_{\mathfrak{j}}^{\mathfrak{t}} = \{\emptyset\}, \mathsf{Z}^{\mathfrak{s}} \neq \mathsf{Z}^{\mathfrak{t}} \in \mathfrak{P}(\Omega^{+})$$

$$\Upsilon \subset \mathfrak{X}: \qquad \bigcup_{j=1}^k \mathfrak{Z}_j^i = \Omega, \qquad \mathsf{Z}^i \in \mathfrak{P}(\Omega^+) \qquad i = 1, \dots, 2^{|\Omega|} - 1$$

- $\Pi$ : All the possible combination of disjoint subsets of  $\mathcal{P}(\Omega^+)$

Now it should be clear that all the possible partition of the universal set  $\Omega$  are:

$$\Pi^{\Omega} = \Pi \bigcap \Upsilon$$

We can then partition the solution space in three sets:

$$\mathfrak{X} = \overline{\Pi} \bigcup \overline{\Upsilon} \bigcup \Pi^{\Omega}$$

Now we must define the solution  $\mathcal{Z}$  more formally. As mentioned above,  $\mathcal{Z}$  is a non-empty sets of zones made up of one or more b.s.u. Therefore, in order to identify the elements that belong to a specific zone, we can establish a bijection relation between the elements of the power set  $\mathcal{P}(\Omega^+)$  and a binary vector **z**. In fact the elements of  $\mathcal{P}(\Omega^+)$  can be seen as vectors in  $\{0, 1\}^{|\Omega^+|}$ . We easily can prove this statement.

position	cba	Ω
1	001	a
2	010	b
3	011	ab
4	100	с
5	101	ac
6	110	bc
7	111	abc

Table 5: Order of the elements of the vectors in  $\Omega = \{\omega_1, \omega_2, \omega_3\} = \{a, b, c\}$ 

**Theorem.** Let  $\mathbf{2}^{\Omega^+} = \{0,1\}^{N^+} = \{(z_1, z_2, \dots, z_N) : z_i \in \{0,1\}, \mathbf{z} \neq \mathbf{0}\}$ then  $f: \mathbf{2}^{\Omega^+} \to \mathcal{P}(\Omega^+) : f((z_1^j, z_2^j, \dots, z_N^j)) = Z^j$  is a bijective function.

Proof. 
$$|\mathbf{z}^{\Omega^+}| = |\{\overline{\{0,1\}}X \dots X\{0,1\}} \setminus \mathbf{o}'\}| = |\{0,1\}^{N^+}| = 2^N - 1$$
  
 $2^N - 1 = 2^{|\Omega|} - 1 = |\mathcal{P}(\Omega^+)|$  then  
 $\forall (z_1, z_2, \dots, z_N) \in \mathbf{z}^{\Omega^+} \exists Z^j \in \mathcal{P}(\Omega^+) : \omega_i \in Z^j \Leftrightarrow z_i^j = 1$ 

It is clear that the number of possible bijections are  $(2^{N} - 1)!$ . The order of the elements can be arbitrary, but one particular order turns out to be extremely practical, and helps enormously in the algorithm design as well as to underline patterns. For pedagogical purpose, many examples are presented on the frames  $\Omega = \{\omega_1, \omega_2, \omega_3\}$  ( $\Omega, 3$ ) or  $(\Omega, 4)$ . Generalization are immediate in the case  $(\Omega, N)$ .

So a natural question is:

How can we choose the function f?

In order to answer at this question, we can observe that an easy way to establish a strictly ordered relation between the elements of  $\mathbf{2}^{\Omega}$  is:

$$\mathbf{z}^s > \mathbf{z}^t \Leftrightarrow \sum_{i=1}^N z_i^s 2^{i-1} > \sum_{i=1}^N z_i^t 2^{i-1} \forall \mathbf{z}^s, \mathbf{z}^t \in \mathbf{2}^{\Omega^+} s \neq t \in \{1, \dots, 2^N - 1\}$$

In the same way we can assign a positional order to the elements of the power set  $\mathcal{P}(\Omega^+)$ . In general, the i – th element of the vector  $z^j$  (i.e  $z_i^j$ ) corresponds to the set which elements are those indicated by a 1 in the binary representation of i. Suppose we have  $(\Omega, 3)$ , consider the vector  $z^3$ , the binary representation of 3 is  $(3)_2 = 110$  and the set is thus  $\{\omega_1, \omega_2\}$  so  $z^3 = Z^3 = \{\omega_1, \omega_2\}$ .

According to this one-to-one and on-to mapping we can enumerate the set of feasible solutions indicating the number of zones. To accomplish this task, we need to introduce further notation.

$ \Omega $	$ \Pi^{\Omega} $
10	10 <sup>5.06437</sup>
50	10 <sup>47.26897</sup>
100	10 <sup>115.67772</sup>
200	10 <sup>275.79631</sup>
300	10 <sup>453.98298</sup>
400	10 <sup>644.10952</sup>
500	10 <sup>843.20762</sup>
600	10 <sup>1049.50792</sup>

Table 6: Set Partitioning Complexity

 $\sigma_n^k$  Stirling number of the second kind (or Stirling partition number). i.e the number of ways to partition a set of n objects into k non empty subsets.

$$\sigma_n^k = \sum_{j=0}^k \frac{(-1)^{k-j} \cdot j^n}{(k-j)! \cdot j!}$$

- $\Pi(\sigma_n^k) \qquad \mbox{ The partion set composed by $k$ sets. In other words all the possible partition with $k$ subsets of $\Omega$. }$

k	$\Pi(\sigma_4^k)$	Z	Z	$\sigma_4^k$
1	$\Pi_{\sigma_{4,1}^1}$	$\{\{1, 2, 3, 4\}\}$	$[\mathbf{z^{15}}]$	
	,	Total ∑		1
2	$\Pi_{\sigma^2_{4,1}}$	$\{\{1, 2, 3\}, \{4\}\}$	$[z^{8}, z^{7}]$	
	$\Pi_{\sigma_{4,2}^2}$	$\{\{1, 2, 4\}, \{3\}\}$	$[z^{11}, z^4]$	
	$\Pi_{\sigma_{4,3}^2}$	$\{\{1,2\},\{3,4\}\}$	$[z^3, z^{12}]$	
	$\Pi_{\sigma_{4,4}^2}$	$\{\{1, 3, 4\}, \{2\}\}$	$[z^{13}, z^2]$	
	$\Pi_{\sigma_{4,5}^2}$	$\{\{1,3\},\{2,4\}\}$	$[z^5, z^{10}]$	
	$\Pi_{\sigma_{4,6}^2}$	$\{\{1,4\},\{2,3\}\}$	[ <b>z<sup>6</sup></b> , <b>z</b> <sup>9</sup> ]	
	$\Pi_{\sigma_{4,7}^2}$	$\{\{1\}, \{2, 3, 4\}\}$	$[z^{1}, z^{14}]$	
		Total ∑		7
3	$\Pi_{\sigma_{4,1}^3}$	$\{\{1,2\},\{3\},\{4\}\}$	$[z^3, z^4, z^8]$	
	$\Pi_{\sigma^3_{4,2}}$	$\{\{1,3\},\{2\},\{4\}\}$	$[z^5, z^2, z^8]$	
	$\Pi_{\sigma^3_{4,3}}$	$\{\{1\}, \{2, 3\}, \{4\}\}$	$[\mathbf{z^1}, \mathbf{z^6}, \mathbf{z^8}]$	
	$\Pi_{\sigma^3_{4,4}}$	$\{\{1,4\},\{2\},\{3\}\}$	$[z^9, z^2, z^4]$	
	$\Pi_{\sigma^3_{4,5}}$	$\{\{1\}, \{2, 4\}, \{3\}\}$	$[z^1, z^{10}, z^4]$	
	$\Pi_{\sigma^3_{4,6}}$	$\{\{1\},\{2\},\{3,4\}\}$	$[z^1, z^2, z^{12}]$	
		Total ∑		6
4	$\Pi_{\sigma_{4,1}^4}$	$\{\{1\},\{2\},\{3\},\{4\}\}$	$[z^1,z^2,z^4,z^8]$	
		Total ∑		1

Table 7: Set Partitioning solution space  $|\Omega| = 4$ 

Now it is immediate to compute the number of feasible solutions.

$$|\Pi^{\Omega}| = \sum_{k=1}^{|\Omega|} \sigma_{|\Omega|}^{k} = \sum_{k=1}^{|\Omega|} \sum_{j=0}^{k} \frac{(-1)^{k-j} \cdot j^{|\Omega|}}{(k-j)! \cdot k!}$$

The formula indicates that one of the reasons why the zone design problem is especially difficult is due to the size of the solution space. The dimension of a usual real world problem makes unfeasible any attempt to explicitly enumerate all the possible solutions. However the solution space dimension reduces its size with the connectivity constraints (not significantly) 6. The numbers of all possible partitions of a set  $|\Omega| = n$  is usually indicated as B(n) (The Bell number).

Suppose we have have  $(\Omega, 4)$ , then the number of feasible solutions are:

Ζ	$\mathbf{s}^{i}$	$\mathbb{Z}_3$	$\mathbb{Z}_2$	$\mathcal{Z}_1$	$\mathbb{Z}^{i}$	Π <sup>i</sup>
[ <b>z</b> <sup>7</sup> , <b>o</b> , <b>o</b> ]	000	Ø	Ø	123	123	1
$[z^3, z^4, o]$	001	Ø	3	12	12 3	2
$[z^5, z^2, 0]$	010	Ø	2	13	13 2	3
$[z^3, z^4, o]$	011	Ø	23	1	1 23	4
$[z^1, z^2, z^4]$	012	3	2	1	1 2 3	5
5	Total $\mathcal{B}_3$					

Table 8: Set Partitioning solution space  $|\Omega| = 3$ 

$$|\Pi^{(\Omega,4)}| = \sum_{k=1}^{4} \sigma_{4}^{k} = \sum_{k=1}^{4} \sum_{j=0}^{k} \frac{(-1)^{k-j} \cdot j^{4}}{(k-j)! \cdot k!} = 15$$

As mentioned in the introduction, areal units can be aggregated into various outputs zones on the same aggregated level. The table 7 shows different outputs zones for each created aggregation level. On the top of the table there is the level of a single output zone; this is the most aggregated level providing only a summary of the individual characteristics and it is the most heterogeneous level. On the other hand, on the bottom there is the level of four output zones the finest one, which preserves homogeneous zone but violates other criteria. However, there is still an open question:

How to represent a set partition inside a computer ?

As repeatedly mentioned in the previous sections, the partitions of a set are the ways to regard that set as a union of non empty, disjoint subsets called 'Zones'. For example, we listed in the table 8 the five essentially different partitions of  $(\Omega, 3)$ , using a vertical line to separate one block (zone) from another. In this list the elements of each block could have been written in any order, and so could the blocks themselves because 13|2 and 31|2 and 2|13 and 2|31 all represent the same partition. But we can standardize the representation by agreeing, for example, to list the elements of each block in increasing order, and to arrange the blocks in increasing order of their smallest elements. With this convention, for example, the 2|31 is then sorted in this way: 2|31- > 2|13- > 13|2.

Following this convention it is straightforward to encode a partition as a *restricted growth string*, namely as a string  $\mathbf{s} = \begin{bmatrix} s_1 & s_2 & s_3 \end{bmatrix}$  in which we have:

**s**: 
$$s_1 = 0, s_{j+1} \le 1 + \max(s_1, \dots, s_j)$$
  $1 \le j < N$ 

The idea is essentially based on the fact that every set partition defines an equivalence relation. If  $\Pi^i$  is a partition of  $(\Omega, N)$  we can write:

$$\omega_{\mathfrak{u}} \equiv \omega_{\mathfrak{v}} \mod \Pi^{\mathfrak{i}} \Leftrightarrow \omega_{\mathfrak{u}}, \omega_{\mathfrak{v}} \in \mathfrak{Z}_k : \mathfrak{Z}_k \in \Pi^{\mathfrak{i}}$$

In other words  $u \equiv v$ , whenever  $\omega_u$  and  $\omega_v$  belong to the same block of  $\Pi^i$ . Therefore the idea is to set  $s_j = s_k$  if and only if  $\omega_j \equiv \omega_k$ , and to choose the smallest available number for  $s_j$  whenever j is smallest in its block. Following this convention we can select any partition using the decision vector **s**.

For example, the restricted growth string for 1|23 is:

$$\mathbf{s}^{1} = \begin{cases} 0, \omega_{1} \in \mathcal{Z}_{1} & \mathcal{Z}_{1} \in \mathcal{Z}^{1} = \Pi^{1} \\ 1, \omega_{2} \in \mathcal{Z}_{2} & \mathcal{Z}_{2} \in \mathcal{Z}^{1} = \Pi^{1} \\ 1, \omega_{3} \in \mathcal{Z}_{2} & \mathcal{Z}_{3} \in \mathcal{Z}^{1} = \Pi^{1} \end{cases}$$

This is an efficient way to represent a solution Z inside the computer. The space Complexity S of this data structure is given by the following formula (it computes the number of bits storage):

$$\mathbb{S}(\mathcal{R}_g) = \begin{cases} \sum_{i=3}^{\lfloor \log_2(N) \rfloor} i \cdot 2^{i-1} & \lfloor \log_2(N) \rfloor \ge 3 \\ 6 & N = 3 \\ 2 & N = 2 \end{cases}$$

It is worth noting that the dimension of the matrix **Z** is NxN. In the case of N = 600, we need only 800.25 B instead of 45 KB; this is an important result as it is crucial to keep in memory a pool of solutions (with specific properties) during the execution of the algorithm. Moreover all the visiting algorithms have linear Complexity  $\Theta(N)$  instead of  $\Theta(N^2)$ . Clearly there is an isomorphism between  $\mathbf{s} \in \mathbb{N}^N : \mathbf{s}_i \in \{0, \dots, N-1\}$  and  $\mathbf{Z} \in \{\mathbf{0}, \mathbf{1}\}^N \mathbf{x}\{\mathbf{0}, \mathbf{1}\}^N$ :

$$\mathbf{z}_{ij} = \begin{cases} 1, & \text{if}\omega_i \in \mathsf{Z}_j \Leftrightarrow s_j = j-1 \\ 0, & \text{otherwise} \end{cases}$$

In this way the elements of  $\Pi^{\Omega}$  can be seen as vectors in  $\mathbb{N}^{\mathbb{N}}$ . We can prove this statement:

**Theorem.** There is a bijection between the restricted growth string functions  $\mathcal{R}_g$  on  $(\Omega, N)$  and  $\Pi^{\Omega}$ . *Proof.* Let  $\mathcal{R}_q$  be the set of all restricted growth functions on  $(\Omega, N)$ and let  $\Pi^{\Omega}$  be the set of all partitions on  $(\Omega, N)$ . We define a map  $\Phi$ :  $\mathfrak{R}_{q} \to \Pi^{\Omega}$  which is the required bijection. Put  $\Phi((s_{1}, s_{2}, \dots, s_{n})) =$  $\mathcal{Z}_1 \bigcup \mathcal{Z}_2 \bigcup \cdots \bigcup \mathcal{Z}_k$  where  $\mathcal{Z}_i = \{j : s_j = i - 1, i \in \{1, \dots, k\}\}$  and the map  $\Phi$  certainly maps  $\mathcal{R}_q$  to  $\Pi^{\Omega}$ . We must verify that it is one-toone and onto. To do this, we explicitly construct the inverse function to  $\Phi, \Phi^{-1}: \Pi^{\Omega} \to \mathcal{R}_q$ . Let  $\mathcal{Z}_1 \bigcup \mathcal{Z}_2 \bigcup \cdots \bigcup \mathcal{Z}_k \in \Pi^{\Omega}$  be a set partition. Assume the blocks have been ordered in the following way:  $0 \in s_1, \min\{\omega_i \in \Omega \setminus \{\mathcal{Z}_1 \cup \mathcal{Z}_2 \cup \ldots \mathcal{Z}_{j-1}\}\} \in \mathcal{Z}_j$ . This just means that we order the blocks so that block  $Z_i$  contains the smallest element not in preceding blocks. We define  $\Phi^{-1}(\mathbb{Z}_1 \cup \mathbb{Z}_2 \cup \cdots \cup \mathbb{Z}_k) =$  $(s_1, s_2, \ldots, s_n)$  by  $s_i = j - 1$  if and only if  $\omega_i \in \mathcal{Z}_j$ . We must check that  $(s_1, s_2, \ldots, s_n)$  is an  $\mathcal{R}_q$  function. Clearly  $s_1 = 0$ . Let  $\omega_i \in \Omega$  and put  $\mathfrak{m} = \max\{s_1, \ldots, s_{i-1}\}$ . Then  $\omega_{i-2} \subset \mathbb{Z}_1 \bigcup \mathbb{Z}_2 \bigcup \cdots \bigcup \mathbb{Z}_m$  and either  $\omega_i \in \mathcal{Z}_1 \bigcup \mathcal{Z}_2 \bigcup \cdots \bigcup \mathcal{Z}_m$  or i is the smallest number outside this union. In the first case  $s_i \leq m$  while in the second case  $\omega_i$  is in the block  $\mathcal{Z}_{m+1}$ , which means that  $s_i = m + 1$ . This verifies that  $s_i \leq \max\{s_1, \dots, s_{i-1}\} + 1$ . It is now easy to verify that  $\Phi \circ \Phi^{-1}$  and  $\Phi^{-1} \circ \Phi$  are identity maps on  $\Pi^{\Omega}$  and  $\mathcal{R}_q$  respectively. This implies that  $\Phi$  is a bijection. 

The bijection between the  $\Re_g$  and  $\Pi^{\Omega}$  enables us to enumerate all the partitions of  $\Omega$ . However, there are several ways to enumerate the elements of a set! Therefore, an important question is: How can we establish an ordered relation between the elements of  $\Pi^{\Omega}$ ?

A natural order for any list of strings or sequences is lexicographic order. Lexicographic order is based on the familiar idea as the ordering of words in dictionaries. The only requirement is that the letters that make up the alphabet of the language be ordered. In the definition below we use  $\prec$  to denote the assumed underlying ordering of the symbols of the alphabet and < to denote orderings of strings. It is worth noting that in most instances the alphabet is the set of natural numbers under the usual numeric ordering  $1 \prec 2 \prec 3 \dots$ 

**Definition.** In lexicographic (or lex) order  $a_1a_2...a_n <_l b_1b_2...b_m$  if either:

- 1. for some k,  $a_k \prec b_k$  and  $a_i = b_i$  for i = 1, 2, ..., k-1
- 2. n < m and  $a_i = b_i$  for i = 1, 2, ..., n

In other terms  $a_1 a_2 ... a_n$  appears in a dictionary before the a sequence  $b_1 b_2 ... b_m$  if and only if at the first i where  $a_i$  and  $b_i$  differ,  $a_i$  comes before  $b_i$  in the alphabet. If the sequences have different length and same symbols than the shorter comes first. Following this ordering between the restricted growth strings, once we set the first digit to 0 all the remaining strings are automatically computed. (Obviously we could use S[1] = 1 instead, but it is just a convention). Therefore this convention suggest the following simple gen-

Algorithm 1 The growth-string partition enumeration algorithm

```
1: procedure RG-Partitions(N : \mathbb{N})
            \triangleright Display all the partitions of |\Omega| = N in lexicographic order
 2:
          for i \leftarrow 1, N do
 3:
               S[i] \leftarrow 0
 4:
          end for
 5:
          for i \leftarrow 1, N-1 do
 6:
               B[i] \leftarrow 1
 7:
          end for
 8:
          \mathfrak{m} \leftarrow 1
 9:
          Done \leftarrow false
10:
          while !Done do
11:
               PRINT(S)
12:
               if S[N] = m then
13:
                   j \leftarrow N-1
14:
                    while S[j] = B[j] do
15:
                         j \leftarrow j - 1
16:
                    end while
17:
                   if j! = 1 then
18:
                         S[j] \leftarrow S[j] + 1
19:
                         \mathfrak{m} \leftarrow B[\mathfrak{j}] + S[\mathfrak{j}]
20:
                         j \leftarrow j + 1
21:
                         while j < N do
22:
                              S[j] \leftarrow 0
23:
                              B[j] \leftarrow \mathfrak{m}
24:
                              j \leftarrow j + 1
25:
                         end while
26:
                         S[N] \leftarrow 0
27:
                    else
28:
                         \texttt{Done} \gets \texttt{true}
29:
                    end if
30:
               else
31:
                    S[N] \leftarrow S[N] + 1
32:
               end if
33:
          end while
34:
35: end procedure
```

eration scheme, due to George Hutchinson 1.

Although lexicographic order is aesthetically pleasing, there is often no particular advantage to use it. For example, suppose that we aren't interested in all of the partitions; we might want only the ones that have exactly m blocks. Can we run through this smaller collection of restricted growth strings, changing only one digit at a time? Yes! a very pretty way to generate such a list has been discovered by Frank Ruskey, and it is listed according to a *co-lexographic order*.

**Definition.** In co-lexicographic (or colex) order  $a_1a_2...a_n <_c b_1b_2...b_m$ if  $a_n...a_2a_1 <_l b_m...b_2b_1$  in lex order.

Algorithm 2 partition enumeration of k blocks algorithm 1: **procedure** RGK-PARTITIONS(N,  $k : \mathbb{N}, k > 1$ ) Display all the partitions of kblocks in colex order 2: for  $i \leftarrow 1$ , N do 3:  $S[i] \leftarrow i - 1$ 4: end for 5: Gen-k(N, k, S)6: **function** GEN-K(N, k, S) 7: ▷ Recursive procedure to print all the partitions. 8: if N=k then 9: Print(S) 10: else 11: for  $i \leftarrow 0, k-1$  do 12:  $A[N] \leftarrow i$ 13: Gen-k(N-1,k,A)14:  $A[N] \leftarrow N - 1$ 15: end for 16: if k > 1 then 17:  $A[N] \leftarrow k-1$ 18: Gen- $\kappa(N - 1, k - 1, A)$ 19:  $A[N] \leftarrow N-1$ 20: end if 21: end if 22: end function 23: 24: end procedure

The 2 function calls the recursive procedure 7 inside.

Sometimes, however, the user might want to restrict the number of basic spatial units in each zone. Therefore, among all the partitions that have m blocks, we are interested only to those that have a minimum (m) and a maximum(M) number of b.s.u for each zone. We

identify this set with the following notation  $\Pi(\sigma_N^k)_m^M$ . According to these constraints we can partition the set of zones

$$Z^{m} = \{ \mathcal{Z}_{i} \equiv \mathcal{Z}_{j} \mod \mathfrak{m} \Leftrightarrow |\mathcal{Z}_{i}|, |\mathcal{Z}_{j}| \ge \mathfrak{m} \}$$
$$Z^{M} = \{ \mathcal{Z}_{i} \equiv \mathcal{Z}_{j} \mod M \Leftrightarrow |\mathcal{Z}_{i}|, |\mathcal{Z}_{j}| \le M \}$$

Then, the set of feasible partitions are:

$$\begin{split} \Pi(\sigma_N^k)_m^M = & \{Z_i \in Z^m \bigcap Z^M : k_m \leqslant k \leqslant k_M\} \\ & k_m = \frac{N}{M} \quad k_M = \frac{N}{m} \end{split}$$

Clearly  $\Pi(\sigma_N^k)_m^M \subseteq \Pi(\sigma_N^k)$ ; So the next question is: How can we identify this subsets of partitions ?

In order to answer at this question we need to introduce a new combinatorial object: *The partition of an integer* In fact a solution is a partition of the study area  $\Omega = \{\omega_1, ..., \omega_N\}$  into k parts and for each part we have a set of basic spatial units.

**Definition.** Partition of an integer: A k-tuple of positive integers  $\mathbf{p} = \begin{bmatrix} p1 & p2 & \dots & p_k \end{bmatrix}$  is an integer partition of N if  $p_1 + p_2 + \dots + p_k = N$  and  $p_1 \ge p_2 \ge \dots \ge p_k \ge 1$ . The number of parts of  $\mathbf{p}$  is k.

An example of a partition of 12 into 6 parts is  $\mathbf{p} = \begin{bmatrix} 4 & 2 & 2 & 2 & 1 & 1 \end{bmatrix}$ . Alternatively, we can completely describe  $\mathbf{p}$  by giving the number of times that a part i occurs, called the multiplicity of i. In this notation  $\mathbf{p} = 4^{1}2^{3}1^{2}$ , because  $\mathbf{p}$  has one 4, three 2's and two 1's. Let P(N,k) denote the number of partitions of N into k parts, then:

$$P(N,k) = \begin{cases} 1 & k = 1, k = N; \\ P(N-1,k-1) + P(N-k,k) & 1 < k < N; \\ 0 & k > N \end{cases}$$

Let P(N) the number of partitions of the integer N. Here's a table of P(N) for  $1 \leq N \leq 7$ :

Ν	1	2	3	4	5	6	7
P(N)	1	2	3	5	7	11	15

For instance, there are 5 different ways to partition the integer 4 9. Suppose we want all the partition with no more than two b.s.u for each zone. Excluding the trivial partitions (k = 1, N):

k	P(4, k)	p	Р	P	$\sigma_4^k$
1	1	4	$\Pi_{\sigma^1_{4,1}}$	1	
		Tota	l ∑		1
2	2	31	$\Pi_{\sigma_{4,1}^2}, \Pi_{\sigma_{4,2}^2}, \Pi_{\sigma_{4,4}^2}, \Pi_{\sigma_{4,7}^2}$	4	
		2 <sup>2</sup>	$\Pi_{\sigma_{4,3}^2}, \Pi_{\sigma_{4,5}^2}, \Pi_{\sigma_{4,6}^2}$	3	
		Tota	I ∑		7
3	1	21 <sup>2</sup>	$\Pi_{\sigma_{4,i}^3} \mathfrak{i} = 1, \dots, 6$	6	
		Tota	I ∑		6
4	1	14	$\Pi_{\sigma_{4,1}^4}$	1	
		Tota	I		1

Table 9: Set Partitioning solution space - cardinality  $|\Omega| = 4$ 

$$\begin{split} \Pi(\sigma_4^k)_1^2 &= P^3 \bigcup P^4 \\ P^3 &= \{\Pi_{\sigma_{4,3}^2}, \Pi_{\sigma_{4,5}^2}, \Pi_{\sigma_{4,6}^2}\} \\ P^4 &= \{\Pi_{\sigma_{4,i}^3} \mathfrak{i} = 1, \dots, 6\} \end{split}$$

We can enumerate all this partition executing the following algorithm 3.

Now that we are more familiar with the notation and have a clear overview of the solution space, we can state the problem more formally.

As already mentioned in the introduction section, the problem of the Catchment Area Identification is to select a set of zones in a way to meet a set of general criteria and to optimise two or more objectives. Therefore, the problem is to define an objective function **f** in order to provide a 'measure of partition performance 'in terms of the model and a predefined target value, so that by optimizing this function an optimum partition will be obtained.

Generally the objective function would be designed to identify a partition with whatever properties are considered. However, as a basis we can define a more general form of what is known as unconstrained *optimal automatic zone design problem* (UAZP). Thus the problem involves finding for any fixed D, A, k a classification Z\* such that  $f(Z^*; D, A, k) = min/max f(Z; D, A, k)$ .

Thus the function f(Z; D, A, k) is a scalar function of the independent variables Z and the constant variables D, A, k. It maps the performance of any partition on the set of real numbers. It is *similar* to a **contiguity-constrained set partitioning problem**. They concern the partitioning of a set of elements in a way which optimizes some objective function defined on the set of all partitions. Many of these

Algorithm 3 partition enumeration of an integer in k parts algorithm 1: **procedure** INTEGER-PARTITIONS(N, k :  $\mathbb{N}$ , N, k  $\geq$  2) Display all the partitions of an integer in k parts 2: for  $j \leftarrow 2, k$  do 3:  $A[i] \gets N-k+1$ 4:  $A[j] \leftarrow 1$ 5: end for 6:  $A[k+1] \leftarrow -1$ 7:  $Done \leftarrow False$ 8: while !Done do 9: PRINT(()A)10: if  $A[2] \ge A[1] - 1$  then 11: j ← 3 12:  $s \leftarrow A[1] + A[2] - 1$ 13: while  $A[j] \ge A[1] - 1$  do 14:  $s \leftarrow s + A[j]$ 15:  $j \leftarrow j + 1$ 16: end while 17:  $\triangleright$  s = A[1] + · · · + A[j - 1] - 1 18: ⊳ increaseA[j] 19: if j > k then 20:  $Done \leftarrow true$ 21: else 22:  $x \leftarrow A[j] + 1$ 23:  $A[j] \gets \boldsymbol{x}$ 24:  $j \leftarrow j - 1$ 25: end if 26: while j > 1 do 27: 28:  $A[j] \leftarrow x$  $s \leftarrow s - x$ 29:  $j \leftarrow j - 1$ 30:  $A[1] \leftarrow s$ 31: end while 32: else 33:  $A[1] \leftarrow A[1] - 1$ 34:  $A[2] \leftarrow A[2] + 1$ 35: end if 36: end while 37: 38: end procedure

problems can be solved by integer linear programming techniques but large problems are nearly always intractable.

Unfortunately, the computational difficulties associated with the AZP are *far more complex than the set partitioning problem*. If it is treated as a mathematical programming problem than the function  $f(Z^*; D, A, k)$  cannot be assumed to be either convex or continuously differentiable or linear in relation to the independent variables. Furthermore, the contiguity constraints are dynamic, depending on the data and the large number of configurations.

In this instance, we assumed a fixed number of zones. Indeed taxonomic procedures in a spatial context operate manipulating the zone system so as to achieve maximum formal or functional homogeneity. Thus it is suggested that there is usually a dependency of k on the zonal data produced by any mapping of  $Z^*$  on to D.

Accordingly, a more general statement of the problem is:

$$\begin{aligned} \mathbf{f}(Z^*, \mathbf{k}^*; \mathbf{D}, \mathbf{A}) &= \min/\max \quad \mathbf{f}(Z, \mathbf{k}; \mathbf{D}, \mathbf{A}) \\ \mathbf{k}^* &= \arg\max \quad \mathbf{k}\{\min/\max \quad \mathbf{f}(Z; \mathbf{D}, \mathbf{A}, \mathbf{k})\} \\ \mathbf{k} &\in \{1, \dots, k-1\} \end{aligned}$$

Therefore we'd like to determine the value of k such that for  $k = k^*$  we have min/maxf(Z; D, A,  $k^*$ ) = Z\*. It now clear that we have only one *scale problem* which regards the value of  $k^*$  whereas we can have (k - 2) *aggregation problems*. In fact considerable complexity is introduced by the need to continually re-estimate Z\* as k changes.

The solution proposed to overcome this issue, is to define a multiobjective function, which enclose all the criteria considered and the homogeneity property.Unfortunately, the non-linearity of the objective function make unfeasible any attempt to solve the problem with any linear programming techniques. Therefore, a first step is to linearize the function in a way that the two formulation are isomorphic.In other words, the objective is to formulate an integer linear model equivalent to the non-linear model. It is a challenging task as we have to prove that the optimal partition of the linear model is exactly the same as the non-linear one.

Let **f** and **f** the objective functions of the non-linear and linear model respectively. In the same way, let **g** and **\hat{g}** the constraints functions. Then the goal is:

#### 1.4 THE OPTIMISATION MODEL

The first step of any optimisation model is the definition of the decision variables, the objective function and the constraints. Regarding the decision variables, we have introduced the classification matrix  $\mathbf{Z}$  (N by N matrix). Although this representation is computationally inefficient, we initially refer to this matrix for a first formulation of the model.

As for the objective function, it is basically composed by two terms:

- J<sub>L</sub> Localization Index: It is the proportion of summed preference fractions for the population residing in a Zone that occurs in provider POA within the same Zone.
- 2.  $J_{\mathcal{H}}$  Homogeneity Index: It is the variation of specified attributes (such as Age,Sex and so on) that occurs within the Zones of the Partition.

The first term captures the fact that users want geographies such that patients in one unit mostly attend services in the same unit. The second term captures the fact that units must be homogeneous along certain user specified dimensions, and variation of certain variables should mostly occur across, but not within, units.

Therefore for each zone  $Z_i$  we have two opposing goals:

- 1. max  $\mathcal{I}_{\mathcal{L}i}$  maximise the number of people served.
- 2. min  $\mathcal{I}_{\mathcal{H}i}$  minimize the population attributes variance.

Finally we need to check feasibility for a set of constraints. Specifically we must ensure that the matrix  $\mathbf{Z}$  constitutes a partition whose zones are spatially contiguous.

It is clear that the next tasks are the definition of:

$$\mathbf{f} = \begin{cases} f_{\mathcal{L}} = \sum_{i=0}^{k} \mathbb{I}_{\mathcal{L}i} & \text{The-Localization} - \text{Index} - \text{function} \\ f_{\mathcal{H}} = \sum_{i=0}^{k} \mathbb{I}_{\mathcal{H}i} & \text{The-Homogeneity} - \text{Index} - \text{function} \end{cases}$$

$$\mathbf{g} = egin{cases} \mathbf{g}_{\mathcal{P}} & ext{The} - ext{Partitioning} - ext{constraints} \ \mathbf{g}_{\mathcal{C}} & ext{The} - ext{Contiguty} - ext{constraints} \end{cases}$$

#### 1.4.1 The Localization Index function

According to the definition of  $\mathcal{I}_{\mathcal{L}}$  it is clear that  $f_{\mathcal{L}}$  depends by the values of Z and O (the Origin Destination matrix).

$$f_{\mathcal{L}}(Z, O) \rightarrow [0 \quad 1] \qquad Z = (Z_1, \dots, Z_N)$$

$$\begin{split} f_{\mathcal{L}}(Z,O) &= \sum_{i=0}^{N} \mathbb{J}_{\mathcal{L}\,i}(Z_{i},O) \qquad Z_{i} \in Z \\ \mathbb{J}_{\mathcal{L}\,i} : \mathbb{J}_{\mathcal{L}\,i}(Z_{i},O) \rightarrow [0 \quad 1] \end{split}$$

In order to understand how to define the  $\mathfrak{I}_{\mathcal{L}i}(Z_i, O)$  we make a simple numeric example first. Suppose we have the following Votes matrix:

$$\mathbf{V} = \begin{bmatrix} 5 & 15 & 0 & 5 \\ 15 & 10 & 5 & 5 \\ 2 & 4 & 20 & 4 \\ 3 & 0 & 2 & 5 \end{bmatrix}$$

And the partition  $\Pi_{\sigma_{4,3}^3} = \mathcal{Z} = \{\{1\}, \{2, 3\}, \{4\}, \emptyset\}$  associated to the classification vector  $\mathbf{Z} = \begin{bmatrix} \mathbf{z}^1 & \mathbf{z}^6 & \mathbf{z}^8 & \mathbf{o} \end{bmatrix}$ .

$$\mathbf{Z} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Then the index localization function value is given by the following computation:

$$f_{\mathcal{L}}(Z, V) = \sum_{i=1}^{4} \mathfrak{I}_{\mathcal{L}i}(Z_i, V) = \mathfrak{I}_{\mathcal{L}1}(z^1) + \mathfrak{I}_{\mathcal{L}2}(z^6) + \mathfrak{I}_{\mathcal{L}3}(z^8) + \mathfrak{I}_{\mathcal{L}4}(o)$$

Thus, the number of patients covered for each zone is:

$$\mathcal{I}_{\mathcal{L}1}(\mathbf{z}^{1}) = v_{11} \qquad \mathbf{V} = \begin{bmatrix} \mathbf{S} & \mathbf{15} & \mathbf{0} & \mathbf{5} \\ \mathbf{15} & \mathbf{10} & \mathbf{5} & \mathbf{5} \\ \mathbf{2} & \mathbf{4} & \mathbf{20} & \mathbf{4} \\ \mathbf{3} & \mathbf{0} & \mathbf{2} & \mathbf{5} \end{bmatrix} \\ = \mathbf{5}$$

$$J_{\mathcal{L}2}(\mathbf{z}^6) = v_{22} + v_{23} + v_{32} + v_{33} \qquad \mathbf{V} = \begin{bmatrix} 5 & 15 & 0 & 5 \\ 15 & 0 & (5) & 5 \\ 2 & (4) & (2) & 4 \\ 3 & 0 & 2 & 5 \end{bmatrix}$$
$$= 10 + 5 + 4 + 20 = \mathbf{39}$$

$$\mathcal{I}_{\mathcal{L}3}(\mathbf{z}^8) = \mathbf{v}_{44} \qquad \mathbf{V} = \begin{bmatrix} 5 & 15 & 0 & 5\\ 15 & 10 & 5 & 5\\ 2 & 4 & 20 & 4\\ 3 & 0 & 2 & 5 \end{bmatrix}$$
$$= \mathbf{5}$$

 $\mathbb{I}_{\mathcal{L}\,4}(o)=0$ 

$$f_{\mathcal{L}}(Z, 3; V) = 5 + 39 + 5 = 49$$

What kind of function  $\mathcal{I}_{\mathcal{L}i}(Z_i, V)$  is ? Let's play with Matrix Algebra !

$$J_{\mathcal{L}2}(\mathbf{z}^{6}) = (\mathbf{z}^{6})' \cdot \mathbf{V} \cdot (\mathbf{z}^{6})$$

$$= \begin{bmatrix} 0 & \mathbf{1} & \mathbf{1} & 0 \end{bmatrix} \cdot \begin{bmatrix} 5 & 15 & 0 & 5 \\ 15 & \mathbf{0} & \mathbf{5} & 5 \\ 2 & \mathbf{4} & \mathbf{20} & 4 \\ 3 & 0 & 2 & 5 \end{bmatrix} \cdot \begin{bmatrix} 0 \\ \mathbf{1} \\ \mathbf{1} \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} 17 & \mathbf{14} & \mathbf{25} & 9 \end{bmatrix} \cdot \begin{bmatrix} 0 \\ \mathbf{1} \\ \mathbf{1} \\ 0 \end{bmatrix}$$

$$= 14 + 25 = 39$$

This is a familiar *quadratic form*:

**Definition.** Given a symmetric square matrix **O** (N by N) and a vector  $\mathbf{z} \in \mathbb{R}^{N}$  ( $\{\mathbf{z}^{N} \subset \mathbb{R}^{N}\}$ ), the expression  $\mathbf{z}' \cdot \mathbf{O} \cdot \mathbf{z}$  identifies a quadratic form over  $\mathbb{R}^{N}$ .

$$\mathbf{O} = \begin{bmatrix} o_{11} & o_{12} & \dots & o_{1N} \\ o_{21} & o_{22} & \dots & o_{2N} \\ \dots & \dots & \dots & \dots \\ o_{N1} & o_{N2} & \dots & o_{NN} \end{bmatrix}; \qquad \mathbf{z} = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_N \end{bmatrix}$$

The expression  $\mathbf{z}' \cdot \mathbf{O} \cdot \mathbf{z}$ :

$$\begin{bmatrix} z_1 & z_2 & \dots & z_N \end{bmatrix} \cdot \begin{bmatrix} o_{11} & o_{12} & \dots & o_{1N} \\ o_{21} & o_{22} & \dots & o_{2N} \\ \dots & \dots & \dots & \dots \\ o_{N1} & o_{N2} & \dots & o_{NN} \end{bmatrix} \cdot \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_N \end{bmatrix}$$

Computing all the cross products:

$$\mathbf{z}' \cdot \mathbf{O} \cdot \mathbf{z} = o_{11}z_1^2 + o_{12}z_1z_2 + o_{13}z_1z_3 + \dots + o_{1N}z_1z_N + o_{21}z_2z_1 + o_{22}z_2^2 + o_{23}z_2z_3 + \dots + o_{2N}z_2z_N + o_{N1}z_Nz_1 + o_{N2}z_Nz_2 + o_{N3}z_Nz_3 + \dots + o_{NN}z_N^2$$

Therefore an **n-ary quadratic form** over a field  $\mathbb{K}$  is a homogeneous polynomial (the non-zero terms all have the same degree) of degree 2 in N variables with coefficient in  $\mathbb{K}$ .

$$q(z_1, z_2, \dots, z_N; \mathbf{O}) = \sum_{i=1}^{N} \sum_{j=1}^{N} o_{ij} z_i z_j \qquad o_{ij} \in \mathbb{K}$$

It is worth noting that the matrix V is generally asymmetric, however it does not matter as we can always make this matrix symmetric:

$$\sum_{i=1}^{N} \sum_{j=1}^{N} o_{ij} z_i z_j = \sum_{i=1}^{N} o_{ii} z_i^2 + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (o_{ij} + o_{ji}) z_i z_j$$

If we replace  $o_{ij}$  and  $o_{ji}$  by  $\frac{o_{ij}+o_{ji}}{2}$  we obtain the same homogeneous polynomial:

$$\hat{o}_{ij} = \hat{o}_{ji} = \frac{o_{ij} + o_{ji}}{2} \quad o_{ij} \in \mathbb{K}$$
$$\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (o_{ij} + o_{ji}) z_i z_j = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (\hat{o}_{ij} + \hat{o}_{ji}) z_i z_j$$

Thus, the Index Localization function is a linear combination of quadratic forms:

$$f_{\mathcal{L}}(Z,V) = \sum_{i=1}^{N} \mathfrak{I}_{\mathcal{L}\,i}(Z_i,V) = \sum_{i=1}^{N} q(Z_i,V) \qquad Z \in \Pi$$

Clearly  $\mathcal{I}_{\mathcal{L}i}(Z_i, V) \ge 0$  as:

$$\sum_{i=1}^{N}\sum_{j=1}^{N}o_{ij}z_{i}z_{j} \ge 0 \qquad o_{ij}, z_{i}, z_{j} \ge 0.$$

#### 34 INTRODUCTION

Although the eigenvalues of the matrix **O** can give us precious information about the network flow, their computation is sometime cumbersome and have some numerical issues. Therefore, an equivalent measure to capture the patients' mobility is given by the statistical indicators mentioned earlier. These indicators have a clear meaning and can be used by anybody.

In order to analyse the energy landscape of the objective function, the problem should be instance independent. Hence, the matrix **V** has to be normalized:

	.05	.15		.05
0 –	.15	.1	.05	.05
0 –	.02	.04	.02	.04
	.03		.02	.05

The table 10 shows the Index Localization function values for all the partitions over  $(\Omega, 4)$ . As can be seen from the table, the maximum and minimum values of the function correspond to the partition  $\Pi_{\sigma_{4,1}^1}$  and  $\Pi_{\sigma_{4,1}^4}$  respectively. Moreover, the function  $f_{\mathcal{L}}(k; Z, V)$  is a monotone decreasing function of the number of zones. We should not be surprised, as the Universal set covers all the study area whereas the latter one (the singletons set) only catches the *non-mover* patients in the basic spatial units. It's now clear why we refer to these basic partitions as trivial solutions. However, in order to give a formal proof of these results, it is crucial to define a partition in terms of the classification matrix Z.

The next steps in our analysis of  $f_{\mathcal{L}}(Z, V)$  are:

- 1. The definition of the **Partitioning constraints**  $g_{\mathcal{P}}$
- 2. The computation of a Lower and Upper Bound; and
- The proof that f<sub>L</sub>(k; Z, V) is a monotone decreasing function; and
- 4. A possible relation between the eigenvalues of the matrix **O** and the **statistical indicators**.

Let's start with the **Partitioning constraints**:

We based the definition of a partition on two basic subsets of the solution space:

$$\Pi^{\Omega} = \Pi \bigcap \Upsilon \quad \Pi, \Upsilon \subset \mathfrak{X}$$

k	$\Pi(\sigma_4^k)$	Z	$f_{\mathcal{L}}(\boldsymbol{Z}_1)$	$f_{\mathcal{L}}(Z_2)$	$f_{\mathcal{L}}(\boldsymbol{Z}_3)$	$f_{\mathcal{L}}(Z_4)$	$f_{\mathcal{L}}(\boldsymbol{Z})$
1	$\Pi_{\sigma^1_{4,1}}$	$[\mathbf{z^{15}}]$	1				1
		$Max f_{\mathcal{L}}(Z;V,1)$	$= f_{\mathcal{L}}(\Pi_{\sigma^1_{4,1}})$				1
2	$\Pi_{\sigma_{4,1}^2}$	[ <b>z</b> <sup>8</sup> , <b>z</b> <sup>7</sup> ]	.76	.05	•	•	.81
	$\Pi_{\sigma_{4,2}^2}$	[ <b>z<sup>11</sup></b> , <b>z</b> <sup>4</sup> ]	.63	.2	•	•	.83
	$\Pi_{\sigma_{4,3}^2}$	$[z^3, z^{12}]$	.45	.31			.76
	$\Pi_{\sigma_{4,4}^2}$	$[z^{13}, z^2]$	.46	.1		•	.56
	$\Pi_{\sigma_{4.5}^2}$	$[z^5, z^{10}]$	.27	.2			.47
	$\Pi_{\sigma_{46}^2}$	$[z^{6}, z^{9}]$	.18	.39			.57
	$\Pi_{\sigma_{4,7}^2}$	$[\mathbf{z^1}, \mathbf{z^{14}}]$	.05	.55			.6
	,	$Max f_{\mathcal{L}}(Z;V,2)$	$= f_{\mathcal{L}}(\Pi_{\sigma_{4,2}^2})$				.83
3	$\Pi_{\sigma_{4,1}^3}$	$[z^3, z^4, z^8]$	.45	.2	.05	•	·7
	$\Pi_{\sigma_{4,2}^3}$	$[z^5, z^2, z^8]$	.27	.1	.05	•	.42
	$\Pi_{\sigma_{4,3}^3}$	$[z^1, z^6, z^8]$	.05	.39	.05	•	.49
	$\Pi_{\sigma_{4,4}^3}$	$[z^9, z^2, z^4]$	.18	.1	.2	•	.48
	$\Pi_{\sigma_{4.5}^3}$	$[z^1, z^{10}, z^4]$	.05	.2	.2	•	.45
	$\Pi_{\sigma_{4.6}^3}$	$[z^1, z^2, z^{12}]$	.05	.1	.13	•	.28
		$Max f_{\mathcal{L}}(Z;V,3)$	$= f_{\mathcal{L}}(\Pi_{\sigma^3_{4,1}})$				.7
4	$\Pi_{\sigma_{4,1}^4}$	$[z^1, z^2, z^4, z^8]$	.05	.1	.2	.05	.4
		$Maxf_{\mathcal{L}}(Z;V,4)$	$= f_{\mathcal{L}}(\Pi_{\sigma_{4,1}^4})$				.4

Table 10: Localization Index energy landscape  $|\Omega| = 4$ 

Therefore, the partitioning constraints can be expressed in terms of two set of constraints:

$$g_{\mathcal{P}} = g_{\Pi} \bigcap g_{\Upsilon}$$
$$g_{\Pi}: \quad \text{bin} - \text{packing} - \text{constraints.}$$
$$g_{\Upsilon}: \quad \text{set} - \text{covering} - \text{constraints.}$$

What kind of constraints the classification matrix Z should satisfy in order to identify:

- $\Pi$ : All the possible combination of disjoint subsets of  $\mathcal{P}(\Omega^+)$
- $\Upsilon$ : All the possible covering of the universal set  $\Omega$

**Theorem.** Let  $\Pi$  be the set of all the possible combination of disjoint subsets of  $\mathcal{P}(\Omega^+)$  and  $Z \in \{0,1\}^N x\{0,1\}^N$ . Then  $\Pi = \{z_{ij} \in Z : \sum_{j=1}^N z_{ij} \leq$  $1, \forall i = 1, \dots, N\}.$ 

*Proof.* Let  $\mathcal{F}^{k}_{\mathcal{P}(\Omega^{+})} \in \mathfrak{X}$  a generic solution composed by k subsets of  $\mathcal{P}(\Omega^+)$ . Let  $Z^s$  and  $Z^t \in \mathcal{P}(\Omega^+)$  such that  $s \neq t \in \mathfrak{i} = \{1, \ldots, |\mathcal{P}(\Omega^+)|\}$ . Then  $\mathfrak{F}^{k}_{\mathfrak{P}(\Omega^{+})} \in \Pi \subset \mathfrak{X} \Leftrightarrow \mathsf{Z}^{s} \bigcap \mathsf{Z}^{t} = \{\emptyset\} \quad \forall \mathsf{Z}^{s}, \mathsf{Z}^{t} \in \mathfrak{F}^{k}_{\mathfrak{P}(\Omega^{+})} : k \geqslant 2$  $Z^{s} \bigcap Z^{t} = \{\emptyset\} \Leftrightarrow \omega_{i} \notin Z^{t} \quad \forall \omega_{i} \in Z^{s} : \omega_{i} \in \Omega, i = 1, \dots, N.$ Let  $z_i^j = \begin{cases} 1, & \text{if}\omega_i \in Z^j \\ 0, & \text{if}\omega_i \notin Z^j \end{cases}$  $\omega_{i} \notin Z^{t} \Leftrightarrow z_{i}^{t} = 0$  $\omega_i \in Z^s \Leftrightarrow z_i^s = 1$  $Z^{s} \bigcap Z^{t} = \{\emptyset\} \Leftrightarrow z^{s}_{i} \land z^{t}_{i} = 0 \Rightarrow (z^{s})' \cdot z^{t} = 0$  $\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} z_{si} z_{sj} = 0 \quad z_{si}, z_{sj} \in Z \quad \forall s = 1, \dots, N$ We would like to use a more compact formulation in terms of linear inequalities. How can we formulate a disjunctive constraint in term of linear inequality?  $z^{s}_{i} \wedge z^{t}_{i} = \mathbf{0} \Leftrightarrow z^{s}_{i} \leqslant \mathbf{1} - z^{t}_{i} \Rightarrow z^{s}_{i} + z^{t}_{i} \leqslant \mathbf{1} \Rightarrow \mathbf{z}^{s} + \mathbf{z}^{t} \leqslant \mathbf{1}$  $\begin{aligned} \mathbf{z}_{i}^{s} & \wedge \mathbf{z}_{i}^{t} = \mathbf{0} \Leftrightarrow \mathbf{z}_{i}^{s} \leqslant \mathbf{1} = \mathbf{z}_{i}^{s} \Rightarrow \mathbf{z}_{i}^{t} + \mathbf{z}_{i}^{s} \leqslant \mathbf{1} \Rightarrow \mathbf{z}^{s} + \mathbf{z}^{s} \\ \mathbf{z}_{s}^{s} + \mathbf{z}^{t} \leqslant \mathbf{1} \quad \forall s \neq t : \mathbf{z}^{s}, \mathbf{z}^{t} \in \mathbf{Z} \\ \sum_{s=1}^{N-1} \sum_{t=s+1}^{N} \mathbf{z}^{s} + \mathbf{z}^{t} \leqslant \mathbf{N} \\ (N-1) \sum_{i=1}^{N} \mathbf{z}_{i}^{i} \leqslant \mathbf{N} \\ (N-1) \sum_{j=1}^{N} z_{ij} \leqslant \mathbf{N} \quad \forall i = 1, \dots, \mathbf{N} : z_{ij} \in \mathbf{Z} \\ (N-1) \sum_{j=1}^{N} z_{ij} \leqslant \mathbf{N} \Leftrightarrow \sum_{j=1}^{N} z_{ij} = \mathbf{0} \lor \sum_{j=1}^{N} z_{ij} = \mathbf{1} \end{aligned}$ 

 $\sum_{i=1}^{N} z_{ij} \leq 1 \quad \forall i = 1, \dots, N \quad z_{ij}$ 

**Theorem.** Let  $\Upsilon$  be the set of all the possible covering of the Universal set  $\Omega \text{ and } Z \in \{0,1\}^N x\{0,1\}^N. \text{Then } \Upsilon = \{z_{ij} \in Z : \sum_{j=1}^N z_{ij} \ge 1, \forall i = 1\}$  $1, \ldots, N$ .

*Proof.* Let  $\mathcal{F}^{k}_{\mathcal{P}(\Omega^{+})} \in \mathcal{X}$  a generic solution composed by k subsets of  $\mathcal{P}(\Omega^+)$  i.e  $\mathcal{F}^k_{\mathcal{P}(\Omega^+)} = \{Z^1, \dots, Z^k\}.$  $\mathcal{F}^{k}_{\mathcal{P}(\Omega^{+})} \in \Upsilon \subset \mathfrak{X} \Leftrightarrow \bigcup_{i=1}^{k} Z^{j} = \Omega \Rightarrow \omega_{i} \in \bigcup_{i=1}^{k} Z^{j} \quad \forall i = 1, \dots, N$  $\omega_i \in \bigcup_{i=1}^k Z^j \Leftrightarrow |\bigcup_{i=1}^k Z^j| = N$ Let  $Z^s$  and  $Z^t \in \mathcal{P}(\Omega^+)$  such that  $s \neq t \in \{1, \dots, |\mathcal{P}(\Omega^+)|\}$  Then  $\omega_i \in Z^s \bigcup Z^t \Leftrightarrow \omega_i \in Z^s \vee \omega_i \in Z^t$  $\omega_{\mathfrak{i}} \in \mathsf{Z}^{s} \Rightarrow z_{\mathfrak{i}}^{s} = 1 \lor \omega_{\mathfrak{i}} \in \mathsf{Z}^{t} \Rightarrow z_{\mathfrak{i}}^{t} = 1$  $\omega_i \in Z^s \bigcup Z^t \Leftrightarrow z_i^s \lor z_i^t = 1$  $z_{i}^{s} \lor z_{i}^{t} = 1 \Leftrightarrow (z_{i}^{s} + z_{i}^{t}) - (z_{i}^{s} \cdot z_{i}^{t}) = 1$  $Z^{s} \bigcup Z^{t} = \{z_{i}^{s} + z_{i}^{t} - z_{i}^{s} \cdot z_{i}^{t} : z_{i}^{s} \in Z^{s}, z_{i}^{t} \in Z^{t}; i = 1, ..., N\}$  $|Z^{s}| = f_{c}(Z^{s}) = \sum_{i=1}^{N} z_{i}^{s}$  $|\mathsf{Z}^{s} \bigcap \mathsf{Z}^{t}| = \mathsf{f}_{c}^{\bigcap}(\mathsf{Z}^{s},\mathsf{Z}^{t}) = \sum_{i=1}^{N} z_{i}^{s} \cdot z_{i}^{t}$  $|\bigcap_{j=1}^{N} Z^{j}| = f_{c}(\bigcap_{j=1}^{N} Z^{j}) = f_{c}^{\cap}(Z^{1}, Z^{2}, \dots, Z^{N}) = \sum_{i=1}^{N} \prod_{j=1}^{N} z_{ij}$  $Z^{s} \bigcup Z^{t} | = f_{c}^{\bigcup}(Z^{s}, Z^{t}) = \sum_{i=1}^{N} z_{i}^{s} + \sum_{i=1}^{N} z_{i}^{t} - \sum_{i=1}^{N} z_{i}^{s} \cdot z_{i}^{t}$  $= |\mathbf{z}^{s}| + |\mathbf{z}^{t}| - (\mathbf{z}^{s})'\mathbf{z}^{t}$ 

$$\begin{split} &= |Z^{s}| + |Z^{t}| - |Z^{s} \bigcap Z^{t}| \\ \text{Therefore according to the Inclusion-Exclusion Principle:} \\ &|\bigcup_{j=1}^{N} Z^{j}| = f_{c}(\bigcup_{j=1}^{N} Z^{j}) = f_{c}(Z^{1}, Z^{2}, \dots, Z^{N}) \\ &= \sum_{i=1}^{N} f_{c}(z^{i}) - \sum_{1 \leqslant i < j \leqslant N} f_{c}(Z^{i} \bigcap Z^{j}) + \sum_{1 \leqslant i < j < k \leqslant N} f_{c}(Z^{i} \bigcap Z^{j} \bigcap Z^{k}) + \\ &\cdots + (-1)^{N-1} f_{c}(\bigcap_{j=1}^{N} Z^{j}) = 1 \\ &= \sum_{j=1}^{N} z_{ij} + \sum_{j=1}^{N-1} \sum_{k=j+1}^{N} z_{ij} z_{ik} - \sum_{j=1}^{N-2} \sum_{k=j+2}^{N} z_{ij} z_{ij+1} z_{ik} + \\ &+ \sum_{j=1}^{N-3} \sum_{k=j+3}^{N} z_{ij} z_{ij+1} z_{ij+2} z_{ik} - \sum_{j=1}^{N-4} \sum_{k=j+4}^{N} z_{ij} z_{ij+1} z_{ij+2} z_{ij+3} z_{ik} + \\ &\cdots + (-1)^{N-1} \prod_{j=1}^{N} z_{ij} = 1 \quad \forall i = 1, \dots, N \\ &= \sum_{j=1}^{N} z_{ij} - \sum_{s=1}^{N-1} (-1)^{S-1} \sum_{j=1}^{N-S} \sum_{k=j+S}^{N} \widehat{z_{ij} z_{ij+1} \dots z_{ik}} = 1 \quad i = 1, \dots, N \\ &= \sum_{j=1}^{N} z_{ij} - \sum_{s=1}^{N-1} (-1)^{S-1} \sum_{j=1}^{N-S} \sum_{k=j+S}^{N} \widehat{z_{ij} z_{ij+1} \dots z_{ik}} \neq 1 \quad \Leftrightarrow \\ &\sum_{j=1}^{N} z_{ij} = 0 \\ &\sum_{j=1}^{N} z_{ij} \geqslant 1 \quad \forall i = 1, \dots, N \end{split}$$

**Lemma.** Let  $\Pi^{\Omega}$  be the set of all the partition of  $\mathcal{P}(\Omega^+)$  and  $Z \in \{0, 1\}^N x\{0, 1\}^N$  then  $\Pi^{\Omega} = \{z_{ij} \in Z : \sum_{j=1}^N z_{ij} = 1, \forall i = 1, \dots, N\}$ 

*Proof.* Let  $g_{\Pi}$  be the constraints of all the possible combination of disjoint subsets of  $\mathcal{P}(\Omega^+)$  and  $g_{\Upsilon}$  the constraint regarding all the possible covering of the Universal set. Then:

$$g_{\mathcal{P}} = g_{\Pi} \bigcap g_{\Upsilon} = \begin{cases} \sum_{j=1}^{N} z_{ij} \leq 1\\ \sum_{j=1}^{N} z_{ij} \geq 1 \end{cases} \Rightarrow \sum_{j=1}^{N} z_{ij} = 1 \quad \forall i = 1, \dots, N. \end{cases}$$

Now we can move on to the computation of a **Lower and Upper Bound** for the Index Localization function.

**Theorem.** Let  $f_{\mathcal{L}}(Z; O)$  be the Index Localization function and  $y_{\mathcal{L}}^{LB} \in \mathbb{R}$  the corresponding Lower Bound Value. (i.e  $f_{\mathcal{L}}(Z; O) \ge y_{\mathcal{L}}^{LB} \forall Z \in \Pi^{\Omega}$ ). Then  $y_{\mathcal{L}}^{LB} = \sum_{i=1}^{N} o_{ii}$  such that  $o_{ii} \in \begin{bmatrix} 0 & 1 \end{bmatrix}$ .

*Proof.* Let  $f_{\mathcal{L}}(Z; O) = q(z_1, z_2, ..., z_N; O)$  be the quadratic form of the Index Localization function. Then

$$\begin{cases} f_{\mathcal{L}}(Z;O) = \sum_{k=1}^{N} q(Z^{k};O) \\ q(Z^{k};O) = \sum_{i=1}^{N} o_{ii} z_{ik}^{2} + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (o_{ij} + o_{ji}) z_{ik} z_{jk} \\ g_{\Pi^{\Omega}} = \sum_{k=1}^{N} z_{ik} = 1 \quad \forall i = 1, \dots, N \quad z_{ik} \in \{0, 1\} \end{cases}$$

We can replace the quadratic terms  $(z_{ij})^2 = z_{ij}$ . Therefore, according to the system of linear equations, it is clear that:

$$\sum_{k=1}^{N} \sum_{i=1}^{N} o_{ii} z_{ik}^{2} = \sum_{k=1}^{N} \sum_{i=1}^{N} o_{ii} z_{ik} = \sum_{i=1}^{N} \sum_{k=1}^{N} o_{ii} z_{ik}$$

$$\sum_{i=1}^{N} \sum_{k=1}^{N} o_{ii} z_{ik} = o_{11} \sum_{k=1}^{N} z_{1k} + o_{22} \sum_{k=1}^{N} z_{2k} + \dots + o_{ii} \sum_{k=1}^{N} z_{ik} +$$

$$\begin{array}{l} & \overbrace{\sum_{k=1}^{N} z_{Nk}}^{N} \\ \sum_{k=1}^{N} z_{ik} = 1 \quad \forall i = 1, \dots, N \\ \text{In other words the first term of the objective function it is a constant.} \\ & \sum_{i=1}^{N} \sum_{k=1}^{N} o_{ii} z_{ik} = \sum_{i=1}^{N} o_{ii} = y_{\mathcal{L}}^{LB} \\ & f_{\mathcal{L}}(Z; O) = y_{\mathcal{L}}^{LB} + \sum_{k=1}^{N} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (o_{ij} + o_{ji}) z_{ik} z_{jk} \\ & \Box \end{array}$$

**Lemma.** Let  $\Pi_{\sigma_{N,1}^N}$  the singleton set partition. (i.e  $\Pi_{\sigma_{N,1}^N} = \{z_{ij} = 1 \Leftrightarrow i = j : z_{ij} \in Z \quad i, j = 1, ..., N\}$ ) and  $\pi_{\sigma_{N,1}^N}$ , the corresponding real value solution. Then  $f_{\mathcal{L}}(\Pi_{\sigma_{N,1}^N}) = \pi_{\sigma_{N,1}^N} = y_{\mathcal{L}}^{LB}$ 

*Proof.* Let  $Z^k = \{z_{ik} \in Z : i = 1, ..., N\}$  and  $Z(\Pi_{\sigma_{N,1}^N})$  the classification matrix associated to the singleton partition.

$$\begin{split} & Z(\Pi_{\sigma_{N,1}^{N}}) = I \\ & z_{ik} = z_{jk} = 0 \quad \forall Z^{k} \in Z(\Pi_{\sigma_{N,1}^{N}}) \quad \forall k = 1, \dots, N \\ & \text{It follows that:} \\ & f_{\mathcal{L}(\Pi_{\sigma_{n,1}^{N}}; O)} = f_{\mathcal{L}(Z(\Pi_{\sigma_{n,1}^{N}}); O)} = y_{\mathcal{L}}^{LB} \end{split}$$

**Theorem.** Let  $f_{\mathcal{L}}(Z; O)$  be the Index Localization function and  $y_{\mathcal{L}}^{UB} \in \mathbb{R}$  the corresponding Upper Bound value. (i.ef\_{\mathcal{L}}(Z; O) \leq y\_{\mathcal{L}}^{UB} \quad \forall Z \in \Pi^{\Omega}). Then  $y_{\mathcal{L}}^{UB} = 1$ .

Proof. 
$$f_{\mathcal{L}}(Z; O) = y_{\mathcal{L}}^{UB} + \sum_{k=1}^{N} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (o_{ij} + o_{ji}) z_{ik} z_{jk}$$
  
If  $z_{is} z_{js} = 1 \rightarrow z_{is} = z_{js} = 1 \rightarrow z_{ik} = z_{jk} = 0 \rightarrow z_{ik} z_{jk} = 0$   
 $\forall k \neq s \in \{1, \dots, N\}, i < j$ 

Therefore the second term of the objective function is bounded:  $\sum_{k=1}^{N}\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}(o_{ij}+o_{ji})z_{ik}z_{jk} =$ 

$$= (o_{12} + o_{21}) \sum_{k=1}^{N} z_{1k} z_{2k} + (o_{13} + o_{31}) \sum_{k=1}^{N} z_{1k} z_{3k} +$$

 $+\dots + (o_{N-1,N} + o_{N,N-1}) \sum_{k=1}^{N} z_{N-1,k} z_{Nk} \leq \sum_{i=1}^{N} \sum_{j=i+1}^{N} (o_{ij} + o_{ji})$ It follows that:

 $f_{\mathcal{L}}(Z; O) = y_{\mathcal{L}}^{UB} + \sum_{k=1}^{N} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (o_{ij} + o_{ji}) z_{ik} z_{jk} \leqslant \sum_{i=1}^{N} o_{ii} + \sum_{i=1}^{N} \sum_{j=i+1}^{N} (o_{ij} + o_{ji}) = \sum_{i=1}^{N} \sum_{j=1}^{N} o_{ij} = 1$ 

**Lemma.** Let  $\Pi_{\sigma_{N,1}^1}$  be the Universal set partition (i.e $\Pi_{\sigma_{N,1}^1} = \{z_{ij} = 1 \Leftrightarrow j = 1 : z_{ij} \in Z \quad i, j = 1, \dots, N\}$ ) and  $\pi_{\sigma_{N,1}^1}$  the corresponding real value solution. Then  $f_{\mathcal{L}}(\Pi_{\sigma_{N,1}^1}) = \pi_{\sigma_{N,1}^1} = y_{\mathcal{L}}^{UB}$ .

*Proof.* Let  $Z^k = \{z_{ik} \in Z : i = 1, ..., N\}$  and  $Z(\Pi_{\sigma_{N,1}^1})$  the classification matrix associated to the Universal set partition.  $Z(\Pi_{\sigma_{N,1}^1}) = (\mathbf{1} \quad \emptyset)$ 

$$\begin{split} &\sum_{k=1}^{N} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (o_{ij} + o_{ji}) z_{ik} z_{jk} = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (o_{ij} + o_{ji}) z_{i1} z_{j1} \\ &= \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (o_{ij} + o_{ji}) \\ \text{Then:} \\ &f_{\mathcal{L}}(\Pi_{\sigma_{N,1}^{1}}; O) = f_{\mathcal{L}}(Z(\Pi_{\sigma_{N,1}^{1}}); O) = y_{\mathcal{L}}^{LB} + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (o_{ij} + o_{ji}) = \\ &y_{\mathcal{L}}^{UB} = 1. \end{split}$$

The computation of a Lower and Upper Bound for the Index Localization function is crucial in the analysis of it's energy landscape. In particular, we prove an important result regarding the 'shape' of the function  $f_{\mathcal{L}}(k; Z, O)$ ; Specifically we show that this function is **monotone decreasing**.

As already mentioned, a solution is a partition of the study area  $\Omega = \{\omega_1, \ldots, \omega_N\}$  into k parts(or zones) made up by one or more basic spatial units. Therefore a partition can be defined formally as a sequence of non negative integers  $n_1 \ge n_2 \ge \cdots \ge n_k \ge 0$  such that  $N = n_1 + n_2 + \cdots + n_k$ . The number of non zero terms is called the cardinality of the zone  $Z^s$  (i.e  $|Z^s| = f_c(Z^s) = \sum_{i=1}^N z_{is} \quad z_{is} \in Z$ ). Clearly there is a mapping between the number of the basic spatial units of a zone and the elements of the Origin-destination matrix.

**Theorem.** Let  $E_k = \{o_{ij} \in Z^k : \omega_i, \omega_j \in Z^k\}$  be the set of elements in the Origin-destination matrix associated to the zone  $Z^k$  and  $n_k = |Z^k|$  the number of basic spatial units inside the zone. Then  $|E_k| = n_k^2$ 

$$\begin{array}{l} \textit{Proof. If } \omega_{i}, \omega_{j} \in \mathsf{Z}^{k} \to \mathsf{E}_{k} = \{ \mathsf{o}_{ii}, \mathsf{o}_{jj}, \mathsf{o}_{ij}, \mathsf{o}_{ji} \} \\ |\mathsf{Z}^{k}| = 2 \text{ and } |\mathsf{E}_{k}| = \mathsf{n}_{k} + 2. \\ \text{It follows that:} \\ |\mathsf{E}_{k}| = 2\binom{\mathsf{n}_{k}}{2} + \mathsf{n}_{k} = 2\frac{\mathsf{n}_{k}!}{(\mathsf{n}_{k}-2)!2!} + \mathsf{n}_{k} \\ \frac{\mathsf{n}_{k}(\mathsf{n}_{k}-1)(\mathsf{n}_{k}-2)!}{(\mathsf{n}_{k}-2)!} + \mathsf{n}_{k} = \mathsf{n}_{k}^{2} - \mathsf{n}_{k} + \mathsf{n}_{k} = \mathsf{n}_{k}^{2} \end{array}$$

For instance, in the case of the trivial solutions it is clear that the total number of elements in the Origin-destination matrix corresponding to the Universal set is N<sup>2</sup> whereas for the singleton partition is N. Let  $\Pi_{\sigma_{N,1}^1}$  be the Universal set and  $E_{\Omega}$  the set of elements in the origin-destination matrix corresponding to  $Z(\Pi_{\sigma_{N,1}^1})$ . Then  $|E_{\Omega}| = N^2$ . Therefore, we have the following mapping:

$$|\mathsf{E}_{\Omega}| = |\mathsf{E}_{1}^{\Omega}| = \mathsf{N}^{2} \rightarrow \sum_{\mathfrak{i}=1}^{\mathsf{N}} \sum_{\mathfrak{j}=1}^{\mathsf{N}} \mathsf{o}_{\mathfrak{i}\mathfrak{j}} = f_{\mathcal{L}}(\Pi_{\sigma_{\mathsf{N},1}^{\mathfrak{l}}})$$

In other words, the Universal set catches all the patient-flow in the Origin-destination matrix. Conversely  $\Pi_{\sigma_{N,N}^1}$  covers the minimum number of elements (patients) in the origin-destination matrix.

$$|\mathsf{E}_{\mathcal{S}}| = \overbrace{|\mathsf{E}_{1}^{\mathcal{S}}|}^{I} + \overbrace{|\mathsf{E}_{2}^{\mathcal{S}}|}^{I} + \dots + \overbrace{|\mathsf{E}_{N}^{\mathcal{S}}|}^{I} = N \rightarrow \sum_{i=1}^{N} \mathsf{o}_{ii} = \mathsf{f}_{\mathcal{L}}(\Pi_{\sigma_{N,N}^{1}})$$

Therefore we have the following inequality:  $f_{\mathcal{L}}(1; Z^*, O) \ge f_{\mathcal{L}}(N; Z^*, O)$ . However, in order to prove that  $f_{\mathcal{L}}(k; Z^*, O)$  is a monotone decreasing function, we must check that  $f_{\mathcal{L}}(k; Z^*, O) \ge f_{\mathcal{L}}(k+1; Z^*, O)$  such that  $1 < k+1 \le N$ .

First of all we prove that  $|E_{\Omega}| > |E_{\Pi(\sigma_N^k)}|$ . In other words the number of elements in the Origin-destination matrix corresponding to the Universal set partition is always grater than any other partition in the solution space.

**Theorem.** Let  $E_{\Pi(\sigma_N^k)}$  be the set of elements in the origin-destination matrix corresponding to  $Z(\Pi_{\sigma_N^k})$ . Then  $|E_{\Omega}| > |E_{\Pi(\sigma_N^k)}| : 2 \le k \le N$ .

$$\begin{split} \textit{Proof.} \ & \mathsf{E}_{\Pi(\sigma_N^k)} = \mathsf{E}_1^{\Pi(\sigma_N^k)} \bigcup \mathsf{E}_2^{\Pi(\sigma_N^k)} \bigcup \cdots \bigcup \mathsf{E}_k^{\Pi(\sigma_N^k)} \\ & |\mathsf{E}_{\Pi(\sigma_N^k)}| = |\mathsf{E}_1^{\Pi(\sigma_N^k)}| + |\mathsf{E}_2^{\Pi(\sigma_N^k)}| + \cdots + |\mathsf{E}_k^{\Pi(\sigma_N^k)}| \\ & \text{We want to prove that:} \\ & |\mathsf{E}_{\Omega}| > |\mathsf{E}_1^{\Pi(\sigma_N^k)}| + |\mathsf{E}_2^{\Pi(\sigma_N^k)}| + \cdots + |\mathsf{E}_k^{\Pi(\sigma_N^k)}| \\ & \mathsf{N} \cdot \mathsf{N} > \mathsf{n}_1 \cdot \mathsf{n}_1 + \mathsf{n}_2 \cdot \mathsf{n}_2 + \cdots + \mathsf{n}_k \cdot \mathsf{n}_k. \end{split}$$

Recalling that a partition of the study area is basically a partition of an integer:

$$\begin{split} &N = n_1 + n_2 + \dots + n_i + \dots + n_k \quad n, n_i \in \mathbb{N}^+, i \in \{1, \dots, k\} \text{ such that } \\ &N \geqslant n_1 \geqslant n_2 \geqslant \dots \geqslant n_k. \text{ It follows that } N \cdot n_i > n_i \cdot n_i \forall k > 1, i \in \\ &1, \dots, k \\ &N \cdot \sum_{i=1}^k n_i = N \cdot n_1 + N \cdot n_2 + \dots + N \cdot n_i + \dots + N \cdot n_k = N \cdot N \\ &\sum_{i=1}^k n_i \cdot n_i = n_1 \cdot n_1 + n_2 \cdot n_2 + \dots + n_i \cdot n_i + \dots + n_k \cdot n_k \\ &\text{It is clear then:} \\ &N \cdot \sum_{i=1}^k n_i > \sum_{i=1}^k n_i \cdot n_i \\ &N \cdot N > \sum_{i=1}^k n_i \cdot n_i \end{split}$$

The previous proof is a consequence of the fact that the set partitions are essentially a partially ordered set (Poset) in which the elements are ordered by reverse refinement.

**Definition.** A partially ordered set  $(P, \leq)$  is a set P with an ordered relation  $\leq$  which has the following properties:

```
1. a \leq a \quad \forall a \in P

2. a \leq b \quad and \quad b \leq a \rightarrow a = b

3. a \leq b \quad and \quad b \leq c \rightarrow a \leq c
```

A number of methods can be used to describe a poset. One is to maintain a list of all pairs (a, b) with a < b (this means  $a \leq b$  and  $a \neq b$ ) we say that b covers a if a < b and there is no c satisfying a < c < b. We shall write a < b for b covers a. Because of property (3), we need only maintain a list of all pairs (a, b) with a < b. These are called the covering relations of P. For ease of use, if

there are more than one cover, we use the following compact notation  $\{(a, b), (a, c)\} = \rho(a, \leqslant) = \{b, c\}$ . We can visualize a poset as a graph with the 'largest' elements of P as vertices at the top, the 'smallest' at the bottom, and the other element of P distributed appropriately in between. An edge connects a and b if and only if a < b. Such a diagram is called a Hasse diagram. However, this kind of representation becomes difficult to visualize even for small values of N. Now that we are more familiar with the concept of partially ordered set, we can introduce the notion of Partition Lattice.

**Definition.** Partition Lattice:  $\mathcal{P}_{\Omega}$  is a poset in which the elements are ordered by reverse refinement. That is:

Given 
$$\Pi_{\sigma_{N,s}^{k}} = \{Z_{1}, \dots, Z_{k}\}$$
 and  $\Pi_{\sigma_{N,q}^{k+1}} = \{Z_{1}, \dots, Z_{k+1}\}$   
 $\Pi_{\sigma_{N,s}^{k}} < \Pi_{\sigma_{N,q}^{k+1}} \Leftrightarrow \exists p, m, t : Z_{p}^{s} = Z_{m}^{q} \bigcup Z_{t}^{q}$   
 $\exists i, j : Z_{i}^{s} = Z_{j}^{q} \quad \forall i \neq p, \quad j \neq \{m, t\}$   
 $i, p \in \{1, \dots, k\} \quad j, m, t \in \{1, \dots, k+1\}$ 

Thus the covering relations are obtained by splitting one block(zone) of  $\Pi_{\sigma_{N,s}^k}$  into two blocks of  $\Pi_{\sigma_{N,q}^{k+1}}$  with all of the other blocks of  $\Pi_{\sigma_{N,s}^k}$  and  $\Pi_{\sigma_{N,q}^{k+1}}$  identical.

For example the partition:

$$\Pi_{\sigma_{4,1}^2} = \{\{123\}, \{4\}\} = \begin{bmatrix} \mathbf{z}^7 & \mathbf{z}^8 \end{bmatrix}$$
$$\rho(\Pi_{\sigma_{4,1}^2}, \leqslant) = \{\Pi_{\sigma_{4,1}^3}, \Pi_{\sigma_{4,2}^3}, \Pi_{\sigma_{4,6}^3}\}$$
$$\Pi_{\sigma_{4,1}^3} = \{\{12\}, \{3\}, \{4\}\} = \begin{bmatrix} \mathbf{z}^3 & \mathbf{z}^4 & \mathbf{z}^8 \end{bmatrix} \quad \{123\} = \{12\} \cup \{3\}$$
$$\Pi_{\sigma_{4,2}^3} = \{\{13\}, \{2\}, \{4\}\} = \begin{bmatrix} \mathbf{z}^5 & \mathbf{z}^2 & \mathbf{z}^8 \end{bmatrix} \quad \{123\} = \{13\} \cup \{2\}$$
$$\Pi_{\sigma_{4,3}^3} = \{\{1\}, \{23\}, \{4\}\} = \begin{bmatrix} \mathbf{z}^1 & \mathbf{z}^6 & \mathbf{z}^8 \end{bmatrix} \quad \{123\} = \{1\} \cup \{23\}$$

It is worth noting that:

$$\begin{array}{l} ({\bf z}^3)\,'\cdot{\bf z}^4=0\to{\bf z}^7={\bf z}^3+{\bf z}^4\\ ({\bf z}^5)\,'\cdot{\bf z}^2=0\to{\bf z}^7={\bf z}^5+{\bf z}^2\\ ({\bf z}^1)\,'\cdot{\bf z}^6=0\to{\bf z}^7={\bf z}^1+{\bf z}^6 \end{array}$$

It is clear that:

$$\begin{split} \rho(\Pi_{\sigma_{N,i}^{1}},\leqslant) &= \{\Pi_{\sigma_{N,i}^{2}}\} \quad i = 1, \dots, \sigma_{N}^{2}\\ \rho(\Pi_{\sigma_{N,i}^{N-1}},\leqslant) &= \{\Pi_{\sigma_{N,i}^{N}}\} \quad i = 1, \dots, \sigma_{N}^{N-1} \end{split}$$

 $\begin{array}{l} \textbf{Theorem. Let } \Pi_{\sigma_{N,s}^k} < \Pi_{\sigma_{N,q}^{k+1}} \textit{ then } \\ f_{\mathcal{L}}(k; Z(\Pi_{\sigma_{N,s}^k}), O) > f_{\mathcal{L}}(k+1; Z(\Pi_{\sigma_{N,q}^{k+1}}), O) \\ s \in \{1, \ldots, k\} \textit{ and } q \in \{1, \ldots, k+1\} \end{array}$ 

*Proof.* if  $\Pi_{\sigma_{N,s}^k} < \Pi_{\sigma_{N,q}^{k+1}}$  then (i)  $\exists p, m, t: Z_p^s \stackrel{\text{ind}}{=} Z_m^q \cup Z_t^q \quad Z_m^q \cap Z_t^q = \emptyset \quad Z_m^q, Z_t^q \neq \emptyset$ (ii) i, j:  $Z_i^s = Z_i^q$   $\forall i \neq p, j \neq \{m, t\}$ Let  $Z^s = \{Z_1, ..., Z_p, ..., Z_k\}$  and  $Z^q = \{Z_1, ..., Z_m, ..., Z_t, ..., Z_{k+1}\}$ the classification matrices of  $\Pi_{\sigma_{N_s}^k}$  and  $\Pi_{\sigma_{N_a}^{k+1}}$  respectively. i.e  $Z(\Pi_{\sigma_{N_s}^k}) =$  $Z^{s}$  and  $Z(\Pi_{\sigma_{N,q}^{k+1}}) = Z^{q}$ . Then according to condition (i):  $z_i^p = z_i^m + z_i^{\text{ind}} z_i^p \in Z_p, z_i^m \in Z_m, z_i^t \in Z_t \quad \forall i = \{1, \dots, N\}$ Let  $E_p^s = \{o_{ij} \in Z_p^s : \omega_i, \omega_j \in Z_p^s\}$  be the set of elements in the origindestination matrix associated to the zone  $Z_p^s$  and  $n_p^s$  =  $|Z^p|.$  Then  $|E_p^s| = n_s^2$ . Similarly  $n_m^q = |Z^m|$  and  $n_t^q = |Z^t|, |E_m^q| = n_{m'}^2 |E_t^q| = n_t^2$ . Then  $n_p^s = n_m^q + n_t^q$  such that  $n_p^s > n_m^q \ge n_t^q$ As proved for the Universal set  $|E_{\Omega}|$  we have  $|E_{p}^{s}| > |E_{m}^{q}| + |E_{t}^{q}| \rightarrow$  $n_s^2 > n_m^2 + n_t^2$  So we are going to prove that:  $f_{\mathcal{L}}(Z_{p}^{s}, O) \ge f_{\mathcal{L}}(Z_{m}^{q}, O) + f_{\mathcal{L}}(Z_{t}^{q}, O)$ In order to verify this inequality we need to prove that:  $\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (o_{ij} + o_{ji}) z_i^p z_j^p \ge \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (o_{ij} + o_{ji}) z_i^m z_j^m + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (o_{ij} + o_{ji}) z_i^t z_j^t$ if  $z_i^p = 1 \rightarrow z_i^m + z_i^t = 1 \leftrightarrow z_i^m \lor z_i^t = 1$ and  $z_j^p = 1 \rightarrow z_j^m + z_j^t = 1 \leftrightarrow z_j^m \lor z_j^t = 1$ According to the following equation:  $n_p^s = n_m^q + n_t^q$  than  $\sum_{i=1}^{N} z_i^p > \sum_{i=1}^{N} z_i^m \rightarrow \exists i : z_i^p = 1 \text{ and } z_i^m = 0$  $\forall j \neq i : z_i^m = 1 \text{ and } z_i^p = 1 \rightarrow z_i^p z_i^p = 1, z_i^m z_i^m = z_i^t z_i^t = 0$  $f_{\mathcal{L}}(Z_p^s, O) \ge f_{\mathcal{L}}(Z_m^q) + f_{\mathcal{L}}(Z_t^q)$ It is worth noting that:  $f_{\mathcal{L}}(Z_p^s, O) = f_{\mathcal{L}}(Z_m^q) + f_{\mathcal{L}}(Z_t^q) \quad \text{if} o_{ii} = o_{ii} = 0$ Clearly for property (ii):  $\sum_{i=1}^{k} f_{\mathcal{L}}(Z_{i}^{s}) = \sum_{j=1}^{k+1} f_{\mathcal{L}}(Z_{j}^{q}) \quad \forall i \neq p, j \neq \{m, t\}$ 

**Lemma.**  $f_{\mathcal{L}}(k; Z^*, O)$  is a monotone decreasing function. i.e  $f_{\mathcal{L}}(k; Z^*, O) \ge f_{\mathcal{L}}(k+1; Z^*, O)$  such that  $1 < k+1 \le N$ .

*Proof.* Let  $\Pi^*(\sigma_{N,s}^k) = Max f_{\mathcal{L}}(Z; =, k)$  and  $\Pi^*(\sigma_{N,q}^{k+1}) = Max f_{\mathcal{L}}(Z; O, k+1)$ . Then according to the previous theorem if  $\Pi^*(\sigma_{N,s}^k) < \Pi^*(\sigma_{N,q}^{k+1})$ . It follows that:  $f_{\mathcal{L}}(k; \mathsf{Z}(\Pi^*(\sigma_{N,s}^k), 0)) \ge f_{\mathcal{L}}(k+1; \mathsf{Z}(\Pi^*(\sigma_{N,q}^{k+1}), 0)$  $f_{\mathcal{L}}(k; Z^*, O) \ge f_{\mathcal{L}}(k+1; Z^*, O)$ if  $\Pi^*(\sigma_{N,s}^k) \ge \Pi^*(\sigma_{N,q}^{k+1})$  then:  $f_{\mathcal{L}}(k, \mathsf{Z}(\Pi^*(\sigma_{N,s}^k)), \mathsf{O}) > f_{\mathcal{L}}(k+1, \mathsf{Z}(\Pi^*(\sigma_{N,s}^{k+1})), \mathsf{O}).$ If it were:  $f_{\mathcal{L}}(k+1, Z(\Pi^{*}(\sigma_{N,q}^{k+1})), O) > f_{\mathcal{L}}(k, Z(\Pi^{*}(\sigma_{N,s}^{k})), O)$ then according to the proved theorem, should exist a partition t such that:  $f_{\mathcal{L}}(k, Z(\Pi^*(\sigma_{N,t}^k)), O) > f_{\mathcal{L}}(k+1, Z(\Pi^*(\sigma_{N,q}^{k+1})), O)$ and this implies:  $f_{\mathcal{L}}(k, \mathsf{Z}(\Pi^*(\sigma_{N,t}^k)), \mathsf{O}) > f_{\mathcal{L}}(k, \mathsf{Z}(\Pi^*(\sigma_{N,s}^k)), \mathsf{O}) = \mathbf{Max} f_{\mathcal{L}}(\mathsf{Z}; \mathsf{O}, k).$ That is a contradiction. 

k	$\Pi(\sigma_4^k)$	$\rho(\Pi(\sigma_4^k),\leqslant)$	$f_{\mathcal{L}}(\rho_1)$	$f_{\mathcal{L}}(\rho_2)$	$f_{\mathcal{L}}(\rho_3)$	$f_{\mathcal{L}}(Z(\Pi_{\sigma_{4,i}^k}))$
2	$\Pi_{\sigma_{4,1}^2}$	$\Pi_{\sigma_{4,1}^3}, \Pi_{\sigma_{4,2}^3}, \Pi_{\sigma_{4,6}^3}$	.7	.42	.49	.81
	$\Pi_{\sigma_{4,2}^2}$	$\Pi_{\sigma_{4,1}^3}, \Pi_{\sigma_{4,4}^3}, \Pi_{\sigma_{4,5}^3}$	.7	.48	.45	.83
	$\Pi_{\sigma^2_{4,3}}$	$\Pi_{\sigma^{3}_{4,1}}, \Pi_{\sigma^{3}_{4,6}}$	.7	.28		.76
	$\Pi_{\sigma^2_{4,4}}$	$\Pi_{\sigma_{4,2}^3}, \Pi_{\sigma_{4,3}^3}, \Pi_{\sigma_{4,4}^3}$	.42	.49	.48	.56
	$\Pi_{\sigma^2_{4,5}}$	$\Pi_{\sigma^{3}_{4,2}}, \Pi_{\sigma^{3}_{4,5}}$	.42	.45		.47
	$\Pi_{\sigma^2_{4,6}}$	$\Pi_{\sigma_{4,3}^3}, \Pi_{\sigma_{4,4}^3}$	.49	.48		.57
	$\Pi_{\sigma^2_{4,7}}$	$\Pi_{\sigma_{4,3}^3},\Pi_{\sigma_{4,5}^3},\Pi_{\sigma_{4,6}^3}$	.49	.45	.28	.6
		$Max f_{\mathcal{L}}(Z; O, 2) =$	$f_{\mathcal{L}}(\Pi_{\sigma^2_{4,2}})$			.83
3	$\Pi_{\sigma^3_{4,1}}$	$\Pi_{\sigma_{4,1}^4}$	.4			.7
	$\Pi_{\sigma^3_{4,2}}$	$\Pi_{\sigma_{4,1}^4}$	.4			.42
	$\Pi_{\sigma^3_{4,3}}$	$\Pi_{\sigma_{4,1}^4}$	.4			.49
	$\Pi_{\sigma^3_{4,4}}$	$\Pi_{\sigma_{4,1}^4}$	.4			.48
	$\Pi_{\sigma^3_{4,5}}$	$\Pi_{\sigma_{4,1}^4}$	.4			.45
	$\Pi_{\sigma^3_{4,6}}$	$\Pi_{\sigma_{4,1}^4}$	.4			.28
		$Max f_{\mathcal{L}}(Z; O, 3) =$	$f_{\mathcal{L}}(\Pi_{\sigma_{4,1}^3})$			.7

Table 11: **Partition set Lattice**  $|\Omega| = 4$ 

Foe example the partition:

$$\Pi_{\sigma_{4,1}^2} = \{\{123\}, \{4\}\} = \begin{bmatrix} \mathbf{z}^7 & \mathbf{z}^8 & \mathbf{o} & \mathbf{o} \end{bmatrix}$$

$$f_{\mathcal{L}}(\mathbf{z}^7) = \mathbf{o}_{11} + \mathbf{0}_{22} + \mathbf{o}_{33} + \mathbf{o}_{12} + \mathbf{o}_{21} + \mathbf{o}_{13} + \mathbf{o}_{31} + \mathbf{o}_{23} + \mathbf{o}_{32}$$

$$\Pi_{\sigma_{4,1}^3} = \{\{12\}, \{3\}, \{4\}\} = \begin{bmatrix} \mathbf{z}^3 & \mathbf{z}^4 & \mathbf{z}^8 & \mathbf{o} \end{bmatrix}$$

$$f_{\mathcal{L}}(\mathbf{z}^3) = \mathbf{o}_{11} + \mathbf{o}_{22} + \mathbf{o}_{12} + \mathbf{o}_{21}$$

$$f_{\mathcal{L}}(\mathbf{z}^4) = \mathbf{o}_{33}$$

$$f_{\mathcal{L}}(\mathbf{z}^7) - (f_{\mathcal{L}}(\mathbf{z}^3) + f_{\mathcal{L}}(\mathbf{z}^4)) = \mathbf{o}_{13} + \mathbf{o}_{31} + \mathbf{o}_{23} + \mathbf{o}_{32} = .11$$

#### 1.4.2 The Homogeneity Index function

The problem of finding the best partition that minimizes the Homogeneity Index function is quite similar, in its formulation, to data partitioning or clustering.

The data partitioning problem consists of merging similar elements into sets that are as distinct as possible. To compare two elements, the notion of distance is used. That brings the data partitioning problem down to the creation of subsets of elements as distinct from each other as possible. Therefore this function is a simple form of  $\mathbf{k}$  – **means clustering** model and it is based on the calculation of attribute distance between two observation. Depending on how the distance is calculated the function model can result: *Euclidean* distance, *Manhattan* distance and the *power* distance.

Therefore, the next steps in the definition of the Homogeneity function are:

- 1. The identification of the independent variables.
- 2. The definition of the three metrics(i.e *Euclidean,Manhattan* and *power*).

In the zone design context, the homogeneity function is structured on the base of the data vector  $d(\omega_i)$ . Recalling that  $d(\omega_i)$  represents the b.s.u data, if we exclude the patient in-flow and out-flow, what we have left are the attributes related to a b.s.u. From now on we identify with **D** the Data array, i.e the array containing the attributes values for each b.s.u.

Let M represent the number of attributes related to a b.s.u. Then let be:

$$\mathbf{d}(\boldsymbol{\omega}_{i}) = \mathbf{d}^{i} = \begin{bmatrix} \mathbf{d}_{1}^{i} \\ \mathbf{d}_{2}^{i} \\ \vdots \\ \mathbf{d}_{M}^{i} \end{bmatrix} \forall i = 1, \dots, N$$

The data vector containing all the information regarding the population attributes in the study area. It's worth noting that the elements of this vector are vectors. In fact for each basic b.s.u we can have more than a single value for a specific variable; specifically there are as many values as the number of people living in the b.s.u. However, in this research we standardise the variables to overcome this issue.

$$\mathbf{d}_{j}^{i} = \begin{bmatrix} d_{j,1}^{i} & d_{j,2}^{i} & \dots & d_{j,P_{i}}^{i} \end{bmatrix} \quad j = 1,\dots,M$$

We can collect all these data in the Data array **D**:

$$\mathbf{D} = \begin{bmatrix} \mathbf{d}_{1}^{\mathbf{1}} & \mathbf{d}_{2}^{\mathbf{1}} & \dots & \mathbf{d}_{M}^{\mathbf{1}} \\ \mathbf{d}_{1}^{\mathbf{2}} & \mathbf{d}_{2}^{\mathbf{2}} & \dots & \mathbf{d}_{M}^{\mathbf{2}} \\ \vdots & & \vdots \\ \mathbf{d}_{1}^{\mathbf{N}} & \mathbf{d}_{2}^{\mathbf{N}} & \dots & \mathbf{d}_{M}^{\mathbf{N}} \end{bmatrix} = \begin{bmatrix} D_{1} & D_{2} & \dots & D_{j} & \dots & D_{M} \end{bmatrix}$$

$$D_j = \begin{bmatrix} d_j^{\scriptscriptstyle \rm I}(V_{\scriptscriptstyle \rm II}) & d_j^{\scriptscriptstyle \rm I}(V_{\scriptscriptstyle \rm I2}) & \dots & d_j^{\scriptscriptstyle \rm I}(V_{\scriptscriptstyle \rm Il}) & \dots & d_j^{\scriptscriptstyle \rm I}(V_{\scriptscriptstyle \rm IN}) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ d_j^k(V_{k \scriptscriptstyle \rm I}) & d_j^k(V_{k \scriptscriptstyle \rm I}) & \dots & d_j^k(V_{k \scriptscriptstyle \rm I}) & \dots & d_j^k(V_{k \scriptscriptstyle \rm N}) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ d_j^N(V_{N \scriptscriptstyle \rm I}) & d_j^N(V_{N \scriptscriptstyle \rm I}) & \dots & d_j^N(V_{N \scriptscriptstyle \rm I}) & \dots & d_j^N(V_{N \scriptscriptstyle \rm N}) \end{bmatrix}$$

It is worth noting that each attribute j has an Origin-destination matrix. Therefore, the vector  $\mathbf{d}_{j}^{k}(\mathbf{V}_{kl})$  contains as many values as the total number of votes moving from the patient postcode (k) to the provider postcode (l).

$$\mathbf{d}_{j}^{k}(\mathbf{V}_{kl}) = \begin{cases} x_{i} \in \mathbb{R} \quad v_{kl} > 0\\ -1 \quad \text{otherwise} \end{cases}$$

$$\mathbf{d}_{j}^{\mathbf{k}}(\mathbf{V}_{\mathbf{k}\mathbf{l}}) = \begin{bmatrix} x_{1} & x_{2} & \dots & x_{\nu_{\mathbf{k}\mathbf{l}}} \end{bmatrix}$$

In order to select this vector, we introduce the following matrix:

$$I(V_{kl}) = \begin{cases} 1 & r = c \quad \sum_{s=1}^{l-1} v_{is} < r \leq \sum_{s=1}^{l-1} v_{is} + v_{kl} \\ 0 & \text{otherwise} \\ \sum_{s=1}^{l-1} v_{is} = 0 \quad l = 1 \end{cases}$$

$$\mathbf{d}_{j}^{\mathbf{k}}(\mathbf{V}_{\mathbf{k}\mathbf{l}}) = \mathbf{d}_{j}^{\mathbf{k}} \cdot \mathbf{I}(\mathbf{v}_{\mathbf{k}\mathbf{l}})$$

Now that we know the Data vector, it is possible to define the three different metrics.

Euclidean distance is the distance between two observations A and B resulting from the sum of squared differences of their x, y coordinates. Structuring a *non-geometric space*, the notion of distance does not represent anymore a measure of geometrical link such as the original Euclidean distance but highlights the **differences of attributes**.

$$d_{E} = \sqrt{(x_{A} - x_{B})^{2} + (y_{A} - y_{B})^{2}}$$
$$d_{E} = \sqrt{\sum_{i=1}^{M} (x_{iA} - x_{iB})^{2}}$$

where,  $x_{iA}$  and  $x_{iB}$  are the values of observations A and B respectively for variable i in a M – dimensional attribute space (M variables in the dataset). The generic formula of Euclidean distance  $d_E$ 

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can be formulated according to the number of variables.

In the case of a single dimension attribute space the distance indicates the sum of squared differences of two observations using one variable (one dimension). In practice, the distance is calculated between the attribute values of each areal unit ( $\omega_i$ ) in zone  $Z_k$  and the mean of zone  $Z_k$  ( $\mu(Z_k)$ ).

Suppose we have only an attribute value for each b.s.u (we are ignoring the origin-destination matrix):

$$D = \begin{bmatrix} d_1^1 \\ d_1^2 \\ \vdots \\ d_1^j \\ \vdots \\ d_1^N \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_j \\ \vdots \\ x_N \end{bmatrix}$$

Then the distance for an areal unit  $\omega_i$  is defined as:

$$\begin{split} d_E^j(Z_k) &= \sqrt{(\mu(Z_k) - x_j)^2} \\ \mu(Z_k) &= \frac{\sum_{j=1}^N x_j}{|Z_k|} \quad x_j \in Z_k \end{split}$$

Suppose we have a partition composed by k zones. Then the Homogeneity Index function is calculated as the sum of the distances expressed as:

$$\mathbf{f}_{\mathcal{H}}(\mathsf{Z},\mathsf{D}) = \frac{\sum_{i=1}^{k} \mathfrak{I}_{\mathcal{H}_{i}}(\mathsf{Z}_{i},\mathsf{D})}{k} \quad \mathsf{Z}_{i} \in \Pi_{\sigma_{\mathsf{N},\mathsf{S}}^{\mathsf{k}}}$$
$$\mathfrak{I}_{\mathcal{H}_{i}}(\mathsf{Z}_{i},\mathsf{D}) = d_{\mathsf{E}}^{j}(\mathsf{Z}_{i})$$

The minimization of distances between the mean of zones and their areal units produce homogeneous output zones consisting of areal units with similar values for the selected variable.

Other variations of Homogeneity are available in the zone design system differing on the method of distance calculation. The *Manhattan* distance (or block distance, taxi-cab distance) is similar to the *Euclidean* distance but the squared differences are replaced with absolute differences of observations. The mathematical definition of *Manhattan* distance ( $d_M$ ) is expressed as:

$$d_M^{AB} = \sum_{i=1}^N |x_{iA} - x_{iB}|$$

And in the zone design system it is defined as:

$$\begin{split} d^j_{\mathcal{M}}(\boldsymbol{Z}_k) &= |\boldsymbol{\mu}(\boldsymbol{Z}_k) - \boldsymbol{x}_j| \\ \boldsymbol{\mu}(\boldsymbol{Z}_k) &= \frac{\sum_{j=1}^N \boldsymbol{x}_j}{|\boldsymbol{Z}_k|} \quad \boldsymbol{x}_j \in \boldsymbol{Z}_k \end{split}$$

In general, the zone design system supports both Homogeneity functions providing two ways for measuring differences between the zones mean and areal unit attributes. In practice, the system copes faster with the *Manhattan* distances in relation to *Euclidean* distance because the process to find the absolute value of a number is calculated much easier than to find the square value of same number. However, the optimisation of an objective function using *Manhattan* distances provides sufficient improvement compared to the Euclidean distance where the attribute differences shrink between the observa-

tions. Moreover, the choice of the Manhattan distance is more convenient if we'd like to formulate an equivalent linear model.

Theoretically speaking, the above attribute distances can be formulated using a generic formula, extending the previous metrics as follows:

$$\mathbf{d}_{p}^{AB} = \sqrt[m]{\sum_{i=1}^{n} |\mathbf{x}_{iA} - \mathbf{x}_{iB}|^{k}}$$

Where, m and k are the two powers. If both powers are equal to 2 then the distance is identical to Euclidean distance. In addition, if both powers are equal to one then the distance is identical to Manhattan distance.

In the zone design context the equation can be expressed as:

$$\begin{split} d_p^j(Z_k) &= \sqrt[m]{(|\mu(Z_k) - x_j|)^k} \\ \mu(Z_k) &= \frac{\sum_{j=1}^N x_j}{|Z_k|} \quad x_j \in Z_k \end{split}$$

where, m and k are the two powers inserted by the user. The powered distance is then calculated for the whole model according to the objective function:

$$\begin{array}{ll} \text{min} \quad \mathbf{f}_{\mathcal{H}}(\mathsf{Z},\mathsf{D}) = \frac{\sum_{i=1}^{k} \mathbb{I}_{\mathcal{H}_{i}}(\mathsf{Z}_{i},\mathsf{D})}{k} \quad \mathsf{Z}_{i} \in \Pi_{\sigma_{\mathsf{N},\mathsf{S}}^{k}} \\ \mathbb{I}_{\mathcal{H}_{i}}(\mathsf{Z}_{i},\mathsf{D}) = d_{\mathsf{F}}^{j}(\mathsf{Z}_{i}) \end{array}$$

Part II

# APPENDIX

# BIBLIOGRAPHY

### COLOPHON

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# DECLARATION

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Sydney, August 2015

Ludovico Pinzari