Spatially Constrained Clusters

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basic principles

indirect solutions

skater

max-p

Basic Principles

- Problem

  grouping contiguous objects that are similar into new aggregate areal units

  tension between

    attribute similarity

      grouping of similar observations

    locational similarity

      group spatially contiguous observations only

- Terminology

  regionalization (special case: redistricting)

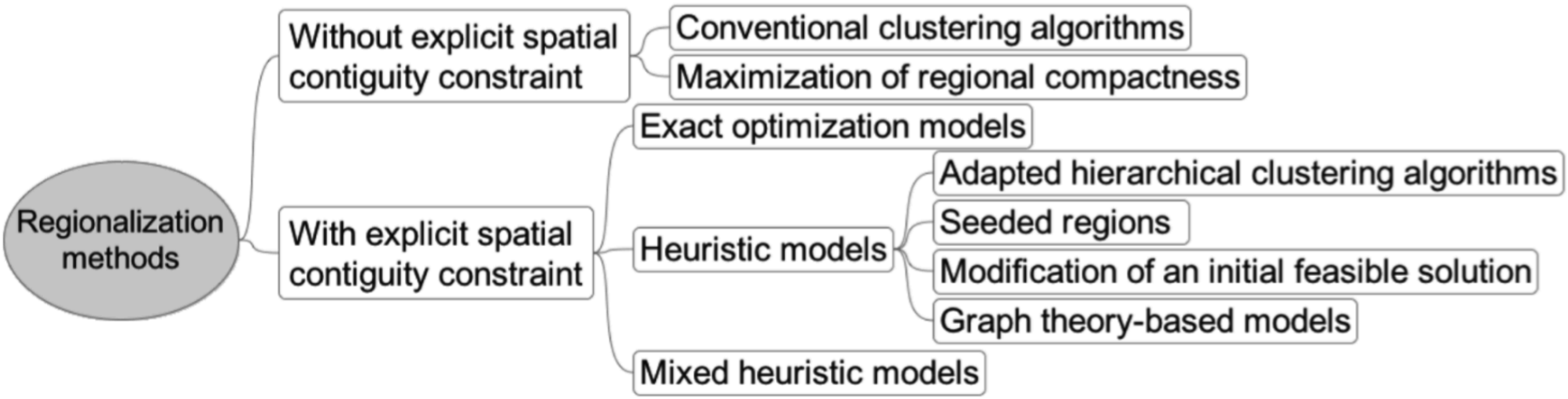
  spatially-constrained clustering

  contiguity-constrained clustering

  clustering under connectivity constraints

    many different terms

- Multiple Objectives
  - classical clustering
    - maximize within-group similarity
    - or, maximize between-group dissimilarity
  - spatial similarity
    - only contiguous objects in same group
  - shape
    - compactness



Solution Strategies (Duque et al. 2007)

- Classical Clustering with Updates

  start with hierarchical clustering or k-means solution

  split/combine clusters that are not contiguous

  inefficient approach

  number of cluster indeterminate

- Multi-Objective Approach

  introduce location (x, y) as variables within the clustering routing

  assign weights to similarity objective vs spatial objective

  difficult to set weights

- Automatic Zoning

    AZP

        automatic zoning procedure (Openshaw and Rao)

        heuristic

            starts from random initial feasible solutions

            optimization (NP-hard problem)

- Graph-Based Approaches

  represent the contiguity structure of the objects as a graph

  graph pruning

    e.g., using minimum spanning tree

    maximize internal similarity objective

- Explicit Optimization

    formulate as an integer programming problem

    decision variables to allocate object i to region j

    formalize adjacency constraints

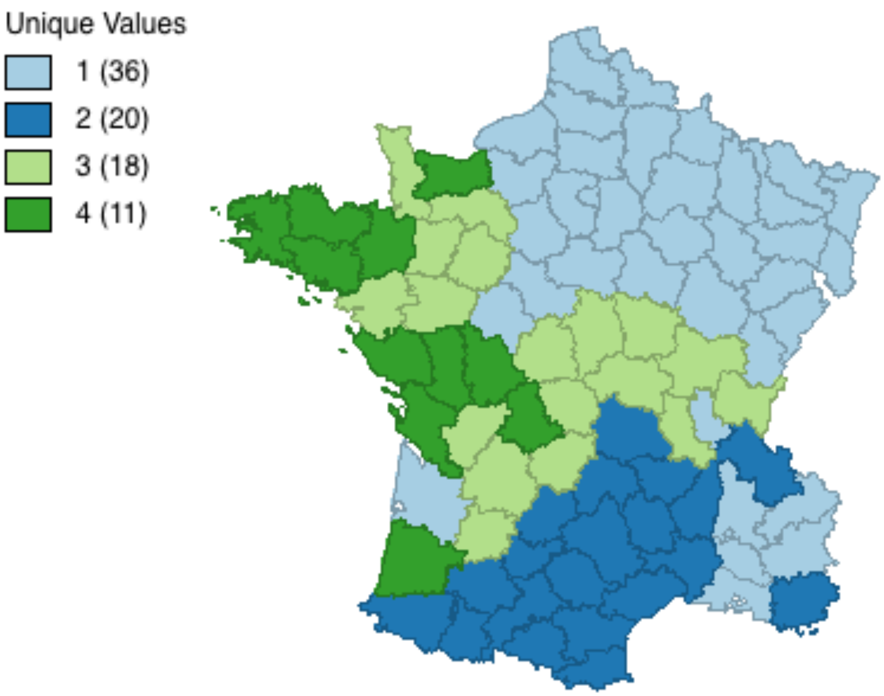
        typically as a graph representation

    several heuristics

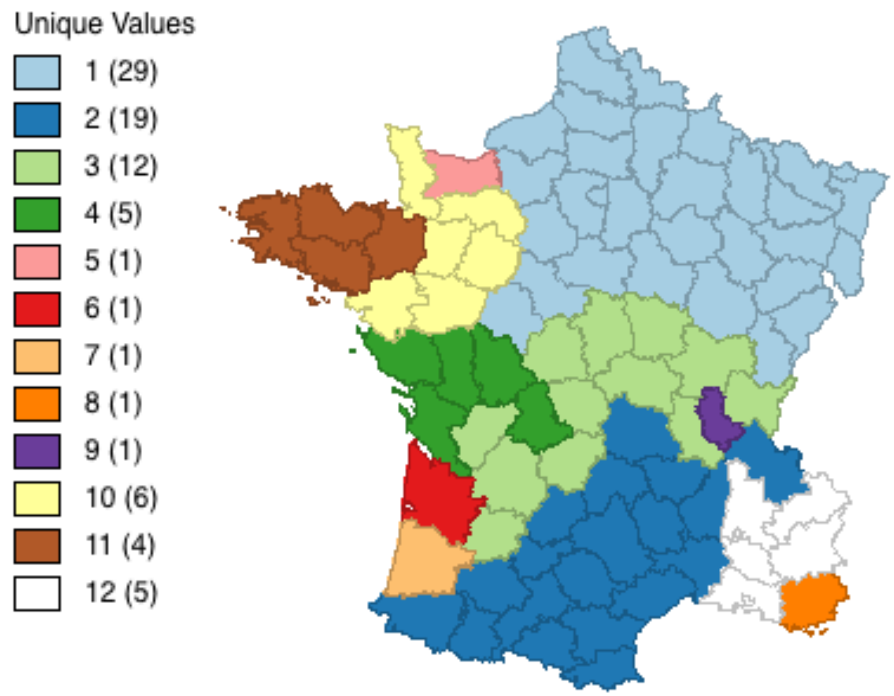
Indirect Solutions

Classic Clustering with Updates

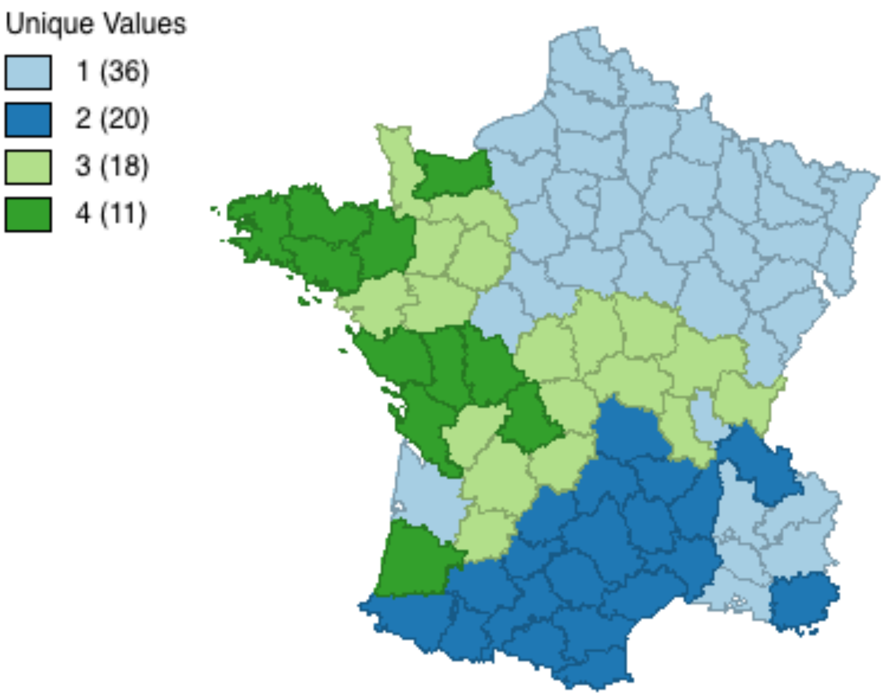
- Point of Departure - k Means Clusters
  - make any non-contiguous part of a cluster into a separate cluster
    - increases the number of clusters
    - fragmented solutions
  - move observations between clusters to achieve contiguity
    - keeps k the same
    - multiple solutions possible

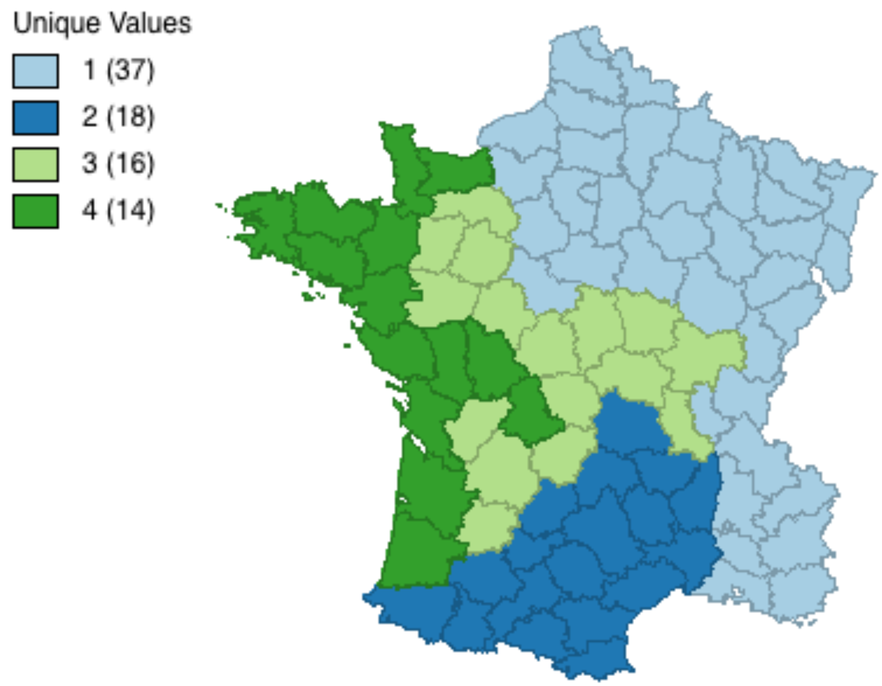


k-means (k=4) solution



12 “contiguous” clusters





k-means (k=4) solution

4 contiguous clusters
six changes

	Total SS	Within SS	Between SS	Ratio B/T
k-means	504	286.8	217.2	0.431
contiguous	504	314.8	189.2	0.375
k=12	504	237.4	266.6	0.529

cluster characteristics

Multi-Objective Optimization

- Weighted Optimization

  w_1(attribute similarity) + w_2(geometric centroids)

    $w_1 + w_2 = 1$

  iterate until contiguity constraint is satisfied

    bisection method

      w_2 is weight for centroids, $w_1 = 1 - w_2$

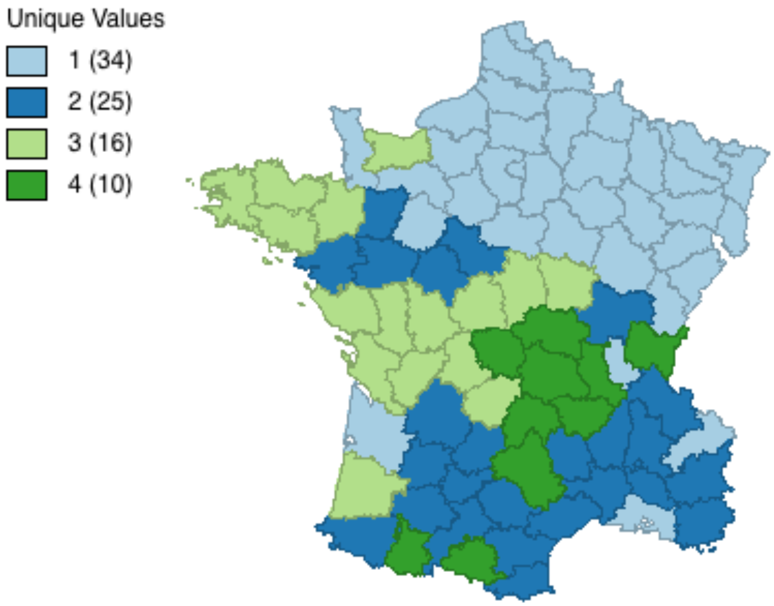
      start with 0.0 and 1.0

      then move to 0.50 - check contiguity

        if contiguous, then to midpoint to the left of 0.50

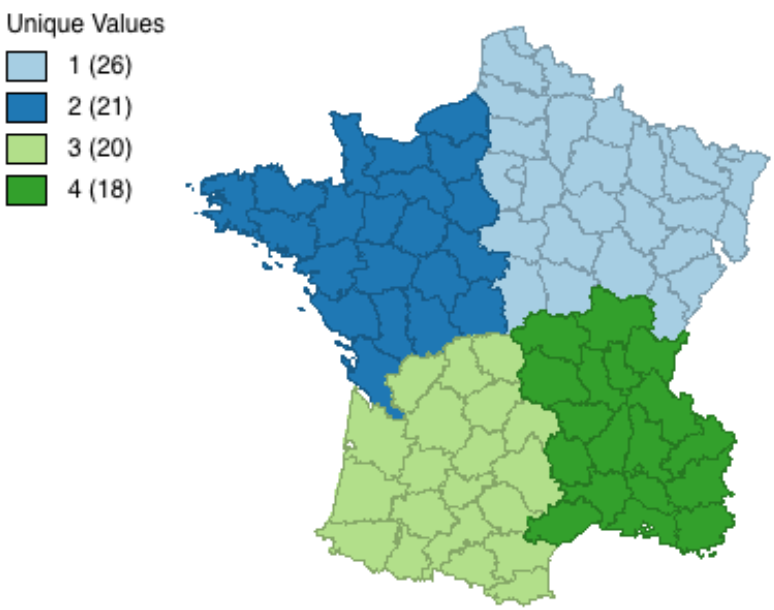
        if not contiguous, then to midpoint to the right of 0.50

      etc… until contiguous with the highest bSS/tSS ratio



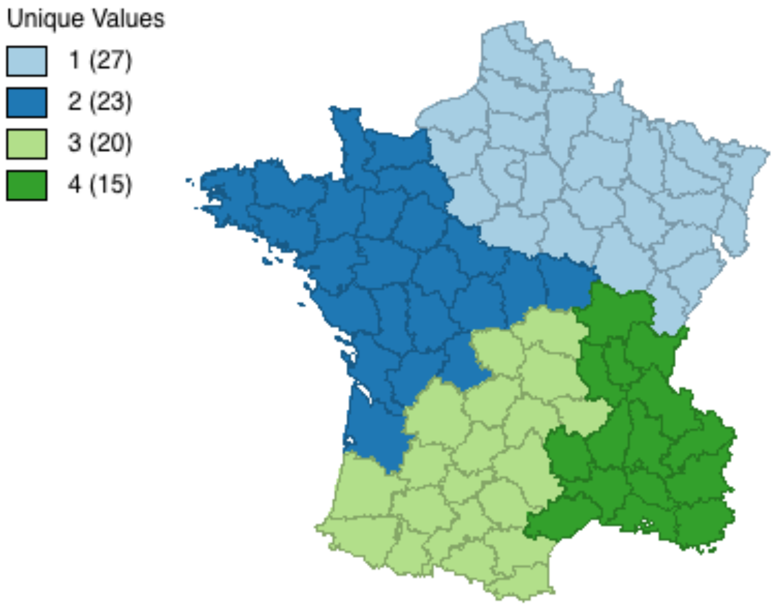
$w_2 = 0$

bSS/tSS = 0.4338



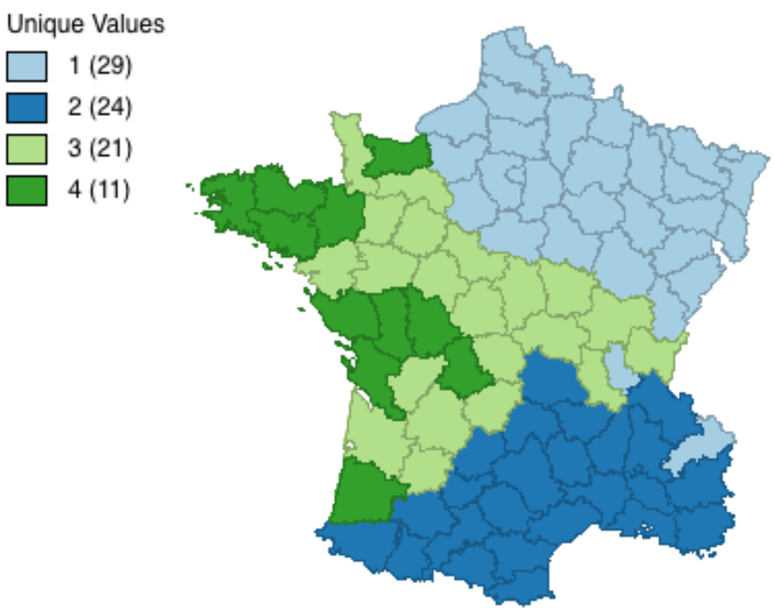
$w_2 = 1$

bSS/tSS = 0.2461



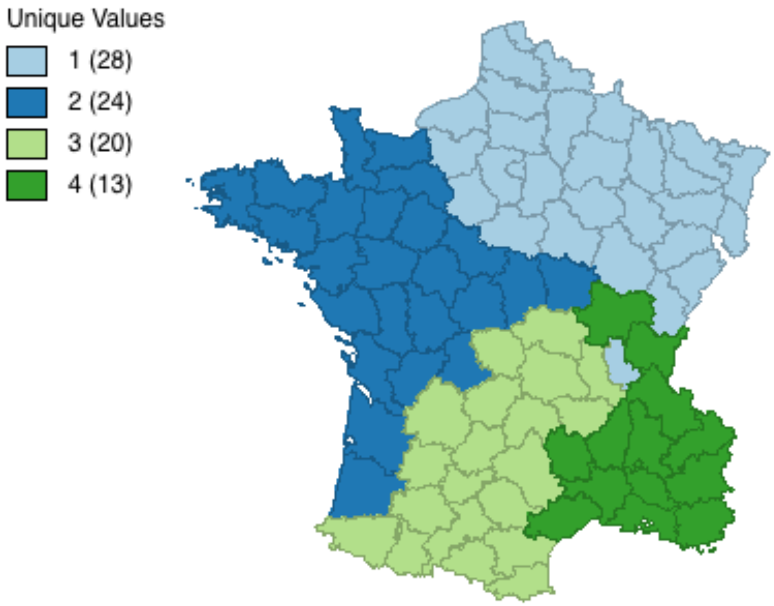
$w_2 = 0.50$

bSS/tSS = 0.3474



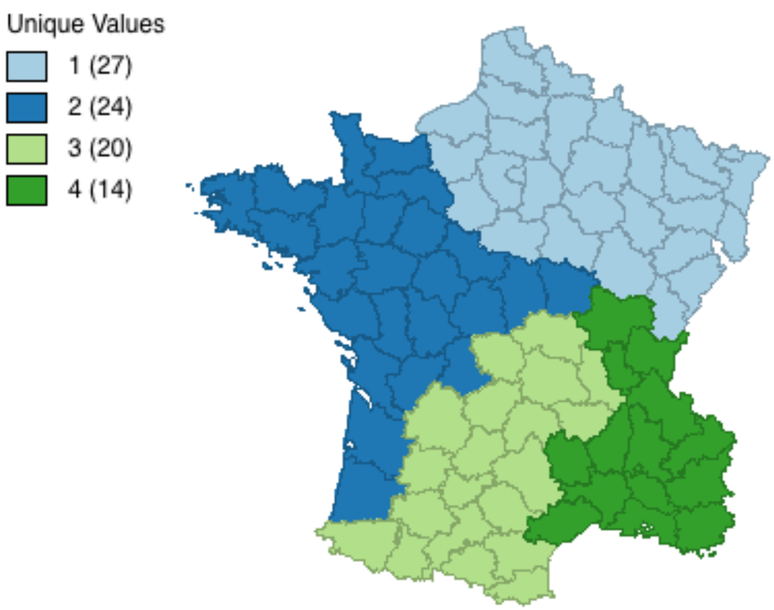
$w_2 = 0.25$

bSS/tSS = 0.4166



$w_2 = 0.375$

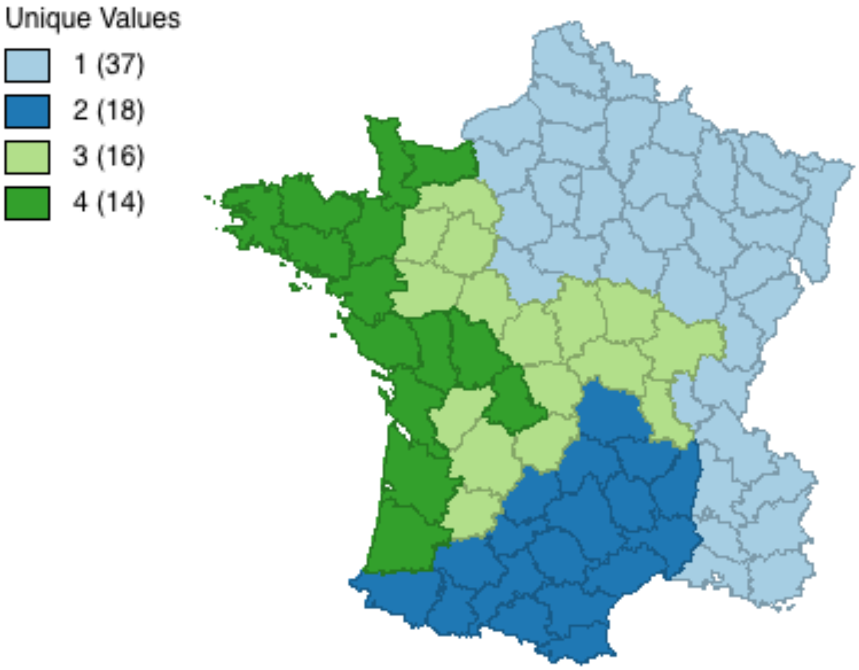
bSS/tSS = 0.3680

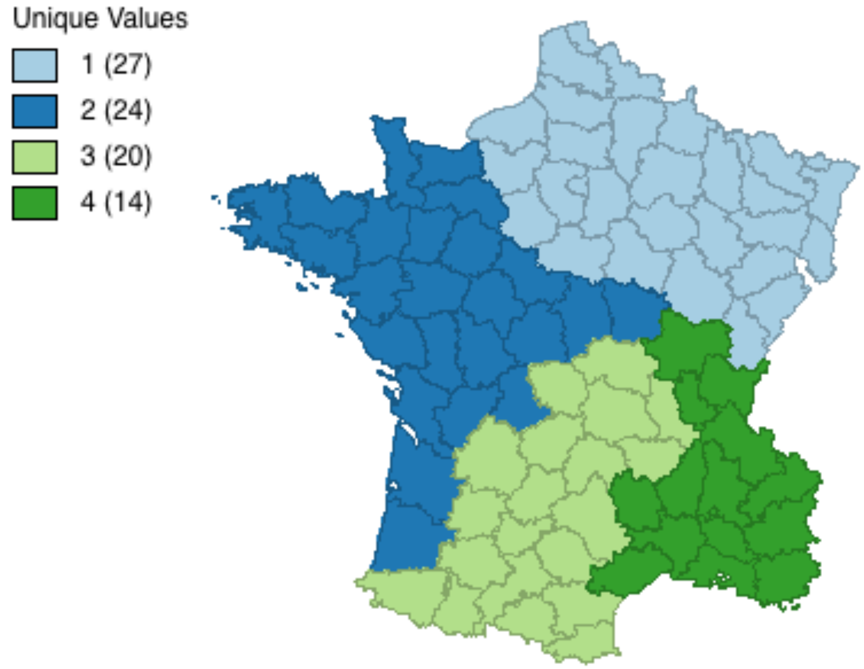


endpoint:

$w_2 = 0.4500$

bSS/tSS = 0.3612





ad hoc solution
ratio= 0.375

centroid solution
ratio= 0.361

skater

- SKATER

  Spatial Kluster analysis by Tree Edge Removal

    Assuncao et al (2006)

  algorithm

    construct minimum spanning tree from adjacency graph

    prune the tree (cut edges) to achieve maximum internal homogeneity

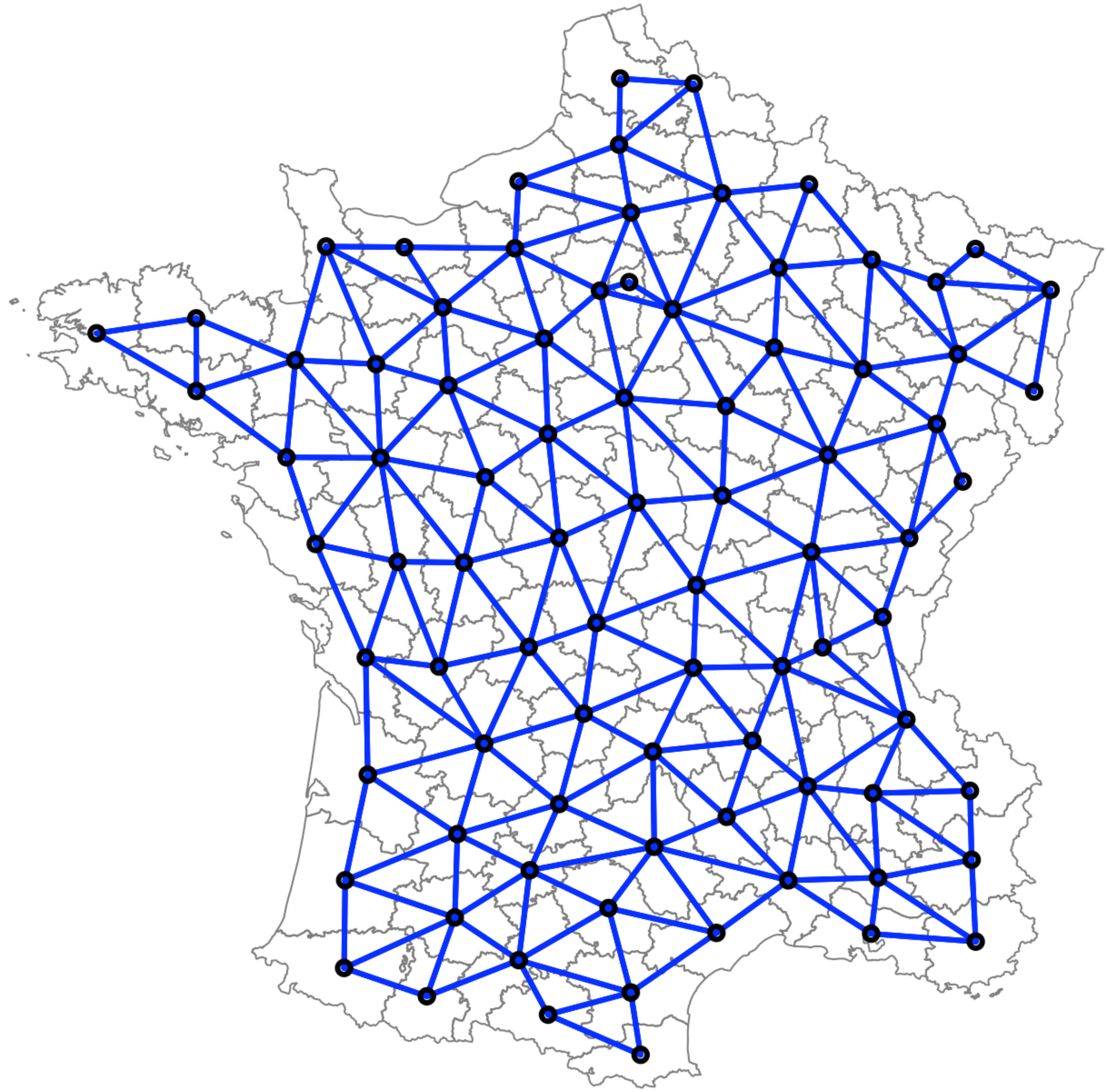
- Contiguity as a Graph

network connectivity based on adjacency between nodes (locations)

edge value reflects dissimilarity between nodes

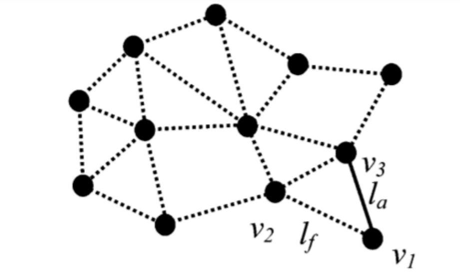
$$d(i,i') = d(x_i,x_{i'}) = \Sigma_p \, (x_{ip} - x_{i'p})^2$$

objective is to minimize within-group dissimilarity (maximize between-group)

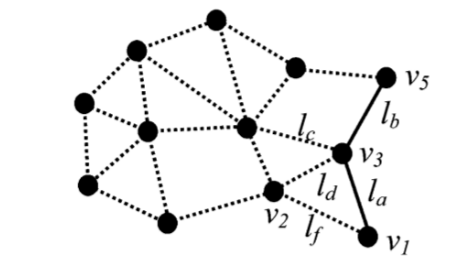


Queen contiguity network graph

- Minimum Spanning Tree
  - connectivity graph G = (V, L)
    - V vertices (nodes), L edges
  - path
    - a sequence of nodes connected by edges
    - v_1 to v_k: $(v_1,v_2), \ldots, (v_{k-1},v_k)$
  - spanning tree
    - tree with n nodes of G
    - unique path connecting any two nodes
    - n-1 edges
  - minimum spanning tree
    - spanning tree that minimizes a cost function
    - minimize sum of dissimilarities over all nodes

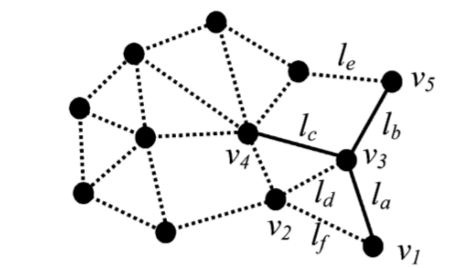


First iteration:
Set $T_1 = (V_1, L_1)$, where $V_1 = \{v_1\}$ and $L_1 = \phi$.
Find the edge of lowest cost ($l_a \langle l_f$).
Step 3: $T_2 \Rightarrow V_2 = \{v_1, v_3\}$ e $L_2 = \{l_a\}$.
Step 4: Repeat Step 2.

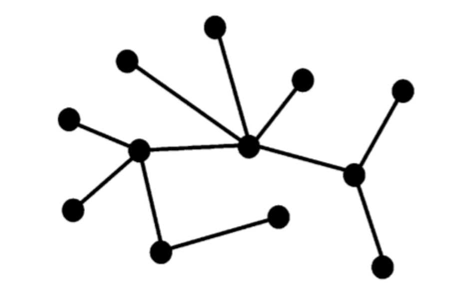


Second iteration:
Find the edge of lowest cost ($l_b \langle l_c \langle l_d \langle l_f$).

Set $T_3 \Rightarrow V_3 = \{v_1, v_3, v_5\}$ and $L3 = \{l_a, l_b\}$.



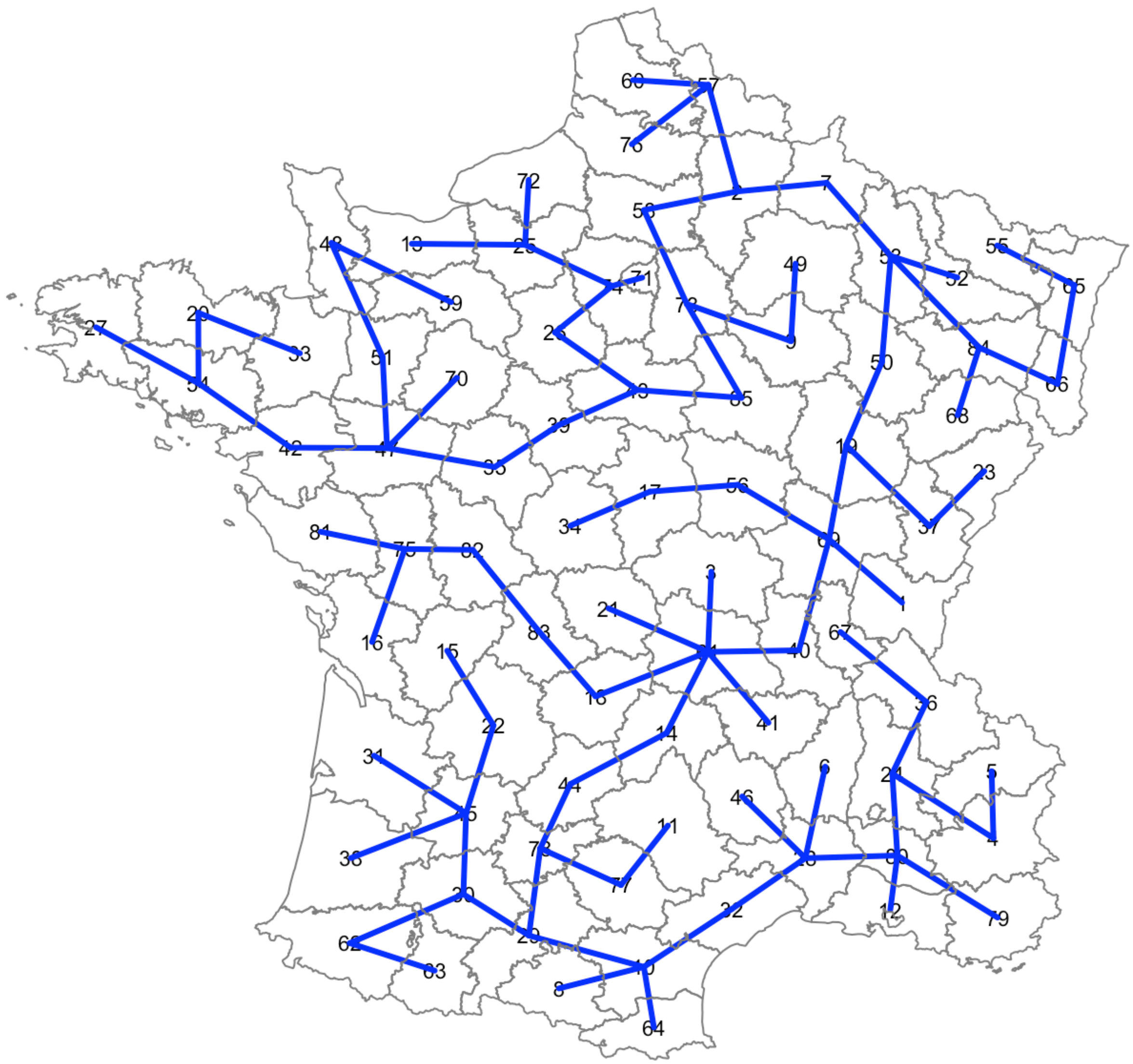
Third iteration:
Find the edge of lowest cost ($l_c \langle l_d \langle l_e \langle l_f$).
Set $T_4 \Rightarrow V_4 = \{v_1, v_3, v_4, v_5\}$ and
$L3 = \{l_a, l_b, l_c\}$.



Final Iteration:
$V_n = V$.

Figure 2. Construction of the minimum spanning tree.

Minimum Spanning Tree Algorithm (Assuncao et al 2006)



Minimum Spanning Tree

- **Tree Pruning**

  finding spatially contiguous clusters as a tree partitioning problem

  to obtain k regions, k-1 edges need to be removed

  - removal of edges results in sub-trees = cluster

  hierarchical approach

  - minimize within-cluster sum of squares

  - cut where max $F(T) - [F(T_a) + F(T_b)]$

    - with $F(T)$ as the within SS for tree T

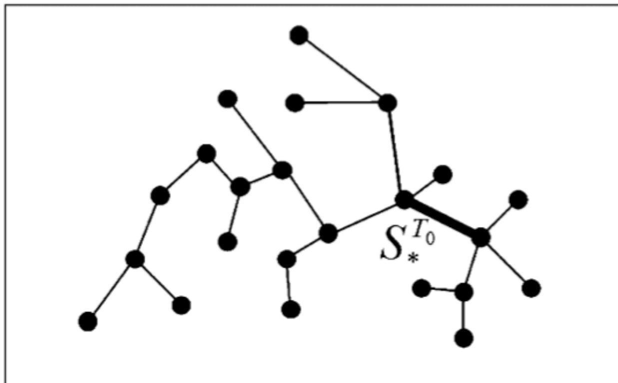
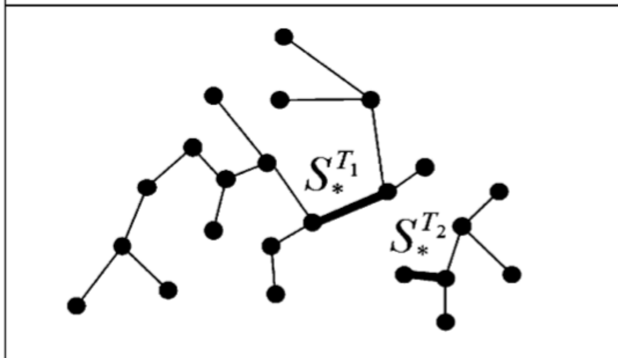
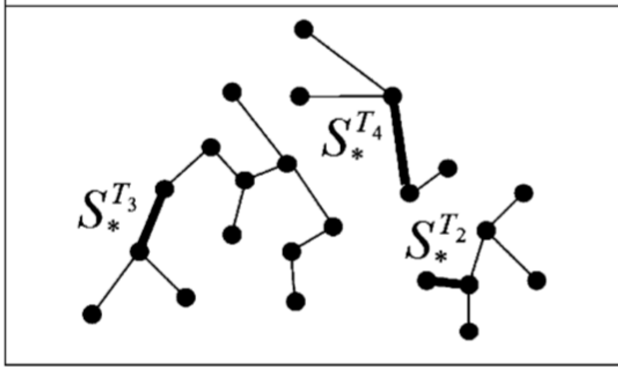
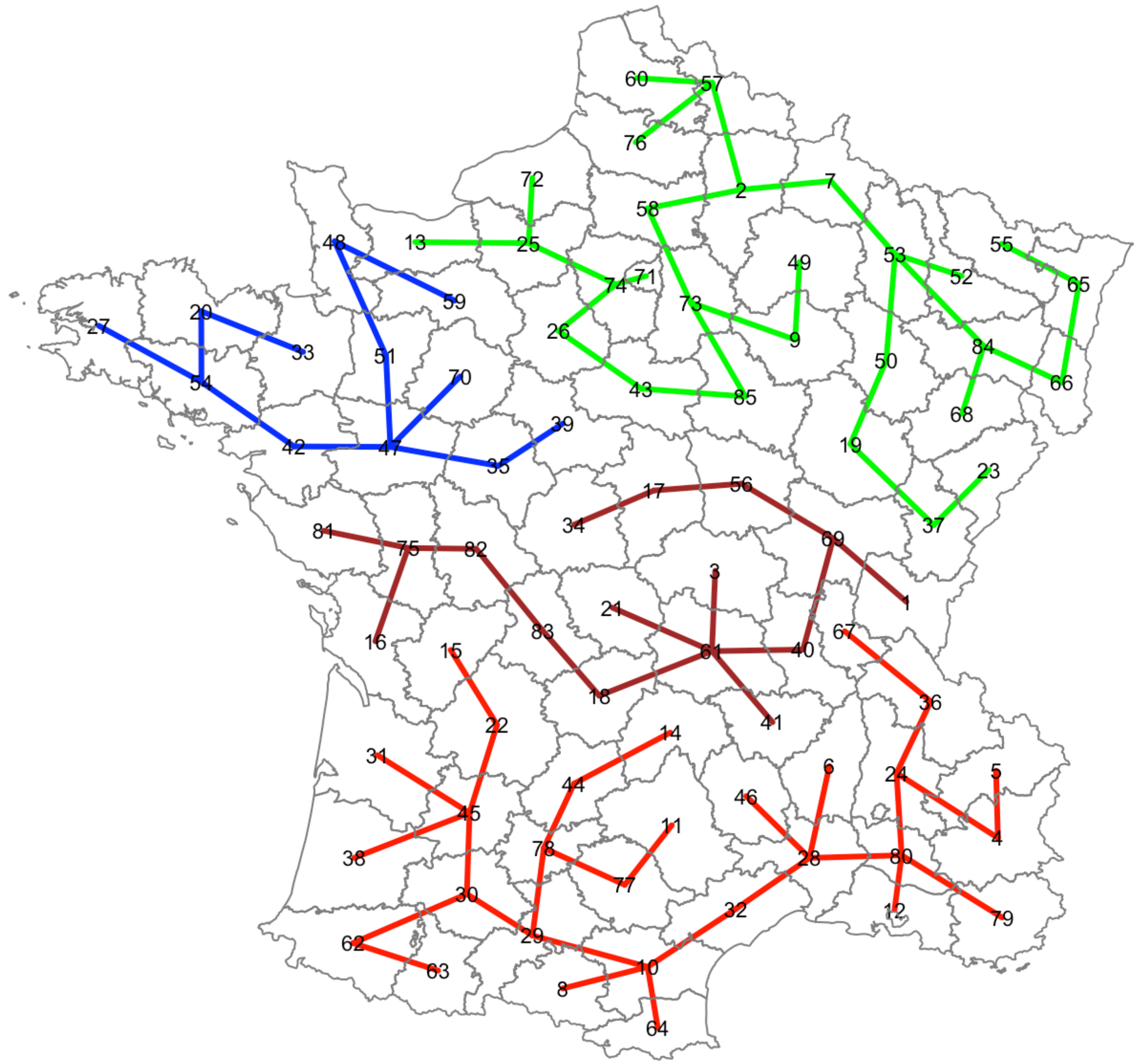
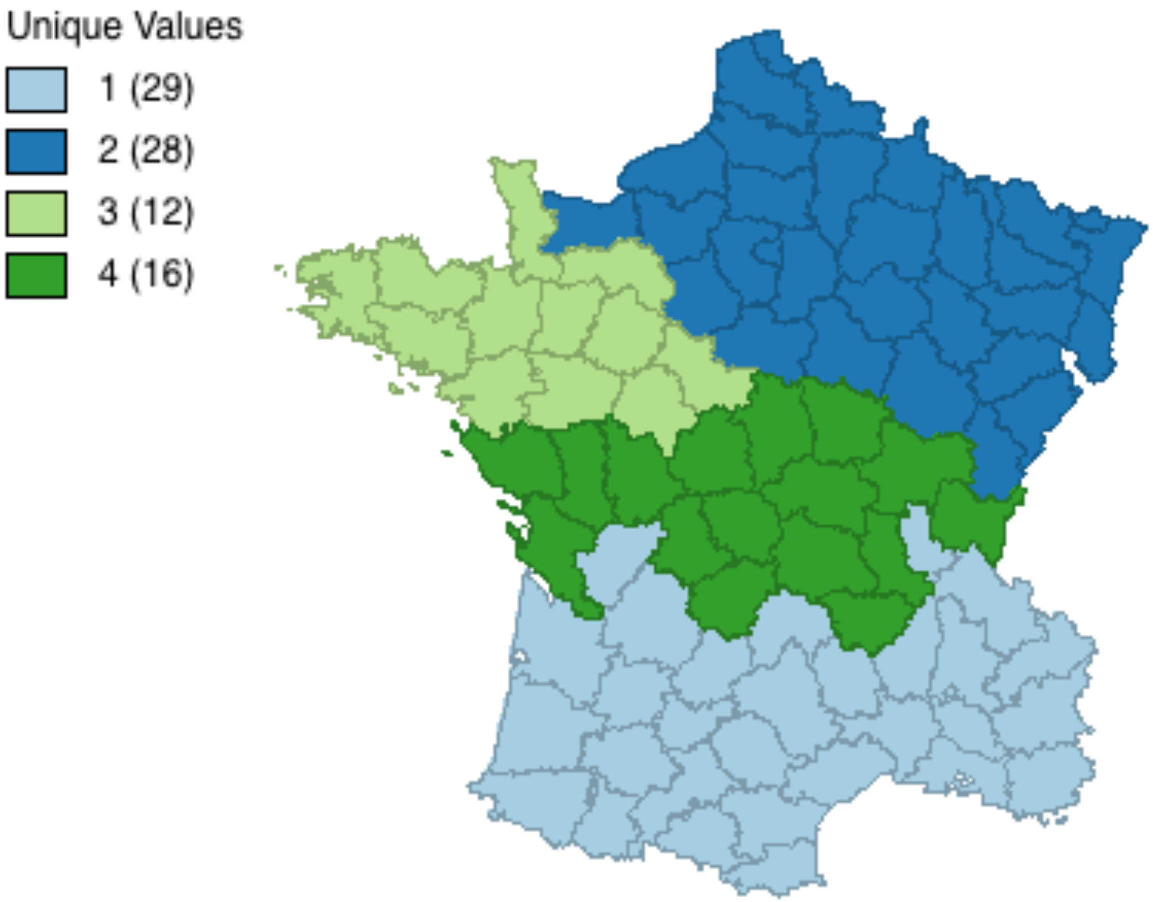
	Iteration 0: G* = MST. We select the edge which has the largest objective function. Cut out this edge leaving two trees (T_1 and T_2).
	Iteration 1: G* = (T_1, T_2). We compare the highest objective functions for T_1 and T_2. We split the tree T_1 since $f_1(S_*^{T_2}) \leq f_1(S_*^{T_1})$
	Iteration 2: G* = (T_2, T_3, T_4). We compare the highest objective functions for T_2, T_3 and T_4. We split the tree T_3 since $f_1(S_*^{T_2}) \leq f_1(S_*^{T_4}) \leq f_1(S_*^{T_3})$

Figure 3. Partitioning of the MST.

skater - pruning the MST (Assuncao et al 2006)



skater clusters k=4

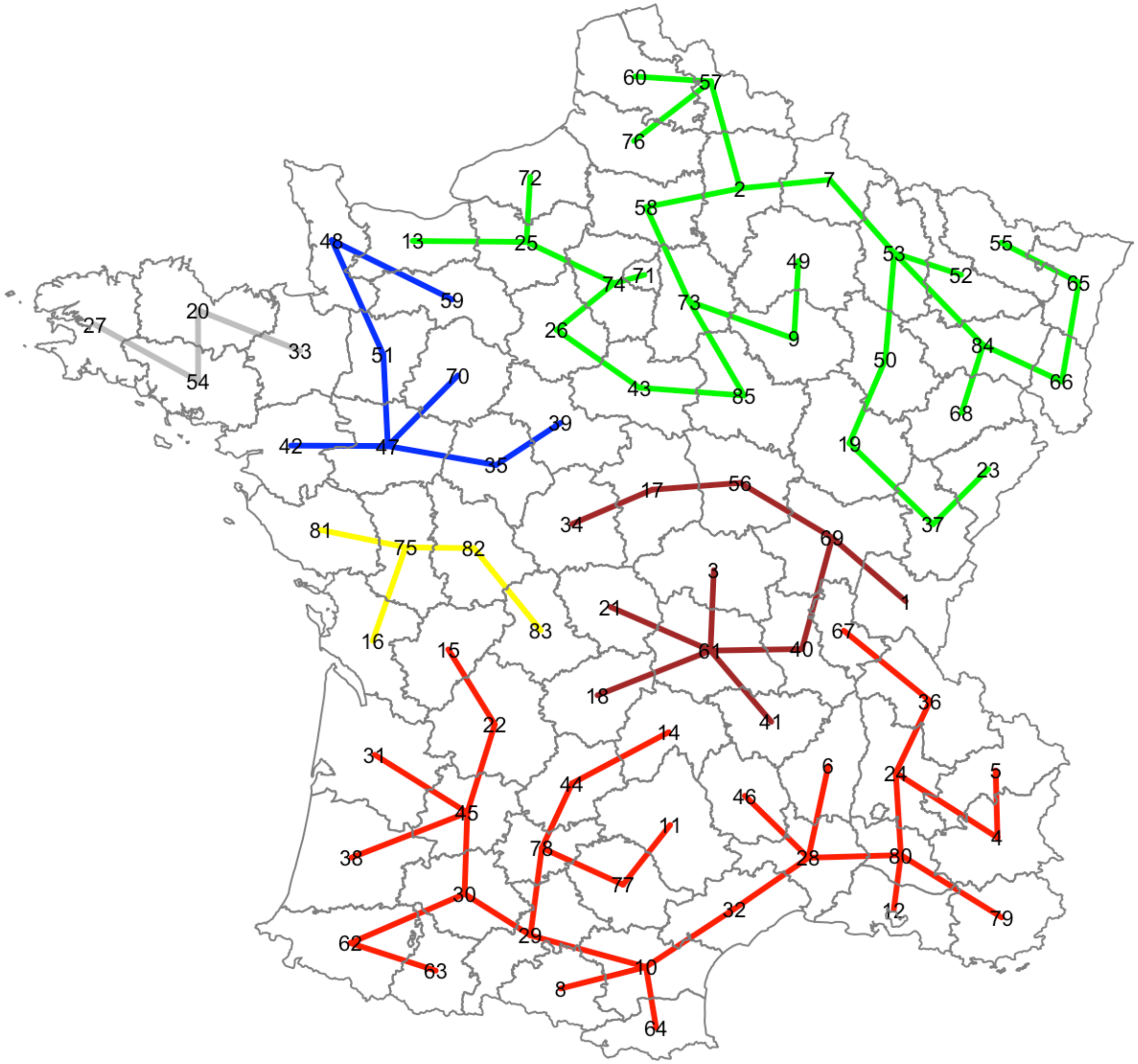


SSw = 344.9

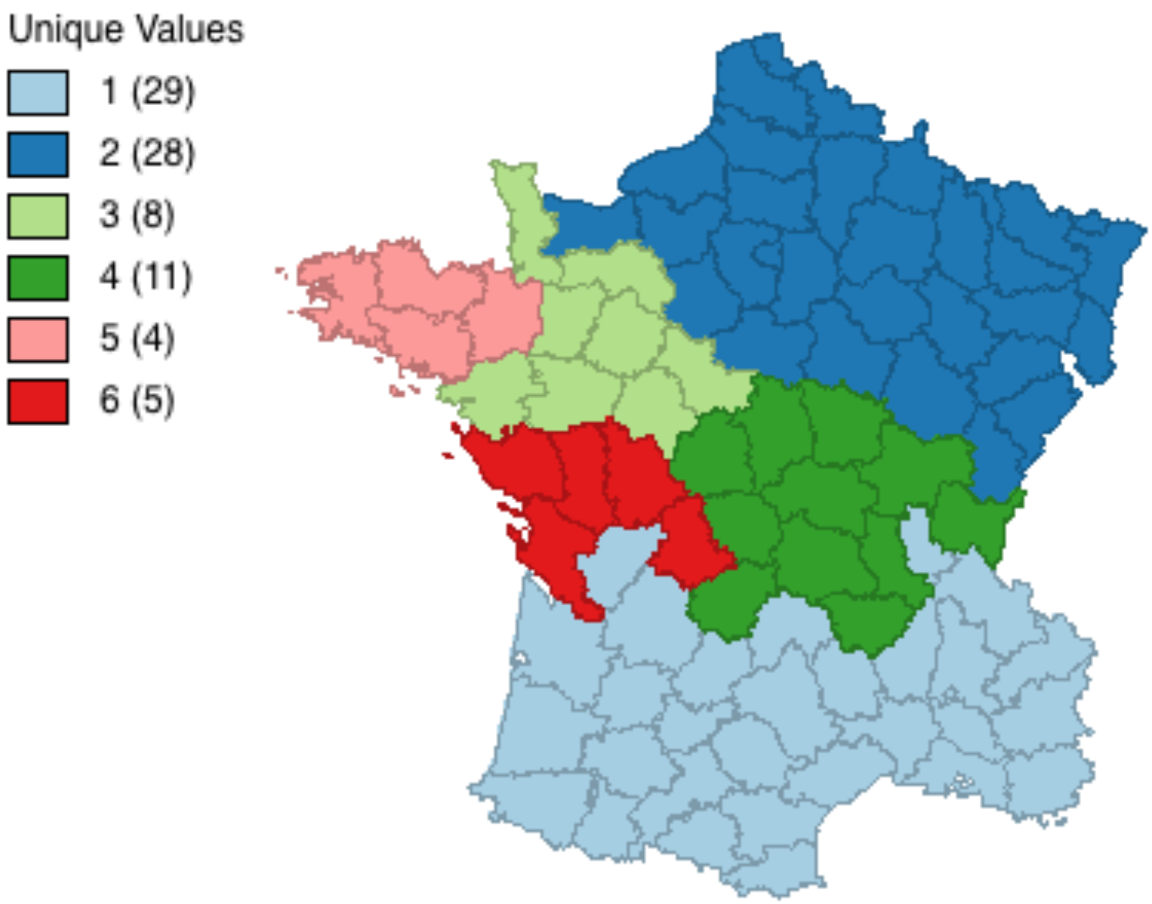
SSb = 159.1

SSb/SSt = 0.316

skater clusters k=4



skater clusters k=6



SSw = 292.6

SSb = 211.4

SSb/SSt = 0.420

skater clusters k=6

- Issues

    constrains solution space

    only cuts in MST and subsets of MST

    local optima

    doesn't scale well

max-p

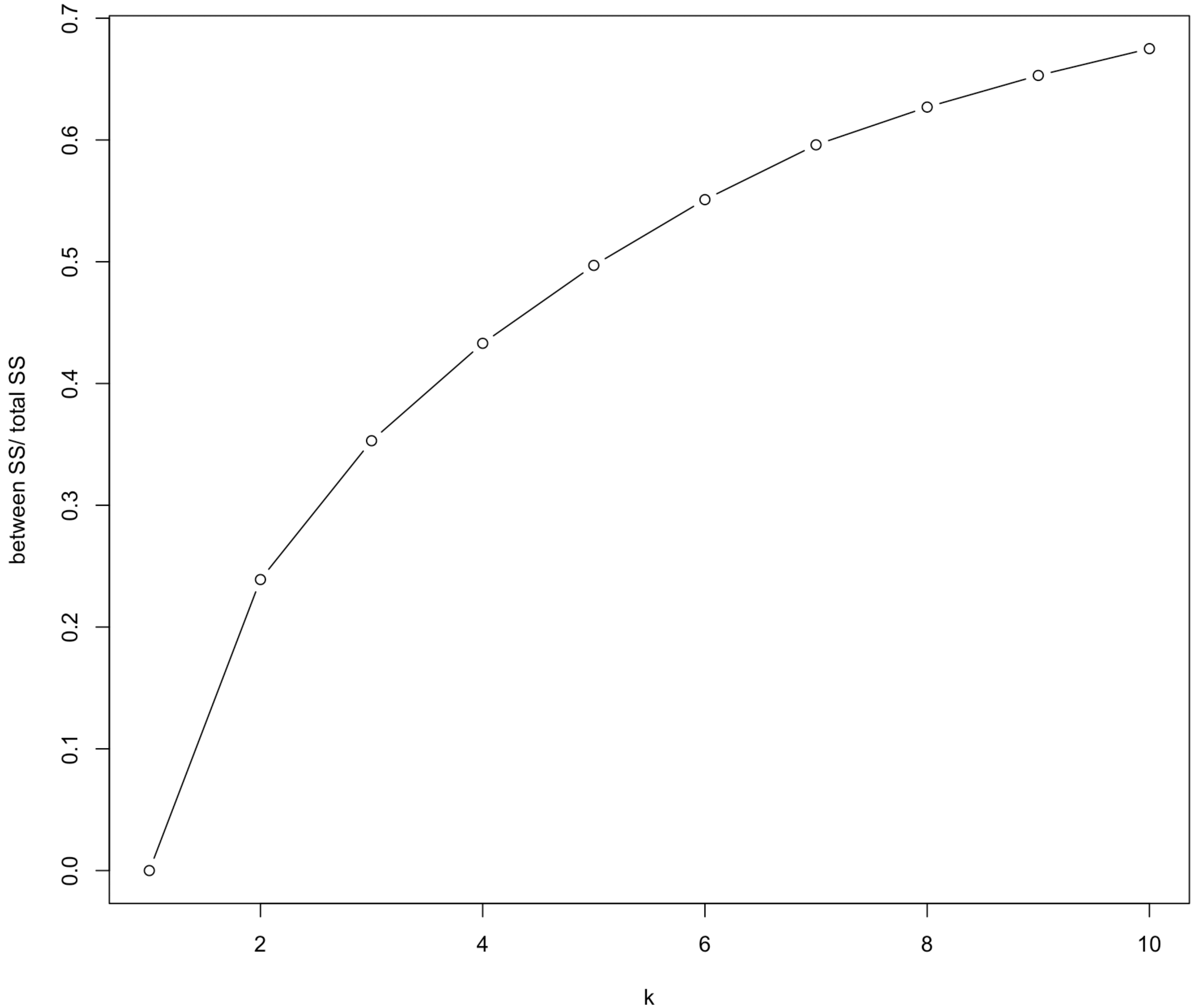
- Selecting k

  ad hoc rules

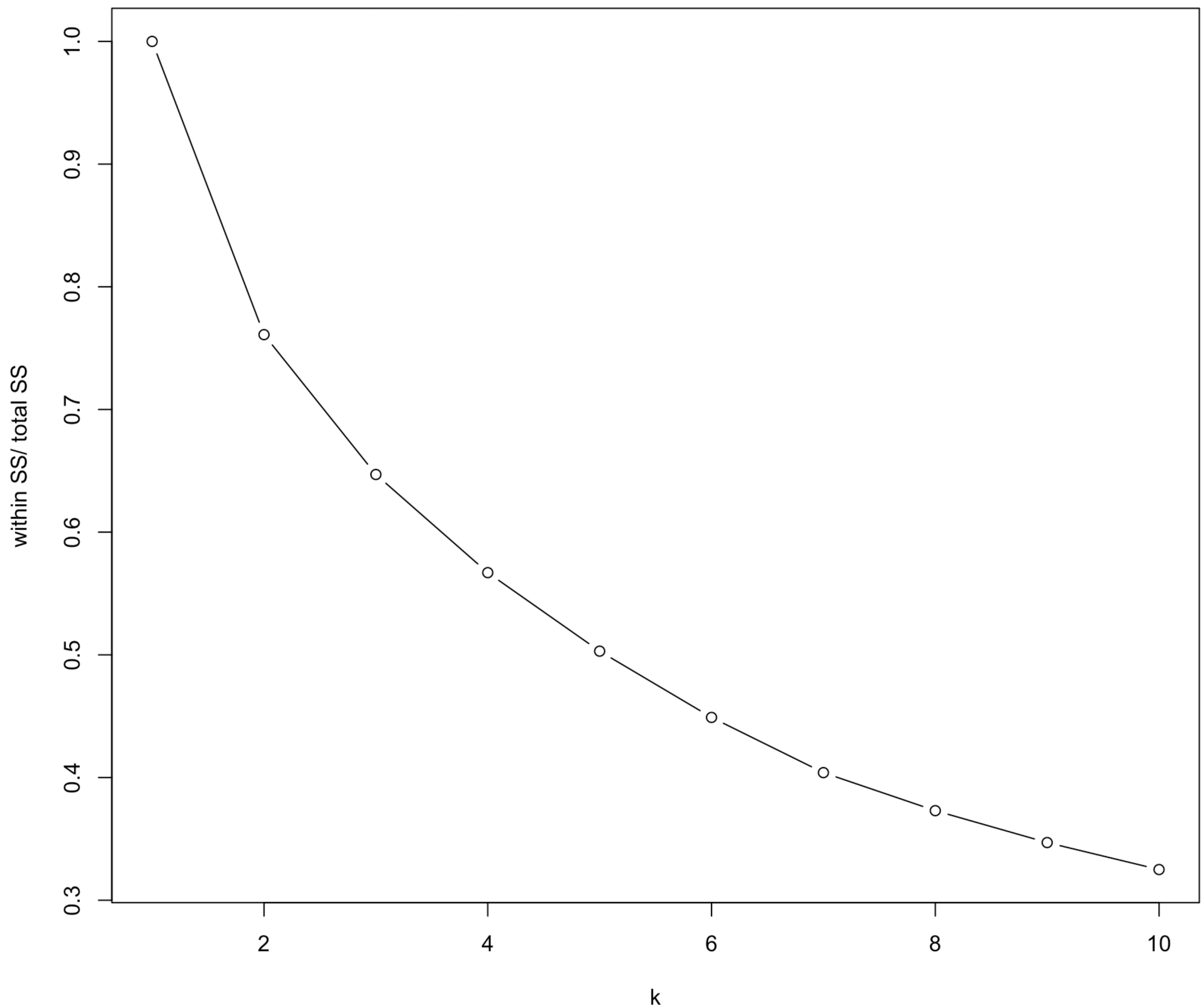
  plot ratio between SS / total SS by k

  plot ratio within SS / total SS by k

  find "elbow" (similar to scree plot for PCA)



ratio between SS / total SS by number of clusters
k-means



ratio within SS / total SS by number of clusters
k-means

- Max-p Regions Problem

    aggregation of n areas into an unknown maximum number (p) of homogenous regions

    each region satisfies a minimum threshold on a spatially extensive variable (e.g., population, area)

  - number of regions is endogenous

    data dictate shape of regions

    contiguity enforced, but not compactness

Problem Formulation

Parameters:

$$
\begin{aligned}
i, I &= \text{Index and set of areas, } I = \{1, \ldots, n\}\,; \\
k &= \text{index of } \textbf{potential} \text{ regions, } k = \{1, \ldots, n\}\,; \\
c &= \text{index of contiguity order, } c = \{0, \ldots, q\}\,, \text{ with } q = (n-1); \\
w_{ij} &= \begin{cases} 1, \text{ if areas } i \text{ and } j \text{ share a border, with } i, j \in I \text{ and } i \neq j \\ 0, \text{ otherwise;} \end{cases} \\
N_i &= \{j | w_{ij} = 1\}, \text{ the set of areas that are adjacent to area } i; \\
d_{ij} &= \text{dissimilarity relationships between areas} \\
&\qquad i \text{ and } j, \text{ with } i, j \in I \text{ and } i < j; \\
h &= 1 + \lfloor \log(\textstyle\sum_i \sum_{j|j>i} d_{ij}) \rfloor, \text{ which is the number of digits of the} \\
&\qquad \text{floor function of } \textstyle\sum_i \sum_{j|j>i} d_{ij}, \text{ with } i, j \in I; \\
l_i &= \text{spatially extensive attribute value of area } i, \text{ with } i \in I; \\
\text{threshold} &= \text{minimum value for attribute } l \text{ at regional} \\
&\quad\ \text{scale.}
\end{aligned}
$$

Decision variables:

$$
t_{ij} = \begin{cases} 1, & \text{if areas } i \text{ and } j \text{ belong to the same region } k, \text{ with } i < j \\ 0, & \text{otherwise;} \end{cases}
$$

$$
x_i^{kc} = \begin{cases} 1, & \text{if areas } i \text{ is assigned to region } k \text{ in order } c \\ 0, & \text{otherwise.} \end{cases}
$$

Problem Formulation (2)

Minimize:

$$Z = \left(- \sum_{k=1}^{n} \sum_{i=1}^{n} x_i^{k0} \right) * 10^h + \sum_{i} \sum_{j|j>i} d_{ij} t_{ij}.$$

Subject to:

(2) $$\sum_{i=1}^{n} x_i^{k0} \leq 1 \qquad \forall k = 1, \ldots, n;$$

(3) $$\sum_{k=1}^{n} \sum_{c=0}^{q} x_i^{kc} = 1 \qquad \forall i = 1, \ldots, n;$$

(4) $$x_i^{kc} \leq \sum_{j \in N_i} x_j^{k(c-1)} \qquad \forall i = 1, \ldots, n;\ \forall k = 1, \ldots, n;\ \forall c = 1, \ldots, q;$$

(5) $$\sum_{i=1}^{n} \sum_{c=0}^{q} x_i^{kc}\, l_i \geq \text{threshold} * \sum_{i=1}^{n} x_i^{k0} \qquad \forall k = 1, \ldots, n;$$

(6) $$t_{ij} \geq \sum_{c=0}^{q} x_i^{kc} + \sum_{c=0}^{q} x_j^{kc} - 1 \qquad \forall i, j = 1, \ldots, n | i < j;\ \forall k = 1, \ldots, n;$$

(7) $$x_i^{kc} \in \{0, 1\} \qquad \forall i = 1, \ldots, n;\ \forall k = 1, \ldots, n;\ \forall c = 0, \ldots, q;$$

(8) $$t_{ij} \in \{0, 1\} \qquad \forall i, j = 1, \ldots, n | i < j.$$

- Logic of Objective Function

  first term controls the number of regions

  second term controls pairwise dissimilarities

  first term dominates (scaling factor)

    solution with higher value of p will always be preferred over lower p in terms of dissimilarity

    for same value of p, solutions with lower heterogeneity are preferred

    avoids comparing heterogeneity between regions for different p

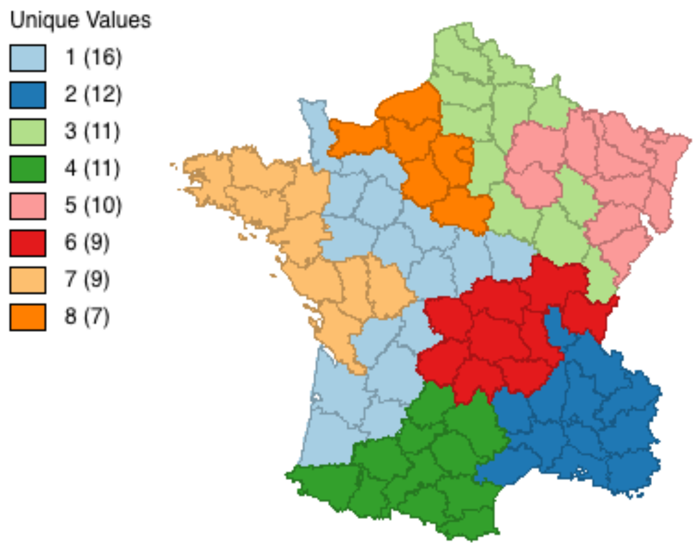
- Logic of Constraints

each region starts with a root area x_i^{k0} to which other areas are added that are contiguous

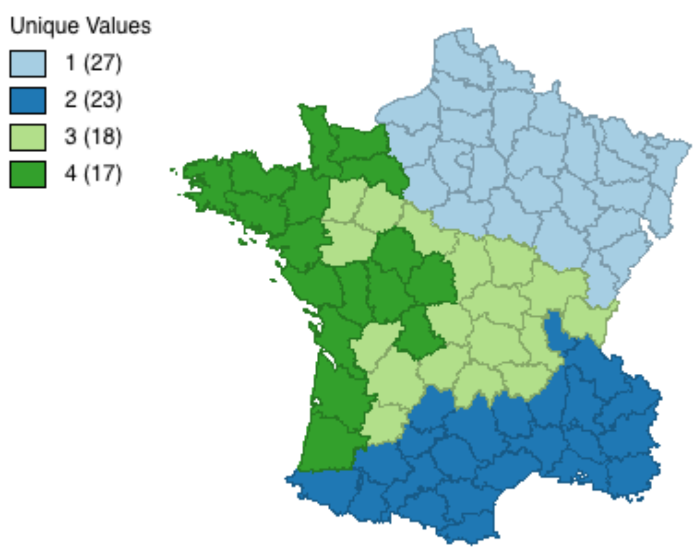
in each region, there can only be one area of a given order of contiguity to the root area

the spatially extensive variable summed over all areas in the region must meet the threshold

- Solution Strategies
    - mixed integer programming
        - exact solution impractical
    - heuristics
        - construction phase: set of feasible solutions
        - local search phase: iterative improvements
            - simulated annealing
            - tabu search
            - greedy algorithm

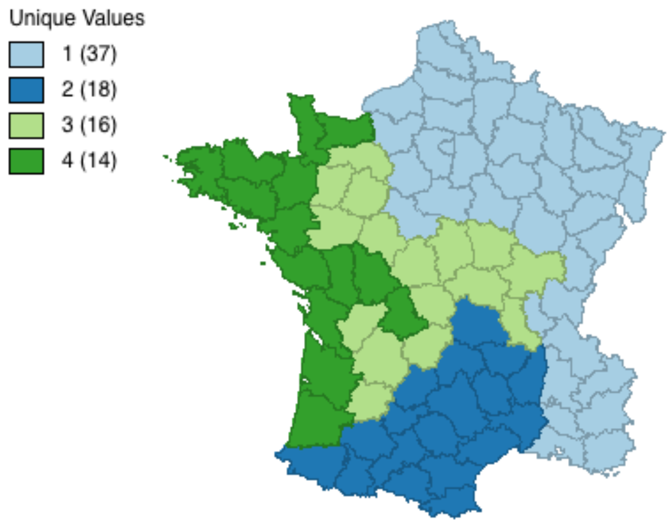


population threshold 10%
p = 8
bSS/tSS = 0.525

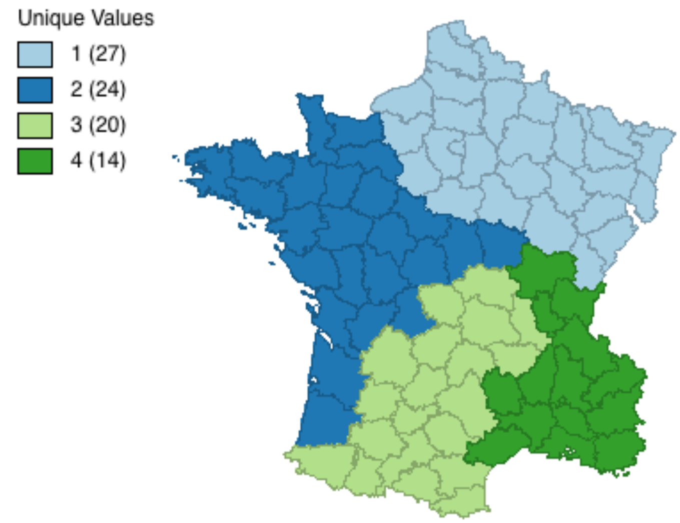


population threshold 20%
p = 4
bSS/tSS = 0.375

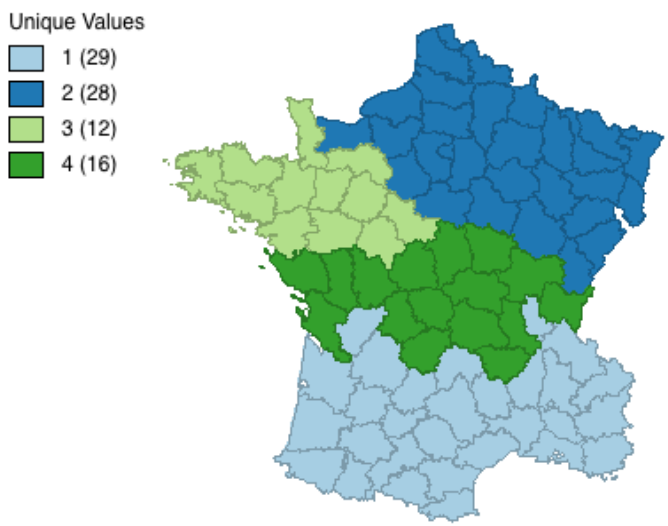
max p results



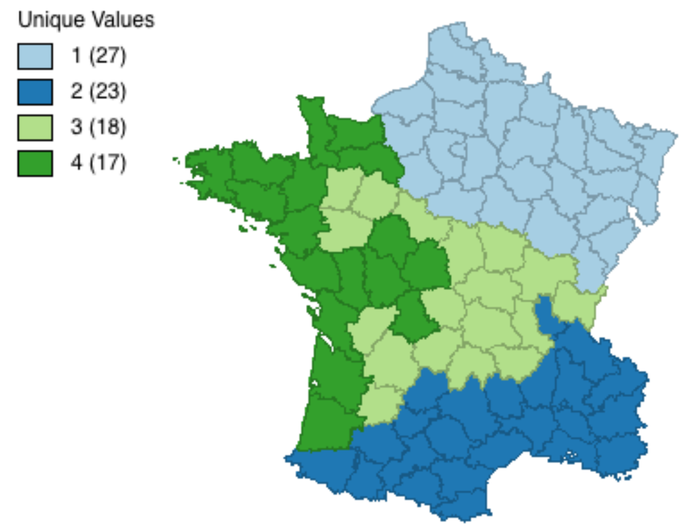
ad hoc — 0.375



centroids — 0.361



skater — 0.316



max p — 0.375

k-means 0.431

- Summary

  trade-off attribute similarity and locational similarity is complex

  no “best” approach

  no mechanical application of one approach

  sensitivity analysis is critical