

## TOWARDS COMBINATORIAL CLUSTERING: Preliminary Research Survey

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The paper describes clustering problems from the combinatorial viewpoint. A brief systemic survey is presented including the following: (i) basic clustering problems (e.g., classification, clustering, sorting, clustering with an order over cluster), (ii) basic approaches to assessment of objects and object proximities (i.e., scales, comparison, aggregation issues), (iii) basic approaches to evaluation of local quality characteristics for clusters and total quality characteristics for clustering solutions, (iv) clustering as multicriteria optimization problem, (v) generalized modular clustering framework, (vi) basic clustering models/methods (e.g., hierarchical clustering, k-means clustering, minimum spanning tree based clustering, clustering as assignment, detection of clique/quasi-clique based clustering, correlation clustering, network communities based clustering), Special attention is targeted to formulation of clustering as multicriteria optimization models.

Combinatorial optimization models are used as auxiliary problems (e.g., assignment, partitioning, knapsack problem, multiple choice problem, morphological clique problem, searching for consensus/median for structures).

Numerical examples illustrate problem formulations, solving methods, and applications. The material can be used as follows: (a) a research survey, (b) a fundamental for designing the structure/architecture of composite modular clustering software, (c) a bibliography reference collection, and (d) a tutorial.

*Keywords:* Clustering, Classification, Combinatorial optimization, Assignment, Multicriteria problems, Decision making, Heuristics, Composite problem frameworks, Applications, Applied artificial intelligence

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## 1. Introduction

Recently clustering/classification problems have been widely used in many domains (Table 1.1).

**Table 1.1.** Main application domains of clustering-like models/problems

| No. | Some applied domains   | Basic applied problem(s)  | Source(s)   |
|-----|--|---|---|
| 1.  | Design/analysis of information systems, information retrieval  | Document clustering/classification, design of hierarchy/ontology/menu, information retrieval  | [32,50,191,418]<br>[453,534,557,593]<br>[598,614,658]                             |
| 2.  | Web systems, web services  | Clustering of Web sites, design of hierarchical Web systems, search   | [67,74,75,85,202]<br>[418,534,550,652]  |
| 3.  | Data mining&knowledge discovery  | Detection of information objects, associations, rules, structures   | [55,137,199,255,262]<br>[265,279,435,446]   |
| 4.  | Medical/technical diagnostics, system testing, maintenance of systems  | Definition of solution classes, diagnostics (assignment/multiple assignment of patients/system components into solution classes), clustering of symptoms/faults, etc. | [214,215,282,341]<br>[369,394,422,488]<br>[565,602,632,665]                       |
| 5.  | Graph partitioning (network design, VLSI design, etc.)   | Grouping of graph vertices  | [19,26,181,218,254]<br>[320,328,582,625]  |
| 6.  | Cell formation in industrial/manufacturing systems   | Grouping of machines  | [122,228,537,555]   |
| 7.  | Anomaly detection (networks, distributed systems, etc.)  | Finding patterns in data that do not conform to expected behavior   | [93,211,487,659]  |
| 8.  | Computer vision (images/scenes, object trajectories)   | Clustering/segmentation of images, shape analysis, detection of events  | [302,310,542,556]<br>[620]  |
| 9.  | Trajectory clustering/classification (e.g., air-traffic control), system testing/maintenance, monitoring                 | Tracking; traces initialization/maintenance; classification/clustering/fusion of streams  | [54,104,213,247]<br>[277,360,365,389]<br>[392,399,400]                            |
| 10. | Chemistry, biology, gene expression data clustering in DNA microarray technology   | Classification/clustering of chemical objects (elements, structures), detection of natural structures, interesting patterns   | [3,35,252,124]<br>[172,306,415,443]<br>[521,522,535,611]<br>[613,641,626]         |
| 11. | Communication/sensor systems/networks, computer networks   | Management, clustering of nodes, clustering based routing, detection of cluster heads, design of hierarchical network   | [1,21,36,37]<br>[38,48,91,98]<br>[101,205,221,223]<br>[335,336,538,644]           |
| 12. | Management, planning, marketing, evaluation of economical objects (e.g., financial instruments, tasks, firms, countries) | Hierarchical management, design of management hierarchy, team design, segmentation of market, segmentation of customers   | [24,49,83,120,160]<br>[163,243,273,274]<br>[329,378,392,442]<br>[463,514,548,605] |
| 13. | Social sciences, political marketing, social network analysis, recognition of communities, econometrics, etc.            | Clustering of social/psychological objects, analysis of networks/hierarchies, evaluation, planning  | [46,176,169,237]<br>[266,395,438,470]<br>[474,507,594,609]                        |
| 14. | Education (evaluation, course design, cluster grouping, planning)  | Evaluation (students, courses), clustering of students, timetabling, educational data mining  | [57,80,113,133]<br>[220,456,499,511]<br>[512,513,616]                             |

The significance of clustering/classification is essentially increased, for example, in the following contemporary fields: data analysis, management and decision making, communication systems, engineering, chemistry, biomedicine, information retrieval, system monitoring, social sciences, network modeling and analysis (e.g., [9,37,98,153,224,302,435,443,518,508,557,666]) (Fig. 1.1).

In two recent decades, excellent well-known surveys and books on clustering problems and methods have been published (e.g., [302,435,623,624,666]). Many research publications including surveys and books are targeted to special clustering approaches, for example: clustering based on fuzzy data (e.g.,

[144,180]), support vector clustering (e.g., [53]), cross-entropy based clustering (e.g., [312,348]), online clustering (e.g., [43,54,92,360]), dynamic clustering (e.g., [48,104]), consensus clustering (e.g., [124,245]), graph-based clustering (e.g., [196,236,340]), clustering ensembles (e.g., [597,224,278]), clustering based on hesitant fuzzy information (e.g., [110,656]), multicriteria clustering (e.g., [156]), correlation clustering (e.g., [159]).

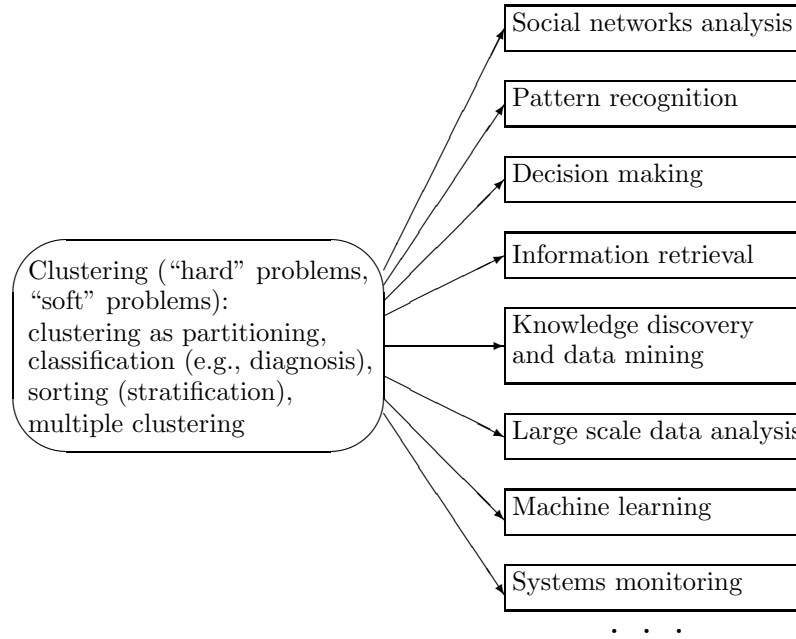


Fig. 1.1. Clustering as basic support problem

In recent decade, the significance of combinatorial approaches to clustering have been increased. In Table 1.2, some research efforts in combinatorial approaches to clustering are pointed out.

This material contains an author’s “architectural” engineering glance to combinatorial clustering problems. A special attention is targeted to formulation of clustering problems as multicriteria optimization models which are based on usage of various quality parameters for clustering solutions (e.g., clusterings as partitions, hierarchical clusterings). Combinatorial optimization models are used as auxiliary problems (e.g., partitioning, assignment, knapsack problem, multiple choice problem, matching problem).

In recent years, various fuzzy clustering methods have been widely studied and used (e.g., [42,109,110,180,238,287,302,330,347,440,467,529,628,656]) and these approaches are not considered in the material.

The presented materials can be useful for educational courses and student projects in computer science, engineering, management, social sciences applications (e.g., [377,380,382]).

**Table 1.2.** Combinatorial approaches to clustering

| No.    | Approaches, algorithmic schemes                      | Source(s)                         |
|--------|--|-----------------------------------|
| 1.     | Some surveys:  |                                   |
| 1.1.   | General  | [218,302,437]                     |
| 1.2.   | Graph clustering                                     | [533]                             |
| 1.3.   | Approximate graph partitioning                       | [189]                             |
| 1.4.   | Cross-entropy method for clustering, partitioning    | [348,520,568]                     |
| 1.5.   | Cell formation (in industrial engineering)           | [228,537,555]                     |
| 1.6.   | Clustering ensemble algorithms                       | [597]                             |
| 1.7.   | Multicriteria classification and sorting methods     | [518,666]                         |
| 2.     | Basic combinatorial optimization problems:           |                                   |
| 2.1.   | Minimal spanning tree approach                       | [244,445,479,492,582,606,626,660] |
| 2.2.   | Partitioning based clustering                        | [26,67,134,166,189,554]           |
| 2.3.   | Assignment/location based clustering                 | [227]                             |
| 2.4.   | Graph matching                                       | [534]                             |
| 2.5.   | Dominant set based clustering                        | [101,263,400,489,643]             |
| 2.6.   | Covering based clustering                            | [9,446,525]                       |
| 2.7.   | Clique based clustering                              | [9,55,81,176,236,340,539]         |
| 2.8.   | Structural clustering (detection of communities)     | [7,459,461,496,625]               |
| 3.     | Correlation clustering                               | [4,40,159,345,564]                |
| 4.     | Graph-based data clustering with overlaps            | [196]                             |
| 5.     | Segmentation problems                                | [334]                             |
| 6.     | Cluster graph modification problems                  | [539,540]                         |
| 7.     | Multi-criteria decision making in clustering-sorting | [214,508,509,666]                 |
| 8.     | Consensus clustering:                                |                                   |
| 8.1.   | Voting-based consensus of cluster ensembles          | [28,522]                          |
| 8.2.   | Consensus partitions                                 | [245]                             |
| 9.     | Algorithmic schemes:                                 |                                   |
| 9.1.   | Enumerative methods:                                 |                                   |
| 9.1.1. | Branch-and-bound methods                             | [111]                             |
| 9.1.2. | Dynamic programming                                  | [640]                             |
| 9.2.   | Local optimization heuristics:                       |                                   |
| 9.2.1. | Simulated annealing algorithms                       | [78,471,536]                      |
| 9.2.2. | Tabu search algorithms                               | [471,561]                         |
| 9.2.3. | Ant colonies algorithms                              | [311,637]                         |
| 9.2.4. | PSO methods  | [102,577,592]                     |
| 9.2.5. | Variable neighborhood search                         | [268,269,270,271]                 |
| 9.3.   | Genetic algorithms, evolutionary strategies          | [30,142,288,477,587]              |
| 9.4.   | Hyper-heuristic approach                             | [129,352,586]                     |

## 2. General Preliminary Glance

### 2.1. Preliminaries

From the structured viewpoint, the following basic clustering problem formulations can be pointed out [153,171,224,231,275,300,302,321,342,343,434,435,443,447,509,518,666]: (i) set partitioning clustering (Fig. 2.1), (ii) classification (i.e., solution classes are predefined as in diagnostics) (Fig. 2.2), (iii) sorting (group ranking, stratification) problem (the obtained clusters are linear ordered) (Fig. 2.3), (iv) hierarchical clustering (Fig. 2.4), (v) multiple clustering (i.e., obtaining  $n$  different clustering solutions while taking into account  $n$  goals/models; alternative clustering) (Fig. 2.5), and (vi) consensus clustering (aggregation of clustering solutions; clustering ensembles) (Fig. 2.6).

Table 2.1 contains initial data for an illustrative numerical example: (a list of item/students and their skill estimates upon parameters/criteria): (1) formal approaches, modeling (i.e., mathematics, physical modeling)  $C_1$ , (2) applied computer science, computing (i.e., software development, software implementation, computing)  $C_2$ , (3) engineering science domain (i.e., information transmission, radio channels, antenna devices, sender/receiver devices, networking)  $C_3$ , (4) measurement radio techniques  $C_4$ , and (5) preparation of the technical documentations (reports, papers, presentations)  $C_5$ . Here ordinal scale [3, 4, 5] is used: excellent (“5”), good (“4”), sufficient (“3”).

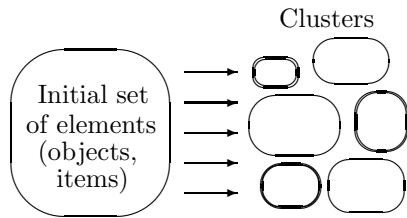


Fig. 2.1. Clustering as partitioning

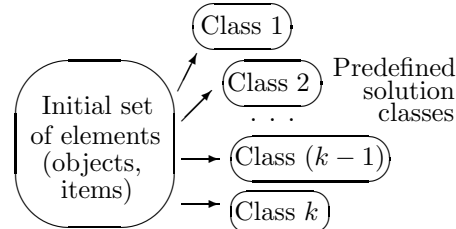


Fig. 2.2. Classification problem

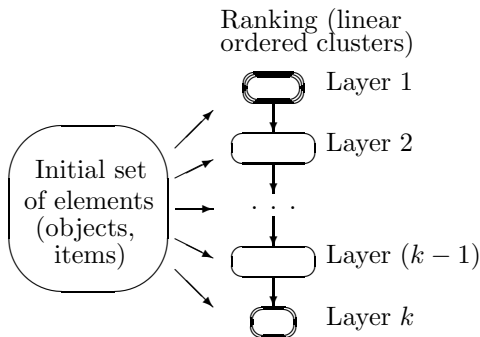


Fig. 2.3. Sorting (stratification) problem

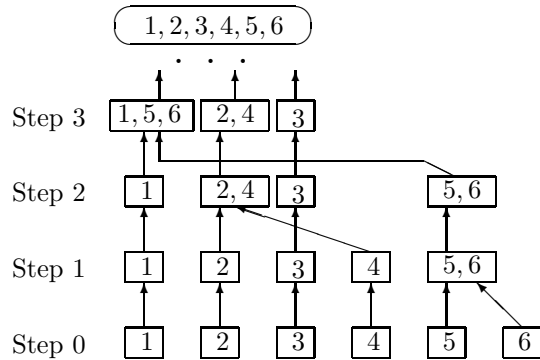


Fig. 2.4. Example of hierarchical clustering

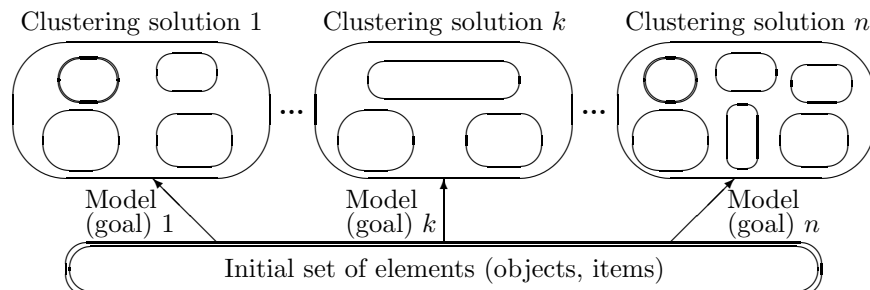


Fig. 2.5. Illustration for multiple clustering

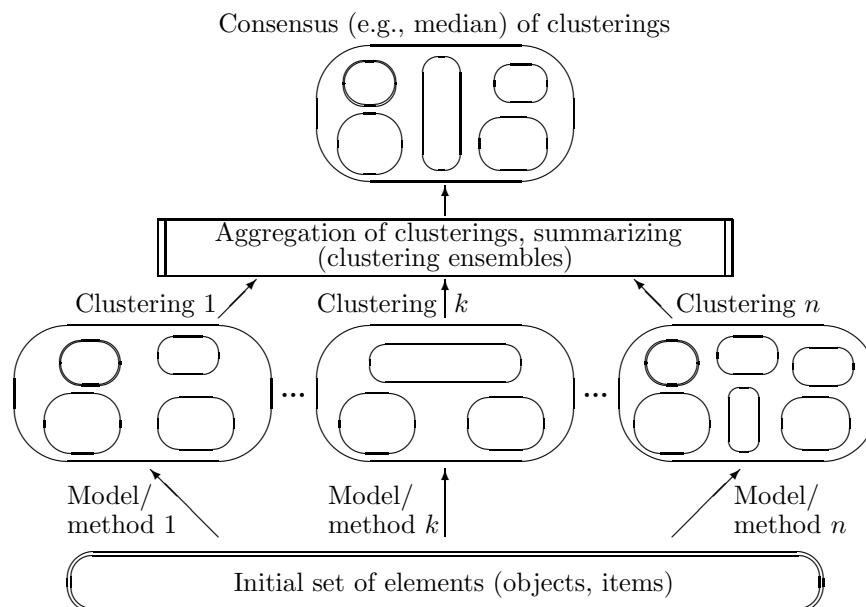


Fig. 2.6. Illustration for consensus clustering, summarizing

This numerical example illustrates the pointed out 5 types of clustering problems on the basis of the same initial data (Table 2.2, for 12 students): (i) clustering as partitioning (Fig. 2.7a), (ii) classification problem (“soft” problem formulation) (Fig. 2.7b), (iii) sorting problem (stratification, multicriteria ranking) (Fig. 2.7c), (iv) hierarchical clustering (Fig. 2.8), and (v) consensus clustering (Fig. 2.9). Note, consensus clustering is based on three initial clustering solutions:

- (a) five clusters (from partitioning problem, Fig. 2.7a):  $\{6, 9, 10\}$ ,  $\{1, 8, 3\}$ ,  $\{2, 5, 7, 11\}$ ,  $\{12, 14\}$ ,  $\{3, 4\}$ ;
- (b) four clusters (from sorting problem, Fig. 2.7c):  $\{6, 9\}$ ,  $\{1, 3, 10\}$ ,  $\{4, 8, 13, 14\}$ ,  $\{2, 5, 7, 11, 12\}$ ;
- (c) four clusters (from hierarchical clustering, Fig. 2.8):  $\{6, 9, 10\}$ ,  $\{1, 3\}$ ,  $\{4, 8, 13, 14\}$ ,  $\{2, 5, 7, 11, 12\}$ .

In recent decade, the significance of the fifth type of clustering problem has been increased: network clustering (e.g., detection of community structures) (Fig. 2.10). Here initial information consists in description of network: i.e., set of vertices/nodes and set of edges. Weights of vertices and/or edges can be used as well.

**Table 2.2.** Items, estimates upon criteria

| Item (student) | $C_1$ | $C_2$ | $C_3$ | $C_4$ | $C_5$ |
|----------------|-------|-------|-------|-------|-------|
| Student 1      | 4     | 4     | 5     | 5     | 4     |
| Student 2      | 3     | 3     | 3     | 4     | 3     |
| Student 3      | 4     | 4     | 4     | 5     | 4     |
| Student 4      | 5     | 4     | 4     | 3     | 5     |
| Student 5      | 3     | 3     | 3     | 4     | 3     |
| Student 6      | 5     | 5     | 5     | 5     | 5     |
| Student 7      | 3     | 3     | 3     | 4     | 3     |
| Student 8      | 4     | 3     | 4     | 4     | 3     |
| Student 9      | 5     | 5     | 5     | 5     | 5     |
| Student 10     | 5     | 5     | 5     | 4     | 5     |
| Student 11     | 3     | 3     | 3     | 5     | 3     |
| Student 12     | 3     | 5     | 3     | 3     | 3     |
| Student 13     | 5     | 3     | 4     | 3     | 3     |
| Student 14     | 3     | 5     | 3     | 5     | 4     |

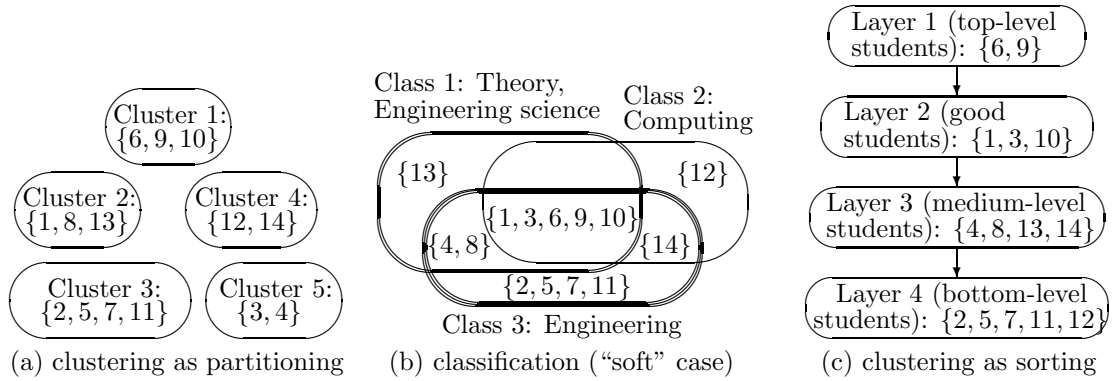


Fig. 2.7. Numerical examples of clustering/classification problems

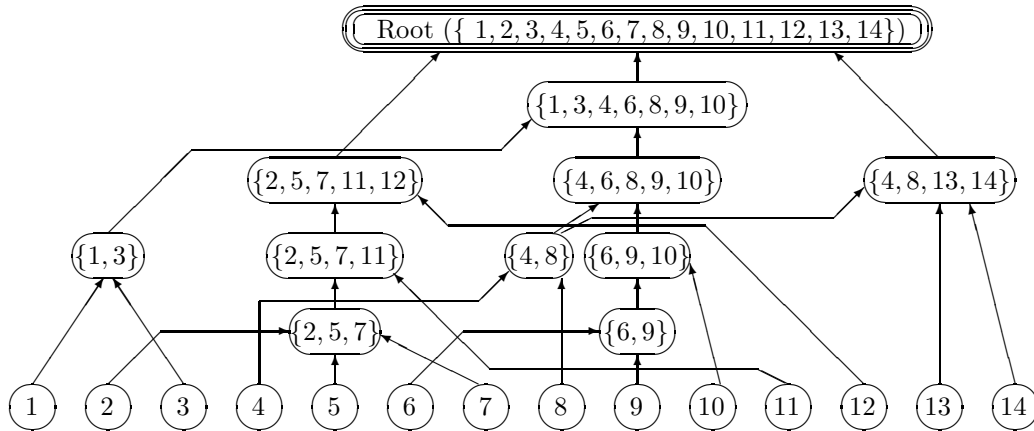


Fig. 2.8. Numerical example of hierarchical clustering

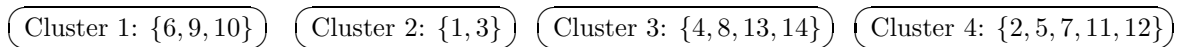


Fig. 2.9. Illustrative numerical example of consensus clustering ("median" clustering solution)

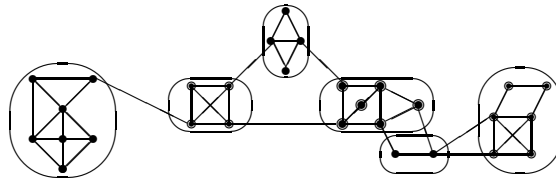


Fig. 2.10. Illustration for network clustering

A generalized scheme of clustering processes consists of the following [22,182,275,300,302,354,435,509, 623,624] (Fig. 2.11):

- Phase 1.* Collection of initial data on the applied situation.
- Phase 2.* Analysis of applied situation(s) and formulation/structuring of clustering problem:
  - (2.1.) generation/detection and description of initial objects/elements;
  - (2.2.) generation/detection of element parameters (i.e., feature selection or extraction);
  - (2.3.) selection/design of proximity measures (for elements, for clusters) and types for inter-cluster criterion and for intra-cluster criterion; and
  - (2.4.) selection of basic clustering model(s) (i.e., hierarchical clustering, partitioning clustering).
- Phase 3.* Selection/design of clustering solving scheme (solving method/procedure).
- Phase 4.* Implementation of clustering procedure(s).
- Phase 5.* Analysis of clustering solution(s) (i.e., clusters validation).



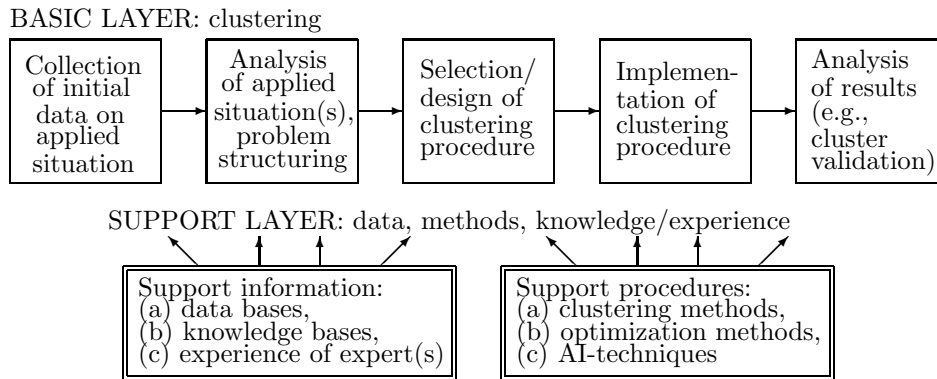


Fig. 2.11. System two-layer scheme for clustering

Fig. 2.12 depicts a structural description for main machine learning paradigms (e.g., [222,313,343, 441,563,607,595]): (a) unsupervised learning, (b) reinforcement learning, and (c) supervised learning. Basic clustering problems/models corresponds to unsupervised learning. Evidently, in complex cases, it is possible to analyze clustering results to correct the clustering solving process (i.e., as in reinforcement learning or in supervised learning).

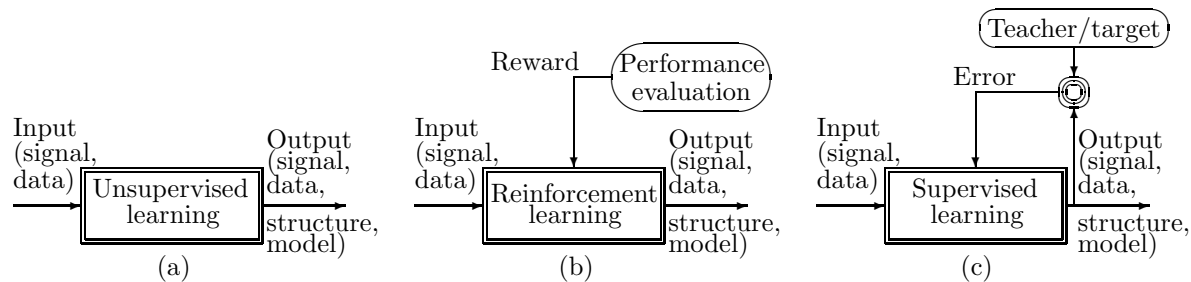


Fig. 2.12. Three learning paradigms [607]

## 2.2. Objects, evaluation, problems

### 2.2.1. Examined objects, parameters

It is reasonable to point out the basic examined objects:

1. item (i.e., element, point),
2. set of items (e.g., initial set of items),
3. subset of items, cluster (e.g., a subset of initial items),
4. clustering solution as partitioning of the initial item set into set of clusters, and
5. clustering solution and an order over its clusters:
  - 5.1. linear order over the clusters (sorting problem),
  - 5.2. hierarchy over the clusters,
  - 5.3. poset over the clusters.

Significant auxiliary problems consist in measurement of proximity for pair of objects: 1. item and item, 2. item and cluster, 3. cluster and cluster, 4. clustering solution and clustering solution, 5. order over clusters and order over clusters, and 6. clustering solution, order over its clusters and clustering solution, order over its clusters.

In recent years, a special research attention is targeted to aggregation of clustering solutions and evaluation of the obtained aggregated clustering solution(s).

Generally, basic problem types, parameters, and criteria are pointed out in Table 2.2 (e.g., [7,6,25,148, 177,229,300,302,333,375,430,435,452,458,459,461,501,502,594,601,623,624,625,648]).

**Table 2.2.** Basic parameters in clustering/classification problems

| No.     | Parameters, requirements  | Description(s) (e.g., type, evaluation scale)   |
|---------|---|---|
| I.      | Elements (items/objects):   |   |
| 1.1.    | Type of element(s)  | One-type/multi-type element(s), whole element(s) or structured/composite element(s)   |
| 1.2.    | Description of element  | Quantitative, nominal, ordinal estimate(s); fuzzy, multiset estimates, vector estimates, binary relation(s) over elements   |
| 1.3.    | Proximity for elements pair   | Metric/proximity, ordinal estimate, fuzzy estimate, multiset estimate, vector estimate  |
| 1.4.    | Proximity between element and element set (e.g., cluster)   | Metric/proximity, ordinal estimate, fuzzy estimate, multiset estimate, vector estimate  |
| 1.5.    | Proximity between element set and element set (e.g., two clusters)  | Metric/proximity, ordinal estimate, fuzzy estimate, multiset estimate, vector estimate  |
| II.     | Clusters/classes (clustering solution):   |   |
| 2.1.    | Definition type for clusters/classes  | 1.Predefined clusters (classification problem)<br>2.Clusters are defined under solving process (clustering problem)   |
| 2.2.    | Constraints for clusters  | Number of clusters, number of cluster elements  |
| 2.3.    | Order over clusters/classes (binary relation(s))  | Independent clusters, linear order/chain, ranking (layered structure), hierarchy (e.g., tree), poset  |
| 2.4.    | Clustering solution validity:   | Quality, correspondence to requirements, etc.   |
| 2.4.1   | Basic criteria (e.g., [6,177,502,648]):   |   |
| 2.4.1.1 | Compactness (minimization):<br>(i) intra-cluster “distance”,<br>(ii) object positioning.  | Uniqueness of objects in each cluster:<br>e.g., closeness to cluster centroid in cluster, maximum distance between objects in each cluster, closeness of object to cluster centroid<br>“good” correspondence of object to cluster |
| 2.4.1.2 | Isolation or separability (maximization):<br>inter-cluster “distance”   | Well-separated clusters: e.g., maximum distances between cluster centroids  |
| 2.4.1.3 | General (maximization):<br>(i) number of correctly positioned objects,<br>(ii) number of “good” clusters (Fig. 2.13),<br>(iii) connectedness. |   |
| 2.4.2   | Quality of structure over clusters  | similar objects are neighboring<br>Similarity to predefined structure   |
| 2.5.    | Modularity (community structure based network clustering, Fig. 2.14 [7,459,496])  | Maximization  |
| III.    | Fuziness/softness of problem/model:   |   |
| 3.1.    | Hard problem  | Assignment of each item to the only one cluster   |
| 3.2.    | Fuzzy/soft problem  | Assignment of each item to many clusters  |
| IV.     | Problem time mode:  |   |
| 4.1.    | Off-line (statical) mode  | Collection of initial data and processing   |
| 4.2.    | On-line mode (dynamics)   | On-line processing (e.g., stream data)  |
| V.      | Complexity of clustering process:   |   |
| 5.1.    | Algorithmic complexity  | Estimate  |
| 5.2.    | Volume of required data   | Estimate of required data   |
| 5.3.    | Volume of required expert’s work  | Estimate of expert/expert knowledge   |

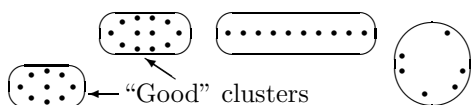


Fig. 2.13. Illustration for “good” clusters

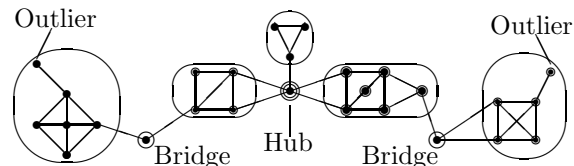


Fig. 2.14. Illustration for community structures

### 2.2.2. Basic scales

Usually, the following main approaches (i.e., scales, types of estimates) for assessment of vector component (i.e.,  $x_i, i = \overline{1, m}$ ) are used (e.g., [275,300,302,375,392,435,623,624]): (i) quantitative estimate (Fig. 2.15a), (ii) ordinal estimate (Fig. 2.15b), (iii) nominal estimate, (iv) poset-like scale (Fig. 2.15c), (v) fuzzy estimate, (vi) multiset based scales: (a) multiset estimate for evaluation of composite system (Fig. 2.16, [372,374,386,392]), (b) interval multiset estimate [386,392], and (vii) vector-like estimate (i.e., multicriteria description) (e.g., [374,392]). Here, traditional fuzzy estimates and hesitant fuzzy estimates are not considered (e.g., [110,628,647,656]).

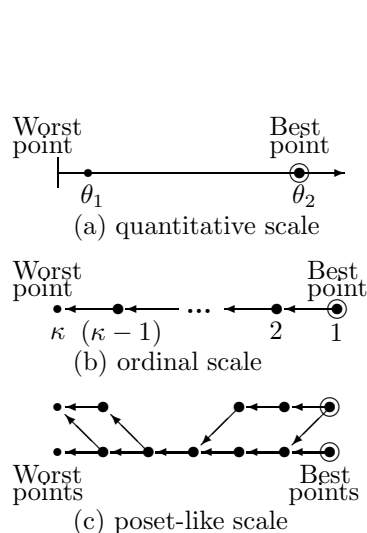


Fig. 2.15. Illustration for scales

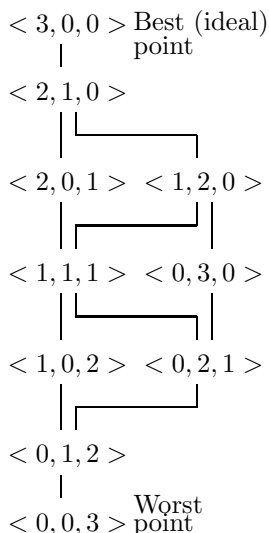


Fig. 2.16. Multiset based scale

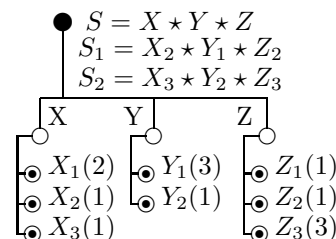


Fig. 2.17. 3-component system

Some fundamentals of multisets and comparison of sets and multisets have been described in ([260,338, 629]). Our brief description of multiset estimates is the following (e.g., [372,374,386,392]). The approach consists in assignment of elements  $(1, 2, 3, \dots)$  into an ordinal scale  $[1, 2, \dots, l]$ . As a result, a multiset based estimate is obtained, where a basis set involves all levels of the ordinal scale:  $\Omega = \{1, 2, \dots, l\}$  (the levels are linear ordered:  $1 \succ 2 \succ 3 \succ \dots$ ) and the assessment problem (for each alternative) consists in selection of a multiset over set  $\Omega$  while taking into account two conditions:

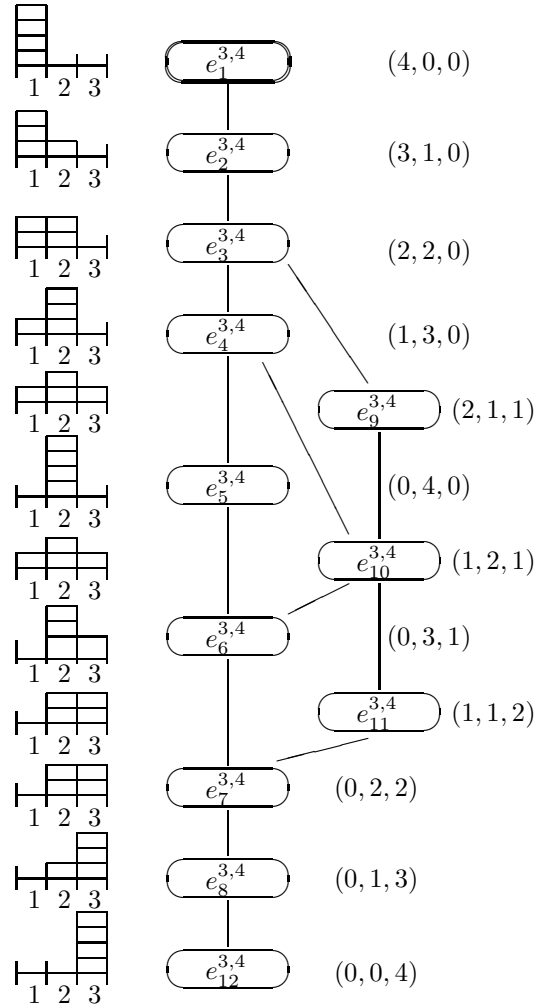
1. cardinality of the selected multiset equals a specified number of elements  $\eta = 1, 2, 3, \dots$  (i.e., multisets of cardinality  $\eta$  are considered);
2. “configuration” of the multiset is the following: the selected elements of  $\Omega$  cover an interval over scale  $[1, l]$  (i.e., “interval multiset estimate”).

Thus, an estimate  $e$  for an alternative  $A$  is (scale  $[1, l]$ , position-based form or position form):  $e(A) = (\eta_1, \dots, \eta_l, \dots, \eta_l)$ , where  $\eta_\iota$  corresponds to the number of elements at the level  $\iota$  ( $\iota = \overline{1, l}$ ), or  $e(A) = \{\underbrace{1, \dots, 1}_{\eta_1}, \underbrace{2, \dots, 2}_{\eta_2}, \underbrace{3, \dots, 3}_{\eta_3}, \dots, \underbrace{l, \dots, l}_{\eta_l}\}$ . The number of multisets of cardinality  $\eta$ , with elements taken from a finite set of cardinality  $l$ , is called the “multiset coefficient” or “multiset number” ([338,629]):  $\mu^{l, \eta} = \frac{l(l+1)(l+2)\dots(l+\eta-1)}{\eta!}$ . This number corresponds to possible estimates (without taking into account interval condition 2). The basic multiset estimate (i.e., without taking into account condition 2) can be used as integration of ordinal estimates to obtain a resultant estimate for a composite system (when system components are evaluated via ordinal scale  $[1, 2, 3]$ ) (e.g., [372,374,392]) (Fig. 2.16, Fig. 2.17).

In the case of condition 2 (i.e., interval multiset estimate), the number of estimates is decreased. Generally, assessment problems based on interval multiset estimates can be denoted as follows:  $P^{l, \eta}$ . A poset-like scale of interval multiset estimates for assessment problem  $P^{3,4}$  is presented in Fig. 2.18. Calculation of multiset estimate is based on transformation of vector ordinal estimate. An illustrative numerical example for obtaining multiset vector estimate is the following:

$$\bar{x} = (0, 3, 1, 0, 2, 1) \implies e(\bar{x}) = (e_o, e_1, e_2, e_3) = (2, 2, 1, 1),$$

where  $e_k$  equals the number of ordinal estimate  $k$  in ordinal vector estimate  $\bar{x}$ .

Fig. 2.18. Scale, estimates ( $P^{3,4}$ ) [386,392]

Brief descriptions of the scales above and their transformations (e.g., mapping, integration) are presented in [386,390,392]. The basic types of operations over estimates above are the following (Table 2.3) (e.g., [390,392]):

1. transformation of an estimate (including transformation into an estimate of another type),
2. calculation the difference (distance/proximity) for two estimates,
3. integrations (e.g., summarization, average estimate or median-like estimate).

A basic approach to integration of qualitative estimates (including vector qualitative estimates) consists in summarization or calculation of an average value. On the other hand, integration of ordinal estimates, poset-like estimates, and multiset estimates (i.e., “structural” estimates) is usually considered as calculation of a median-like estimate (i.e., as agreement/consensus structure). This kind of problems is formulated as an optimization (or multicriteria optimization) (e.g., [372,384,392]). Sometimes, the resultant integrated estimate can be considered as a “fuzzy” structure (e.g., interval-like integrated ranking for integration of rankings in [372,392]).

The above-mentioned operations (integration as summarization, calculation of proximity, calculation of a median estimate) for multiset estimates are presented in [386,392].

**Table 2.3.** Basic operations over estimate(s)

| No. | Type of initial estimate(s) | Transformation of estimate (resultant estimate)     | Difference (proximity) of two estimates (resultant estimate) | Integration of several estimates (resultant estimate)                  |
|-----|-----------------------------|---|--|--|
| 1.  | Quantitative                | 1.Qualitative<br>2.Ordinal                          | 1.Quantitative<br>2.Ordinal                                  | 1.Quantitative (average value)<br>2.Vector estimate                    |
| 2.  | Ordinal                     | 1.Ordinal   | 1.Ordinal  | 1.Ordinal (average/median)<br>2.Vector estimate<br>3.Multiset estimate |
| 3.  | Nominal                     | 1.Nominal   | 1.Ordinal  | 1.Vector estimate  |
| 4.  | Vector                      | 1.Vector<br>2.Ordinal<br>3.Multiset                 | 1.Qualitative<br>2.Ordinal<br>3.Vector                       | 1.Vector (average/median)  |
| 4.  | Poset-like                  | 1.Poset-like<br>2.Vector<br>3.Multiset<br>4.Ordinal | 1.Qualitative<br>2.Ordinal<br>3.Vector                       | 1.Poset-like (average/median)<br>2.Multiset                            |
| 5.  | Multiset                    | 1.Multiset<br>2.Ordinal                             | 1.Ordinal<br>2.Multiset<br>3.Vector                          | 1.Multiset (average/median)  |

### 2.2.3. Assessment/evaluation problems

Generally, the following measurement approaches are under examination (for solutions as clustering, ranking, consensus clustering, and their components): 1. metrics/proximities: (i) for objects/clusters, (ii) for orders over clusters, (iii) for clustering solutions; 2. total measures for clustering solution(s) (total quality); 3. measure for an aggregation structure (i.e., median, consensus, agreement structure, covering structure). Table 2.4 involves a list of basic types of the assessment/evaluation problems.

### 2.2.4. Calculation of objects/clusters proximities

The initial set of items (objects) under examination is  $A = \{a_1, \dots, a_j, \dots, a_n\}$ . There are  $m$  parameters of  $x \in A$  and vector estimate  $\bar{x} = (x_1, \dots, x_1, \dots, x_m)$  (Fig. 2.19). Here, the following cases of metrics/proximities for objects/clusters are considered:

*Case 1.* objects/points - object/point (Fig. 2.20, Fig. 2.21a).

*Case 2.* object - cluster (subset) (Fig. 2.21b).

*Case 3.* Intra-cluster proximity (distance): for all elements in cluster.

*Case 4.* Inter-cluster proximity (distance): cluster - cluster (Fig. 2.21c).

Further, the above-mentioned cases are examined.

#### Case 1. Metrics/proximity for two objects (points) (Fig. 2.20, Fig. 2.21a).

Two objects are examined while taking into account  $m$  parameters (criteria): (i) the first object  $x \in A$ : vector estimate  $\bar{x} = (x_1, \dots, x_i, \dots, x_m)$ , (ii) the second object  $y \in A$ : vector estimate  $\bar{y} = (y_1, \dots, y_i, \dots, y_m)$ . Here,  $x_i, y_i$  ( $i = \overline{1, m}$ ) are real numbers. The basic types of proximities/distances (as an integration of vector-like difference between vector element estimate upon quantitative scales) between two objects  $x$  and  $y$  ( $D(x, y)$ ) are the following (e.g., [231,275,300,302,321,343,392,434,435,490,623,624,666]):

1. Euclidean distance:  $D(x, y) = [ \sum_{i=1}^m |x_i - y_i|^2 ]^{1/2}$ .

2. Minkowski distance:  $D^{mink}(x, y) = [ \sum_{i=1}^m |x_i - y_i|^r ]^{1/r}$  ( $r > 0$ ).

3. Manhattan distance:  $D^{manh}(x, y) = \sum_{i=1}^m |x_i - y_i|$ .

4. Tchebyshev distance:  $D^{cheb}(x, y) = \max_{i \in \{1, \dots, m\}} |x_i - y_i|$ .

5. Canberra distance:  $D^{can}(x, y) = \sum_{i=1}^m \frac{|x_i - y_i|}{|x_i + y_i|}$  ( $x_i > 0$  and  $y_i > 0$ ).

6. Vector proximity:  $\overline{D(x, y)} = (|x_1 - y_1|, \dots, |x_i - y_i|, \dots, |x_m - y_m|)$ ;

7. Ordinal estimate (for example, scale [0, 1, 2, 3, 4]: 0 corresponds to the same objects or equivalent ones, 1 corresponds to the “very close” objects, 2 corresponds to the “close” objects, 3 corresponds to

the “different” objects, 4 corresponds to the “very different” objects).

**Table 2.4.** Assessment/evaluation problems

| No. | Analyzed object(s)  | Goal  | Approach   | Estimate type (scales)  |
|-----|---|---|--|---|
| 1.  | Element (item)  | Description   | Assessment<br>(e.g., expert,<br>statistics)            | Quantitative, ordinal,<br>nominal, fuzzy, multiset,<br>vector |
| 2.  | Two elements/items  | Proximity/distance  | Calculation  | Quantitative, ordinal,<br>fuzzy, multiset, vector             |
| 3.  | Element,<br>cluster (subset)  | Proximity/distance  | Calculation  | Quantitative, ordinal,<br>fuzzy, multiset, vector             |
| 4.  | Two clusters<br>(subsets)   | Proximity/distance  | Calculation  | Quantitative, ordinal,<br>fuzzy, multiset, vector             |
| 5.  | All elements of<br>cluster (subset)   | Intra-cluster proximity<br>(quality of cluster as<br>element proximity)                         | Calculation  | Quantitative, ordinal,<br>fuzzy, multiset, vector             |
| 6.  | All elements in all<br>clusters (clustering<br>solution)                                    | Total intra-cluster<br>proximity (generalized<br>element proximity<br>in all clusters)          | Calculation  | Quantitative, ordinal,<br>fuzzy, multiset, vector             |
| 7.  | All clusters of<br>clustering solution  | Inter-cluster proximity<br>(quality of solution as<br>integrated proximity<br>between clusters) | Calculation  | Quantitative, ordinal,<br>fuzzy, multiset, vector             |
| 8.  | Clustering solution   | Criteria, requirements/<br>constraints  | Constraint<br>satisfaction/<br>optimization            | Quantitative, ordinal,<br>fuzzy, multiset, vector             |
| 9.  | Two rankings (two<br>sorting solutions)   | Proximity/distance  | Calculation  | Quantitative, ordinal,<br>fuzzy, multiset, vector             |
| 10. | Ranking (sorting)<br>solution   | Proximity to standard<br>solution, correspon-<br>dence to requirements<br>(quality of solution) | Constraint<br>satisfaction/<br>optimization<br>problem | Quantitative, ordinal,<br>fuzzy, multiset, vector             |
| 11. | Two hierarchies (e.g.,<br>trees) over clusters  | Proximity/distance  | Calculation  | Quantitative, ordinal,<br>fuzzy, multiset, vector             |
| 12. | Hierarchy over<br>clusters (solution)   | Proximity to standard<br>solution, correspon-<br>dence to requirements                          | Constraint<br>satisfaction/<br>optimization            | Quantitative, ordinal,<br>fuzzy, multiset, vector             |
| 13. | Aggregated item(s):<br>“median item/set”,<br>“center”, covering<br>object (e.g., ellipsoid) | Quality of aggregated<br>item(s) (value,<br>vector)   | Calculation  | Quantitative, ordinal,<br>fuzzy, multiset, vector             |
| 14. | Consensus clustering<br>(median/agreement)  | Quality of consensus<br>solution (value,<br>vector)   | Constraint<br>satisfaction/<br>optimization            | Quantitative, ordinal,<br>fuzzy, multiset, vector             |
| 15. | Consensus ranking/<br>sorting solution  | Quality of consensus<br>solution (value,<br>vector)   | Constraint<br>satisfaction/<br>optimization            | Quantitative, ordinal,<br>fuzzy, multiset, vector             |
| 16. | Consensus hierarchi-<br>cal clustering<br>solution  | Quality of consensus<br>solution  | Constraint<br>satisfaction/<br>optimization            | Quantitative, ordinal,<br>fuzzy, multiset, vector             |

8. Fuzzy estimate of object proximity and/or vector fuzzy estimate of object proximity. Fuzzy estimates are widely used in clustering methods (e.g., [42,109,180,238,287,302,330,347,440,467,529]) including clustering based on hesitant fuzzy estimates (e.g., [110,628,656]) (here they are not considered).

9. Multiset estimate of object proximity [386,392].

10. Angular separation (e.g., [490], Fig. 2.20):  $D^{angular}(x, y) = \frac{\sum_{i=1}^m x_i y_i}{[\sum_{i=1}^m x_i^2 \sum_{i=1}^m y_i^2]^{1/2}}$ .

The similarity measure corresponds to the angle between the item vectors in directions of  $x$  and  $y$  [490].

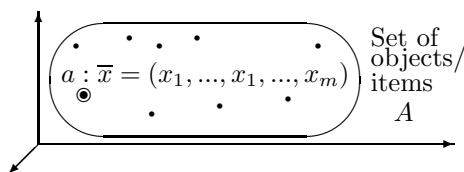


Fig. 2.19. Illustration for object/item

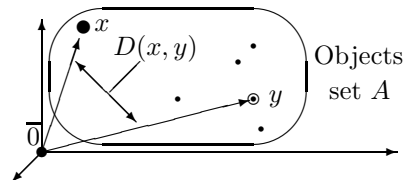


Fig. 2.20. Angle proximity

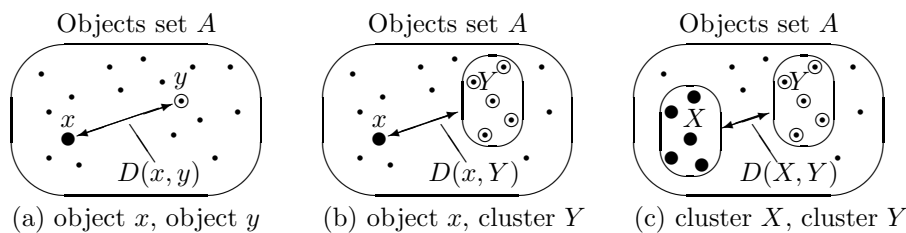


Fig. 2.21. Object/cluster proximities

Illustrative numerical examples are the following.

**Example 2.1.** An ordinal vector proximity can be used for calculation of the proximity of two ordinal vectors  $\bar{x}$  and  $\bar{y}$  (ordinal scale [1, 5] for vector estimates, ordinal scale [0, 4] for vector proximity):

(a) ordinal vector estimates are:  $x : \bar{x} = (3, 4, 1, 1, 2, 5)$ ,  $y : \bar{y} = (3, 1, 2, 1, 4, 4)$ ;

(b) ordinal proximities are:

(i)  $\overline{D(x, y)} = (x_1 - y_1, x_2 - y_2, x_3 - y_3, x_4 - y_4, x_5 - y_5, x_6 - y_6) = (0, 3, -1, 0, -2, 1)$ ,

(ii)  $D'(x, y) = (|x_1 - y_1|, |x_2 - y_2|, |x_3 - y_3|, |x_4 - y_4|, |x_5 - y_5|, |x_6 - y_6|) = (0, 3, 1, 0, 2, 1)$ .

**Example 2.2.** An ordinal vector proximity can be used for calculation of the proximity of two quantitative vectors  $\bar{x}$  and  $\bar{y}$  (quantitative scale (0, 5) for vector estimates, ordinal scale [0, 4] for vector proximity). Two initial quantitative vector estimates are: (a)  $\bar{x} = (0.3, 3.5, 1.4, 1.5, 2.3, 4.9)$ , (b)  $\bar{y} = (0.3, 0.8, 2.2, 1.6, 3.9, 4.1)$ . Examples for calculation of proximities are:

(1) The quantitative proximity is:

$\overline{D(x, y)} = (|x_1 - y_1|, |x_2 - y_2|, |x_3 - y_3|, |x_4 - y_4|, |x_5 - y_5|, |x_6 - y_6|) = (0.0, 2.7, 0.8, 0.1, 1.6, 0.8)$ .

(2) Calculation of the vector ordinal proximity  $D'(x, y) = (d_1, d_2, d_3, d_4, d_5, d_6)$  can be based on rule:

$$d_i = \begin{cases} 0, & \text{if } 0.0 \leq |x_i - y_i| \leq 0.2, \\ 1, & \text{if } 0.2 < |x_i - y_i| \leq 0.5, \\ 2, & \text{if } 0.5 < |x_i - y_i| \leq 0.8, \\ 3, & \text{if } 0.8 < |x_i - y_i| \leq 3.5, \\ 4, & \text{if } 3.5 < |x_i - y_i| \leq 5.0. \end{cases}$$

The resultant vector ordinal proximity is (based on  $\overline{D(x, y)}$ ):  $\overline{D'(x, y)} = (0, 3, 2, 0, 3, 2)$ .

**Example 2.3.** In the case when quantitative vector estimates are transformed into ordinal vector estimates, the example 1 is obtained.

**Case 2.** Object-cluster (subset) (Fig. 2.21b). The following initial information is considered:

(i) object  $x \in A$ :  $\bar{x} = (x_1, \dots, x_i, \dots, x_m)$  (vector estimate);

(ii) elements of cluster  $Y = \{y^1, \dots, y^\zeta, \dots, y^n\} \subset A$ ,  $y^\zeta$ :  $\bar{y}^\zeta = (y_1^\zeta, \dots, y_i^\zeta, \dots, y_m^\zeta)$  (vector estimate) ( $\forall y^\zeta \in Y$ ).

Proximity  $D(x, Y)$  between object  $x$  and cluster  $Y$  can be considered, for example, as the following:

- (1)  $D^{min}(x, Y) = \min_{\forall y^\zeta \in Y} D(x, y^\zeta)$ ;
- (2)  $D^{max}(x, Y) = \max_{\forall y^\zeta \in Y} D(x, y^\zeta)$ ;
- (3)  $D^{av}(x, Y) = 1/\eta \sum_{\forall y^\zeta \in Y} D(x, y^\zeta)$ ;
- (4)  $D^{cent}(x, Y) = D(x, \hat{y})$ , where  $\hat{y}$  is centroid (or median point) of cluster  $Y$ .

Clearly, various measurement approaches (i.e., metric/proximity) described for case 1 can be used.

**Example 2.4.** Let us consider item  $x$ :  $\bar{x} = (0.3, 3.5, 1.4, 1.5)$  and cluster  $Y$ :  $\bar{y}^1 = (1.1, 4.0, 3.2, 4.3)$ ,  $\bar{y}^2 = (2.0, 5.1, 2.5, 5.2)$ ,  $\bar{y}^3 = (1.3, 4.7, 4.2, 1.6)$ .

For four case above, the following proximities are obtained (Euclidean distance of two items is used):

- (1)  $D^{min}(x, Y) = \min_{\forall y^\zeta \in Y} D(x, y^\zeta) = \min\{D(x, y^1), D(x, y^2), D(x, y^3)\} = \min\{3.4, 4.5, 3.3\} = 3.3$ ;
- (2)  $D^{max}(x, Y) = \max_{\forall y^\zeta \in Y} D(x, y^\zeta) = \max\{D(x, y^1), D(x, y^2), D(x, y^3)\} = \max\{3.4, 4.5, 3.3\} = 4.5$ ;
- (3)  $D^{av}(x, Y) = \frac{1}{3} \sum_{\forall y^\zeta \in Y} D(x, y^\zeta) = \frac{1}{3}(D(x, y^1) + D(x, y^2) + D(x, y^3)) = 1/3(3.4 + 4.5 + 3.3) = 3.7$ ;
- (4)  $D^{cent}(x, Y) = D(x, \hat{y}) = D((0.3, 3.5, 1.4, 1.5), (1.16, 1.1, 1.9, 2.2)) = 2.7$ .

In the case of vector proximity  $\overline{D}(x, y^\zeta)$  the following calculation schemes can be used:

*Scheme 1.* Preliminary transformation of vector proximities  $D(x, y^\zeta)$  ( $\forall y^\zeta$ ) into ordinal vector proximity and usage of the measurement methods above (e.g., proximity to the closest point of cluster);

*Scheme 2.* Integration of proximities  $D(x, y^\zeta)$  ( $\forall y^\zeta$ ) to obtain a general vector proximity  $D(x, Y)$  and transformation the general vector proximity into a number (quantitative or ordinal).

**Example 2.5.** Numerical examples for the above-mentioned two cases (i) and (ii) are the following:

*Scheme 1:*  $\overline{D}(x, y^\zeta) = (|x_1 - y_1^\zeta|, |x_2 - y_2^\zeta|, |x_3 - y_3^\zeta|, |x_4 - y_4^\zeta|)$ .

Thus,  $\overline{D}(x, y^1) = (0.8, 0.5, 1.8, 2.8)$ ,  $\overline{D}(x, y^2) = (1.7, 1.6, 1.1, 3.7)$ ,  $\overline{D}(x, y^3) = (1.0, 1.2, 2.8, 0.1)$ .

Transformed vector proximities (into ordinal vector estimates, rules from example 2) are:

$\overline{D'}(x, y^1) = (2, 1, 3, 3)$ ,  $\overline{D'}(x, y^2) = (3, 3, 3, 4)$ ,  $\overline{D'}(x, y^3) = (3, 3, 3, 0)$ .

Evidently, point  $y^1$  can be considered as the closest point for item  $x$  (version of proximity between point  $x$  and cluster  $Y$  as proximity of point  $x$  and the closest point of the cluster  $Y$ ), i.e.,  $\overline{D'}(x, Y) = \overline{D'}(x, y^1) = (2, 1, 3, 3)$ .

*Scheme 2:* Let us integrated general vector proximity is:  $D(x, Y) = \overline{D'}(x, Y) = (2, 1, 3, 3)$  (from scheme 1 above). A transformation process of the ordinal vector into an ordinal estimate can be based on the following simplified rule (for ordinal vector  $(\beta_1, \dots, \beta_i, \dots, \beta_m)$ ):

$$\alpha' = \begin{cases} 0, & \text{if } 0 \leq \sum_{i=1, \dots, m} \beta_i \leq m, \\ 1, & \text{if } m < \sum_{i=1, \dots, m} \beta_i \leq 2m, \\ 2, & \text{if } 2m < \sum_{i=1, \dots, m} \beta_i \leq 3m, \\ 3, & \text{if } 3m < \sum_{i=1, \dots, m} \beta_i \leq 4m, \\ 4, & \text{if } 4m < \sum_{i=1, \dots, m} \beta_i. \end{cases}$$

Here,  $m = 4$  and the resultant ordinal estimate for  $\overline{D'}(x, Y)$  is: 2. In general, it may be reasonable to use a multiset estimate, for example,  $e(x, Y) = (0, 1, 1, 2)$  because in  $\overline{D'}(x, Y) = (2, 1, 3, 3)$ : 0 estimates at the level 0, 1 estimate at the level 1, 1 estimate at the level 2, 2 estimate at the level 3.

**Case 3.** Intra-cluster proximity (distance) (for all element pair in cluster). The following initial information is considered: elements of cluster  $Y = \{y^1, \dots, y^\zeta, \dots, y^\eta\} \subset A$ ,  $y^\zeta$ :  $\overline{y^\zeta} = (y_1^\zeta, \dots, y_i^\zeta, \dots, y_m^\zeta)$  (vector estimate) ( $\forall y^\zeta \in Y$ ).

Intra-cluster proximity for cluster  $Y$ :  $I(Y)$ ,  $Y \subseteq A$  can be considered, for example, as the following:

- (1) minimum distance  $I^{intra, min}(Y) = \min_{\zeta=1, \dots, \eta, \xi=1, \dots, \eta, \zeta \neq \xi} D(y^\zeta, y^\xi)$ ;
- (2) maximum distance  $I^{intra, max}(Y) = \max_{\zeta=1, \dots, \eta, \xi=1, \dots, \eta, \zeta \neq \xi} D(y^\zeta, y^\xi)$ ;
- (3) average distance  $I^{intra, av}(Y) = \frac{1}{\eta} \sum_{\zeta=1, \dots, \eta, \xi=1, \dots, \eta, \zeta \neq \xi} D(y^\zeta, y^\xi)$ .

Various measurement approaches (i.e., metric/proximity) from case 1 can be used as well.

**Example 2.6.** Let us consider cluster  $Y = \{y^1, y^2, y^3\}$  (from example 2.4).

Euclidean distances between cluster elements are:  $D(y^1, y^2) = 1.8$ ,  $D(y^1, y^3) = 3.0$ ,  $D(y^2, y^3) = 4.0$ .

Thus, versions of intra-cluster proximities for cluster  $Y$  are:



$$I^{intra,min}(Y) = 1.8, \quad I^{intra,max}(Y) = 4.0, \quad I^{intra,av}(Y) = 2.9.$$

On the other hand, element distances

$$\overline{D}(y^1, y^2) = (0.9, 1.1, 0.7, 0.9), \quad \overline{D}(y^1, y^3) = (0.2, 0.7, 1.0, 2.7), \quad \overline{D}(y^2, y^3) = (0.7, 0.4, 1.7, 3.6)$$

can be transformed into ordinal vector proximities (by rule above)

$$\overline{D}'(y^1, y^2) = (3, 3, 2, 3), \quad \overline{D}'(y^1, y^3) = (0, 2, 3, 3), \quad \overline{D}'(y^2, y^3) = (2, 1, 3, 4).$$

After transformation of ordinal vector proximities into integrated ordinal estimates, the following estimates are obtained (by rule above):  $\overline{D}'(y^1, y^2) \Rightarrow 2$ ,  $\overline{D}'(y^1, y^3) \Rightarrow 1$ ,  $\overline{D}'(y^2, y^3) \Rightarrow 2$ . Here, minimum ordinal intra-cluster proximity equals 1, maximum ordinal intra-cluster proximity equals 2.

Transformation of ordinal vector proximities into multiset estimates leads to the following estimates:  $e(y^1, y^2) = (0, 1, 1, 3, 0)$ ,  $e(y^1, y^3) = (1, 0, 1, 2, 0)$ ,  $e(y^2, y^3) = (0, 1, 1, 1, 1)$ . Note, the average multiset estimate can be computed as a median estimate [386,392].

**Case 4.** Inter-cluster proximity (distance) (for two clusters, Fig. 2.21c). The following initial information is considered: (i) elements of cluster  $X = \{x^1, \dots, x^\xi, \dots, x^\phi\} \subset A$ ,  $x^\xi: \overline{x^\xi} = (x_1^\xi, \dots, x_i^\xi, \dots, x_m^\xi)$  (vector estimate) ( $\forall x^\xi \in X$ ); (ii) elements of cluster  $Y = \{y^1, \dots, y^\zeta, \dots, y^n\} \subset A$ ,  $y^\zeta: \overline{y^\zeta} = (y_1^\zeta, \dots, y_i^\zeta, \dots, y_m^\zeta)$  (vector estimate) ( $\forall y^\zeta \in Y$ ). In the main, the following basic types of inter-cluster distances are considered: (a) minimum element proximity (distance) (“single link”), (b) maximum element proximity (distance) (“complete link”), (c) average element proximity (distance), (d) median element proximity (distance), (e) proximity (distance) between cluster centroids. For example, inter-cluster proximity for two clusters  $X, Y$ :  $I^{inter}(X, Y)$ ,  $X, Y \subseteq A$  can be considered as the following:

- (1)  $I^{inter,min}(X, Y) = \min_{\xi=1, \phi, \zeta=1, \eta} D(x^\xi, y^\zeta)$ ;
- (2)  $I^{inter,max}(X, Y) = \max_{\xi=1, \phi, \zeta=1, \eta} D(x^\xi, y^\zeta)$ ;
- (3)  $I^{inter,av}(X, Y) = \frac{1}{\phi \times \eta} \sum_{\xi=1, \phi, \zeta=1, \eta} D(x^\xi, y^\zeta)$ .

Clearly, various measurement approaches (i.e., metric/proximity) described for case 1 can be used. In the case of vector proximity  $D(x^\xi, y^\zeta)$ , the following calculation scheme can be used:

(a) preliminary transformation of vector proximity  $D(x^\xi, y^\zeta)$  ( $\forall x^\xi, y^\zeta$ ) into a number (quantitative or ordinal) and usage of the above-mentioned measurement methods;

(b) integration of proximities  $D(x^\xi, y^\zeta)$  ( $\forall x^\xi, y^\zeta$ ) to obtain a general vector proximity  $D(X, Y)$  and transformation the general vector proximity into a number (quantitative or ordinal).

**Example 2.7.** Let us consider cluster  $Y = \{y^1, y^2, y^3\}$  (from example 2.4) and cluster and cluster  $X$ :  $\overline{x^1} = (0.1, 1.0, 0.2, 0.3)$ ,  $\overline{x^2} = (0.3, 0.9, 0.5, 0.6)$ . Distances between elements of  $X$  and  $Y$  are presented in Table 2.5 ( $\overline{D}(x^\xi, y^\zeta)$ ), Table 2.6 (Euclidean distance  $D(x^\xi, y^\zeta)$ ), and Table 2.7 (ordinal distance  $\overline{D}'(x^\xi, y^\zeta)$ , by rule above).

**Table 2.5.** Vector distance  $\overline{D}(x^\xi, y^\zeta)$

|       | $y^1$                | $y^2$                | $y^3$                |
|-------|----------------------|----------------------|----------------------|
| $x^1$ | (1.0, 3.0, 3.0, 4.0) | (1.9, 4.1, 2.3, 4.9) | (1.2, 3.7, 4.0, 1.3) |
| $x^2$ | (0.8, 3.1, 2.7, 3.7) | (1.7, 4.2, 2.0, 4.6) | (1.0, 3.8, 3.7, 1.0) |

**Table 2.6.** Euclidean distance  $D(x^\xi, y^\zeta)$

|       | $y^1$ | $y^2$ | $y^3$ |
|-------|-------|-------|-------|
| $x^1$ | 6.0   | 7.0   | 5.8   |
| $x^2$ | 5.7   | 6.8   | 5.4   |

**Table 2.7.** Ordinal vector distance  $\overline{D}'(x^\xi, y^\zeta)$

|       | $y^1$        | $y^2$        | $y^3$        |
|-------|--------------|--------------|--------------|
| $x^1$ | (3, 3, 3, 4) | (3, 4, 3, 4) | (3, 4, 4, 3) |
| $x^2$ | (2, 3, 3, 4) | (3, 4, 3, 4) | (3, 4, 4, 3) |

Thus, versions of inter-cluster proximities for clusters  $X$  and  $Y$  are:

$$I^{inter,min}(X, Y) = 5.4, \quad I^{inter,max}(X, Y) = 7.0, \quad I^{inter,av}(X, Y) = 6.1.$$

Results of transformation of ordinal vector proximities into integrated ordinal estimates (by rule above) are presented in Table 2.8. Here, minimum ordinal inter-cluster proximity equals 2, maximum ordinal inter-cluster proximity equals 3. Resultant multiset estimates are presented in Table 2.9.

**Table 2.8.** Integrated ordinal estimates

|       | $y^1$ | $y^2$ | $y^3$ |
|-------|-------|-------|-------|
| $x^1$ | 3     | 3     | 3     |
| $x^2$ | 2     | 3     | 3     |

**Table 2.9.** Resultant multiset estimates  $e(x^\xi, y^\zeta)$ 

|       | $y^1$           | $y^2$           | $y^3$           |
|-------|-----------------|-----------------|-----------------|
| $x^1$ | (0, 0, 0, 3, 1) | (0, 0, 0, 2, 2) | (0, 0, 0, 2, 2) |
| $x^2$ | (0, 0, 1, 2, 1) | (0, 0, 0, 2, 2) | (0, 0, 0, 2, 2) |

### 2.2.5. Quality of clustering solution

Here “hard” clustering problem is examined. Consider initial items/elements of element set  $A = \{a_1, \dots, a_j, \dots, a_n\}$  (Fig. 2.19). Two types of initial information for clustering can be examined: 1. there are  $m$  parameters/criteria and measurement of  $a$  is based on vector estimate  $\bar{x} = (x_1, \dots, x_1, \dots, x_m)$  (Fig. 2.19); 2. binary relation(s) over element set  $A$  (including weighted binary relation(s); this is a structure over obtained clusters of a graph). Note, the first type of initial information can be transformed into the second type. A clustering solution consists of the following two parts:

(1) Clusters  $\hat{X} = \{X_1, \dots, X_\iota, \dots, X_\lambda\}$ , i.e. dividing set  $A$  into clusters:  $X_\iota \subseteq A \quad \forall \iota = \overline{1, \lambda}$ ;  $\eta_\iota = |X_\iota|$  is the cluster size (i.e., cardinality for cluster  $X_\iota$ ,  $\iota = \overline{1, \lambda}$ ).

(2) Structure over clusters (if needed). Let  $\Gamma(\hat{X})$  be a structure over the clusters of the clustering solution  $\hat{X}$ , i.e., there exists digraph  $G = \hat{X}, \Gamma(\hat{X})$ . Let  $\Gamma(X_\iota)$  be the structure over the elements of cluster  $X_\iota$  ( $\forall X_\iota \in \hat{X}$ ).

The list of basic quality characteristics is the following (Table 2.10):

**Table 2.10.** List of quality characteristics

| No.  | Quality type                         | Notation             | Description   |
|------|--------------------------------------|----------------------|---|
| I.   | Cluster                              | $X_\iota$            | $1 \leq \iota \leq \lambda$   |
| 1.1. | Intra-cluster distance               | $I^{intra}(X_\iota)$ | Proximity between elements of cluster   |
| 1.2. | Size of cluster                      | $ X_\iota $          | Number of elements in cluster $X_\iota$   |
| 1.3. | Quality of cluster form              |                      | Closeness to predefined form (e.g., ball, ellipsoid) (if needed)  |
| 1.4. | Size of cluster region               |                      | Difference between “max” and “min” coordinates (by parameters)  |
| 1.5. | Quality of cluster content/structure |                      | Configuration of element types (if needed)  |
| 1.6. | Quality of cluster structure         |                      | Proximity of structure over cluster elements to predefined structure (if needed)  |
| II.  | Clustering solution                  | $\hat{X}$            | $\hat{X} = \{X_1, \dots, X_\iota, \dots, X_\lambda\}$   |
| 2.1. | Total intra-cluster quality          | $Q^{intra}(\hat{X})$ | Integration of intra-cluster parameters ( $I^{intra}(X_\iota)$ , by $\iota = \overline{1, \lambda}$ )                                   |
| 2.2. | Total inter-cluster quality          | $Q^{inter}(\hat{X})$ | Integration of inter-cluster parameters ( $I^{inter}(X_{\iota_1}, X_{\iota_2})$ , by $\iota_1, \iota_2, \iota_1 \neq \iota_2$ )         |
| 2.3. | Number of clusters ( $\lambda$ )     | $Q^{num}(\hat{X})$   | Number of clusters in clustering solution   |
| 2.4. | Closeness to cluster size            | $Q^{bal}(\hat{X})$   | Balance by cluster size, closeness to predefined balance vector   |
| 2.5. | Quality by forms of clusters         | $Q^{form}(\hat{X})$  | Integration of cluster form parameters  |
| 2.6. | Parameter of cluster regions         | $Q^{reg}(\hat{X})$   | Integration of cluster regions sizes (by coordinates)   |
| 2.7. | “Correlation clustering functional”  | $Q^{corr}(\hat{X})$  | Integration of maximum agreement (in each cluster) and minimum disagreements (between clusters) [39,40]                                 |
| 2.8. | Quality of modularity                | $Q^{mod}(\hat{X})$   | Parameter of network modularity [226,459]   |
| III. | Quality of structure over clusters   | $Q^{struc}(\hat{X})$ | Closeness to predefined structure   |
| IV.  | Multicriteria quality                | $\bar{Q}(\hat{X})$   | Integrated vector of quality (e.g., $\bar{Q}(\hat{X}) = (Q^{intra}(\hat{X}), Q^{inter}(\hat{X}), Q^{bal}(\hat{X}), Q^{reg}(\hat{X}))$ ) |

**1. Quality of clusters** (i.e., local quality parameters in clustering solution):

**1.1. Intra-cluster distance** (i.e., general proximity between elements in each cluster):

$$I^{intra}(X_\iota) \ (\iota = \overline{1, \lambda}).$$

*Version 1.* Quantitative parameter as integration of quantitative element proximities (distances) in the cluster (this is described in previous section, case 3).

*Version 2.* Multiset parameter as integration of ordinal estimates of element proximities. The approach is illustrated by example.

**Example 2.8.** Example for three clusters is depicted in Fig. 2.22:  $X_1 = \{1, 2, 3, 4\}$ ,  $X_2 = \{5, 6, 7\}$ ,  $X_3 = \{8, 9, 10, 11, 12\}$ . Ordinal scale  $[1, 2, 3]$  for estimates of element similarity is used:

1 corresponds to “very similar”,

2 corresponds to “medium level”,

3 corresponds to “very different” (in this case the edge in Fig. 2.22 is absent).

Ordinal proximities of edges are presented in Table 2.11. The resultant multiset intra-cluster parameters for clusters are:  $I^{intra}(X_1) = (2, 3, 1)$ ,  $I^{intra}(X_2) = (1, 1, 1)$ ,  $I^{intra}(X_3) = (4, 2, 4)$ .

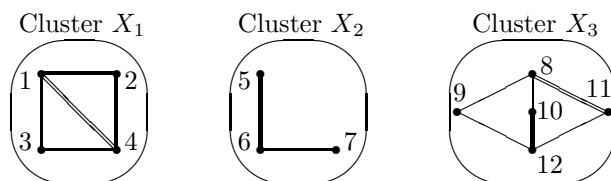


Fig. 2.22. Local intra-cluster quality (for cluster)

**Table 2.11.** Ordinal proximities (intra-cluster, edge  $(i_1, i_2)$ )

| $i_1$ | $i_2$ | 2 | 3 | 4 | 6 | 7 | 9 | 10 | 11 | 12 |
|-------|-------|---|---|---|---|---|---|----|----|----|
| 1     |       | 2 | 1 | 2 |   |   |   |    |    |    |
| 2     |       |   | 3 | 2 |   |   |   |    |    |    |
| 3     |       |   |   | 1 |   |   |   |    |    |    |
| 5     |       |   |   |   | 2 | 3 |   |    |    |    |
| 6     |       |   |   |   |   | 1 |   |    |    |    |
| 8     |       |   |   |   |   |   | 1 | 1  | 2  | 3  |
| 9     |       |   |   |   |   |   |   | 3  | 3  | 1  |
| 10    |       |   |   |   |   |   |   |    | 3  | 2  |
| 11    |       |   |   |   |   |   |   |    |    | 1  |

**1.2.** Number of elements in cluster (or in each cluster, i.e., cluster size) corresponds to constraints, for example:  $\pi^- \leq \eta_\iota = |X_\iota| \leq \pi^+$  ( $\pi^-, \pi^+$  are predefined limits of the cluster size) ( $\forall X_\iota \in \widehat{X}$ ).

The quality parameter corresponds to external requirement (from the viewpoint of applied problem(s), e.g., teams, communication systems).

**1.3.** Quality of cluster form (e.g., body, envelope, cover), for example: sphere/ball, ellipsoid, globe (i.e., closeness to the required cluster form).

**1.4.** Quality as constraint for size of cluster region (limits for interval for coordinates of cluster elements). Let us consider cluster  $X = \{x^1, \dots, x^\xi, \dots, x^\phi\}$ , parameter estimates of each cluster element  $x^\xi$  are (vector estimate, parameters  $i = \overline{1, m}$ ):  $\overline{x^\xi} = (x_1^\xi, \dots, x_i^\xi, \dots, x_m^\xi)$ . Constraints are (by each parameter  $\forall i = \overline{1, \phi}$ ) (Fig. 2.23):

$$|\max_{\xi=1, \phi} x_i^\xi - \min_{\xi=1, \phi} x_i^\xi| \leq d_i, \quad \forall i = \overline{1, m}.$$

The quality parameter corresponds to external requirement (from the viewpoint of applied problem(s), e.g., communication systems).

**1.5.** Quality of the cluster contents/structure (if needed), for example (a composite “team”): 1 element of the 1st type, 3 elements of the 2nd type, 2 elements of the 3rd type, 1 element of the 4th type. Here proximity of the obtained cluster content to the required content can be considered.

**1.6.** Quality of cluster structure (if needed) for cluster  $X_\iota$  ( $\forall X_\iota \in \widehat{X}$ ), i.e., proximity  $\delta(\Gamma(X_\iota), \Gamma^0(X_\iota))$ , where  $\Gamma^0(X_\iota)$  is the predefined structure over the cluster elements.

**2. Total quality for clustering solution** (i.e., for cluster set):

**2.1.** Total intra-cluster quality for clustering solution  $Q^{intra}(\widehat{X})$  is an integrated measure of intra-cluster parameters ( $I^{intra}(X_\iota)$ ) of all clusters in clustering solution (i.e.,  $\iota = \overline{1, \lambda}$ ).

*Version 1.* Total qualitative quality parameter for qualitative local estimates:

$$Q^{intra}(\widehat{X}) = \frac{1}{\lambda} \sum_{\iota=\overline{1, \lambda}} I^{intra}(X_\iota).$$

Note, integration process can be based on summarization and some other operations (maximization, minimization, etc.).

*Version 2.* Total multiset quality parameter for multiset local estimates. The approach is illustrated by example.

**Example 2.9.** Example for three clusters is depicted in Fig. 2.24 (for simplification the cardinality of clusters is the same):  $X_1 = \{1, 2, 3\}$ ,  $X_2 = \{4, 5, 6\}$ ,  $X_3 = \{7, 8, 9\}$ ; clustering solution is:  $\widehat{X} = \{X_1, X_2, X_3\}$ . Ordinal scale  $[1, 2, 3]$  for estimates of element similarity is used: 1 corresponds to “very similar”, 2 corresponds to “medium level”, 3 corresponds to “very different” (in this case the corresponding edge is absent). Ordinal proximities of edges in clusters are presented in Table 2.12.

The resultant multiset intra-cluster parameters for clusters are:

$$I^{intra}(X_1) = (1, 2, 0), \quad I^{intra}(X_2) = (2, 1, 0), \quad I^{intra}(X_3) = (2, 1, 0).$$

These multiset estimates correspond to poset (lattice) from Fig. 2.16.

Integration of the above-mentioned intra-cluster multiset estimates can be based on two methods (e.g., [386,392]):

(a) summarization (by the vector components):  $Q^{intra}(\widehat{X}) = (5, 4, 0)$ , the obtained integrate estimate corresponds to an extended lattice (not to lattice from Fig. 2.16);

(b) searching for a median multiset estimate:  $Q^{intra}(\widehat{X}) = (2, 1, 0)$  (lattice from Fig. 2.16).

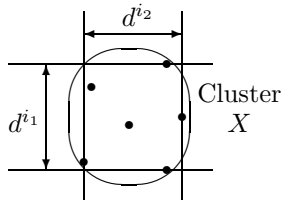


Fig. 2.23. Size of cluster region

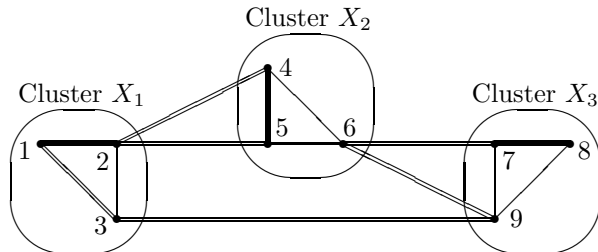


Fig. 2.24. Intra- and inter-cluster qualities

**Table 2.12.** Ordinal proximities (intra-cluster, edge  $(i_1, i_2)$ )

| $i_1$ | $i_2 :$ | 2 | 3 | 5 | 6 | 8 | 9 |
|-------|---------|---|---|---|---|---|---|
| 1     |         | 2 | 2 |   |   |   |   |
| 2     |         |   | 1 |   |   |   |   |
| 4     |         |   |   | 2 | 1 |   |   |
| 5     |         |   |   |   | 1 |   |   |
| 7     |         |   |   |   |   | 2 | 1 |
| 8     |         |   |   |   |   |   | 1 |

**2.2.** Total inter-cluster quality for clustering solution  $Q^{inter}(\widehat{X})$  is an integrated measure of inter-cluster parameters ( $I^{intra}(X_{\iota_1}, X_{\iota_2})$ ) of all cluster pairs in clustering solution (i.e.,  $\iota_1 = \overline{1, \lambda}$ ,  $\iota_2 = \overline{1, \lambda}$ ,  $\iota_1 \neq \iota_2$ ).

*Version 1.* Total qualitative quality parameter for qualitative local estimates as integration of all qualitative two-cluster inter-cluster proximities/distances (from previous section, case 4):

$$Q^{inter}(\widehat{X}) = \frac{1}{\lambda(\lambda - 1)} \sum_{\substack{\iota_1 = \overline{1, \lambda}, \iota_2 = \overline{1, \lambda}, \\ \iota_1 \neq \iota_2}} I^{inter}(X_{\iota_1}, X_{\iota_2}).$$

Note, integration process can be based on summarization and some other operations (maximization, minimization, etc.).

*Version 2.* Total multiset quality parameter for multiset local estimates. The approach is illustrated by example.

**Example 2.10.** The example is based on data from previous example 2.9 (i.e., Fig. 2.24). Table 2.13 contains inter-cluster ordinal proximities.

**Table 2.13.** Ordinal proximities (inter-cluster, edge  $(i, j)$ )

| $i$ | $j$ : | 4 | 5 | 6 | 7 | 8 | 9 |
|-----|-------|---|---|---|---|---|---|
| 1   |       | 3 | 3 | 3 | 3 | 3 | 3 |
| 2   |       | 2 | 2 | 3 | 3 | 3 | 3 |
| 3   |       | 3 | 3 | 3 | 3 | 3 | 2 |
| 4   |       |   |   |   | 3 | 3 | 3 |
| 5   |       |   |   |   | 3 | 3 | 3 |
| 6   |       |   |   |   | 2 | 3 | 2 |

Inter-cluster multiset estimates are:

$$I^{inter}(X_1, X_2) = (0, 2, 7), \quad I^{inter}(X_1, X_3) = (0, 1, 8), \quad I^{inter}(X_2, X_3) = (0, 2, 7).$$

Integration of the above-mentioned intra-cluster multiset estimates can be based on two methods (e.g., [386,392]):

- (a) summarization (by the vector components):  $Q^{inter}(\widehat{X}) = (0, 5, 22)$ ;
- (b) searching for a median multiset estimate:  $Q^{inter}(\widehat{X}) = (0, 2, 7)$ .

**2.3.** Total number of clusters in clustering solution  $Q^{num}(\widehat{X})$ , for example:  $\Upsilon^- \leq \lambda(\widehat{X}) \leq \Upsilon^+$  ( $\Upsilon^-, \Upsilon^+$  are predefined limits of the total cluster number). The quality parameter corresponds to external requirement (from the viewpoint of applied problem(s)). This is connected to 1.2

**2.4.** Closeness of element cluster sizes in clustering solution to the predefined cluster size constraints, i.e., balance (or imbalance) of cluster cardinalities  $Q^{bal}(\widehat{X})$ , for example:  $\pi^- \leq |X_l| \leq \pi^+$  ( $\pi^-, \pi^+$  are general limits of each cluster size. Evidently, here the balance/imbalance (i.e., out-of-balance) estimate of a clustering solution can be consider as the number of clusters that corresponds (or does not correspond) to the constraints. The estimates can be examined as a vector-like estimate or a multiset estimate, for example: the number of “good” clusters (with “good/right” cluster size), the number of quasi-good clusters (with quasi-right cluster size), and the number of other clusters. This parameter corresponds to external requirement (from the viewpoint of applied problem(s)). Now let us describe the version of the vector-like estimate. The notations are as follows: (a)  $\pi^0(\widehat{X})$  is the number of clusters in  $\widehat{X}$  in which the cluster size  $X_l$  complies with the predefined limits, (b)  $\pi^{+l}(\widehat{X})$  is the number of clusters in  $\widehat{X}$  where the cluster size  $X_l$  more then  $\widehat{\pi}^+$  (upper limit) by  $l$  elements, (c)  $\pi^{-l}(\widehat{X})$  be the number of clusters in  $\widehat{X}$  where the cluster size  $X_l$  less then  $\widehat{\pi}^-$  (bottom limit) by  $l$  elements. As a result, the following vector estimate can be considered:

$$Q^{bal}(\widehat{X}) = (\pi^{-l}(\widehat{X}), \dots, \pi^{-1}(\widehat{X}), \pi^0(\widehat{X}), \pi^1(\widehat{X}), \dots, \pi^{+l}(\widehat{X})).$$

Note, a close type of the vector estimate (vector proximity) has been suggested for comparison of rankings in [372]. The approach is illustrated by example.

**Example 2.11.** Initial set of objects is:  $A = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17\}$ , clustering solution is:  $\widehat{X}: X_1 = \{1, 5, 7\}, X_2 = \{2\}, X_3 = \{3, 6, 10, 13, 17\}, X_4 = \{11, 12\}, X_5 = \{4, 12, 14, 15\}, X_6 = \{8, 16\}$ . The following constrains for cluster size are considered:  $\widehat{\pi}_1 = 2, \widehat{\pi}_2 = 3$ . Vector estimate for balance of cluster cardinalities is:  $Q^{bal}(\widehat{X}) = (\pi^{-1}(\widehat{X}), \pi^0(\widehat{X}), \pi^1(\widehat{X}), \dots, \pi^2(\widehat{X})) = (1, 3, 1, 1)$ .

The considered approach is close to  $\Upsilon$ -balanced partitioning (clustering solution  $\widehat{X}$ ) when size of each obtained cluster  $|X_\iota| \approx \frac{n}{\Upsilon(\widehat{X})}$  ( $\forall X_\iota \in \widehat{X}$ ) where  $\Upsilon(\widehat{X})$  (i.e.,  $\lambda$ ) is the number of obtained clusters.

**2.5.** Total quality for balance (or imbalance) of cluster forms (i.e., cluster bodies/covers) in a clustering solution  $Q^{form}(\widehat{X})$ , for example: majority of clusters of a clustering solution have the same (or about the same) bodies (e.g., spheres/balls, ellipsoids, globes).

Evidently, it is possible to consider a measure of imbalance, analogically as in parameter 2.3.

**2.6.** Total quality  $Q^{reg}(\widehat{X})$  as constraints for size of cluster regions (limits for interval of cluster element coordinates for each cluster). Let us consider cluster  $X_\iota = \{x^{\iota,1}, \dots, x^{\iota,\xi}, \dots, x^{\iota,\phi_\iota}\}$ . Parameter estimates of each cluster element  $x^{\iota,\xi}$  are (vector estimate, parameters  $i = \overline{1, m}$  and clusters  $\iota = \overline{1, \lambda}$ ):  $\overline{x^{\iota,\xi}} = (x_1^{\iota,\xi}, \dots, x_i^{\iota,\xi}, \dots, x_m^{\iota,\xi})$ . Constraints are (by each parameter  $\forall i = \overline{1, m}$ ) (Fig. 2.23):

$$|\max_{\xi=\overline{1, \phi_\iota}} x_i^{\xi} - \min_{\xi=\overline{1, \phi_\iota}} x_i^{\xi}| \leq d_i, \quad \forall i = \overline{1, m} \text{ (each coordinate/parameter)}, \quad \forall \iota = \overline{1, \lambda} \text{ (each cluster)}.$$

The quality parameter corresponds to external requirement (from the viewpoint of applied problem(s), e.g., communication systems).

**2.7.** The ‘‘correlation clustering functional’’ to maximize the intra-cluster agreement (attraction) and the inter-cluster disagreement (repulsion) has been proposed in [39,40] ( $Q^{corr}(\widehat{X})$ ). Here, partitioning a fully connected labeled graph is examined (label ‘‘+’’ corresponds to edge between similar vertices, label ‘‘-’’ corresponds to edge between different vertices). The optimization functional  $Q^{corr}(\widehat{X})$  is an integration (i.e., summarization) of two components: (i) the maximizing number of ‘‘-’’ edges between clusters (i.e., minimizing disagreements), (b) the number of ‘‘+’’ edges insides the clusters (i.e., maximizing agreements) (e.g., [4,33,39,40,159,345,564,662]). Weighted versions of the ‘‘correlation clustering functional’’ are considered as well (e.g., [94,95,159]).

**2.8.** Modularity of clustering solution  $Q^{mod}(\widehat{X})$  is defined as follows (e.g., [226,457,459,461]) (Fig. 2.25). Let  $G = (A, E)$  be an initial graph, where  $A$  is the set of nodes,  $E$  is the set of edges. Clustering solution for graph  $G$  is:  $\widehat{X} = \{X_1, \dots, X_\iota, \dots, X_\lambda\}$ . Let  $A^\iota$  be the set of nodes in cluster  $X_\iota$  ( $\iota = \overline{1, \lambda}$ ). Let  $E^\iota$  be the set of internal edges in cluster  $X_\iota$  ( $\iota = \overline{1, \lambda}$ ), i.e., all corresponding nodes belong to  $A^\iota$ . Let  $\widetilde{E}^\iota$  be the set of external edges for cluster  $X_\iota$  ( $\iota = \overline{1, \lambda}$ ), i.e., the only one corresponding node belong to  $A^\iota$ . The definitions are illustrated in Fig. 2.25 for a four cluster solution (cluster  $X_3$ ).

Thus, the following parameters for each cluster  $X_\iota$  can be used:

(a)  $e_\iota = \frac{|E^\iota|}{|E|}$  (% edges in module  $\iota$ ),

(b)  $a_\iota = \frac{|\widetilde{E}^\iota| + |E^\iota|}{|E|}$  (% edges with at least one end in module  $\iota$ ).

Further, general modularity of clustering solution for graph  $G$  is:

$$Q^{mod}(\widehat{X}) = \sum_{\iota=1}^{\lambda} (e_\iota - (a_\iota)^2).$$

Clustering problem to maximize the modularity is NP-hard [73]. The approach is illustrated by example.

**Example 2.12.** Let us consider modularity parameters for clustering solution from Fig. 2.25. Here,  $|E| = 26$ . Parameters for clusters are:

(1)  $|E^1| = 6, |\widetilde{E}^1| = 4, e_1 = 0.23, a_1 = 0.38$ ; (2)  $|E^2| = 4, |\widetilde{E}^2| = 4, e_2 = 0.15, a_2 = 0.3$ ;

(3)  $|E^3| = 3, |\widetilde{E}^3| = 4, e_3 = 0.115, a_3 = 0.27$ ; (4)  $|E^4| = 4, |\widetilde{E}^4| = 2, e_4 = 0.15, a_4 = 0.23$ .

The resultant modularity parameter for clustering solution is:  $Q^{mod}(\hat{X}) = (0.23 - 0.14) + (0.15 - 0.09) + (0.115 - 0.073) + (0.15 - 0.053) = 0.09 + 0.06 + 0.42 + 0.097 = 0.667$ .

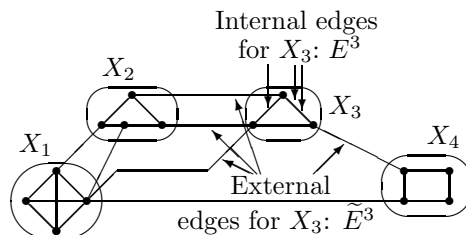


Fig. 2.25. Modularity in graph clustering

**3. Quality of structure over clusters** (e.g., tree, hierarchy) (if needed) ( $Q^{struc}(\hat{X})$ ). Here a proximity of the obtained structure  $\Gamma(\hat{X})$  in clustering solution  $\hat{X}$  and a predefined structure  $\Gamma^0$  is examined:  $Q^{struc}(\hat{X}) = \delta(\Gamma(\hat{X}), \Gamma^0)$ . Clearly, various scales for assessment of the proximities can be used (e.g., qualitative, ordinal, vector-like, multiset) (e.g., [384,392]).

**4.** Generally, it is reasonable to consider multicriteria quality of clustering solutions that integrates the above-mentioned clustering characteristics, for example:  $Q(\hat{X}) = (Q^{inter}(\hat{X}), Q^{intra}(\hat{X}), \pi(\hat{X}))$ .

Evidently, general integrated vector-like estimate for assessment of total quality of clustering solution can be examined, for example:  $\bar{Q}(\hat{X}) = (Q(\hat{X}), \delta(\Gamma(\hat{X}), \Gamma^0))$ . As a result, the clustering problem can be formulated as generalized multicriteria optimization problem (i.e., Pareto-efficient solutions have to be searched for), for example:

$$\min Q^{intra}(\hat{X}), \quad \max Q^{inter}(\hat{X}), \quad s.t. \quad Q^{bal}(\hat{X}) \preceq \pi^0, \quad Q^{struc} = \delta(\Gamma(\hat{X}), \Gamma^0) \leq \delta^0.$$

In the case of multiset estimates, the multiple criteria optimization clustering problem can be considered on the basis of quality lattices (poset-like scales) as follows (i.e., Pareto-efficient solutions over posets have to be searched for):

$$\min Q^{intra}(\hat{X}), \quad (by \ lattice, \ Fig. \ 2.26a)$$

$$\max Q^{inter}(\hat{X}), \quad (by \ lattice, \ Fig. \ 2.26b)$$

$$s.t. \quad I^{intra}(X_l) \succeq I^0, \quad \forall l = \overline{1, \lambda}, \quad I^0 \text{ is reference multiset estimate } \forall X_l \text{ (by lattice, Fig. 2.26c),}$$

$$Q^{bal}(\hat{X}) \preceq \pi^0, \quad \pi^0 \text{ is reference multiset estimate (balance by cluster size, by lattice, Fig. 2.26d),}$$

$$Q^{struc} = \delta(\Gamma(\hat{X}), \Gamma^0) \leq \delta^0, \quad (closeness \ to \ predefined \ general \ structure \ \Gamma^0).$$

Thus, Fig. 2.26 illustrates the integrated “discrete space” (poset) for total multiset based vector quality of clustering solution  $\hat{X}$ .

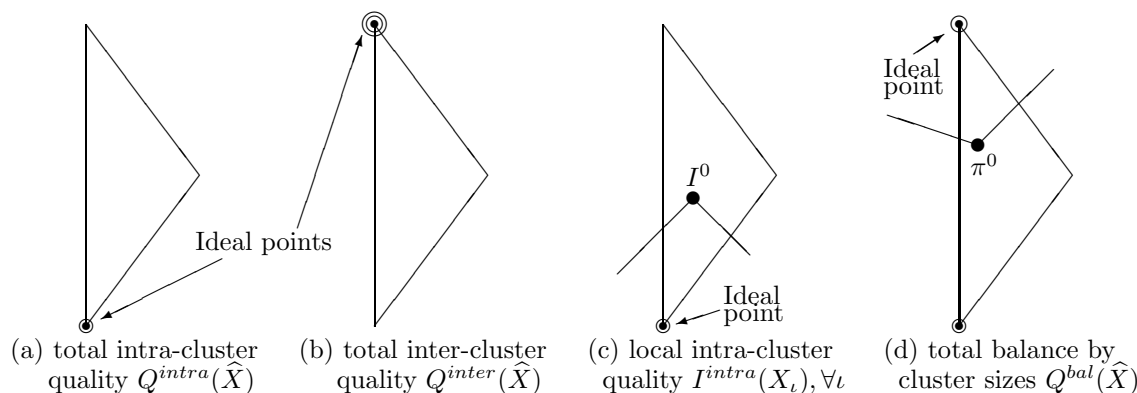


Fig. 2.26. Illustration for quality posets (lattices)

In the case of “soft” clustering problems, it is necessary to examine measures of solution “softness” (e.g., total parameter for intersection of clusters).

### 2.2.6. Comparison of two clustering solutions

Comparing methods for clustering solutions (e.g., partitions, hierarchical clustering solutions) have been studied many years (e.g., [31,51,207,293,294,428,434,501,661]). The main methods are the following: (a) pair counting methods (i.e., how likely two solutions group an elements pair together, or, separate them in different clusters); (b) set matching, (c) variation of information. Here, the following kinds of clustering solution are considered:

- (1) basic clustering solution  $\hat{X}$  as a set of clusters  $\hat{X} = \{X_1, \dots, X_l, \dots, X_\lambda\}$  (i.e., partition of initial elements  $A = \{1, \dots, i, \dots, n\}$ );
- (2) clustering and order over the cluster set  $\{X_1, \dots, X_l, \dots, X_\lambda\}$ :
  - (2.1) clustering and linear order over the cluster set, i.e. ranking  $R$ ,
  - (2.2) hierarchy over the cluster set  $\hat{H} = \langle H, \hat{X} \rangle$ , where  $H$  is hierarchy over clusters of basic clustering solution (partition of elements)  $\hat{X}$ .

Evidently, general graph over the cluster set can be examined as well.

Generally, two approaches can be examined for comparison of two clustering solutions:

- (a) difference by structures (“structural” comparison), e.g., a cost of transformation:

$$\hat{X}_1 \Rightarrow \hat{X}_2, R_1 \Rightarrow R_2, \hat{H}_1 \Rightarrow \hat{H}_2.$$

- (b) difference by quality criterion (or criteria), for example:

$$Q'(\hat{X}_1) - Q'(\hat{X}_2), Q''(R_1) - Q''(R_2), Q'''(\hat{H}_1) - Q'''(\hat{H}_2).$$

Here “structural” comparison is considered. The following comparison cases are examined:

Case 1. Proximity of two clustering solutions  $\hat{X}_1$  and  $\hat{X}_2$  (Fig. 2.27):  $D(\hat{X}_1, \hat{X}_2)$ .

Case 2. Proximity of two rankings  $R_1$  and  $R_2$  (Fig. 2.28):  $D(R_1, R_2)$ .

Case 3. Proximity (auxiliary ) of two hierarchies  $H_1$  and  $H_2$  (over clusters, Fig. 2.29):  $D(H_1, H_2)$ .

Case 4. Proximity of two hierarchical clusterings  $\hat{H}_1$  and  $\hat{H}_2$  (e.g., vector; Fig. 2.30):

$$D(\hat{H}_1, \hat{H}_2) = (D(H_1, H_2), D(\hat{X}_1, \hat{X}_2)).$$

Fig. 2.31 depicts an illustrative numerical example for 7 elements:  $A = \{1, 2, 3, 4, 5, 6, 7\}$  (“hard” clustering problems).

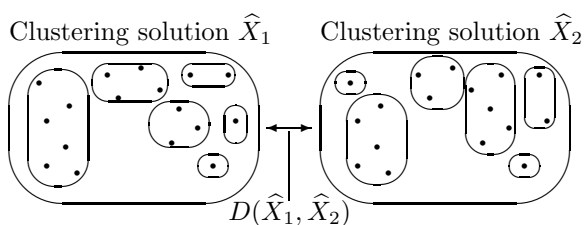


Fig. 2.27. Proximity for two clustering solutions

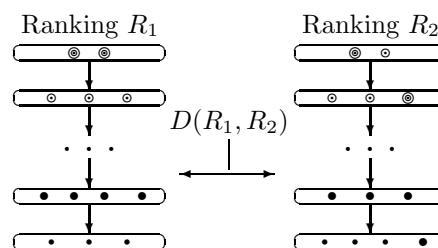


Fig. 2.28. Proximity of rankings

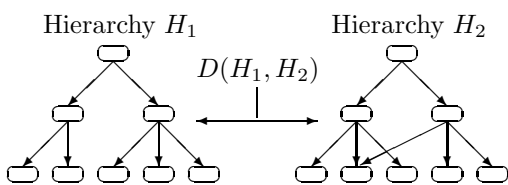


Fig. 2.29. Proximity of hierarchies

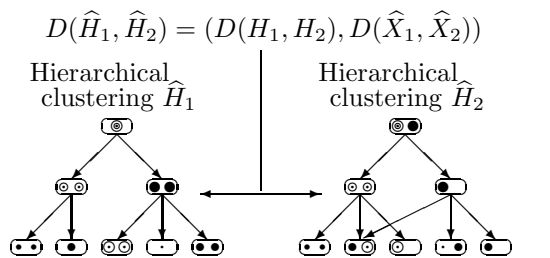


Fig. 2.30. Proximity of hierarchical clusterings

Further, some simplified versions of comparing methods for clusterings solutions are described (for “hard” clustering).

For case 1 (proximity for clustering solutions, i.e., partitions) the following main approaches are considered (e.g., [44,51,153,293,294,428,433,434,436,501]): Misclassification Error distance,  $\chi^2$  distance, Hamming distance, Rand index, Mirkin metric, ordered sets, consensus. Generally, it is possible to use



vector and multiset estimates as well. Let us consider a simplified edit proximity as number of steps for transformation (i.e., cost of transformation):

$$D(\widehat{X}_1 \Rightarrow \widehat{X}_2): \widehat{X}_1 = \{X_{1,1}, \dots, X_{1,\iota_1}, \dots, X_{1,\lambda_1}\} \implies \widehat{X}_2 = \{X_{2,1}, \dots, X_{2,\iota_2}, \dots, X_{2,\lambda_2}\}.$$

The value of proximity will be based on ordinal interval  $[0, \dots, n]$  (i.e., the number of relocated elements in  $\widehat{X}_1$ ). The following simple algorithm (heuristic) can be used (i.e.,  $\widehat{X}_1 \Rightarrow \widehat{X}'_1 = \widehat{X}_2$ ):

*Stage 1.* Definition:  $D(\widehat{X}_1 \Rightarrow \widehat{X}_2) = 0$ .

If  $\lambda_1 < \lambda_2$  then extension of solution  $\widehat{X}_1$  by  $(\lambda_2 - \lambda_1)$  empty clusters.

*Stage 2.* Calculation of the number of common elements for clusters of the clustering solutions (the number corresponds to cluster proximity)  $X_{1,\iota_1}$ ,  $\iota_1 = \overline{1, \lambda_1}$  and  $X_{2,\iota_2}$ ,  $\iota_2 = \overline{1, \lambda_2}$  as intersection (as cardinality of the same elements set). As a result, the intersection matrix will be obtained:  $M(\widehat{X}_1, \widehat{X}_2) = \|\mu(X_{1,\iota_1}, X_{2,\iota_2})\|$ ,  $\iota_1 = \overline{1, \lambda_1}$ ,  $\iota_2 = \overline{1, \lambda_2}$ .

*Stage 3.* Finding the maximum element in matrix  $M$ :

$$\mu^{max} = \mu(X_{1,\iota'}, X_{2,\iota''}) = \max_{\substack{\iota_1=1, \lambda_1, \iota_2=1, \lambda_2}} \{\mu(X_{1,\iota_1}, X_{2,\iota_2})\}.$$

*Stage 4.* Selection the cluster  $X_{1,\iota'}$  in solution  $\widehat{X}_1$  as cluster of new (transformed from  $\widehat{X}_1$ ) solution  $\widehat{X}'_1$ .

*Stage 5.* Relocation for set  $X_{1,\iota'}$  the following elements:  $\iota \in X_{2,\iota''} | \iota \notin X_{2,\iota''}$  (with deletion of the elements from other clusters of solution  $\widehat{X}_1$ ).

Increasing  $D(\widehat{X}_1 \Rightarrow \widehat{X}_2)$  by the number of the relocated elements.

*Stage 6.* Deletion of cluster  $X_{1,\iota'}$  and  $X_{2,\iota''}$  from the examination and recalculation of matrix  $M$  (i.e., deletion of the corresponding line and column).

*Stage 7.* If matrix  $M$  is empty (i.e., resultant transformed cluster  $\widehat{X}'_1$  is built) then GO TO Stage 9.

*Stage 8.* GO TO stage 3.

*Stage 9.* Stop.

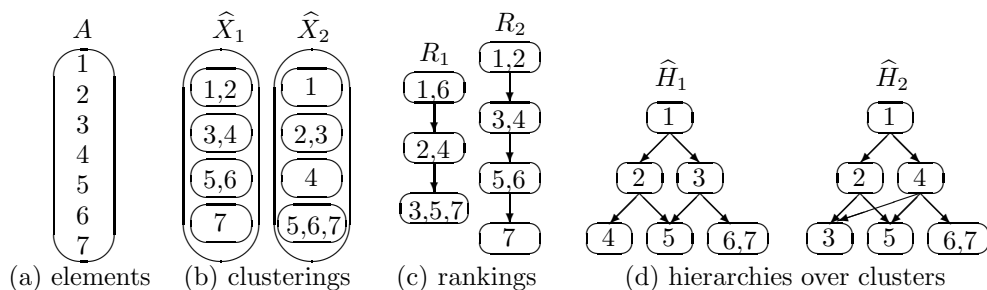


Fig. 2.31. Illustrative numerical example

**Example 2.13.** The usage of algorithm above for example from Fig. 2.31b is the following.

Two clustering solutions are under examination:

(i)  $\widehat{X}_1 = \{X_{1,1}, X_{1,2}, X_{1,3}, X_{1,4}\}$ ,  $X_{1,1} = \{1, 2\}$ ,  $X_{1,2} = \{3, 4\}$ ,  $X_{1,3} = \{5, 6\}$ ,  $X_{1,4} = \{7\}$ ,

(ii)  $\widehat{X}_2 = \{X_{2,1}, X_{2,2}, X_{2,3}, X_{2,4}\}$ ,  $X_{2,1} = \{1\}$ ,  $X_{2,2} = \{2, 3\}$ ,  $X_{2,3} = \{4\}$ ,  $X_{2,4} = \{5, 6, 7\}$ .

Table 2.14 presents the number of common elements for cluster pairs. Fig. 2.32 depicts step-by-step building the clustering solution  $\widehat{X}'_1 = \widehat{X}_2$ . Thus,  $D(\widehat{X}_1 \Rightarrow \widehat{X}'_1) = 3$  (three elements have been re-located: 7, 2, 4).

**Table 2.14.** Common elements for clusters of solutions  $\widehat{X}_1, \widehat{X}_2$

|                      | $X_{2,1} = \{1\}$ | $X_{2,2} = \{2, 3\}$ | $X_{2,3} = \{4\}$ | $X_{2,4} = \{5, 6, 7\}$ |
|----------------------|-------------------|----------------------|-------------------|-------------------------|
| $X_{1,1} = \{1, 2\}$ | 1                 | 1                    | 0                 | 0                       |
| $X_{1,2} = \{3, 4\}$ | 0                 | 1                    | 1                 | 0                       |
| $X_{1,3} = \{5, 6\}$ | 0                 | 0                    | 0                 | 2                       |
| $X_{1,4} = \{7\}$    | 0                 | 0                    | 0                 | 1                       |

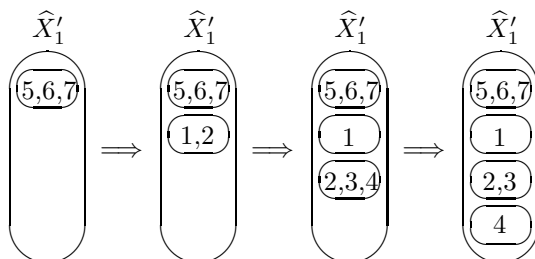


Fig. 2.32. Steps for solution  $\widehat{X}_1 \Rightarrow \widehat{X}_1 = \widehat{X}_2$

For case 2 (proximity for rankings), the following approaches are often considered (e.g., [135,136,326, 384,392,433]): 1. Kendall tau distance [327], 2. distances for partial rankings [41,190], and 3. vector-like proximity [372].

Further, proximity measure as a transformation cost will be used:  $D(R_1, R_2) = D(R_1 \Rightarrow R_2)$  (i.e., the number of element re-allocations while taking into account linear ordering over clusters) (this is similar to Kendall tau distance). Let  $\alpha(i, R_1)$  be the number of layer of element  $i \in A$  in ranking  $R_1$  and  $\alpha(i, R_2)$  be the number of layer of element  $i \in A$  in ranking  $R_2$ . Thus, re-location parameter for  $i \in A$  is:  $\Delta(i, R_1 \Rightarrow R_2) = \alpha(i, R_2) - \alpha(i, R_1)$ . Generally, the following proximity is obtained (an analogue of Kendall tau distance, ordinal scale  $[0, (n-1)n]$ ):

$$D(R_1 \Rightarrow R_2) = \sum_{i \in A} |\Delta(i, R_1 \Rightarrow R_2)| = \sum_{i \in A} |\alpha(i, R_2) - \alpha(i, R_1)|.$$

For vector-like proximity (e.g., [372,384,392]), the following parameter is considered:  $\beta^\kappa$  ( $\kappa \in [-(n-1), (n-1)]$ ) which equals the number of elements with  $\Delta(i, R_1 \Rightarrow R_2) = \kappa$ . Then, integrated vector-like proximity is:  $\overline{D}(R_1 \Rightarrow R_2) = (\beta^{-(n-1)}, \dots, \beta^{-1}, \beta^0, \beta^1, \dots, \beta^{(n-1)})$ .

**Example 2.14.** Example of two rankings from Fig. 2.31 is considered. Table 2.15 contains numbers of re-locations for each element of ranking  $R_1$  to obtain ranking  $R_2$ .

**Table 2.15.** Re-location of elements for transformation  $R_1 \Rightarrow R_2$

| $i \in A$ | Re-location | $\Delta(i, R_1 \Rightarrow R_2)$ |
|-----------|-------------|----------------------------------|
| 1         | 0           | 0                                |
| 2         | 1           | 1                                |
| 3         | 1           | 1                                |
| 4         | 0           | 0                                |
| 5         | 0           | 0                                |
| 6         | 1           | -2                               |
| 7         | 1           | -1                               |

Thus, the resultant transformation cost (the number of re-location) is:  $D(R_1 \Rightarrow R_2) = 5$ . For vector-like proximity [372,384,392], the following result is obtained:  $\overline{D}(R_1 \Rightarrow R_2) = (0, 0, 0, 0, 0, 1, 1, 3, 2, 0, 0, 0, 0, 0)$ .

For case 3 (proximity for hierarchies, e.g., trees), the following main approaches are in use (e.g., [69,218,384,392]): 1. metrics/distances (e.g., alignment distance, top-down distance, bottom-up distance) (e.g., [305,419,571,591]), 2. tree edit distances (i.e., correction algorithms) (e.g., [100,526,569,572]), 3. largest common subtree, median tree or tree agreement/consensus (e.g., [12,20,603]), and 4. vector proximity (e.g., [384,392]). For the simplification, the following correction algorithm will be considered as the number of addition and deletion of edges/arcs to transform initial tree (hierarchy)  $H_1$  into the resultant hierarchy (tree)  $H_2$ :  $D(H_1 \Rightarrow H_2)$ . For example in Fig. 2.31d,  $D(H_1 \Rightarrow H_2) = 1$  (i.e., deletion of the only one arc).

In case 4, it may be reasonable to use an integrated vector-like resultant including two main components: proximity for clustering solution and proximity for hierarchies. For example in Fig. 2.31d, the following initial information is examined:  $\widehat{H}_1 = \langle \widehat{X}_1, H_1 \rangle$  and  $\widehat{H}_2 = \langle \widehat{X}_2, H_2 \rangle$ . Thus, the following resultant two-component proximity is obtained:  $\overline{D}(\widehat{H}_1 \Rightarrow \widehat{H}_2) = (D(\widehat{X}_1 \Rightarrow \widehat{X}_2), D(H_1 \Rightarrow H_2)) = (2, 1)$ .

### 2.2.7. Aggregation of objects/clustering solutions

The aggregation problem for  $N$  initial objects is depicted in Fig. 2.33 (e.g., [384,392]):

$$\{S_1, \dots, S_\theta, \dots, S_N\} \implies S^{agg}.$$

The basic types of aggregation problems are listed in Table 2.16. Two notes can be pointed out:

1. There are aggregation problems in which the resultant (agreement) structure has another type than the initial structures, for example: (a) trees are aggregated by graph, (b) trees are aggregated by forest, (c) rankings are aggregated by fuzzy ranking, (d) rankings are aggregated by poset (e.g., [97,259,392]).

2. Separation of two-object aggregation problems is based some situations when these problems can have more simple level of algorithmic complexity than many object aggregation problems.

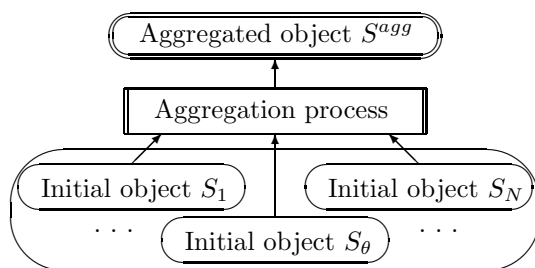


Fig. 2.33. Aggregation of objects

**Table 2.16.** Types of aggregation problems

| No. | Type of objects   | Result   | Description                   | Some) source(s)     |
|-----|---|--|-------------------------------|---------------------|
| 1.  | Two elements (i.e., two parameters vectors)                             | 1. Aggregated element                          | 1. Median                     |                     |
| 2.  | $N$ elements (i.e., $N$ parameters vectors)                             | 2. Integration (cluster)                       | 1. Integration                | [300,302]           |
| 3.  | 1 element and cluster $X$   | 1. Aggregated element                          | 1. Centroid/median            |                     |
| 4.  | 2 clusters $X_1, X_2$ ,   | 2. Integration (cluster)                       | 2. Integration                |                     |
| 5.  | $N$ clusters $\{X_1, \dots, X_N\}$                                      | Extended cluster                               | Addition                      |                     |
| 6.  | 2 clustering solutions $\hat{X}_1, \hat{X}_2$                           | 1. Agreement cluster                           | 1. Median/agreement/consensus |                     |
| 7.  | $N$ clustering solutions $\{\hat{X}_1, \dots, \hat{X}_N\}$              | 2. Aggregated cluster                          | 2. Integration                |                     |
| 8.  | 2 rankings $R_1, R_2$   | 1. Agreement cluster                           | 1. Median/agreement/consensus | [28,44,107,264,293] |
| 9.  | $N$ rankings $\{R_1, \dots, R_N\}$                                      | 2. Aggregated cluster                          | 2. Integration                | [443,447,560,579]   |
| 10. | 2 hierarchies (trees) $H_1, H_2$  | Aggregated clustering solution $\hat{X}^{agg}$ | Median/agreement/consensus    |                     |
| 11. | $N$ hierarchies (trees) $\{H_1, \dots, H_N\}$                           | Aggregated clustering solution $\hat{X}^{agg}$ | Median/agreement/consensus    | [47,135,136,574]    |
| 12. | 2 hierarchical clustering solutions $\hat{H}_1, \hat{H}_2$              | Aggregated ranking $R^{agg}$                   | Median, agreement/consensus   |                     |
| 13. | $N$ hierarchical clustering solutions $\{\hat{H}_1, \dots, \hat{H}_N\}$ | Aggregated ranking $R^{agg}$                   | Median, agreement/consensus   | [12,20,192,603]     |

The aggregation problems are formulated as a calculation procedure (e.g., calculation of a median point) or as an optimization problem to find a set/structure which is median/agreement/consensus for the set of initial structures:  $S^{agg} = \arg \min_{\forall S} \sum_{\theta=1, \overline{N}} D(S_\theta \Rightarrow S)$ . On the other hand, the aggregation problem can be considered on the basis of optimization approach:

Find an aggregation object (set, structure)  $S^{agg}$  for the initial set of objects  $\{S_1, \dots, S_\theta, \dots, S_N\}$  to obtain maximum/minimum for quality estimates of  $S^{agg}$  while taking into account requirements (as some constraints, e.g., transformation costs) for  $S^{agg}$ .

Here, the problem is ( $D^0$  is a limit for transformation cost):

$$\max_{\forall S^{agg}} \overline{Q}(S^{agg}) \quad s.t. \quad D(S_\theta \Rightarrow S^{agg}) \leq D^0, \quad \theta = \overline{1, N}.$$

The basic cases for aggregation of  $N$  objects are the following:

*Case 1.* Aggregation of  $N$  objects (i.e., points/clusters). Here, calculations of an average object/centroid or a covering object are usually used.

*Case 2.* Aggregation of  $N$  clustering solutions:  $\{\widehat{X}_1, \dots, \widehat{X}_\theta, \dots, \widehat{X}_N\} \Rightarrow \widehat{X}^{agg}$ .

*Case 3.* Aggregation of  $N$  rankings:  $\{R_1, \dots, R_\theta, \dots, R_N\} \Rightarrow R^{agg}$ .

Here the following three methods can be used: (i) median consensus method based on assignment problem (e.g., [135,136]), (ii) heuristic approach (e.g., [47,574], and (iii) method based on multiple choice problem (e.g., [372]).

*Case 4.* Aggregation of  $N$  hierarchies (trees):  $\{H_1, \dots, H_\theta, \dots, H_N\} \Rightarrow H^{agg}$ .

The following methods are often considered for trees: (1) maximum common subtree (e.g., [12]), (2) median/agreement tree (e.g., [20,192]), (3) compatible tree (e.g., [261]), and (4) maximum agreement forest (e.g., [97,259]).

*Case 5.* Aggregation of  $N$  hierarchical clustering solutions:  $\{\widehat{H}_1, \dots, \widehat{H}_\theta, \dots, \widehat{H}_N\} \Rightarrow \widehat{H}^{agg}$ .

Here, a composition of case 2 and case 4 can be considered. This aggregation problem is very prospective for future study.

Mainly (e.g., cases 2, 3, 4, 5), the aggregation problems above belong to class of NP-hard problems (e.g., [135,261]). A simplified illustrative numerical example for case 2 is as follows.

**Example 2.15.** Three initial clustering solutions for set  $A = \{1, 2, 3, 4, 5, 6, 7\}$  are examined:

(i)  $\widehat{X}_1 = \{X_{11}, X_{12}, X_{13}, X_{14}\}$ ,  $X_{11} = \{1, 2\}$ ,  $X_{12} = \{3, 4\}$ ,  $X_{13} = \{5, 6\}$ ,  $X_{14} = \{7\}$  (Fig. 2.31b);

(ii)  $\widehat{X}_2 = \{X_{21}, X_{22}, X_{23}, X_{24}\}$ ,  $X_{21} = \{1\}$ ,  $X_{22} = \{2, 3\}$ ,  $X_{23} = \{4\}$ ,  $X_{24} = \{5, 6, 7\}$  (Fig. 2.31b);

(iii)  $\widehat{X}_3 = \{X_{31}, X_{32}, X_{33}\}$ ,  $X_{31} = \{1, 2\}$ ,  $X_{32} = \{3, 4\}$ ,  $X_{33} = \{5, 6, 7\}$ .

The following aggregation problem is under examination (with constraint for cluster size):

$$\widehat{X}^{agg} = \arg \min_{2 \leq |\widehat{X}| \leq 3} \sum_{\theta=1, \overline{N}} D(\widehat{X}_\theta \Rightarrow \widehat{X}).$$

In our problem ( $N = 3$ ), the number of admissible partitions (i.e., clustering solutions) equals 90 ( $C_6^2 \times C_4^2$ ). For the simplified calculation, the following admissible aggregated clustering solution is considered:  $\widehat{X}'^{agg} = \{\widehat{X}'_1^{agg}, \widehat{X}'_2^{agg}, \widehat{X}'_3^{agg}\}$ . Numbers of common elements for clusters of initial clustering solutions  $\widehat{X}_1, \widehat{X}_2, \widehat{X}_3$  and considered aggregated solution  $\widehat{X}'^{agg}$  are presented in Table 2.17, Table 2.18, Table 2.19. The transformation costs are (i.e., numbers of re-allocations):

$$D(\widehat{X}_1 \Rightarrow \widehat{X}'^{agg}) = 1, \quad D(\widehat{X}_2 \Rightarrow \widehat{X}'^{agg}) = 2, \quad D(\widehat{X}_3 \Rightarrow \widehat{X}'^{agg}) = 0.$$

**Table 2.17.** Common elements for clusters of solutions  $\widehat{X}_1, \widehat{X}'^{agg}$ 

|                      | $X_{1,1}^{agg} = \{1, 2\}$ | $X_{3,4}^{agg} = \{3, 4\}$ | $X_{1,3}^{agg} = \{5, 6, 7\}$ |
|----------------------|----------------------------|----------------------------|-------------------------------|
| $X_{1,1} = \{1, 2\}$ | 2                          | 0                          | 0                             |
| $X_{1,2} = \{3, 4\}$ | 0                          | 2                          | 0                             |
| $X_{1,3} = \{5, 6\}$ | 0                          | 0                          | 2                             |
| $X_{1,4} = \{7\}$    | 0                          | 0                          | 1                             |

**Table 2.18.** Common elements for clusters of solutions  $\widehat{X}_2, \widehat{X}'^{agg}$ 

|                         | $X_{1,1}^{agg} = \{1, 2\}$ | $X_{3,4}^{agg} = \{3, 4\}$ | $X_{1,3}^{agg} = \{5, 6, 7\}$ |
|-------------------------|----------------------------|----------------------------|-------------------------------|
| $X_{2,1} = \{1\}$       | 1                          | 0                          | 0                             |
| $X_{2,2} = \{2, 3\}$    | 1                          | 1                          | 0                             |
| $X_{2,3} = \{4\}$       | 0                          | 1                          | 0                             |
| $X_{2,4} = \{5, 6, 7\}$ | 0                          | 0                          | 3                             |

**Table 2.19.** Common elements for clusters of solutions  $\widehat{X}_3, \widehat{X}'^{agg}$ 

|                         | $X_{1,1}^{agg} = \{1, 2\}$ | $X_{1,2}^{agg} = \{3, 4\}$ | $X_{1,3}^{agg} = \{5, 6, 7\}$ |
|-------------------------|----------------------------|----------------------------|-------------------------------|
| $X_{3,1} = \{1, 2\}$    | 2                          | 0                          | 0                             |
| $X_{3,2} = \{3, 4\}$    | 0                          | 2                          | 0                             |
| $X_{3,3} = \{5, 6, 7\}$ | 0                          | 0                          | 3                             |

## 2.3. Basic clustering models and general framework

### 2.3.1. Basic clustering problems/models

Table 2.20 contains the list of basic types of well-known clustering problems/models: (e.g., [25,22,139, 156,179,218,231,275,300,302,321,328,342,345,435,451,509,533,594,623,624]):

- (1) connectivity models (e.g., hierarchical clustering),
- (2) centroid models (e.g., k-means algorithms, i.e. *exclusive clustering*),
- (3) distribution models (based on statistical distribution),
- (4) subspace models (e.g., bi-clustering or two-mode clustering while taking into account elements and attributes),
- (5) graph-based models (e.g., detection of cliques or quasi-cliques/community structures, graph partitioning), etc.

Note, clustering procedures based on combinatorial optimization problems and/or their composition are widely studied [27,267,300,302,437]:

- (i) spanning trees based clustering (e.g., [235,244,445,479,492,606,626,660]);
- (ii) assignment/location problems based clustering (e.g., [227,323]);
- (iii) set covering problem based clustering (e.g., [9,446,525]);
- (iv) partitioning problem based clustering (e.g., [134,166,189,328,554,625]) including correlation clustering (e.g., [4,159,345]);
- (v) dominant sets/dominating sets based clustering (e.g., [101,263,400,489,643]); and
- (vi) clique/community based clustering (e.g., [9,55,170,176,236,340,426,458,459,461,496,539]).

Important contemporary clustering problems are targeted to clustering of complex (e.g., composite, modular, structured) objects, for example:

- (a) words/chains/sequence clustering (e.g., in bioinformatics) [188],
- (b) trajectory clustering [213,365,400],
- (c) data stream clustering [277,247,389],
- (d) subspace clustering [9,345,446], and
- (e) clustering of structured objects (e.g., trees, graph-based models) [201,421,534,558].

On the other hand, clustering is widely used in complex combinatorial optimization problems, for example:

- (1) clustering/partitioning of an initial problem for decreasing the problem dimension,
- (2) clustering as local auxiliary problem(s) (e.g., [332,356,372,392]).

**Table 2.20.** Basic types of clustering problems/models

| No.   | Model type   | Some sources   |
|-------|--|--|
| I.    | Basic problem formulations   |  |
| 1.1.  | Connectivity models (hierarchical/agglomerative clustering)  | [146,275,232,355,509,468,630]  |
| 1.2.  | Centroid models (k-means algorithms, <i>exclusive clustering</i> )   | [161,276,300,302,299,318,435]  |
| 1.3.  | Distribution models (based on statistical distribution)  | [300,301,302,435]  |
| 1.4.  | Subspace models (e.g., bi-clustering or two-mode clustering while taking into account elements and attributes)   | [300,302,345,415]  |
| 1.5.  | Pattern-based clustering   | [17,345,476,491,604]   |
| 1.6.  | Combinatorial optimization models in clustering:<br>(i) minimal spanning tree based clustering,<br>(ii) partitioning based clustering,<br>(iii) correlation clustering,<br>(iv) detection of communities structures (clique, etc.),<br>(v) assignment/location based clustering. | [111,218,437]<br>[302,235,244,445,479,492,606]<br>[626,660]<br>[134,166,189,328,437]<br>[4,40,159,345,564]<br>[218,170,302,459,461,496,588]<br>[227,292] |
| 1.7.  | Overlapping clustering   | [23]   |
| 1.8.  | Modularity clustering  | [7,73,459,461,625]   |
| 1.9.  | Support vector clustering  | [53,118,401]   |
| 1.10. | Spectral clustering models   | [161,254,317,414]  |
| 1.11. | Symbolic approach in clustering  | [58,63,165,233,234,364,530]  |
| 1.12. | AI-based clustering (e.g., knowledge bases, heuristics, evolutionary approaches)   | [14,30,78,142,346,453,536]<br>[544,561,587]  |
| 1.13. | Clustering based on Variable Neighborhood Search   | [268,269,271]  |
| 1.14. | Neural networks based clustering   | [186,216,315]  |
| 1.15. | Robust clustering  | [149,188,212,246,310]  |
| 1.16. | Clustering of structured objects   | [252,558]  |
| II.   | Fuzzy (soft) clustering problems/models  |  |
| 2.1.  | Fuzzy clustering   | [42,238,287,302,347,440]<br>[467,490]  |
| 2.2.  | Fuzzy k-means clustering   | [138,180,287,297]  |
| 2.3.  | Kernel-based fuzzy clustering  | [109,118,238,529]  |
| 2.4.  | Fuzzy clustering for symbolic data/categorical data  | [184,290,330]  |
| 2.5.  | Clustering based on hesitant fuzzy information   | [108,110,628,656]  |
| III.  | Stochastic clustering  |  |
| 3.1.  | Probabilistic clustering   | [62,72,302,347,412,570]  |
| 3.2.  | Probability-based graph partitioning, Markov random works  | [67,181,358,410,553,566]   |
| 3.3.  | Cross-entropy method for clustering  | [155,348,312,520,568,567]  |
| IV.   | Dynamic clustering, online clustering, restructuring   |  |
| 4.1.  | Dynamic clustering   | [48,84,104,164,316,644,652]  |
| 4.2.  | Dynamic fuzzy clustering   | [144,464,480,528]  |
| 4.3.  | Online clustering  | [43,54,92,654]   |
| 4.4.  | Restructuring in clustering (i.e., changing of clustering)   | [381,392], this paper  |
| 4.5.  | Multistage clustering, cluster trajectories  | this paper   |
| V.    | Very large clustering problems/models  |  |
| 5.1.  | Clustering of large data sets  | [55,543,653,667]   |
| 5.2.  | K-means clustering for large data sets   | [289,291,299]  |
| VI.   | Multiple clustering, framework-based clustering  |  |
| 6.1.  | Multiple clustering, cluster ensembles, aggregation clustering, consensus clustering   | [3,28,153,224,245,278,443]<br>[447,560,597,637]  |
| 6.2.  | Unified frameworks, parallel clustering, hybrid strategies   | [146,298,452,468,477,527,657]  |

**2.3.2. Systems problems**

Generally, the following vital clustering system problems can be pointed out (e.g., [52,196,300,302,435, 540,539,552,577,594,650]) (Table 2.21).

**Table 2.21.** Basic systems problems in clustering

| No.   | Systems problem  | Some source(s)   |
|-------|--|--|
| 1.    | Formulation/structuring of clustering problem(s)   | [275,300,302,433,434,435,594]                          |
| 2.    | Comparison of models/methods/techniques  | [427,501,557,650]                                      |
| 3.    | Selection/design of model/method/technique   | [117,209,541]  |
| 4.    | Evaluation of clustering solution(s)   | [4,33,39,40,94,95,159]<br>[226,345,457,459,564,662]    |
| 5.    | Validation of clustering solution  | [56,177,257,258,359,424,452]                           |
| 6.    | Stability of clustering solution   | [51,359,541,552]                                       |
| 7.    | Robustness of clustering solution  | [4,109,149,188,212,246,310]                            |
| 8.    | Cluster editing, cluster graph modification,<br>transformation of clustering solution  | [64,65,66,147,157,251]<br>[500,539,540]                |
| 9.    | Identification/selection/assignment of cluster heads<br>(e.g., sensor networks, mobile networks, target tracking)                            | [82,98,103,119,280,307,577,583]<br>[589,638]           |
| 10.   | Prospective clustering problems/approaches:  |  |
| 10.1. | Online clustering, clustering data streams   | [43,54,92,247,360,389]                                 |
| 10.2. | Multiple clustering, consensus clustering  | [3,28,153,224,245,278,443]                             |
| 10.3. | Hybrid (by methods, by data types) clustering methods<br>composite, multistage/multilevel clustering methods<br>(including adaptation modes) | [115,303,314,357,404,416,576,584]<br>[562,617,618,642] |
| 10.4. | Expert knowledge based clustering/classification<br>(including expert judgment based clustering)   | [125,126,214,215,453,490]                              |
| 10.5. | Multicriteria optimization clustering  | [156,197,368,392,551,666]                              |
| 10.6. | Clustering with multi-type elements (each cluster is<br>composed by compatible elements of different types)                                  | this paper   |
| 10.7. | Clustering with hesitant fuzzy sets data   | [627,628,108]  |
| 10.8. | Fast clustering methods  | [218,170,302,457,459,461]                              |

In addition, the following system stage can be used:

“Modification of clustering process (if needed), for example, by the following ways:” (a) modification of type(s) of element description(s), (b) modification of element parameters/features, (c) modification of element estimates types (or scales), (d) modification of criteria for inter-cluster proximity and intra-cluster proximity, (e) modification of criteria for quality of clustering solution(s), (f) modification of clustering method(s), and (g) searching for additional expert(s).

### 2.3.3. General framework

Fig. 2.6 depicts an example of a clustering framework for multiple clustering. Another generalized clustering/classification framework (the viewpoint of a simplified information processing morphology) is presented in Fig. 2.34 (an extension of framework in Fig. 2.11):

*Stage 1.* Collection of initial data.

*Stage 2.* Analysis of applied situation, problem structuring/formulation: (2.1) selection/generation of features/parameters/criteria, (2.2) definition and description (assessment) of the set of objects/items, (2.3) selection/design of basic clustering model(s).

*Stage 3.* Preliminary data processing: (3.1) calculation of element proximities (distances), (3.2) definition of very close elements (i.e., definition of a small element proximity/distance), (3.3) definition of basic relation(s) over element set (a basic relation graph(s)), (3.4) revelation of basic preliminary groups of interconnected elements (i.e., some preliminary kernels of clusters).

*Stage 4.* Basic clustering: (4.1) selection/definition of basic groups of interconnected elements (i.e., some candidates-clusters), (4.2) definition of the basic cluster set, (4.3.) extension of the basic cluster set (within framework of feedback).

*Stage 5.* Classification (if needed): (5.1) assignment of elements into clusters, (5.2) multiple assignment of elements into clusters.

*Stage 6.* Aggregation of cluster solutions (i.e., consensus clustering/clustering ensemble) (if needed).

*Stage 7.* Analysis of clustering/classification results (clustering solution(s)) (e.g., cluster validity).

Here, a special support layer can include the following: 1. additional data, 2. expert(s) and expert(s) knowledge, 3. additional models (e.g., vertex covering problem, assignment/matching problems, multiple criteria sorting/ranking problems, clique/quasi clique problem(s), multiple clique/quasi clique problem(s), median/consensus/agreement problems).

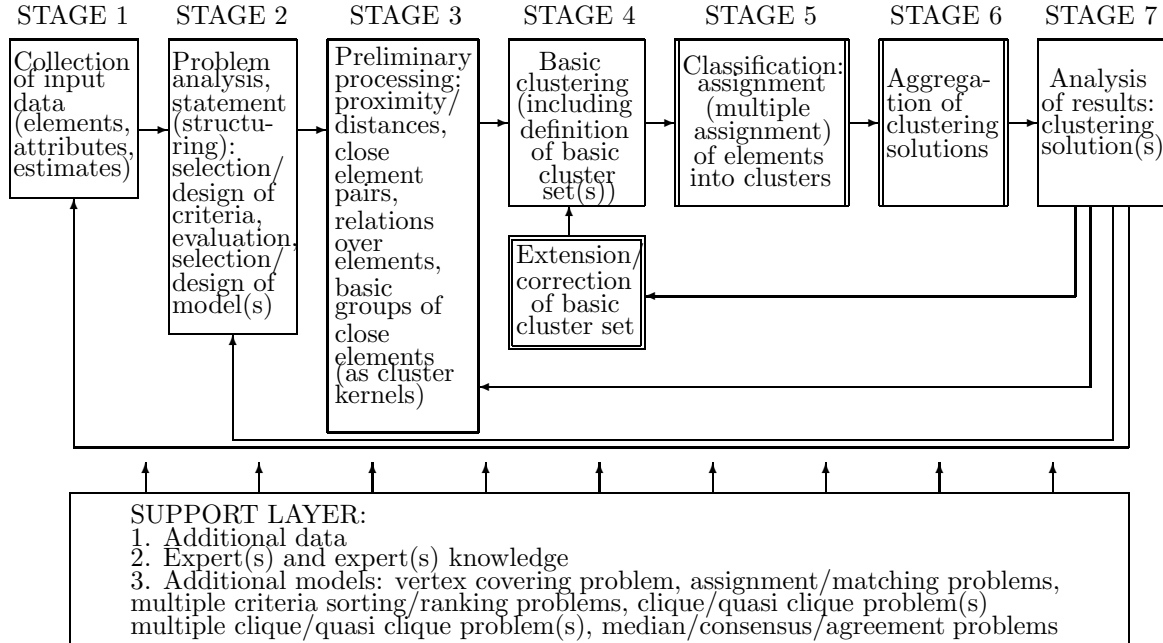


Fig. 2.34. General framework for clustering/classification

Note, the following can be used as alternative morphological components:

(i) various problem analysis and formulation approaches (e.g., selection of well-known problem statement(s), design of a new problem formulation(s)), (ii) various element metrics/proximities, (iii) various cluster metrics/proximities, (iv) various item assessment techniques (e.g., usage of statistical data, usage of expert-based techniques), (v) various clustering methods, (v) various clustering solution aggregation methods.

### 2.3.4. Example of solving morphological scheme

A simplified example of morphological scheme for clustering process presented in Fig. 2.34 (an analogue of composite strategy for multicriteria ranking/sorting problem [387,392]) is the following (Fig. 2.35):

**0.** Compressed solving framework  $S = H \star P \star M \star G \star Q$  :

**1.** Analysis of situation, problem statement and structuring (i.e., parameters/criteria, scales, etc.), assessment  $H = X \star Y$  (stage 3):

(1.1) problem formulation  $X$ : classification (“hard”)  $X_1$ , classification (“soft”)  $X_2$ , clustering (i.e., partitioning) (“hard”)  $X_3$ , clustering (i.e., partitioning) (“soft”)  $X_4$ , sorting (“hard”)  $X_5$ , sorting (“soft”)  $X_6$ , a composite problem  $X_7$ .

(1.2) assessment of objects/items  $Y$ : usage of statistical data  $Y_1$ , expert based procedures  $Y_2$ , statistical data and expert based procedures  $Y_3 = Y_1 \& Y_2$ .

**2.** Criteria/proximities and preliminary processing  $P = U \star V$  (stage 3):

(2.1) proximity/metric for element pair (i.e., similarity measure)  $U$ : Euclidean distance ( $L_2$ )  $U_1$ , ordinal estimate  $U_2$ , multicriteria estimate  $U_3$ , interval multiset estimate  $U_4$ ,

(2.2) intra-cluster quality (criterion for intra-cluster “distance”, to minimize)  $V$ : maximum of element pair proximity (single link)  $V_1$ , maximum of all element pair proximities (all links or average link)  $V_2$ ;

(2.3) criterion for inter-cluster “distance” (to maximize)  $W$ : minimum “distance” between clusters  $W_1$ , average “distance” between clusters  $W_2$ .



3. Clustering method/model  $M$  (stage 4): hierarchical clustering  $M_1$ ,  $K$ -means clustering  $M_2$ , spanning tree based clustering  $M_3$ , graph method based on detection of cliques/quasi-cliques  $M_4$ , correlation clustering  $M_5$ , composite method (parallel processing)  $M_6 = M_2 \& M_3 \& M_4$ , composite method (parallel processing)  $M_7 = M_2 \& M_4 \& M_5$ .

4. Aggregation of clustering solutions  $G$  (stage 6): none  $G_1$ , median-based solving process  $G_2$ , extension of common clustering solution part (i.e., a solution kernel)  $G_3$ .

5. Analysis of resultant clustering solution(s) (i.e., cluster validity)  $Q$  (stage 7): none  $Q_1$ , expert-based process  $Q_2$ , special calculation procedure(s)  $Q_3$ .

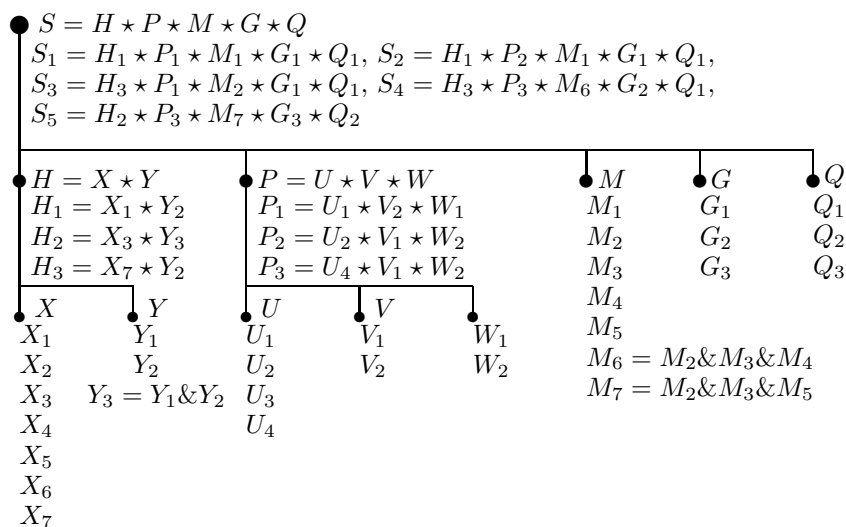


Fig. 2.35. Illustration for morphological scheme of clustering

Thus, five illustrative alternative examples of the composite (series-parallel) solving strategies for clustering are the following (Fig. 2.35):

$$\begin{aligned}
 S_1 &= H_1 \star P_1 \star M_1 \star G_1 \star Q_1 = (X_1 \star Y_2) \star (U_1 \star V_2 \star W_1) \star M_1 \star G_1 \star Q_1; \\
 S_2 &= H_1 \star P_2 \star M_1 \star G_1 \star Q_1 = (X_1 \star Y_2) \star (U_2 \star V_1 \star W_2) \star M_1 \star G_1 \star Q_1; \\
 S_3 &= H_3 \star P_1 \star M_2 \star G_1 \star Q_1 = (X_7 \star Y_2) \star (U_1 \star V_2 \star W_1) \star M_2 \star G_1 \star Q_1; \\
 S_4 &= H_3 \star P_3 \star M_6 \star G_2 \star Q_1 = (X_7 \star Y_2) \star (U_4 \star V_1 \star W_2) \star (M_2 \& M_3 \& M_4) \star G_2 \star Q_1; \text{ and} \\
 S_5 &= H_2 \star P_3 \star M_7 \star G_3 \star Q_2 = (X_3 \star (Y_1 \& Y_2)) \star (U_4 \star V_1 \star W_2) \star (M_2 \& M_3 \& M_5) \star G_3 \star Q_1.
 \end{aligned}$$

In Fig. 2.36, a graphical illustration for three composite strategies above is depicted.

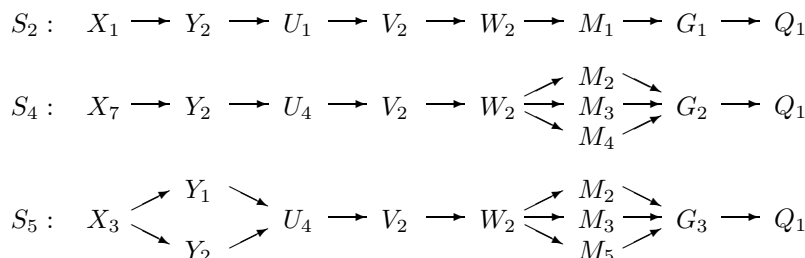


Fig. 2.36. Examples of composite solving strategies

## 2.4. On clustering in large scale data sets/networks

In recent years, the significance of clustering in large-scale data bases and analysis and modeling in large networks has been increased, for example:

- (i) clustering of large data sets (e.g., [55,289,291,299,543,653,667]);
- (ii) detection of communities in large networks (e.g., [127,230,285,286,370,495,636]);
- (iii) detection of communities in mega-scale networks (e.g., [59,600]);
- (iv) tracking evolving communities in large networks (e.g., [286]).

Table 2.22 illustrates some dimensional layers (classification) of data sets/networks.

**Table 2.22.** Dimensional layers of data sets/networks

| No. | Type of studied data sets/networks                    | Number of objects/network nodes | Examples of applications   | Some source(s) |
|-----|---|---------------------------------|--|----------------|
| 1.  | Simplified data sets/networks<br>(e.g., small groups) | ~ 10...60                       | (i) student group,<br>(ii) sport club network,<br>(iii) laboratory group,<br>(iv) Web page structure,<br>(v) product assortment<br>(product variety)   | [646]          |
| 2.  | Simple data sets/networks                             | ~ 100                           | (i) university department,<br>(ii) animal network,<br>(iii) big firm department,<br>(iv) department of government organization,<br>(v) network of books/articles<br>(close by topic(s))<br>(vi) social network of bottlenose dolphins,<br>(vii) supply chain network,<br>(viii) network of software system components,<br>(ix) molecular structures,<br>(x) manufacturing structures | [461]          |
| 3.  | Traditional data sets/networks                        | ~ 1 k                           | (i) citation networks,<br>(ii) university network,<br>(iii) collaboration network,<br>(iv) urban systems,<br>(v) consumers bases,<br>(vi) multiple server computer systems   | [226]          |
| 4.  | Large data sets/networks                              | ~ 10 k                          | (i) research society network,<br>(ii) sensor networks,<br>(iii) manufacturing technology networks,<br>(iv) Microarrays   | [461]          |
| 5.  | Very large data sets/networks                         | ~ 100 k                         | (i) client bases,<br>(ii) VLSI,<br>(iii) medical patients bases,   | [127]          |
| 6.  | Mega-scale data sets/networks                         | ~ 1 M                           | (i) university library,<br>(ii) bases of editorial houses,   | [600]          |
| 7.  | Super-scale data sets/networks                        | ~ 10 M                          | (i) library networks,<br>(ii) Internet-based shops,<br>(iii) protein sequence databases  | [59]           |
| 8.  | To-day's/prospective Web-based data sets/networks     | ~ 100 M ...1 B                  | (i) World Wide Web,<br>(ii) social networks<br>(e.g., Twitter, Facebook)   |                |

### 2.5. Note on multidimensional scaling

Many decades, multidimensional scaling approach is widely used in many domains (e.g., [70,86,143, 150,580,645]). Here, an initial space of object parameters is transformed and simplified (by increasing its dimension, on the basis of optimization). As a result, obtained clusters are more "good". Table 2.23 contains some basic directions in multidimensional scaling researches.

**Table 2.23.** Directions in multidimensional scaling (methods, clustering, CS applications)

| No.    | Approaches, models   | Source(s)                   |
|--------|--|-----------------------------|
| 1.     | Basic methods in multidimensional scaling:   |                             |
| 1.1.   | Multidimensional scaling, general  | [70,86,143,150,240,349,580] |
| 1.2.   | Nonmetric multidimensional scaling   | [284,350]                   |
| 1.3.   | Least-squares multidimensional scaling   | [242]                       |
| 1.4.   | Application of convex analysis to multidimensional scaling   | [366]                       |
| 1.5.   | Global optimization in multidimensional scaling  | [241,241]                   |
| 1.6.   | Probabilistic multidimensional scaling   | [663]                       |
| 1.7.   | Genetic algorithms, evolutionary methods<br>in multidimensional scaling  | [575]                       |
| 1.8.   | Multigrid multidimensional scaling   | [77]                        |
| 1.9.   | Configural synthesis in multidimensional scaling   | [239]                       |
| 1.10.  | Functional approach to data structure<br>in multidimensional scaling   | [99]                        |
| 1.11.  | Convergence of methods in multidimensional scaling   | [367]                       |
| 1.12.  | Distributed multidimensional scaling   | [141]                       |
| 2.     | Multidimensional clustering:   |                             |
| 2.1.   | Multidimensional clustering algorithms   | [451]                       |
| 2.2.   | Multidimensional scaling and data clustering:  |                             |
| 2.2.1. | Multidimensional scaling and data clustering   | [283]                       |
| 2.2.2. | Multidimensional scaling: tree-fitting, and clustering   | [545]                       |
| 2.3.   | Multidimensional data clustering utilizing<br>hybrid search strategies   | [298]                       |
| 3.     | Contemporary applications in CS:   |                             |
| 3.1.   | Multidimensional clustering in data mining   | [55]                        |
| 3.2.   | Graph drawing by multidimensional scaling  | [337]                       |
| 3.3.   | Visualization  | [619]                       |
| 3.4.   | Multidimensional scaling in communication, sensor<br>networks (node localization, location, positioning, etc.) | [116,141,362]               |

### 3. Basic Structured Clustering Combinatorial Schemes

#### 3.1. Auxiliary problems

Table 3.1 contains a list of main auxiliary problems for combinatorial clustering methods/procedures.

**Table 3.1.** Auxiliary problems

| No.   | Problem   | Clustering model(s)/stage(s)      | Solving schemes  | Some source(s)   |
|-------|---|-----------------------------------|--|--|
| 1.    | Transformation of scales  | Data processing                   | 1.Calculation<br>2.Expert judgment   |  |
| 2.    | Calculation of proximity matrix   | Main clustering schemes           | 1.Direct calculation<br>2.Calculation with scale transformation                              |  |
| 3.    | Multicriteria ranking/sorting   | 1.Data processing<br>2.Clustering | 1.Utility function<br>2.Pareto approach<br>3.Outranking technique<br>4.Expert judgment, etc. | [71,198,324,387,392]<br>[485,518,666]                                |
| 4.    | Minimum spanning tree   | Graph-based clustering            | 1.Kruskal's algorithms<br>2.Boruvka's algorithms   | [10,139,174,217,218]<br>[599,606,493,626,639]                        |
| 5.    | Knapsack-like problems (basic problem, multiple choice problem, multicriteria problems) | k-means clustering, restructuring | 1.Dynamic programming (e.g., FPTAS)<br>2.Approximation<br>3.Heuristics                       | [174,218,295,325,420]<br>[523]                                       |
| 6.    | Assignment problems (basic problem, generalized problem, multicriteria problem)         | k-means clustering                | 1.Fast algorithms<br>2.Heuristics<br>3.Enumerative methods                                   | [16,79,90,174,218]<br>[292,323,351,392,396]<br>[482,483,494,519,532] |
| 7.    | Covering problems   | Set covering based clustering     | 1.Enumerative methods<br>2.Heuristics  | [9,446,525]  |
| 8.    | Dominating sets problem   | Dominating set based clustering   | 1.Enumerative methods<br>2.Heuristics  | [101,263,400,489,643]  |
| 9.    | Partitioning problems:  |                                   |  |  |
| 9.1.  | Graph partitioning  | Partitioning based clustering     | 1.Approximation<br>2.Heuristics  | [134,166,189,328,554]<br>[625]                                       |
| 9.2.  | Graph partitioning  | Correlation clustering            | 1.Enumerative methods<br>2.Heuristics  | [4,33,39,40,110]<br>[159,345,564,662]                                |
| 10.   | Communities detection:  |                                   |  |  |
| 10.1. | Detection of clique/quasi-clique  | Clique based clustering           | 1.Enumerative methods<br>2.Heuristics  | [2,81,152,176,174,218]<br>[236,309,340,426]                          |
| 10.2. | Detection of network communities  | Communities detection             | 1.Enumerative methods<br>2.Heuristics  | [7,226,371,457,458]<br>[459,460,461,478,496]                         |
| 13.   | Finding agreement/median/consensus for:   | Consensus clustering              | 1.Approximation<br>2.Heuristics  |  |
| 13.1. | Partitions  |                                   |  | [28,44,107,264,293]<br>[443,447,560,579]                             |
| 13.2. | Rankings  |                                   |  | [47,135,136,392,574]   |
| 13.3. | Trees   |                                   |  | [12,20,192,603]  |
| 14.   | Morphological clique problem  | Clustering of multi-type objects  | 1.Heuristic<br>2.Enumerative methods   | [152,372,374,385,392]  |

Fig. 3.1 depicts main stages for processing of initial data:

1. Collection of initial information, i.e., set of objects  $A = \{A_1, \dots, A_l, \dots, A_n\}$ , set of parameters  $C = \{C_1, \dots, C_i, \dots, C_m\}$ , estimates of objects upon parameters  $x_l = (x_{l,1}, \dots, x_{l,i}, \dots, x_{l,m})$  ( $l = \overline{1, n}$ ).
2. Calculation of distance matrix  $Z = \|z_{\iota_1, \iota_2}\|$  ( $\iota_1 = \overline{1, n}, \iota_2 = \overline{1, n}$ ); (usually: complexity estimate equals  $O(m \times n^2)$ ).
3. Transformation of distance matrix into a spanning graph (if needed):

$Z = \|z_{\iota_1, \iota_2}\| \implies G(A, \Gamma)$ ; (usually: complexity estimate equals  $O(n^2)$ ).

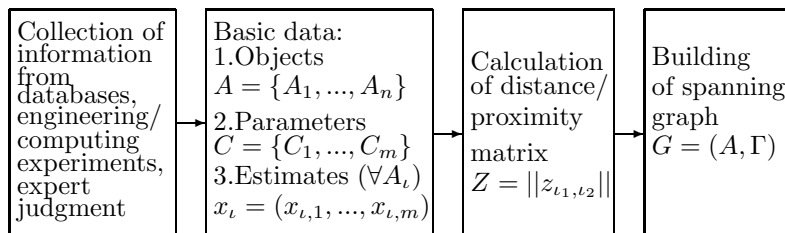


Fig. 3.1. Preliminary data processing

Procedures for transformation of scales (e.g., transformation of ordinal scale into ordinal scale, transformation of vector-like scale into ordinals scale, transformation of vector scale into multiset based scale) can be useful for processing of proximity matrix and for design of covering graph (to obtain a simple covering graph, e.g., by the use of thresholds for edge/arcs estimates/weights). On the other hand, transformation of vector-like estimates into ordinal estimates can be based on multicriteria ranking (sorting problem).

Minimum spanning tree problem is an important part of many effective solving schemes for many combinatorial optimization problems (e.g., [139,218]): (a) polynomial approximation of initial graph by tree, (b) effective solving a combinatorial problem over the obtained tree. Here, several well-known algorithms for design of minimum spanning tree can be used, for example: Borovka's algorithm Prim's algorithm, Kruskal's algorithm [10,217,218,139,493,639]. Complexity estimate of the algorithms is:  $O(p \log n)$  (or less [639]) ( $p$  is the number of edges,  $n$  is the number of vertices).

Other auxiliary combinatorial problems (Table 3.1) are more complicated (i.e., they belong to class of NP-hard problems). Only in some simple cases polynomial algorithms can be used:

- (i) polynomial algorithms for basic assignment problem (e.g., [218,351]);
- (ii) polynomial approximate solving schemes for basic knapsack problem and multiple choice problem (e.g., [218,295,325,420,523]);
- (iii) polynomial algorithms for some network partition problems (e.g., cores decomposition of networks [45]);
- (iv) polynomial approximate solving schemes for simple cases of partitioning problems, network community detection problems, covering problems.

Thus, it is necessary to use polynomial heuristics or enumerative methods for the above-mentioned auxiliary combinatorial problems (i.e., generalized assignment problem, clique problems, morphological clique problem, dominating set problem, covering problems, graph partitioning problems, finding agreement/median/consensus problems, multicriteria combinatorial problems). In the case of fast clustering schemes, fast heuristics (e.g., some analogues of greedy algorithms) have to be used for auxiliary combinatorial problems.

Some basic clustering models (e.g., hierarchical clustering, k-means clustering) are often used as auxiliary problems of multi-stage clustering schemes (e.g., for preliminary definition of a cluster set or cluster centroids).

The significance of balanced clustering problems (by cluster size) has been increased in many domains (e.g., communication systems). As a result, balanced partition of tree problem can be useful components of contemporary clustering schemes. Generally, the problem of  $k$ -balanced partitioning a tree is NP-hard ( $k$  is the number of elements in each cluster of clustering solution) [195]. Here, it may be reasonable to use  $k$ -balanced agglomerative algorithm over a tree (i.e., under restriction on cluster sizes in obtained solution).

### 3.2. Hierarchical clustering

Hierarchical clustering is widely used in many domains (e.g., [146,232,275,300,302,355,375,468,509,630]). The approach consists in agglomerative (i.e., hierarchical, "Bottom-Up") scheme (e.g., [275,300,302,375]):

1. Calculate the proximity (distance) matrix between elements.
2. Start with  $n$  clusters containing one element.

3. Find the most similar pair of clusters from the proximity matrix and merge them into a single cluster
4. Update the proximity matrix (reduce its order by one, by replacing the individual clusters with the merged clusters)
5. Repeat steps 3,4 until a single cluster is obtained (i.e.,  $n - 1$  times).

### 3.2.1. Basic agglomerative algorithm

The basic agglomerative algorithm (*algorithm 1*) is the following (e.g., [375,392]):

*Stage 1.* Calculate the matrix of element pair  $\forall(A(i_1), A(i_2))$ ,  $A(i_1) \in A$ ,  $A(i_2) \in A$ ,  $i_1 \neq i_2$  “distances” (a simple case, metric  $l_2$ ):

$$z_{i_1 i_2} = \sqrt{\sum_{j=1}^m (x_{i_1, j} - x_{i_2, j})^2}.$$

*Stage 2.* Searching for the minimum element pair “distance”  $z^{min} = \min_{i_1, i_2 \in \{1, \dots, n\}} \{z_{i_1, i_2}\}$ , integration of the corresponding two elements into a resultant “integrated” element, extension of the corresponding cluster.

*Stage 3.* If all elements are processed than GO TO Stage 5.

*Stage 4.* Recalculate the matrix of pair “distances”  $Z$  (initial element set is decreased by 1 element) and Go To Stage 2.

*Stage 5.* Stop.

As result, a tree-like structure for the element pair integration process (Bottom-Up) is obtained (one element pair integration at each integration step). A basic simplified procedure for aggregation of items (aggregation as average values) is as follows ( $J_{i_1, i_2} = A_{i_1} \& A_{i_2}$ ):  $\forall j = \overline{1, m} \quad x_{J_{i_1, i_2}, j} = \frac{x_{i_1, j} + x_{i_2, j}}{2}$ .

Complexity estimates for the above-mentioned version hierarchical clustering algorithm (by stages) is presented in Table 3.2.

**Table 3.2.** Complexity estimates for stages of basic hierarchical clustering algorithm

| Stage    | Description  | Complexity estimate (running time) |
|----------|--|------------------------------------|
| Stage 1  | Calculate the distance matrix $Z$  | $O(n^2)$                           |
| Stage 2  | Searching for the minimum element pair “distance”, integration of the corresponding element pair, extension of the corresponding cluster | $O(n^2)$                           |
| Stage 3. | Checking the condition for stopping (all elements are processed)   | $O(n)$                             |
| Stage 4  | Recalculate the “distance” matrix $Z$  | $O(n^2)$                           |
| Stage 5. | Stopping   | $O(1)$                             |

Here there exists a computing cycle (stages 2,3,4) that can contain  $(n - 1)$  steps. Thus, the general complexity (running time) of this hierarchical clustering algorithm equals  $O(n^3)$ . Generally, hierarchical clustering methods have the following problems: (a) sensitivity to noise and outliers, (b) difficulty handling different sized clusters and convex shapes, and (c) breaking large clusters.

### 3.2.2. Balancing by cluster size

Now let us consider a modified version of hierarchical clustering with a special requirement to cluster size (as balancing of cluster sizes) to obtain about the same (close) cluster sizes. Let  $B = \{B_1, \dots, B_l, \dots, B_\kappa\}$  be the obtained set of clusters. Let  $\alpha_\iota = |B_\iota|$  ( $\iota = \overline{1, \kappa}$ ) be the size (i.e., number of elements) for cluster  $B_\iota$ .

Thus for each cluster the following constraints are considered:  $\alpha' \leq \alpha_\iota \leq \alpha''$ . For example:  $\alpha' = 3$ ,  $\alpha'' = 4$ . Evidently, one cluster of the obtained cluster set can contain less elements (i.e., 1, 2, ...,  $(\alpha' - 1)$ ). Generally, the above-mentioned requirement leads to balanced clustering solution by cluster size. This is

significant in many applications (e.g., local areas in communication networks, student teams in educational process). Our modified balanced by cluster size hierarchical clustering algorithm is:

*Stage 1.* Calculate the matrix of element pair  $\forall(A(i_1), A(i_2)), A(i_1) \in A, A(i_2) \in A, i_1 \neq i_2$  “distances” (a simple case, metric  $l_2$ ):

$$z_{i_1 i_2} = \sqrt{\sum_{j=1}^m (x_{i_1, j} - x_{i_2, j})^2}.$$

*Stage 2.* Searching for the minimum element pair “distance”  $z^{min} = \min_{i_1, i_2 \in \{1, \dots, n\}} \{z_{i_1, i_2}\}$ , integration of the corresponding two elements into a resultant “integrated” element, extension of the corresponding cluster.

*Stage 3.* Analysis of the obtained extended cluster  $B_i$  by new size  $\alpha_i$ . If  $\alpha_i = \alpha''$  then deleting the cluster and its elements for the future processing (as a part of the resultant solution).

*Stage 4.* If all elements are processed than GO TO Stage 6.

*Stage 5.* Recalculate the matrix of pair “distances”  $Z$  (initial element set is decreased by 1 element) and Go To Stage 2.

*Stage 6.* The other elements are organized as additional separated clusters (if needed). Stop.

Complexity estimates for the above-mentioned version hierarchical clustering algorithm (by stages) is presented in Table 3.3.

**Table 3.3.** Complexity estimates of stages for balanced (by cluster size) hierarchical algorithm

| Stage    | Description  | Complexity estimate (running time) |
|----------|--|------------------------------------|
| Stage 1  | Calculate distance matrix $Z$  | $O(n^2)$                           |
| Stage 2  | Searching for the minimum element pair “distance”, integration of the corresponding element pair, extension of the corresponding cluster | $O(n^2)$                           |
| Stage 3. | Checking the condition for stopping (all elements are processed)   | $O(n)$                             |
| Stage 4. | Analysis of the obtained cluster by cluster size   | $O(1)$                             |
| Stage 5  | Recalculate the “distance” matrix $Z$  | $O(n^2)$                           |
| Stage 6. | Stopping   | $O(1)$                             |

Here there exists a computing cycle (stages 2,3,4,5) that can contain  $(n - 1)$  steps. Thus, the general complexity (running time) of this hierarchical clustering algorithm equals  $O(n^3)$ . Note the average complexity estimate is less.

**Example 3.1.** A numerical example of tree with weights of edges (i.e., proximity between element pairs) is presented in Fig. 3.2: tree  $T = (A, E)$ ,  $A = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14\}$ . The constraint for cluster size is:  $\leq 3$ . Table 3.4. contains the corresponding proximity matrix, i.e., weights of edges (a very large proximity is denoted by symbol “\*”, proximity is symmetric).

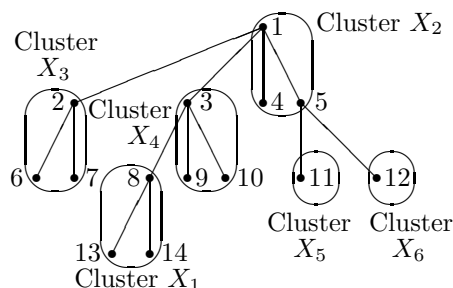


Fig. 3.2. Balanced clustering of tree

**Table 3.4.** Proximities for tree-like example (edge  $(i_1, i_2)$ )

| $i_1$ | $i_2$ : | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  | 11  | 12  | 13  | 14  |
|-------|---------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 1     |         | 1.5 | 1.7 | 0.5 | 0.2 | *   | *   | *   | *   | *   | *   | *   | *   | *   |
| 2     |         |     | *   | *   | *   | 0.1 | 0.6 | *   | *   | *   | *   | *   | *   | *   |
| 3     |         |     |     | *   | *   | *   | *   | 3.1 | 1.0 | 0.9 | *   | *   | *   | *   |
| 4     |         |     |     |     | *   | *   | *   | *   | *   | *   | *   | *   | *   | *   |
| 5     |         |     |     |     |     | *   | *   | *   | *   | *   | 2.5 | 2.1 | *   | *   |
| 6     |         |     |     |     |     |     | *   | *   | *   | *   | *   | *   | *   | *   |
| 7     |         |     |     |     |     |     |     | *   | *   | *   | *   | *   | *   | *   |
| 8     |         |     |     |     |     |     |     |     | *   | *   | *   | *   | 0.3 | 0.4 |
| 9     |         |     |     |     |     |     |     |     |     | *   | *   | *   | *   | *   |
| 10    |         |     |     |     |     |     |     |     |     |     | *   | *   | *   | *   |
| 11    |         |     |     |     |     |     |     |     |     |     |     | *   | *   | *   |
| 12    |         |     |     |     |     |     |     |     |     |     |     |     | *   | *   |
| 13    |         |     |     |     |     |     |     |     |     |     |     |     |     | *   |

In the considered case (i.e., tree), proximity information can be presented as a list of  $(n-1)$  components: number of vertex, number of “son”-vertex, weight of the corresponding edge (Table 3.5).

**Table 3.5.** Initial list if proximities

| Vertex $i_1$ | Vertex $i_2$<br>(“son” of $i_1$ ) | Weight of<br>edge $(i_1, i_2)$ |
|--------------|-----------------------------------|--------------------------------|
| 1            | 2                                 | 1.5                            |
| 1            | 3                                 | 1.7                            |
| 1            | 4                                 | 0.5                            |
| 1            | 5                                 | 0.2                            |
| 2            | 6                                 | 0.1                            |
| 2            | 7                                 | 0.6                            |
| 3            | 8                                 | 3.1                            |
| 3            | 9                                 | 1.0                            |
| 3            | 10                                | 0.9                            |
| 5            | 11                                | 2.5                            |
| 5            | 12                                | 2.1                            |
| 8            | 13                                | 0.3                            |
| 8            | 14                                | 0.4                            |

In the example, proximity between element  $x$  and cluster  $Y$  (or integrated element)  $D^{min}(x, Y)$  is used (case 2 from previous section 2). The steps of agglomerative algorithms to obtain the balanced clustering (cluster size is  $\leq 3$ ) are the following:

*Step 1.* Integration of elements 2 and 6 into  $J(2, 6)$ . As a result, Table 3.6 is obtained.

**Table 3.6.** List of proximities after step 1

| Vertex $i_1$ | Vertex $i_2$<br>(“son” of $i_1$ ) | Weight of<br>edge $(i_1, i_2)$ |
|--------------|-----------------------------------|--------------------------------|
| 1            | $J(2, 6)$                         | 1.5                            |
| 1            | 3                                 | 1.7                            |
| 1            | 4                                 | 0.5                            |
| 1            | 5                                 | 0.2                            |
| $J(2, 6)$    | 7                                 | 0.6                            |
| 3            | 8                                 | 3.1                            |
| 3            | 9                                 | 1.0                            |
| 3            | 10                                | 0.9                            |
| 5            | 11                                | 2.5                            |
| 5            | 12                                | 2.1                            |
| 8            | 13                                | 0.3                            |
| 8            | 14                                | 0.4                            |



*Step 2.* Integration of elements 1 and 5 into  $J(1, 5)$ . As a result, Table 3.7 is obtained.

**Table 3.7.** List of proximities after step 2

| Vertex $i_1$ | Vertex $i_2$<br>("son" of $i_1$ ) | Weight of<br>edge $(i_1, i_2)$ |
|--------------|-----------------------------------|--------------------------------|
| $J(1, 5)$    | $J(2, 6)$                         | 1.5                            |
| $J(1, 5)$    | 3                                 | 1.7                            |
| $J(1, 5)$    | 4                                 | 0.5                            |
| $J(2, 6)$    | 7                                 | 0.6                            |
| 3            | 8                                 | 3.1                            |
| 3            | 9                                 | 1.0                            |
| 3            | 10                                | 0.9                            |
| $J(1, 5)$    | 11                                | 2.5                            |
| $J(1, 5)$    | 12                                | 2.1                            |
| 8            | 13                                | 0.3                            |
| 8            | 14                                | 0.4                            |

*Step 3.* Integration of elements 8 and 13 into  $J(8, 13)$ . As a result, Table 3.8 is obtained.

**Table 3.8.** List of proximities after step 3

| Vertex $i_1$ | Vertex $i_2$<br>("son" of $i_1$ ) | Weight of<br>edge $(i_1, i_2)$ |
|--------------|-----------------------------------|--------------------------------|
| $J(1, 5)$    | $J(2, 6)$                         | 1.5                            |
| $J(1, 5)$    | 3                                 | 1.7                            |
| $J(1, 5)$    | 4                                 | 0.5                            |
| $J(2, 6)$    | 7                                 | 0.6                            |
| 3            | $J(8, 13)$                        | 3.1                            |
| 3            | 9                                 | 1.0                            |
| 3            | 10                                | 0.9                            |
| $J(1, 5)$    | 11                                | 2.5                            |
| $J(1, 5)$    | 12                                | 2.1                            |
| $J(8, 13)$   | 14                                | 0.4                            |

*Step 4.* Integration of elements  $J(8, 13)$  and 14 into  $J(8, 13, 14)$ . Thus, cluster 1 is designed  $X_1 = \{8, 13, 14\}$ . The corresponding elements (i.e.,  $J(8, 13), 14$ ) can be deleted from the next analysis. As a result, Table 3.9 is obtained.

**Table 3.9.** List of proximities after step 4

| Vertex $i_1$ | Vertex $i_2$<br>("son" of $i_1$ ) | Weight of<br>edge $(i_1, i_2)$ |
|--------------|-----------------------------------|--------------------------------|
| $J(1, 5)$    | $J(2, 6)$                         | 1.5                            |
| $J(1, 5)$    | 3                                 | 1.7                            |
| $J(1, 5)$    | 4                                 | 0.5                            |
| $J(2, 6)$    | 7                                 | 0.6                            |
| 3            | 9                                 | 1.0                            |
| 3            | 10                                | 0.9                            |
| $J(1, 5)$    | 11                                | 2.5                            |
| $J(1, 5)$    | 12                                | 2.1                            |

*Step 5.* Integration of elements  $J(1, 5)$  and 4 into  $J(1, 4, 5)$ . Thus, cluster 2 is designed  $X_2 = \{1, 4, 5\}$ . The corresponding elements (i.e.,  $J(1, 5), 4$ ) can be deleted from the next analysis. As a result, Table 3.10 is obtained.

**Table 3.10.** List of proximities after step 5

| Vertex $i_1$ | Vertex $i_2$<br>("son" of $i_1$ ) | Weight of<br>edge $(i_1, i_2)$ |
|--------------|-----------------------------------|--------------------------------|
| $J(2, 6)$    | 7                                 | 0.6                            |
| 3            | 9                                 | 1.0                            |
| 3            | 10                                | 0.9                            |

*Step 6.* Integration of elements  $J(2, 6)$  and 7 into  $J(2, 6, 7)$ . Thus, cluster 3 is designed  $X_3 = \{2, 6, 7\}$ . The corresponding elements (i.e.,  $J(2, 6), 7$ ) can be deleted from the next analysis. As a result, Table 3.11 is obtained.

**Table 3.11.** List of proximities after step 6

| Vertex $i_1$ | Vertex $i_2$<br>("son" of $i_1$ ) | Weight of<br>edge $(i_1, i_2)$ |
|--------------|-----------------------------------|--------------------------------|
| 3            | 9                                 | 1.0                            |
| 3            | 10                                | 0.9                            |

*Step 7.* Integration of elements 3 and 10 into  $J(3, 10)$ . As a result, Table 3.12 is obtained.

**Table 3.12.** List of proximities after step 7

| Vertex $i_1$ | Vertex $i_2$<br>("son" of $i_1$ ) | Weight of<br>edge $(i_1, i_2)$ |
|--------------|-----------------------------------|--------------------------------|
| $J(3, 10)$   | 9                                 | 1.0                            |

*Step 8.* Integration of elements  $J(3, 10)$  and 9 into  $J(3, 9, 10)$ . Thus, cluster 4 is designed  $X_4 = \{3, 9, 10\}$ . The corresponding elements (i.e.,  $J(3, 10), 9$ ) can be deleted from the next analysis.

Two separated elements 11 and 12 can be organized as two clusters:  $X_5 = \{11\}$  and  $X_6 = \{12\}$ .

**3.2.3. Improvements of hierarchical clustering scheme [375]**

First, let us point out some properties of the considered clustering process as follows:

1. The matrix of element pair proximity can contain several "minimal" elements. Thus there are problems as follows: (i) selection of the best unit pair for integration; (ii) possible integration of several unit pair at each algorithm stage.

2. Computing the matrix of element pair distances often does not correspond to the problem context and it is reasonable to consider a "softer" approach for computing element pair proximity.

3. The obtained structure of the clustering process is a tree. Often the clustering problem is used to get a system structure that corresponds to the above-mentioned clustering process (e.g., evolution trees, system architecture). Thus, it is often reasonable to organize the clustering process as a hierarchy, e.g., for modular systems in which the same modules can be integrated into different system components/parts.

Fig. 3.3 illustrates concurrent integration of element pairs at the same step of the algorithm when some elements can be integrated into different system components parts, i.e., obtaining a hierarchical system structure (common modules/parts, e.g., 3 and 4). In this case, obtained clusters can have intersections (Fig. 3.4).

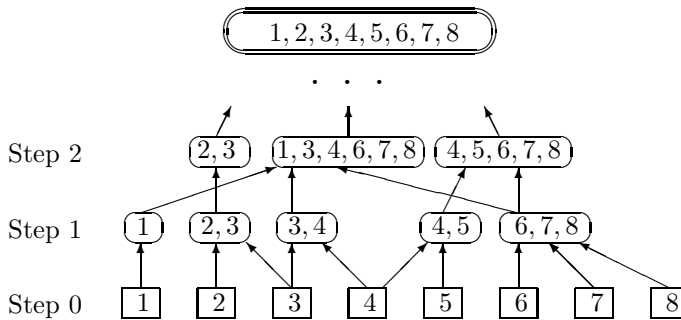


Fig. 3.3. Illustration for hierarchy

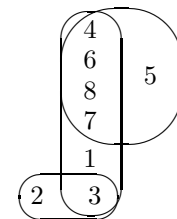


Fig. 3.4. Clusters for Step 2 (Fig. 3.2)

Now, let us describe some possible algorithm improvements.

**Improvement 1** (algorithm 2):

*Stage 1.* Computing an ordinal distance/proximity (0 corresponds to equal or the more similar elements). Here it is possible to compute the pair distance/proximity via the previous approach and mapping the pair distance to the ordinal scale.

*Stage 2.* Revelation of the smallest pair distance and integration of the corresponding elements.

*Note 1.* It is possible to reveal several close element pairs and execution several pair integration.

*Note 2.* It is possible to include the same element into different integrated pairs.

*Stage 3.* The stage corresponds to stage 3 in *algorithm 1*.

Here, a hierarchical structure for the element pair integration (Bottom-Up) is obtained (several element pair integration at each integration step). The complexity of the problem may consist in revelation of many subcliques (in graph over elements and their proximity). In the process of computing the ordinal proximity it is reasonable to use a limited number of element pairs for each level of the proximity ordinal scale. As a result, the limited number of integrated element pairs (or complete subgraphs or cliques) will be revealed at each integration stage. This provides polynomial complexity of the algorithm (number of operations, volume of required memory)  $O(m n^2)$ .

**Improvement 2** (algorithm 3): This algorithm is close to *algorithm 2*, but the computing process for the ordinal element pairs proximity is based on multicriteria analysis, *e.g.*, Pareto-approach or outranking technique (*i.e.*, Electre-like methods). Complexity of the algorithm is  $O(m n^4)$ .

The algorithms 2 and 3 implement the following trend:

*from tree-like structure (of clustering process) to hierarchy.*

An analysis of obtained clique(s) can be included into the algorithms as well.

### 3.3. K-means clustering

K-means clustering approach is widely used [161,276,300,302,299,318,435]. The basic simplified version of the algorithm is:

*Stage 1.* Select  $K$  points as initial centroids (*e.g.*, mean points) (*e.g.*, selection is based on random process).

*Stage 2.* Cycle by all  $n$  points:

(2.1) Form  $K$  clusters by assigning all points to the closest centroid.

(2.2) Recalculate the centroid of each cluster.

(2.3) If all points are assigned GO TO stage 3.

(2.4) GO TO (2.1).

*Stage 3.* Stop.

Complexity estimates for  $K$ -mean clustering algorithm (by stages) is presented in Table 3.13.

**Table 3.13.** Complexity estimates of stages of  $K$ -means clustering algorithm

| Stage      | Description  | Complexity estimate<br>(running time) |
|------------|--|---------------------------------------|
| Stage 1    | Selection of $K$ centroids   | $O(K)$                                |
| Stage 2.2  | Assignment of all $n$ points to $K$ centroids<br>(by $m$ attributes) | $O(n \times K \times m)$              |
| Stage 2.2  | Recalculation of the centroids (for $K$ clusters)                    | $O(K \times n \times m)$              |
| Stage 2.3. | Checking the condition for stopping<br>(all elements are processed)  | $O(1)$                                |
| Stage 3.   | Stopping   | $O(1)$                                |

Thus, the general complexity of this algorithm equals  $O(K \times n \times m)$ .

This approach has some problems when initial object set contains “outlier”-like point(s). (Fig. 2.14). A general framework of k-means clustering is shown in Fig. 3.5.

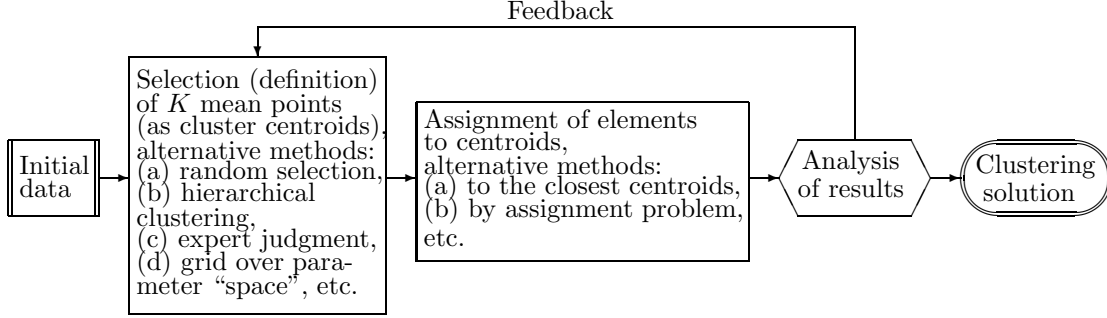


Fig. 3.5. General framework of k-means clustering process

### 3.4. Clustering as assignment

Generally, the k-means clustering approaches involve a stage to assignment the items to preliminary defined clusters. Thus assignment problems can be used at this stage and, as a result, special assignment based clustering methods are obtained (e.g., [227,292]).

In basic assignment problem (bipartite matching problem) there are the following: items/elements  $\{1, \dots, i, \dots, n\}$ , agents  $\{1, \dots, j, \dots, \mu\}$ , positive  $c_{ij}$  profit for assignment of item  $i$  to agent  $j$ , binary variable  $x_{ij}$  equals 1 if item  $i$  is assigned to agent  $j$  and 0 otherwise. The basic assignment problem is (e.g., [218]):

$$\max \sum_{j=1}^{\mu} \sum_{i=1}^n c_{ij} x_{ij} \quad \text{s.t.} \quad \sum_{i=1}^n a_{ij} x_{ij} \leq 1, \quad j = \overline{1, \mu}, \quad \sum_{j=1}^{\mu} x_{ij} \leq 1, \quad i = \overline{1, n}, \quad x_{ij} \in \{0, 1\}, \quad i = \overline{1, n}, \quad j = \overline{1, \mu}.$$

Here each item has to be assigned to the only one cluster (agent). There exist several well-known polynomial algorithms for the problem above (e.g., [183,139,167,218,351]).

The generalized assignment problem GAP can be described as a multiple knapsack (or multiple agents) problem. Analogically, given  $n$  items/elements ( $i = \overline{1, n}$ ) and  $\mu$  knapsacks (agents) ( $j = \overline{1, \mu}$ ). The following notations are used:  $c_{ij}$  is a profit of item  $i$  if it is assigned to knapsack (agent),  $a_{ij}$  is a weight (e.g., required resource) of item  $i$  if it assigned to knapsack (agent)  $j$ ,  $b_j$  is a capacity (volume of resource) of knapsack (agent)  $j$ , binary variable  $x_{ij}$  equals 1 if item  $i$  is assigned to agent  $j$  and 0 otherwise. Clearly, the knapsack (agent) capacity can be considered as multiple recourse (i.e, a vector-like parameter) as well (e.g., [219]). The problem is [218,420]:

*Assign each item to exactly one knapsack so as to maximize the total profit assigned, without assigning to any knapsack a total weight greater than its capacity.*

The basic problem statement is:

$$\max \sum_{j=1}^{\mu} \sum_{i=1}^n c_{ij} x_{ij} \quad \text{s.t.} \quad \sum_{i=1}^n a_{ij} x_{ij} \leq b_j, \quad j = \overline{1, \mu}, \quad \sum_{j=1}^{\mu} x_{ij} \leq 1, \quad i = \overline{1, n}, \quad x_{ij} \in \{0, 1\}, \quad i = \overline{1, n}, \quad j = \overline{1, \mu}.$$

The problem is known to be NP-hard (e.g., [524]). Evidently, the objective function can be minimized as well (e.g., minimum cost assignment of a set of items/objects to a set of agents). In the case of  $a_{ij} = 1 \forall i, \forall j$ , each agent has an integer restriction of assigned elements as restriction for cluster size). In multiple assignment problem constraint  $\sum_{j=1}^{\mu} x_{ij} \leq 1$  ( $i = \overline{1, n}$ ) is replaced by  $\sum_{j=1}^{\mu} x_{ij} \leq \lambda_i$  ( $i = \overline{1, n}$ ) where  $\lambda_i$  is restriction for the number of admissible assignment to different agents for elements  $i$ . In applications, knapsack/agents can be considered as service centers (e.g., access points in communication networks) which have limited service resource(s) (e.g., [396,397]).

Generally, the following kinds of algorithms have been used for basic generalized assignment problems (e.g., [87,325,420]): (i) exact algorithms as enumerative methods (e.g., branch-and-bound algorithms)

(e.g., [503,515,531]), (ii) relaxation methods, reduction algorithms (e.g., relaxations to linear programming models, relaxation heuristics) (e.g., [219,408,581]), (iii) approximation schemes (e.g., [130,151,200,466, 547]), (iv) various heuristics (e.g., [253,455]) including greedy algorithms (e.g., [455,510]), set partitioning heuristic (e.g., [88]) genetic algorithms (e.g., [123]), tabu search algorithms (e.g., [162,281]). Fig. 3.6 illustrates the generalized assignment problem.

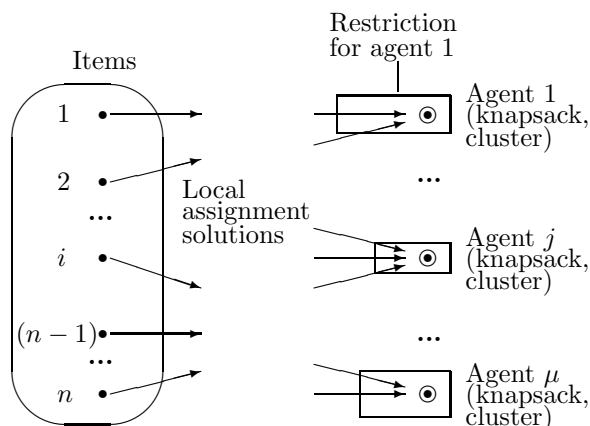


Fig. 3.6. Illustration of generalized assignment

In multiple criteria generalized assignment problem, vector-like profit is considered for each item  $i$  (e.g., [396,392,532,655]):  $c_{ij} = (c_{ij}^1, \dots, c_{ij}^l, \dots, c_{ij}^k)$  (criteria:  $\{C_1, \dots, C_l, \dots, C_k\}$ ).

A simplified multicriteria problem statement can be examined as follows:

$$\max \sum_{j=1}^{\mu} \sum_{i=1}^n c_{ij}^1 x_{ij}, \dots, \max \sum_{j=1}^{\mu} \sum_{i=1}^n c_{ij}^l x_{ij}, \dots, \max \sum_{j=1}^{\mu} \sum_{i=1}^n c_{ij}^k x_{ij}, \quad l = \overline{1, k}$$

$$s.t. \quad \sum_{i=1}^n a_{ij} x_{ij} \leq b_i, \quad j = \overline{1, \mu}, \quad \sum_{j=1}^{\mu} x_{ij} \leq 1, \quad i = \overline{1, n}, \quad x_{ij} \in \{0, 1\}, \quad i = \overline{1, n}, \quad j = \overline{1, \mu}.$$

Here it is reasonable to search for Pareto-efficient solutions.

**Example 3.2.** A modified numerical example for connection of end-users and access points in a wireless telecommunication network is based on the example from [396,397,392]. Four access points are considered as cluster centroids and 14 end-users are examined as initial objects (example from [396] is compressed, Fig. 3.7).

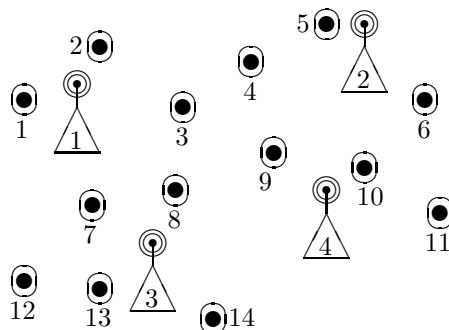


Fig. 3.7. Example: 4 access points, 14 users

Let  $\{1, \dots, i, \dots, n\}$  be a set of users (here: 14) and  $\{1, \dots, j, \dots, \mu\}$  be a set of access points (here: 4).

Each user  $i$  is described by parameters (a compressed set of parameters): (i) coordinates  $(x_i, y_i, x_i)$ ; (ii) parameter corresponding to required frequency bandwidth (e.g., 1 Mbit/s ... 10 Mbit/s)  $f_i$ ; (iii)

maximal possible number of access points for connection  $\kappa_i \leq \mu$  (here  $\kappa_i = 1 \forall i$ , i.e., each user is assigned to the only one access point/cluster); (iv) required reliability of information transmission  $r_i$ . Note, in multi-assignment problem  $\kappa_i \geq 1$ .

Each access point is described by parameters (a compressed set of parameters): (a) coordinates of access point  $(x_j, y_j, z_j)$ , (b) parameter corresponding to maximal possible traffic (i.e., maximum of possible bandwidth)  $f_j$ , (c) maximal possible number of users under service  $k_j$ , (d) reliability of channel for data transmission  $r_j$ , (e) admissible proximity (distance)  $d_j$ . Table 3.14 and Table 3.15 contains parameters estimates of the access points and users.

**Table 3.14.** Parameter estimates of access points

| Access point<br>$j$ | Coordinates:<br>$x_j$ $y_j$ $z_j$ | Bandwidth<br>$f_j$ | Number<br>of users<br>$n_j$ | Reliability<br>$r_j$ | Admissible<br>distance<br>$d_j$ |
|---------------------|-----------------------------------|--------------------|-----------------------------|----------------------|---------------------------------|
| 1                   | 50   157   10                     | 30                 | 4                           | 10                   | 10                              |
| 2                   | 150   165   10                    | 30                 | 5                           | 15                   | 10                              |
| 3                   | 72   102   10                     | 42                 | 6                           | 10                   | 6                               |
| 4                   | 140   112   10                    | 32                 | 5                           | 8                    | 9                               |

**Table 3.15.** Parameter estimates of end users

| User<br>$i$ | Coordinates:<br>$x_j$ $y_j$ $z_j$ | Bandwidth<br>$f_i$ | Reliability<br>$r_i$ |
|-------------|-----------------------------------|--------------------|----------------------|
| 1           | 30   165   5                      | 10                 | 5                    |
| 2           | 58   174   5                      | 5                  | 9                    |
| 3           | 88   156   0                      | 6                  | 6                    |
| 4           | 110   169   5                     | 7                  | 5                    |
| 5           | 145   181   3                     | 5                  | 4                    |
| 6           | 170   161   5                     | 7                  | 4                    |
| 7           | 52   134   5                      | 6                  | 8                    |
| 8           | 86   134   3                      | 6                  | 7                    |
| 9           | 120   140   6                     | 4                  | 6                    |
| 10          | 150   136   3                     | 6                  | 7                    |
| 11          | 175   125   1                     | 8                  | 5                    |
| 12          | 27   109   7                      | 8                  | 5                    |
| 13          | 55   105   2                      | 7                  | 10                   |
| 14          | 98   89   3                       | 10                 | 10                   |

As a result, each pair “user-access point” can be described by the following parameters (a compressed set of parameters): (1) proximity (e.g., Euclidean distance)  $d_{ij}$ , (2) level of reliability  $r_{ij}$ , (3) parameter of using bandwidth  $f_{ij}$ .

Clearly, Euclidean distances between users and access points  $\{d_{ij}\}$  can be calculated on the basis coordinates from Table 3.14 and Table 3.15. Thus, the following parameter vector is obtained  $\widehat{c}_{ij} = (d_{ij}, r_{ij}, f_{ij})$  ( $i = \overline{1, n}, j = \overline{1, \mu}$ ). Further, the parameter vector can be transformed into a profit  $c_{ij}$  (i.e., mapping of vector estimate into ordinal scale [1, 2, 3], 3 corresponds to the best level, multicriteria ranking based on outranking ELECTRE technique can be used).

The assignment of user  $i$  to access point  $j$  is defined by Boolean variable  $x_{ij}$  ( $x_{ij} = 1$  in the case of assignment  $i$  to  $j$  and  $x_{ij} = 0$  otherwise). The assignment solution is defined by Boolean matrix  $X = \|x_{ij}\|$ ,  $i = \overline{1, n}$ ,  $j = \overline{1, \mu}$ . Finally, the problem is:

$$\max \sum_{j=1}^{\mu} \sum_{i=1}^n c_{ij} x_{ij}$$

$$s.t. \quad \sum_{i=1}^n f_{ij} x_{ij} \leq f_j \quad \forall j = \overline{1, \mu}; \quad \sum_{i=1}^n x_{ij} \leq k_j \quad \forall j = \overline{1, \mu}; \quad \sum_{j=1}^{\mu} x_{ij} \leq 1 \quad \forall i = \overline{1, n};$$

$$x_{ij} = 0 \quad \text{if} \quad d_{ij} > d_j \quad \forall i = \overline{1, n}, \quad \forall j = \overline{1, \mu}; \quad x_{ij} = 0 \quad \text{if} \quad r_{ij} > r_j \quad \forall i = \overline{1, n}, \quad \forall j = \overline{1, \mu};$$

$$x_{ij} \in \{0, 1\} \quad \forall i = \overline{1, n}, \forall j = \overline{1, \mu}.$$

A numerical example of the assignment solution (i.e., clustering solution) is depicted in Fig. 3.8. In [396], the described problem is examined as generalized multiple assignment problem (extended version).

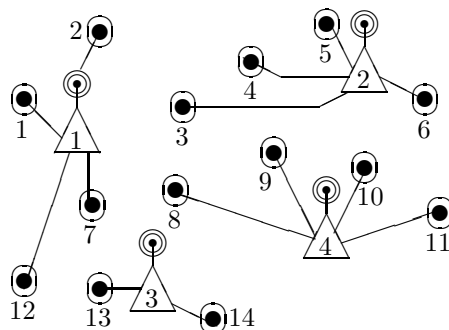


Fig. 3.8. Assignment of users to access points

### 3.5. Graph based clustering

#### 3.5.1. Minimum spanning tree based clustering

The preliminary building of minimum trees is widely used in many combinatorial problems (e.g., [218]). The algorithmic complexity estimate for this spanning problem over graph equals  $O(n \log n)$  ( $n$  is the number of graph vertices). Minimum spanning tree based clustering algorithms have been studied and applied by many researchers (e.g., [235,244,353,445,479,492,555,606,626,660]). The basic stages of the algorithms are as follows:

*Stage 1.* Calculation of distance/proximity matrix  $Z$ .

*Stage 2.* Design of the corresponding graph  $G$ .

*Stage 3.* Building of the minimum spanning tree  $T$  for graph  $G$ .

*Stage 4.* Clustering of the vertices of tree  $T$  (e.g., by algorithm of deletion of branches, by algorithm of hierarchical clustering).

*Stage 5.* Stopping.

Further, the usage of hierarchical clustering at stage 4 is considered. Complexity estimates for minimum spanning tree clustering algorithm (by stages) are presented in Table 3.16.

**Table 3.16.** Complexity estimates of stages for minimum spanning tree based clustering

| Stage    | Description                        | Complexity estimate<br>(running time) |
|----------|------------------------------------|---------------------------------------|
| Stage 1. | Calculate distance matrix $Z$      | $O(n^2)$                              |
| Stage 2. | Design the corresponding graph $G$ | $O(n^2)$                              |
| Stage 3. | Building the minimum spanning tree | $O(n \log n)$                         |
| Stage 4. | Clustering of the tree vertices    | $O(n \log n)$                         |
| Stage 5. | Stopping                           | $O(1)$                                |

Stages 3, 4, 5 correspond to the situation when a graph is examined as initial data. In this case, complexity of the algorithm equals  $O(n \log n)$ .

**Example 3.3.** A numerical example for elements  $A = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12\}$  illustrates building of graph  $G = (A, E)$  (corresponding proximity matrix  $Z$ ), minimum spanning tree  $T = (A, E')$ , and clustering solution  $\widehat{X} = \{X_1, X_2, X_3\}$  (cluster size  $\leq 4$ ). The following is implemented:

$$\text{Proximity matrix } Z \Rightarrow \text{Graph } G = (A, E) \Rightarrow \text{Tree } T = (A, E') \Rightarrow \text{Clustering solution } \widehat{X} = \{X_1, X_2, X_3\}.$$

The method for building the spanning tree is used as in example 3.1. Table 3.17 contains proximity matrix (symbol “ $\star$ ” corresponds to a very big value).

**Table 3.17.** Proximities for example (edge  $(i_1, i_2)$ )

| $i_1$ | $i_2 :$ | 2   | 3   | 4    | 5   | 6   | 7    | 8    | 9    | 10   | 11  | 12  |
|-------|---------|-----|-----|------|-----|-----|------|------|------|------|-----|-----|
| 1     |         | 0.3 | 1.4 | 1.45 | *   | *   | *    | *    | *    | *    | *   | *   |
| 2     |         |     | 0.3 | *    | *   | 2.6 | 0.2  | 1.8  | *    | *    | *   | *   |
| 3     |         |     |     | 0.4  | *   | *   | 1.65 | 0.25 | *    | *    | *   | *   |
| 4     |         |     |     |      | 0.4 | *   | *    | 0.45 | 1.9  | *    | *   | *   |
| 5     |         |     |     |      |     | *   | *    | *    | 0.35 | 1.5  | *   | *   |
| 6     |         |     |     |      |     |     | 0.1  | *    | *    | *    | 1.4 | *   |
| 7     |         |     |     |      |     |     |      | 0.41 | *    | *    | 0.4 | *   |
| 8     |         |     |     |      |     |     |      |      | 0.9  | *    | 2.1 | *   |
| 9     |         |     |     |      |     |     |      |      |      | 0.15 | *   | 0.5 |
| 10    |         |     |     |      |     |     |      |      |      |      | *   | 2.0 |
| 11    |         |     |     |      |     |     |      |      |      |      |     | 2.5 |

Fig. 3.9 depicts corresponding graph,  $G = (A, E)$ , Fig. 3.10 depicts spanning tree  $T = (A, E')$ , and clustering solution. Generally, it is reasonable to point out threshold based modification of graph  $G = (A, E)$  over object set  $A$ : deletion of edges by condition: the weight “>” the threshold. Decreasing the threshold leads to decreasing the cardinality of  $E$ . This process can be very useful for analysis and processing of initial data in clustering. Let us consider an illustration of the above-mentioned process on the basis graph from example 3.3 (basic proximity matrix from Table 3.17): (i) threshold equals 2.6: graph  $G = (A, E)$  in Fig. 3.9; (ii) threshold equals 1.4: graph  $G^1 = (A, E^1)$  in Fig. 3.11; (iii) threshold equals 0.5: graph  $G^2 = (A, E^2) = T = (A, E')$  in Fig. 3.10 (here: spanning tree); (iv) threshold equals 0.3: graph  $G^3 = (A, E^3)$  in Fig. 3.12.

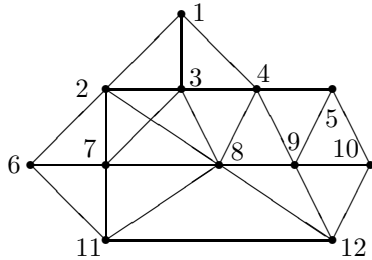


Fig. 3.9. Graph  $G = (A, E)$

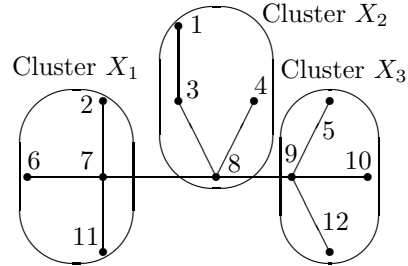


Fig. 3.10. Spanning tree  $T = (A, E')$

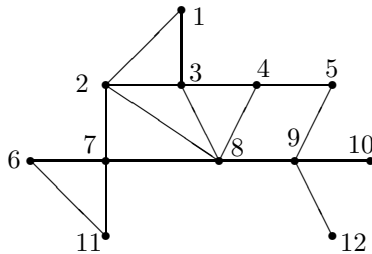


Fig. 3.11. Graph  $G^1 = (A, E^1)$

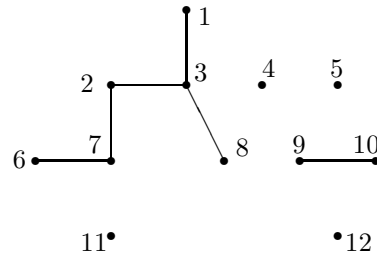


Fig. 3.12. Graph  $G^3 = (A, E^3)$

As a result, a useful structure can be found. The described by example procedure is an important auxiliary problem. An additional significant problem consists in analysis of the obtained graph, for example: (a) connectivity, (b) similarity to tree (or hierarchy, clique). Further, a modified version of adaptive minimum spanning tree clustering algorithm is examined as follows. Initial data are: (a) set of objects/alternatives  $A = \{A_1, \dots, A_i, \dots, A_n\}$ , (b) set of parameters/criteria  $\overline{C} = \{C_1, \dots, C_j, \dots, C_m\}$ , (c) estimate matrix  $X = \{x_{ij}\}$ ,  $i = 1, n, j = 1, m$ , where  $x_{ij}$  is estimate of  $A_i$  upon criterion  $C_j$  (a qualitative scale is considered). The algorithm consists of the following stages:



*Stage 1.* Calculation of proximity matrix  $Z = \{z_{ik}\}$ ,  $i = \overline{1, n}$ ,  $k = \overline{1, n}$ , where  $z_{ik}$  is estimate of proximity (distance) between  $A_i$  and  $A_k$  (e.g., Euclidean metric is used). Evidently,  $z_{ii} = 0, \forall i = \overline{1, n}$ .

*Stage 2.* Transformation of matrix  $Z$  into ordinal matrix  $Y = \{y_{ik}\}$ . Let us consider the maximum and minimum values of elements of matrix  $Z$ :  $z^{min} = \min_{\substack{i=\overline{1, n}, \\ i=\overline{1, k}}} \{z_{ik}\}$ ,  $z^{max} = \max_{\substack{i=\overline{1, n}, \\ i=\overline{1, k}}} \{z_{ik}\}$ . Thus an interval is obtained  $[z^{min}, z^{max}]$  and  $d = z^{max} - z^{min}$ . Now an additional integer parameter  $\delta$  (e.g., 3, 4, 5, 6) is used. Let  $\delta = 5$ . Then elements of new matrix  $Y$  (i.e, adjacency matrix) are based on the following calculation:

$$y_{ik} = \begin{cases} 0, & \text{if } 0.0 \leq z_{ik} \leq d/\delta, \\ 1, & \text{if } d/\delta < z_{ik} \leq 2d/\delta, \\ 2, & \text{if } 2d/\delta < z_{ik} \leq 3d/\delta, \\ 3, & \text{if } 3d/\delta < z_{ik} \leq 4d/\delta, \\ 4, & \text{if } 4d/\delta < z_{ik} \leq d. \end{cases}$$

*Stage 3.* Obtaining an interconnected graph over elements  $A$  (iterative approach):

Let  $\Delta = 1, 2, \dots$  be an integer algorithmic parameter (for the algorithm cycle).

*Step 3.1.* Initial value  $\Delta = 1$ .

*Step 3.2* Transformation of ordinal matrix  $Y$  into Boolean matrix  $B = \{b_{ik}\}$ :

$$b_{ik} = \begin{cases} 1, & \text{if } y_{ik} < \Delta, \\ 0, & \text{if } y_{ik} \geq \Delta. \end{cases}$$

*Step 3.3.* Building a graph over elements  $A$ :  $G^\Delta = (A, \Gamma^\Delta)$ , where  $\Gamma^\Delta$  is the set of edges, edge  $(A_i, A_k)$  exists if  $b_{ik} = 1$ .

*Step 3.4.* Analysis of connectivity for graph  $G^\Delta = (A, \Gamma^\Delta)$ . If the graph is connected, then GOTO *Step 3.6*.

*Step 3.5.*  $\Delta = \Delta + 1$  and GOTO *Step 3.2*

*Step 3.6.* Building of minimum spanning tree for graph  $G^\Delta = (A, \Gamma^\Delta)$ :  $T^\Delta = (A, \widehat{E}^\Delta)$ .

Here, several well-known algorithms can be used, for example: Borovka's algorithm Prim's algorithm, Kruskal's algorithm [10,217,218,139,493,639]. Complexity estimate of the algorithms is:  $O(p \log n)$  (or less [639]) ( $p$  is the number of edges,  $n$  is the number of vertices). It is necessary to take into account for each edge  $\gamma \in \Gamma$  its weight as follows: proximity value  $z_{ik}$  for corresponding element of  $Z$ .

*Step 3.7.* Clustering set  $A$  on the basis of spanning tree  $T^\Delta = (A, \widehat{E}^\Delta)$  while taking into account an algorithmic parameter: a number of elements  $\alpha$  in each obtained cluster  $\alpha' \leq \alpha \leq \alpha''$ , for example  $\alpha' = 4$ ,  $\alpha'' = 6$ . The constrains above have to be based on the engineering analysis of the applied problem.

*Stage 4.* Stop.

Complexity estimates for the described adaptive algorithm (by stages) is presented in Table 3.18. Thus, the general complexity estimate (running time) of the described adaptive algorithm equals  $O(n^2)$ .

Generally, the problem of  $k$ -balanced partitioning a tree is NP-hard ( $k$  is the number of elements in each cluster of clustering solution) [195].

Note, the obtained clustering solution has a property: "modularity". This can be very important for many applied problems (e.g., close cardinalities of clusters/groups: local region elements in communication network, student teams).

**Table 3.18.** Complexity estimates for adaptive minimum spanning tree based algorithm

| Stage/step | Description   | Complexity estimate (running time) |
|------------|---|------------------------------------|
| Stage 1    | Calculate the distance matrix $Z$   | $O(n^2)$                           |
| Stage 2    | Transformation of matrix $Z$ into ordinal matrix $Y$  | $O(n^2)$                           |
| Stage 3    | Design of interconnected graph over elements $A$  | $O(n^2)$                           |
| Step 3.1   | Specifying the start of the cycle   | $O(1)$                             |
| Step 3.2   | Transformation of matrix $Y$ into Boolean matrix $B$  | $O(n^2)$                           |
| Step 3.3   | Building the graph $G$ that corresponds to matrix $B$   | $O(n^2)$                           |
| Step 3.4   | Analysis of connectivity of graph $G$   | $O(n)$                             |
| Step 3.5   | Correction of cycle parameter   | $O(1)$                             |
| Step 3.6   | Building the minimum spanning tree $T$ for graph $G$  | $O(p \log n)$                      |
| Step 3.7   | Clustering the vertices (elements $A$ ) of the spanning tree $T$ while taking into account the constraints for cluster size | $O(n)$                             |
| Stage 4.   | Stopping  | $O(1)$                             |

### 3.5.2. Clique based clustering

Here, an initial graph  $G = (A, E)$  is examined as initial data. In a clique (complete graph/subgraph), each vertex is connected to all other the vertices (Fig. 3.13). A quasi-clique can be examined, for example, as a clique without one-two edges. The cliques (or quasi-cliques) form a very strong clusters (from the viewpoint of interconnection). The problem of finding a maximal clique in a graph is a well-known NP-hard problem (e.g., [218,319]). Thus, heuristics or enumerative methods have been used for the problem.

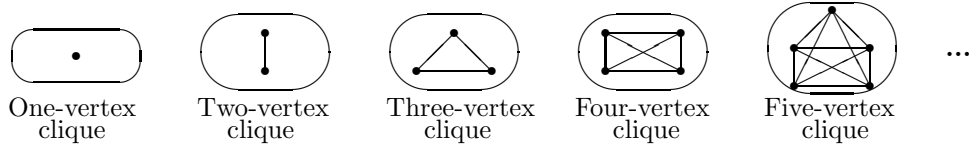


Fig. 3.13. Illustration of cliques

Clique-based clustering process can be organized as a series of clique problems [218]:

*Stage 1.* Finding the “maximal clique” (or maximal “quasi-clique”) in graph  $G = (A, E)$ : subgraph  $H = (B, V)$  ( $H \subseteq A, V \subseteq E$ ).

*Stage 2.* Forming a cluster from subgraph  $H$  and compression of initial graph  $G$ :  $G' = (A', E')$ , ( $A' = A \setminus H, E' = E \setminus \{V \cup W\}$ , where  $W$  is a set of external edges of clique, i.e., the only one vertex belongs to set  $H$ ) (Fig. 3.14).

*Stage 3.* If  $G'$  is empty GO TO Stage 4 otherwise GO TO Stage 1.

*Stage 4.* Stop.

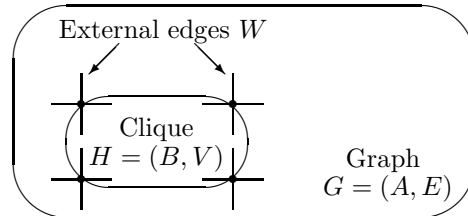


Fig. 3.14. Illustration of clique in graph

The above-mentioned solving scheme is based on series of NP-hard problems. Evidently, it is possible to find several “maximal cliques” concurrently. Some sources on researches on clique finding and clique based clustering are presented in Table 3.19.

Clique partitioning problem for a given graph  $G = (A, E)$  with edge weights consists in partitioning the graph into cliques such that the sum of the edge weights over all cliques formed is as large as possible (e.g., [340,469]).

There are some close problems over graphs/digraphs, for example, independent set problems and dominating set problems which are used in clustering as well (e.g., [105,131,132,140,263,296,489]). Recently, the significance of dynamic problems over data streams has been increased including clique/quasi-clique finding in graph streams (e.g. [8,128,247,389]).

On the other hand, clique-based approaches can be considered as density-based and grid-based clustering methods. In some recent works, subgraph as clique/quasi-clique is considered as one of network community structures (network community based clustering [226,459,460,496]).

**Table 3.19.** Detection of cliques/quasi-cliques and clustering

| No.  | Research  | Source(s)                          |
|------|---|------------------------------------|
| 1.   | Detection and analysis of cliques in graphs:                        |                                    |
| 1.1  | Cliques in graphs   | [309,444]                          |
| 1.2. | Finding of clique/quasi-clique in graphs                            | [2,18,81,193,218,472,484]          |
| 1.3. | Maximum-weight clique problem                                       | [29,34,68,473,481]                 |
| 1.4. | Finding all cliques of undirected graph                             | [76]                               |
| 1.5. | Enumeration maximal cliques of large graph                          | [13]                               |
| 2.   | Clustering based on cliques:  |                                    |
| 2.1. | Clique based clustering   | [9,55,176,236,302,426,437,539,588] |
| 2.2. | Clique partitioning problem<br>(clique partition of maximum weight) | [154,340,469]                      |
| 3.   | Clique-based multiple clustering:                                   |                                    |
| 3.1. | Ensemble clustering with voting active clusters                     | [590]                              |
| 3.2. | Cliques for combining multiple clusterings                          | [431]                              |
| 4.   | Clique based methods over data streams:                             |                                    |
| 4.1. | K-clique clustering in dynamic networks                             | [176]                              |
| 4.2. | Clique-based fusion of graph streams                                | [389]                              |

In recent decades, several new combinatorial problems as clique clustering in multipartite graphs have been suggested (e.g., [96,152,272,372,374,392,596]). Fig. 3.15. illustrates this kind of problems. Table 3.20 contains a list of the research directions in the above-mentioned field.

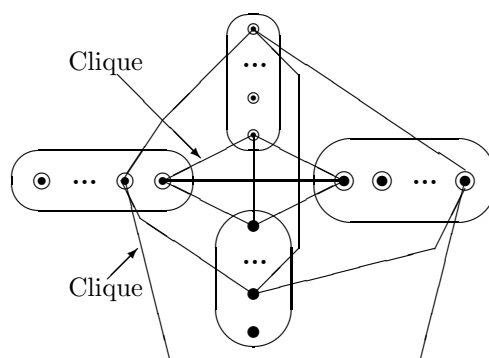


Fig. 3.15. Cliques in four-partite graph

**Table 3.20.** Research directions in multi-partite graphs

| No. | Research                                   | Source(s)     |
|-----|--|---------------|
| 1.  | Problem of compatible representatives      | [339]         |
| 2.  | Morphological clique (ordinal estimates)   | [372,374,392] |
| 3.  | Morphological clique (multiset estimates)  | [386,392]     |
| 4.  | Clustering in multipartite graph           | [96,596]      |
| 5.  | Bipartite and multipartite clique problems | [152]         |
| 6.  | Morphological clique over graph streams    | [389]         |
| 7.  | Coreset problems                           | [194,272]     |
| 8.  | Coresets in dynamic data streams           | [208]         |

### 3.5.3. Correlation clustering

Correlation clustering provides a method for partitioning a fully connected labeled graph (label “+” corresponds to edge for similar vertices, label “-” corresponds to edge for different vertices) while taking into account two objectives for the obtained clusters:

- (i) minimizing disagreements (i.e., minimizing the number of “-” edges within the clusters ( $Q^{disagr}(\hat{X}) \rightarrow \min$ ) or maximizing the number of “-” between clusters),
- (ii) maximizing agreements (i.e., the number of “+” edges inside the clusters) ( $Q^{agr}(\hat{X}) \rightarrow \max$ ) (e.g., [4,33,40,52,159,345,564,662]).

In the basic above-mentioned problem formulation, the objective functions are summarized. In other words, binary scale  $[-1, +1]$  is used for each edge as a weight (zero value is not used). Here it is not necessary to specify the preliminary number of clusters (e.g., as in  $k$ -means clustering). The correlation clustering problem formulation is motivated from documents/web pages clustering. This combinatorial model belongs to NP-complete class (e.g., [11,39,40]).

Various versions of correlation problem formulations are examined:

- (a) weighted versions of the “correlation clustering functional” are considered as well (e.g., [94,95,159]),
- (b) correlation clustering with partial information (e.g., [158]),
- (c) correlation clustering with noisy input (e.g., [423]), etc.

Let us consider the weighted version of the problem. Let  $A = \{A_1, \dots, A_j, \dots, A_n\}$  be the initial set of elements. As a result,  $(n - 1)^2$  elements pairs can be considered:  $G = \{g_1, \dots, g_{(n-1)^2}\}$ . Each element of  $G$  corresponds to element pair  $(A_{j_1}, A_{j_2})$  and an element of proximity matrix  $Z = \|z_{j_1, j_2}\|$ . Further, it is possible to replace scale  $[-1, +1]$  for each edge (i.e., for each element from  $G$  or element of proximity matrix  $Z$ ) by two quantitative scales for weights: negative quantitative (or ordinal) scale  $[-w^-, \dots, 0]$  instead of “-1” and positive quantitative scale  $(0, \dots, w^+]$  instead of “+1”. Evidently, element pair set is divided into two separated subsets  $G = G^- \cup G^+$  (without intersection, i.e.,  $|G^- \cap G^+| = 0$ ) where  $\forall g^- \in G^-$  weight estimate corresponds to negative quantitative scale above, where  $\forall g^+ \in G^+$  weight estimate corresponds to positive quantitative scale above. The clustering solution is:  $\hat{X} = \{X_1, \dots, X_\nu, \dots, X_\lambda\}$ . For this solution, two total quality parameters above are examined:

- (i) total agreements quality as (summarization by all intra-cluster pairs with positive edge weight)  $Q^{agr}(\hat{X})$  (maximization);
- (ii) total disagreements quality (summarization by all intra-cluster pairs with negative edge weight)  $Q^{disagr}(\hat{X})$  (for minimization, by module).

As a result, the weighted version of correlation clustering problem is (Fig. 3.16):

Find clustering solution  $\hat{X}$  such that: (i)  $Q^{agr}(\hat{X}) \rightarrow \max$  and (ii)  $|Q^{disagr}(\hat{X})| \rightarrow \min$ .

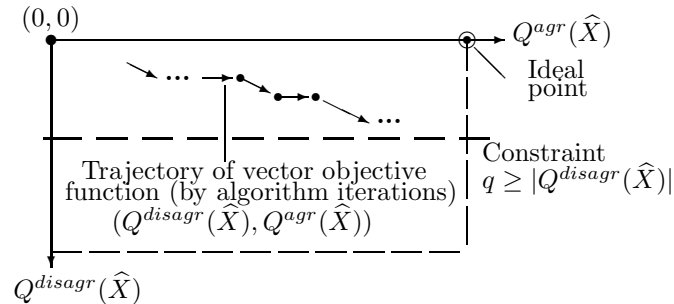


Fig. 3.16. “Space” of solution quality

Heuristics and approximation algorithms (e.g., PTAS) have been proposed for the problem versions (e.g., [33,39,40,662]). Clearly, agglomerative (hierarchical) clustering scheme (i.e., selection of an element pair from set  $B$  for next joining for improvement of a current clustering solution) can be used here as a simple greedy algorithm (Bottom-Up process of selection of element pair with the best improvement of objective vector function and corresponding joining the elements), for example (Fig. 3.16):

*Stage 1.* Calculation of the matrix of element pair  $\forall(A(j_1), A(j_2))$ ,  $A(j_1) \in A$ ,  $A(j_2) \in A$ ,  $j_1 \neq j_2$  proximities (“distances”).

*Stage 2.* Transformation of element pair proximities into positive (for similar elements) or negative (for dissimilar elements) weights (e.g., mapping).

*Stage 3.* Specifying the initial clustering solution  $\widehat{X}^0$  as composition of initial elements, vector objective function  $\overline{f}^0 = (Q^{disagr}(\widehat{X}^0), Q^{agr}(\widehat{X}^0)) = (0, 0)$  (initial value, initial index  $\gamma = 0$ ).

*Stage 4.* Searching for the element pair with the best improvement of vector objective function  $\overline{f}$  (i.e., searching for Pareto-efficient point(s)). Integration of the corresponding both elements into a cluster or inclusion of the corresponding element into the cluster with the second element (i.e., new clustering solution)  $\widehat{X}^q$  ( $q$  is parameter of algorithm iteration). Recalculation of the current value of vector objective function:  $\overline{f}^\gamma = (Q^{disagr}(\widehat{X}^\gamma), Q^{agr}(\widehat{X}^\gamma))$ .

*Stage 5.* If all elements are processed then GO TO Stage 7.

*Stage 6.* Increasing index  $\gamma = \gamma + 1$ , while constraint  $|Q^{disagr}(\widehat{X})| \leq q$  is satisfied Go To Stage 4, else GO TO Stage 7.

*Stage 7.* Stop.

Complexity estimates of greedy heuristic above for two-objectives correlation clustering (by stages) are presented in Table 3.21.

**Table 3.21.** Complexity estimates of stages for greedy agglomerative heuristic

| Stage    | Description   | Complexity estimate (running time) |
|----------|---|------------------------------------|
| Stage 1. | Calculation of distance matrix $Z$  | $O(n^2)$                           |
| Stage 2. | Calculation of positive/negative weights  | $O(n^2)$                           |
| Stage 3. | Specifying the initial solution   | $O(1)$                             |
| Stage 4. | Searching for the best element pair (by Pareto-efficient improvement of objective function) | $O(n^2)$                           |
| Stage 5. | Analysis of algorithm end, recalculation of objective function                              | $O(n)$                             |
| Stage 6. | Transition of computing process   | $O(1)$                             |
| Stage 7. | Stopping  | $O(1)$                             |

**Example 3.4.** The examined element set involves 11 elements:  $A = \{A_1, \dots, A_j, \dots, A_{11}\}$ . The weights of all edges are presented in Table 3.22. Here, two quantitative scales are used:  $[-6.5, 0)$  and  $(0, 3.5]$ .

**Table 3.22.** Weights of edges  $\{(A_{j_1}, A_{j_2})\}$

| $j_1$ | $j_2 :$ | 2    | 3    | 4    | 5    | 6    | 7    | 8    | 9    | 10   | 11   |
|-------|---------|------|------|------|------|------|------|------|------|------|------|
| 1     |         | -3.0 | 1.4  | -0.6 | -5.1 | -5.5 | -3.5 | -1.2 | -3.4 | -4.5 | -6.5 |
| 2     |         |      | -0.8 | -1.3 | -3.3 | -1.4 | 3.1  | -2.9 | -3.6 | -5.1 | -4.9 |
| 3     |         |      |      | -1.1 | -2.0 | -2.7 | -2.1 | 3.2  | -3.0 | -4.5 | -4.1 |
| 4     |         |      |      |      | -0.5 | -3.7 | -2.5 | 2.6  | -0.9 | -1.3 | -2.2 |
| 5     |         |      |      |      |      | -6.5 | -5.6 | -1.1 | 2.8  | -0.5 | -6.1 |
| 6     |         |      |      |      |      |      | 3.5  | 0.4  | -1.8 | -3.2 | -0.3 |
| 7     |         |      |      |      |      |      |      | 0.5  | -0.3 | -0.8 | 2.9  |
| 8     |         |      |      |      |      |      |      |      | 1.0  | -0.8 | -2.8 |
| 9     |         |      |      |      |      |      |      |      |      | 3.0  | -5.5 |
| 10    |         |      |      |      |      |      |      |      |      |      | -6.0 |

Initial information is the following (iteration index equals  $\gamma = 0$ ): (a)  $\widehat{X}^0 = \{X_1^0, \dots, X_l^0, \dots, X_{11}^0\}$  where  $X_1^0 = \{A_1\}$ ,  $X_2^0 = \{A_2\}$ ,  $X_3^0 = \{A_3\}$ ,  $X_4^0 = \{A_4\}$ ,  $X_5^0 = \{A_5\}$ ,  $X_6^0 = \{A_6\}$ ,  $X_7^0 = \{A_7\}$ ,  $X_8^0 = \{A_8\}$ ,  $X_9^0 = \{A_9\}$ ,  $X_{10}^0 = \{A_{10}\}$ ,  $X_{11}^0 = \{A_{11}\}$ ; (b)  $\overline{f}^0(\widehat{X}^0) = (0, 0)$ ; (c) improvement operations (i.e., inclusion of element (cluster)  $A_j$  into cluster  $X_\iota$ ) as  $O_{j,\iota}(A_j \rightarrow X_\iota)$  ( $j = \overline{1, 10}$ ,  $\iota = \overline{j, 11}$ ) and corresponding improvements (by positive component or by negative component) of objective function  $\overline{f}$  as  $\Delta\overline{f}(O_{j,\iota})$  are presented in Table 3.23 (component 0 of the vector is not pointed out).

**Table 3.23.** Improvements of objective function  $\Delta\bar{f}(O_{j,\ell})$  (iteration index  $\gamma = 0$ )

| $A_j$    | $X_\ell :$ | $X_2$ | $X_3$ | $X_4$ | $X_5$ | $X_6$ | $X_7$ | $X_8$ | $X_9$ | $X_{10}$ | $X_{11}$ |
|----------|------------|-------|-------|-------|-------|-------|-------|-------|-------|----------|----------|
| $A_1$    |            | -3.0  | 1.4   | -0.6  | -5.1  | -5.5  | -3.5  | -1.2  | -3.4  | -4.5     | -6.5     |
| $A_2$    |            |       | -0.8  | -1.3  | -3.3  | -1.4  | 3.1   | -2.9  | -3.6  | -5.1     | -4.9     |
| $A_3$    |            |       |       | -1.1  | -2.0  | -2.7  | -2.1  | 3.2   | -3.0  | -4.5     | -4.1     |
| $A_4$    |            |       |       |       | -0.5  | -3.7  | -2.5  | 2.6   | -0.9  | -1.3     | -2.2     |
| $A_5$    |            |       |       |       |       | -6.5  | -5.6  | -1.1  | 2.8   | -0.5     | -6.1     |
| $A_6$    |            |       |       |       |       |       | 3.5   | 0.4   | -1.8  | -3.2     | -0.3     |
| $A_7$    |            |       |       |       |       |       |       | 0.5   | -0.3  | -0.8     | 2.9      |
| $A_8$    |            |       |       |       |       |       |       |       | 1.0   | -0.8     | -2.8     |
| $A_9$    |            |       |       |       |       |       |       |       |       | 3.0      | -5.5     |
| $A_{10}$ |            |       |       |       |       |       |       |       |       |          | -6.0     |

**Iteration 1.** Selection of the best (Pareto-efficient) improvement operation  $O_{6,7}$  with the best improvement  $\Delta\bar{f}(O_{j,\ell}) = (0, 3.5)$ . As a result, the following information is used for the next algorithm step: (a)  $\hat{X}^1 = \{X_1^1, X_2^1, X_3^1, X_4^1, X_5^1, X_7^1, X_8^1, X_9^1, X_{10}^1, X_{11}^1\}$  where  $X_1^1 = \{A_1\}$ ,  $X_2^1 = \{A_2\}$ ,  $X_3^1 = \{A_3\}$ ,  $X_4^1 = \{A_4\}$ ,  $X_5^1 = \{A_5\}$ ,  $X_7^1 = \{A_6, A_7\}$ ,  $X_8^1 = \{A_8\}$ ,  $X_9^1 = \{A_9\}$ ,  $X_{10}^1 = \{A_{10}\}$ ,  $X_{11}^1 = \{A_{11}\}$ ; (b)  $\bar{f}^1(\hat{X}^1) = (0, 3.5)$ ; (c) improvement operations (i.e., inclusion of element/cluster  $X_{\ell_1}$  into cluster  $X_{\ell_2}$ ) as  $O_{\ell_1, \ell_2}(X_{\ell_1} \rightarrow X_{\ell_2})$  and corresponding improvements (by positive component or by negative component) of objective function  $\bar{f}$  as  $\Delta\bar{f}(O_{\ell_1, \ell_2})$  are presented in Table 3.24 (component 0 of the vector is not pointed out).

**Table 3.24.** Improvements of objective function  $\Delta\bar{f}(O_{j,\ell})$  (iteration index  $\gamma = 1$ )

| $X_{\ell_1}$           | $X_{\ell_2} :$ | $X_2^1$ | $X_3^1$ | $X_4^1$ | $X_5^1$ | $X_7^1$     | $X_8^1$ | $X_9^1$ | $X_{10}^1$ | $X_{11}^1$  |
|------------------------|----------------|---------|---------|---------|---------|-------------|---------|---------|------------|-------------|
| $X_1^1$                |                | -3.0    | 1.4     | -0.6    | -5.1    | -9.0        | -1.2    | -3.4    | -4.5       | -6.5        |
| $X_2^1$                |                |         | -0.8    | -1.3    | -3.3    | (-1.4, 3.1) | -2.9    | -3.6    | -5.1       | -4.9        |
| $X_3^1$                |                |         |         | -1.1    | -2.0    | -4.8        | 3.2     | -3.0    | -4.5       | -4.1        |
| $X_4^1$                |                |         |         |         | -0.5    | -6.2        | 2.6     | -0.9    | -1.3       | -2.2        |
| $X_5^1$                |                |         |         |         |         | -12.2       | -1.1    | 2.8     | -0.5       | -6.1        |
| $X_7^1 = \{A_6, A_7\}$ |                |         |         |         |         |             | 0.9     | -2.1    | -4.0       | (-0.3, 2.9) |
| $X_8^1$                |                |         |         |         |         |             |         | 1.0     | -0.8       | -2.8        |
| $X_9^1$                |                |         |         |         |         |             |         |         | 3.0        | -5.5        |
| $X_{10}^1$             |                |         |         |         |         |             |         |         |            | -6.0        |

**Iteration 2.** Selection of the best (Pareto-efficient) improvement operation  $O_{3,8}$  with the best improvement  $\Delta\bar{f}(O_{j,\ell}) = (0, 3.2)$ . As a result, the following information is used for the next algorithm step: (a)  $\hat{X}^2 = \{X_1^2, X_2^2, X_4^2, X_5^2, X_7^2, X_8^2, X_9^2, X_{10}^2, X_{11}^2\}$  where  $X_1^2 = \{A_1\}$ ,  $X_2^2 = \{A_2\}$ ,  $X_4^2 = \{A_4\}$ ,  $X_5^2 = \{A_5\}$ ,  $X_7^2 = \{A_6, A_7\}$ ,  $X_8^2 = \{A_3, A_8\}$ ,  $X_9^2 = \{A_9\}$ ,  $X_{10}^2 = \{A_{10}\}$ ,  $X_{11}^2 = \{A_{11}\}$ ; (b)  $\bar{f}^2(\hat{X}^2) = (0, 9.9)$ ; (c) improvement operations (i.e., inclusion of element/cluster  $X_{\ell_1}$  into cluster  $X_{\ell_2}$ ) as  $O_{\ell_1, \ell_2}(X_{\ell_1} \rightarrow X_{\ell_2})$  and corresponding improvements (by positive component or by negative component) of objective function  $\bar{f}$  as  $\Delta\bar{f}(O_{\ell_1, \ell_2})$  are presented in Table 3.25 (component 0 of the vector is not pointed out).

**Table 3.25.** Improvements of objective function  $\Delta\bar{f}(O_{j,\ell})$  (iteration index  $\gamma = 2$ )

| $X_{\ell_1}$           | $X_{\ell_2} :$ | $X_2^2$ | $X_4^2$ | $X_5^2$ | $X_7^2$     | $X_8^2$     | $X_9^2$ | $X_{10}^2$ | $X_{11}^2$  |
|------------------------|----------------|---------|---------|---------|-------------|-------------|---------|------------|-------------|
| $X_1^2$                |                | -3.0    | -0.6    | -5.1    | -9.0        | (-1.2, 1.4) | -3.4    | -4.5       | -6.5        |
| $X_2^2$                |                |         | -1.3    | -3.3    | (-1.4, 3.1) | -3.7        | -3.6    | -5.1       | -4.9        |
| $X_4^2$                |                |         |         | -0.5    | -6.2        | (-1.1, 2.6) | -0.9    | -1.3       | -2.2        |
| $X_5^2$                |                |         |         |         | -12.2       | -3.1        | 2.8     | -0.5       | -6.1        |
| $X_7^2 = \{A_6, A_7\}$ |                |         |         |         |             | (-4.8, 0.9) | -2.1    | -4.0       | (-0.3, 2.9) |
| $X_8^2 = \{A_3, A_8\}$ |                |         |         |         |             |             | 1.0     | -0.8       | -2.8        |
| $X_9^2$                |                |         |         |         |             |             |         | 3.0        | -5.5        |
| $X_{10}^2$             |                |         |         |         |             |             |         |            | -6.0        |

**Iteration 3.** Selection of the best (Pareto-efficient) improvement operations:  $O_{2,7}$  and  $O_{9,10}$ . The corresponding Pareto-efficient improvements are:  $\Delta\bar{f}(O_{2,7}) = (-1.4, 3.1)$  and  $\Delta\bar{f}(O_{9,10}) = (0, 3.0)$ . Operation  $O_{9,10}$  is selected. As a result, the following information is used for the next algorithm step:

(a)  $\widehat{X}^3 = \{X_1^3, X_2^3, X_4^3, X_5^3, X_7^3, X_8^3, X_{10}^3, X_{11}^3\}$  where  $X_1^3 = \{A_1\}$ ,  $X_2^3 = \{A_2\}$ ,  $X_4^3 = \{A_4\}$ ,  $X_5^3 = \{A_5\}$ ,  $X_7^3 = \{A_6, A_7\}$ ,  $X_8^3 = \{A_3, A_8\}$ ,  $X_{10}^3 = \{A_9, A_{10}\}$ ,  $X_{11}^3 = \{A_{11}\}$ ; (b)  $\bar{f}^3(\widehat{X}^3) = (0, 12.9)$ ; (c) improvement operations (i.e., inclusion of element/cluster  $X_{l_1}$  into cluster  $X_{l_2}$ ) as  $O_{l_1, l_2}(X_{l_1} \rightarrow X_{l_2})$  and corresponding improvements (by positive component or by negative component) of objective function  $\bar{f}$  as  $\Delta\bar{f}(O_{l_1, l_2})$  are presented in Table 3.26 (component 0 of the vector is not pointed out).

**Table 3.26.** Improvements of objective function  $\Delta\bar{f}(O_{j, l})$  (iteration index  $\gamma = 3$ )

| $X_{l_1}$                    | $X_{l_2} :$ | $X_2^3$ | $X_4^3$ | $X_5^3$ | $X_7^3$     | $X_8^3$     | $X_{10}^3$  | $X_{11}^3$  |
|------------------------------|-------------|---------|---------|---------|-------------|-------------|-------------|-------------|
| $X_1^3$                      |             | -3.0    | -0.6    | -5.1    | -9.0        | (-1.2, 1.4) | -7.9        | -6.5        |
| $X_2^3$                      |             |         | -1.3    | -3.3    | (-1.4, 3.1) | -3.7        | -8.7        | -4.9        |
| $X_4^3$                      |             |         |         | -0.5    | -6.2        | (-1.1, 2.6) | -2.2        | -2.2        |
| $X_5^3$                      |             |         |         |         | -12.2       | -3.1        | (-0.5, 2.8) | -6.1        |
| $X_7^3 = \{A_6, A_7\}$       |             |         |         |         |             | (-4.8, 0.9) | -6.1        | (-0.3, 2.9) |
| $X_8^3 = \{A_3, A_8\}$       |             |         |         |         |             |             | (-8.3, 1.0) | -2.8        |
| $X_{10}^3 = \{A_9, A_{10}\}$ |             |         |         |         |             |             |             | -8.8        |

**Iteration 4.** Selection of the best (Pareto-efficient) improvement operations:  $O_{2,7}$  and  $O_{7,11}$ . The corresponding Pareto-efficient improvements are:  $\Delta\bar{f}(O_{2,7}) = (-1.4, 3.1)$  and  $\Delta\bar{f}(O_{7,11}) = (-0.3, 2.9)$ . Operation  $O_{7,11}$  is selected. As a result, the following information is used for the next algorithm step: (a)  $\widehat{X}^4 = \{X_1^4, X_2^4, X_4^4, X_5^4, X_8^4, X_{10}^4, X_{11}^4\}$  where  $X_1^4 = \{A_1\}$ ,  $X_2^4 = \{A_2\}$ ,  $X_4^4 = \{A_4\}$ ,  $X_5^4 = \{A_5\}$ ,  $X_8^4 = \{A_3, A_8\}$ ,  $X_{10}^4 = \{A_9, A_{10}\}$ ,  $X_{11}^4 = \{A_6, A_7, A_{11}\}$ ; (b)  $\bar{f}^4(\widehat{X}^4) = (-0.3, 15.8)$ ; (c) improvement operations (i.e., inclusion of element/cluster  $X_{l_1}$  into cluster  $X_{l_2}$ ) as  $O_{l_1, l_2}(X_{l_1} \rightarrow X_{l_2})$  and corresponding improvements (by positive component or by negative component) of objective function  $\bar{f}$  as  $\Delta\bar{f}(O_{l_1, l_2})$  are presented in Table 3.27 (component 0 of the vector is not pointed out).

**Table 3.27.** Improvements of objective function  $\Delta\bar{f}(O_{j, l})$  (iteration index  $\gamma = 4$ )

| $X_{l_1}$                    | $X_{l_2} :$ | $X_2^4$ | $X_4^4$ | $X_5^4$ | $X_8^4$     | $X_{10}^4$  | $X_{11}^4 = \{A_6, A_7, A_{11}\}$ |
|------------------------------|-------------|---------|---------|---------|-------------|-------------|-----------------------------------|
| $X_1^4$                      |             | -3.0    | -0.6    | -5.1    | (-1.2, 1.4) | -7.9        | -15.5                             |
| $X_2^4$                      |             |         | -1.3    | -3.3    | -3.7        | -8.7        | (-6.3, 3.1)                       |
| $X_4^4$                      |             |         |         | -0.5    | (-1.1, 2.6) | -2.2        | -8.4                              |
| $X_5^4$                      |             |         |         |         | -3.1        | (-0.5, 2.8) | -18.2                             |
| $X_8^4 = \{A_3, A_8\}$       |             |         |         |         |             | (-8.3, 1.0) | (-14.8, 0.9)                      |
| $X_{10}^4 = \{A_9, A_{10}\}$ |             |         |         |         |             |             | -17.6                             |

**Iteration 5.** Selection of the best (Pareto-efficient) improvement operations:  $O_{2,11}$  and  $O_{5,10}$ . The corresponding Pareto-efficient improvements are:  $\Delta\bar{f}(O_{2,11}) = (-6.3, 3.1)$  and  $\Delta\bar{f}(O_{5,10}) = (-0.5, 2.8)$ . Operation  $O_{5,10}$  is selected. As a result, the following information is used for the next algorithm step: (a)  $\widehat{X}^5 = \{X_1^5, X_2^5, X_4^5, X_8^5, X_{10}^5, X_{11}^5\}$  where  $X_1^5 = \{A_1\}$ ,  $X_2^5 = \{A_2\}$ ,  $X_4^5 = \{A_4\}$ ,  $X_8^5 = \{A_3, A_8\}$ ,  $X_{10}^5 = \{A_5, A_9, A_{10}\}$ ,  $X_{11}^5 = \{A_6, A_7, A_{11}\}$ ; (b)  $\bar{f}^5(\widehat{X}^5) = (-0.8, 18.6)$ ; (c) improvement operations (i.e., inclusion of element/cluster  $X_{l_1}$  into cluster  $X_{l_2}$ ) as  $O_{l_1, l_2}(X_{l_1} \rightarrow X_{l_2})$  and corresponding improvements (by positive component or by negative component) of objective function  $\bar{f}$  as  $\Delta\bar{f}(O_{l_1, l_2})$  are presented in Table 3.28 (component 0 of the vector is not pointed out).

**Table 3.28.** Improvements of objective function  $\Delta\bar{f}(O_{j, l})$  (iteration index  $\gamma = 5$ )

| $X_{l_1}$                         | $X_{l_2} :$ | $X_2^5$ | $X_4^5$ | $X_8^5$     | $X_{10}^5$   | $X_{11}^5 = \{A_6, A_7, A_{11}\}$ |
|-----------------------------------|-------------|---------|---------|-------------|--------------|-----------------------------------|
| $X_1^5$                           |             | -3.0    | -0.6    | (-1.2, 1.4) | -13.0        | -15.5                             |
| $X_2^5$                           |             |         | -1.3    | -3.7        | -12.0        | (-6.3, 3.1)                       |
| $X_4^5$                           |             |         |         | (-1.1, 2.6) | -2.7         | -8.4                              |
| $X_8^5 = \{A_3, A_8\}$            |             |         |         |             | (-11.4, 1.0) | (-14.8, 0.9)                      |
| $X_{10}^5 = \{A_5, A_9, A_{10}\}$ |             |         |         |             |              | -35.8                             |

**Iteration 6.** Selection of the best (Pareto-efficient) improvement operations:  $O_{2,11}$  and  $O_{4,8}$ . The corresponding Pareto-efficient improvements are:  $\Delta\bar{f}(O_{2,11}) = (-6.3, 3.1)$  and  $\Delta\bar{f}(O_{4,8}) = (-1.1, 2.6)$ . Operation  $O_{4,8}$  is selected. As a result, the following information is used for the next algorithm step: (a)  $\widehat{X}^6 = \{X_1^6, X_2^6, X_8^6, X_{10}^6, X_{11}^6\}$  where  $X_1^6 = \{A_1\}$ ,  $X_2^6 = \{A_2\}$ ,  $X_8^6 = \{A_3, A_4, A_8\}$ ,  $X_{10}^6 = \{A_5, A_9, A_{10}\}$ ,

$X_{11}^6 = \{A_6, A_7, A_{11}\}$ ; (b)  $\bar{f}^6(\hat{X}^6) = (-1.9, 21.2)$ ; (c) improvement operations (i.e., inclusion of element/cluster  $X_{l_1}$  into cluster  $X_{l_2}$ ) as  $O_{l_1, l_2}(X_{l_1} \rightarrow X_{l_2})$  and corresponding improvements (by positive component or by negative component) of objective function  $\bar{f}$  as  $\Delta\bar{f}(O_{l_1, l_2})$  are presented in Table 3.29 (component 0 of the vector is not pointed out).

**Table 3.29.** Improvements of objective function  $\Delta\bar{f}(O_{j, l})$  (iteration index  $\gamma = 6$ )

| $X_{l_1}$                         | $X_{l_2} :$ | $X_2^6$ | $X_8^6$     | $X_{10}^6$   | $X_{11}^6 = \{A_6, A_7, A_{11}\}$ |
|-----------------------------------|-------------|---------|-------------|--------------|-----------------------------------|
| $X_1^6$                           |             | -3.0    | (-1.8, 1.4) | -13.0        | -15.5                             |
| $X_2^6$                           |             |         | -5.7        | -12.0        | (-6.3, 3.1)                       |
| $X_8^6 = \{A_3, A_4, A_8\}$       |             |         |             | (-14.1, 1.0) | (-20.1, 0.9)                      |
| $X_{10}^6 = \{A_5, A_9, A_{10}\}$ |             |         |             |              | -35.8                             |

**Iteration 7.** Selection of the best (Pareto-efficient) improvement operations:  $O_{2,11}$  and  $O_{1,8}$ . The corresponding Pareto-efficient improvements are:  $\Delta\bar{f}(O_{2,11}) = (-6.3, 3.1)$  and  $\Delta\bar{f}(O_{1,8}) = (-1.8, 1.4)$ . Operation  $O_{1,8}$  is selected. As a result, the following information is used for the next algorithm step: (a)  $\hat{X}^7 = \{X_2^7, X_8^7, X_{10}^7, X_{11}^7\}$  where  $X_2^7 = \{A_2\}$ ,  $X_8^7 = \{A_1, A_3, A_4, A_8\}$ ,  $X_{10}^7 = \{A_5, A_9, A_{10}\}$ ,  $X_{11}^7 = \{A_6, A_7, A_{11}\}$ ; (b)  $\bar{f}^7(\hat{X}^7) = (-3.7, 22.6)$ ; (c) improvement operations (i.e., inclusion of element/cluster  $X_{l_1}$  into cluster  $X_{l_2}$ ) as  $O_{l_1, l_2}(X_{l_1} \rightarrow X_{l_2})$  and corresponding improvements (by positive component or by negative component) of objective function  $\bar{f}$  as  $\Delta\bar{f}(O_{l_1, l_2})$  are presented in Table 3.30 (component 0 of the vector is not pointed out).

**Table 3.30.** Improvements of objective function  $\Delta\bar{f}(O_{j, l})$  (iteration index  $\gamma = 7$ )

| $X_{l_1}$                         | $X_{l_2} :$ | $X_8^7$ | $X_{10}^7$   | $X_{11}^7 = \{A_6, A_7, A_{11}\}$ |
|-----------------------------------|-------------|---------|--------------|-----------------------------------|
| $X_2^7$                           |             | -8.0    | -12.0        | (-6.3, 3.1)                       |
| $X_8^7 = \{A_1, A_3, A_4, A_8\}$  |             |         | (-27.1, 1.0) | (-35.6, 0.9)                      |
| $X_{10}^7 = \{A_5, A_9, A_{10}\}$ |             |         |              | -35.8                             |

**Iteration 8.** Selection of the best (Pareto-efficient) improvement operation  $O_{2,11}$ . The corresponding Pareto-efficient improvement is:  $\Delta\bar{f}(O_{2,11}) = (-6.3, 3.1)$ . As a result, the following information is used for the next algorithm step: (a)  $\hat{X}^8 = \{X_8^8, X_{10}^8, X_{11}^8\}$  where  $X_8^8 = \{A_1, A_3, A_4, A_8\}$ ,  $X_{10}^8 = \{A_5, A_9, A_{10}\}$ ,  $X_{11}^8 = \{A_2, A_6, A_7, A_{11}\}$ ; (b)  $\bar{f}^8(\hat{X}^8) = (-10.0, 25.7)$ ; (c) improvement operations (i.e., inclusion of element/cluster  $X_{l_1}$  into cluster  $X_{l_2}$ ) as  $O_{l_1, l_2}(X_{l_1} \rightarrow X_{l_2})$  and corresponding improvements (by positive component or by negative component) of objective function  $\bar{f}$  as  $\Delta\bar{f}(O_{l_1, l_2})$  are presented in Table 3.31 (component 0 of the vector is not pointed out).

**Table 3.31.** Improvements of objective function  $\Delta\bar{f}(O_{j, l})$  (iteration index  $\gamma = 8$ )

| $X_{l_1}$                         | $X_{l_2} :$ | $X_8^8$ | $X_{10}^8$   | $X_{11}^8 = \{A_6, A_7, A_{11}\}$ |
|-----------------------------------|-------------|---------|--------------|-----------------------------------|
| $X_8^8 = \{A_1, A_3, A_4, A_8\}$  |             |         | (-27.1, 1.0) | (-43.8, 0.9)                      |
| $X_{10}^8 = \{A_5, A_9, A_{10}\}$ |             |         |              | -47.8                             |

Finally, it is reasonable to consider the result of iteration 8 as the clustering solution:  
 $\hat{X} = \hat{X}^8 = \{X_8^8, X_{10}^8, X_{11}^8\}$ .

Table 3.32 contains a list of main research directions in correlation clustering.

On the other hand, it is possible to use a multiset based problem formulation. It is possible to replace scale  $[-1, +1]$  (or two quantitative scales above) for each edge (i.e., for each element from  $G$  or element of proximity matrix  $Z$ ) by two ordinal scales: negative ordinal scale  $[-k^-, \dots, -1]$  instead of “-1” and positive ordinal scale  $[+1, \dots, k^+]$  instead of “+1”. Note, calculation of edge weights upon the above-mentioned scales is sufficiently easy (e.g., mapping of the quantitative estimate into the ordinal scale). For the clustering solution  $\hat{X} = \{X_1, \dots, X_\lambda\}$  two total quality parameters can be calculated as follows: (i) total agreements quality as multiset estimate (summarization by the component for all intra-cluster pairs with positive edge weight)  $Q^{agr}(\hat{X})$  (maximization); (ii) total disagreements quality as multiset estimate (summarization by the component for all intra-cluster pairs with negative edge weight)  $Q^{disagr}(\hat{X})$  (for minimization). As a result, the multiset based correlation clustering problem is (Fig. 3.17):

Find clustering solution  $\hat{X}$  such that  $Q^{agr}(\hat{X}) \rightarrow \max$  and  $|Q^{disagr}(\hat{X})| \rightarrow \min$ .



**Table 3.32.** Correlation clustering

| No. | Research direction                                    | Source(s)                |
|-----|---|--------------------------|
| 1.  | Basic problem formulations and complexity             | [11,33,39,40,52,345,662] |
| 2.  | Surveys   | [11,40,345,662]          |
| 3.  | Comparing methods for correlation clustering          | [185]                    |
| 4.  | Approximation algorithms (including PTAS)             | [33,39,40,225,662]       |
| 5.  | Weighted versions of correlation clustering problems  | [94,95,159]              |
| 6.  | Correlation clustering with fixed number of clusters  | [225]                    |
| 7.  | Maximizing agreements via semidefinite programming    | [564]                    |
| 8.  | Minimizing disagreements on arbitrary weighted graphs | [187]                    |
| 9.  | Global correlation clustering                         | [5]                      |
| 10. | Correlation clustering with partial information       | [158]                    |
| 11. | Correlation clustering with noisy input               | [423]                    |
| 12. | Error bounds for correlation clustering               | [308]                    |
| 13. | Robust correlation clustering                         | [4,344]                  |
| 14. | Correlation clustering in image segmentation          | [331]                    |

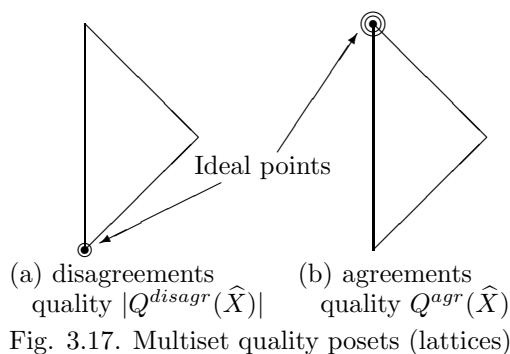


Fig. 3.17. Multiset quality posets (lattices)

### 3.5.4. Network communities based clustering

In recent decades, “network communities based clustering” as a new research direction has been organized (e.g., [206,226,285,370,457,458,459,460,461,496]). The largest connected components are examined as “network communities”, for example: cliques, quasi-cliques, cliques/quasi-cliques with leaves, chains of cliques/quasi-cliques, integrated groups of cliques/quasi-cliques (Fig. 3.18).

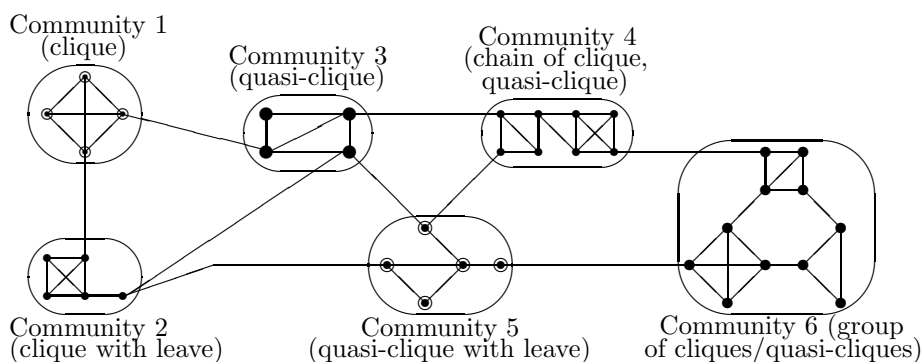


Fig. 3.18. Illustration for network communities

The network example in Fig. 3.18 does not contain overlaps (i.e., without intersection of community structures). Fig. 3.19 illustrates the overlaps.

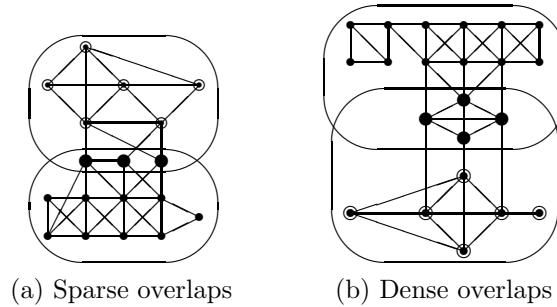


Fig. 3.19. Illustration for overlaps in structures

The detection of “network communities structures” corresponds to complex combinatorial optimization models (e.g., linear/nonlinear integer programming, mixed integer programming). The models belong to NP-hard problems (e.g., [73,127,206,460]). Table 3.33 contains a list of basic research directions in community network based clustering.

A list of basic algorithmic approaches for finding communities involves the following (e.g., [206,459,460,461]): (i) graph partitioning (e.g., minimum-cut method), (ii) hierarchical clustering (greedy agglomerative algorithms), (iii) Girvan-Newman algorithm (edge betweenness), (iv) modularity maximization approaches, (v) spectral clustering methods, (vi) methods based on statistical inference, (vii) clique based methods.

Modularity of a graph can be defined as a normalized tradeoff between edges covered by clusters and squared cluster degree sums [73,461]. The problem is formulated as combinatorial optimization model. For the modularity maximization, several main algorithms are pointed out [73]: (a) greedy agglomeration [127,457], (b) spectral division [459,610], (c) simulated annealing [249,504], (d) extremal optimization [178]. An example of modularity algorithm as greedy agglomerative heuristic is the following [457]:

*Stage 1.* Trivial clustering: each node corresponds to its own cluster.

*Stage 2.* Cycle by cluster pairs:

*Stage 2.1.* Calculation of possible increase of modularity for merging each cluster pairs.

*Stage 2.2.* Merging the two clusters with maximum possible increase.

*Stage 2.3.* If increasing of modularity by merges of cluster pair is impossible then GO TO Stage 3.

*Stage 2.4.* Go To Stage 2.2.

*Stage 3.* Stop.

In this algorithm, algorithmic complexity estimate equals  $O((p+n)n)$  or  $O(n^2)$  [457].

The general scheme of Girvan-Newman (GN) algorithm based on edge betweenness is [226]:

*Step 1.* Calculation of the betweenness score for each the edges.

*Step 2.* Deletion of the edges with the highest score.

*Step 3.* Performance analysis for the network’s components.

*Step 4.* If all edges are deleted and the system breaks up into  $N$  non-connected nodes Go TO Step 5. Otherwise GO TO Step 1.

*Step 5.* Stop.

Algorithmic complexity estimate of the algorithm equals  $O(p^2n)$  ( $p$  is the number of edges) [226]).

### 3.6. Towards fast clustering

Many applications based on very large data sets/networks require fast clustering approaches (e.g., [127,457,546,585,600,662]). In Table 3.34, basic ideas for fast clustering schemes are pointed out. Generally, many fast clustering schemes consist of two basic levels (global level and local level): (a) partition of the initial problems into local problems (i.e., decreased dimension, limited type of objects/elements) (global level), (b) clustering of local clustering problems (local level), (c) composition/integration of local clustering solutions into a resultant global clustering solution (global level).

In Table 3.35, a list of basic fast local clustering algorithms (i.e., fast sub-algorithms) is presented.

**Table 3.33.** Community network based clustering

| No.   | Research direction   | Source(s)                                    |
|-------|--|--|
| 1.    | Basic issues:  |  |
| 1.1.  | Basic problem formulations   | [73,206,226,370,461,459,460,496,608,635,636] |
| 1.2.  | Basic surveys  | [73,61,206,370,439,461,459,460,496]          |
| 1.3.  | Problems complexity  | [73,127,206,460]                             |
| 1.4.  | Overlapping (fuzzy) community structures   | [230,608,622,633,634,635]                    |
| 1.5.  | Analysis/evaluation of community structures  | [370,461,608,636]                            |
| 2.    | Main algorithms/solving schemes:   |  |
| 2.1.  | Algorithm based on edge betweenness<br>(divisive algorithm)                                | [226]  |
| 2.2.  | Modularity algorithm as greedy agglomerative<br>heuristic                                  | [457,475]                                    |
| 2.3.  | “Karate Club” algorithm  | [461]  |
| 2.4.  | Kernighan-Lin method and variants  | [328]  |
| 2.5.  | Overlapping communities (clique percolation,<br>local expansion, dynamic algorithms, etc.) | [230,622,633,634,635]                        |
| 2.6.  | Spectral clustering algorithms, modifications  | [636]  |
| 2.7.  | Genetic algorithms   | [405]  |
| 2.8.  | Agent-based algorithms   | [250]  |
| 3.    | Modularity clustering (maximum modularity):  |  |
| 3.1.  | Surveys  | [73,459,664,636]                             |
| 3.2.  | Tripartite modularity (three vertex types)   | [448,449]                                    |
| 3.3.  | Modularity in $k$ -partite networks  | [406]  |
| 3.4.  | Greedy agglomeration algorithm   | [127,457]                                    |
| 3.5.  | Spectral division algorithm  | [459,610]                                    |
| 3.6.  | Simulated annealing algorithms   | [249,504]                                    |
| 3.7.  | Detecting communities by merging cliques   | [631]  |
| 3.8.  | Extremal optimization scheme<br>(mathematical programming)                                 | [7,178]                                      |
| 3.9.  | Global optimization approach   | [425]  |
| 3.10. | Memetic algorithm  | [454]  |
| 3.11. | Random works algorithms  | [495]  |
| 3.12. | Multi-level algorithms   | [168,465,517]                                |
| 4.    | Large networks:  |  |
| 4.1.  | Communities in large networks  | [59,127,230,285,286,370,495,636]             |
| 4.2.  | Communities in mega-scale networks   | [600]  |
| 4.3.  | Communities in super-scale networks  | [59]   |
| 4.4.  | Tracking evolving communities in large networks  | [286]  |
| 5.    | Applications:  |  |
| 5.1.  | World Wide Web   | [168,370,448]                                |
| 5.2.  | Journal/article networks, citation networks, etc.  | [106,206,516]                                |
| 5.3.  | Social networks (friendship, collaboration, etc.)  | [206,226,248,457,460,461,600,636]            |
| 5.4.  | Biological networks  | [206,226,461]                                |
| 5.5.  | Purchasing network   | [127]  |
| 5.6.  | CAD applications   | [461]  |
| 5.7.  | Antenna-To-Antenna network<br>(mobile phone network)                                       | [60,407]                                     |

**Table 3.34.** Main approaches to fast clustering

| No.    | Approach  | Solving schemes  | Source(s)                   |
|--------|---|--|-----------------------------|
| 1.     | Aggregation of object/network nodes   | Hierarchical clustering (Bottom-Up, step-by-step node aggregation)   | [300,302,546]               |
| 2.     | Division of objects/network nodes (partition/decomposition):  | Top-Down scheme  |                             |
| 2.1.   | Pruning of objects/network nodes (Fig. 3.20)  | 1.Selection of basic edge betweenness in graph and decoupling (Top-Down scheme)<br>2.Clustering in each graph part (if needed)   | [226,546]                   |
| 2.2.   | Multi-level schemes (partition, clustering, integration of solutions):  | 1.Partition of object set/network<br>2.Clustering of local regions<br>3.Composition of local solutions   | [584,585,662]<br>this paper |
| 2.2.1. | “Basic” objects (special “key” objects/nodes) based clustering (Fig. 3.21)  | 1.Detection of “basic” objects/nodes (e.g., by filtering)<br>2.Clustering of “basic” objects/nodes,<br>3.Joining other elements/nodes to obtained clusters   | this paper                  |
| 2.2.2. | Grid-based clustering   | Dividing the space into cells  | [345,402,662]               |
| 2.2.3. | Grid-based clustering in data streams   | Online clustering of data streams  | [411,486]                   |
| 2.2.4. | Grid-based clustering (composition): multiple division of objects “space”/network into cells/regions (e.g., axis-parallel subspaces), region-based clustering, composition of local solutions (Fig. 3.22) | 1.Grid over object “space”/network<br>2.Analysis of grid regions<br>3.Selection of “non-empty” regions<br>4.Clustering in “dense” regions<br>5.Clustering in “sparse” regions (while taking into account solutions in “dense” regions)<br>6.Composition of regions solutions | this paper                  |
| 2.2.5. | Grid-based clustering (extension): multiple division of objects “space”/network and “extension” of clustering solutions (with condensing of clusters, as in dynamic programming) (Fig. 3.22)              | 1.Grid over object “space”/network<br>2.Analysis of grid regions<br>3.Selection of “non-empty” regions<br>4.Clustering in “dense” regions<br>5.Extension of “dense” regions by neighbor region(s) and extension of clustering solution(s)                                    | this paper                  |
| 2.2.6. | Division of object “space”/network by types ( $k$ -partite network) (close to 2.2.1)  | 1.Detection of objects by types<br>2.Clustering for each part<br>3.Composition of clustering solutions   | [406,448,449]<br>this paper |
| 3.     | Composite (multistage, concurrent, multi-techniques) approaches   | Composition/combination of various approaches  | [357]<br>this paper         |

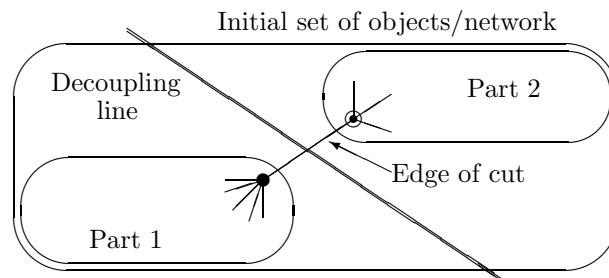


Fig. 3.20. Edge betweenness for decoupling

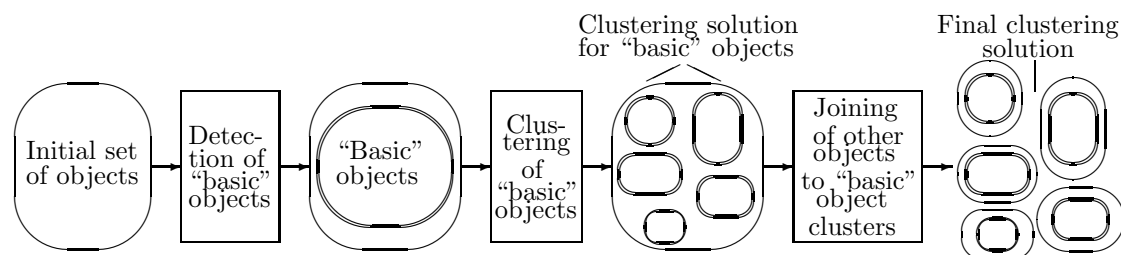


Fig. 3.21. “Basic” objects based clustering framework

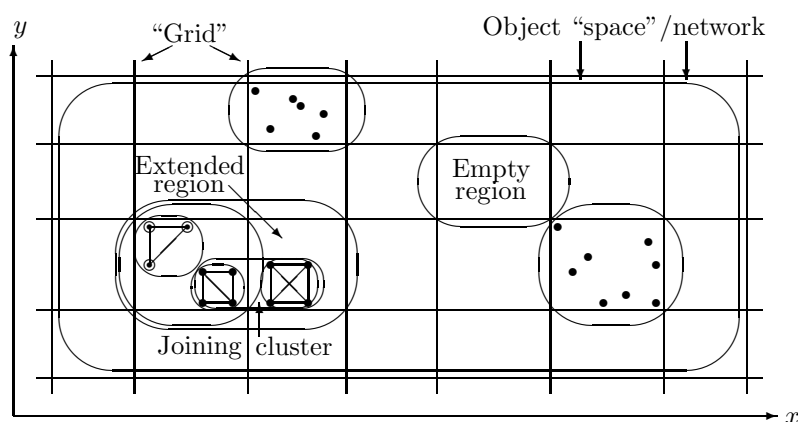


Fig. 3.22. “Grid” over object “space”/network

**Table 3.35.** List of some fast local clustering algorithms

| No. | Fast scheme  | Description  | Complexity estimate (running time)                  | Source(s)                                       |
|-----|--|--|---|---|
| 1.  | Basic agglomerative (hierarchical) algorithm   | Bottom-up joining the closest object pair                                    | $O(n^3)$  | [302]   |
| 2.  | Balanced by cluster size hierarchical algorithm  | Bottom-up joining the closest object pair under constraints for cluster size | $O(n^3)$  |   |
| 3.  | Minimum spanning tree based algorithm  | Clustering the spanning tree nodes   | $O(n \log n)$                                       | [235,244,445]<br>[479,492,555]<br>[606,626,660] |
| 4.  | Balanced by cluster size minimum spanning tree based algorithm                           | Clustering the spanning tree nodes under constraints for cluster size        | $O(n \log n)$                                       |   |
| 5.  | Graph clustering algorithm   | Detection of network communities (edge betweenness of the graph)             | $O(p^2n)$   | [226]   |
| 6.  | Modularity graph clustering algorithm  | Modularity based detection of network communities                            | $O((p+n)n)$ or $O(n^2)$                             | [457]   |
| 7.  | Algorithms based on grid over “space of object coordinates” (partition space techniques) | Assignment of objects into local regions of “space of object coordinates”    | $O(n + n' \times n'')$<br>( $n' \ll n, n'' \ll n$ ) | [585]   |
| 8.  | Clustering based on cores decomposition of networks                                      | Preliminary cores decomposition of covering graph                            | $O(n^2) + O(h)$                                     | [45]  |

## 4. Some Combinatorial Clustering Problems

### 4.1. Clustering with interval multiset estimates

#### 4.1.1. Some combinatorial optimization problems with multiset estimates

Multiset estimates are a simplification of multicriteria (vector) estimates. As a result, a simple scale (a little more complicated as an ordinal scale) is used. On the other hand, multiset estimate is a simple generalization of well-known binary voting procedure. Thus, multiset estimate can be used for simplification of multicriteria (multi-parameter) measurement in various problems/procedures.

In [386,392], basic operations over multiset estimates have been described: integration, vector-like proximity, aggregation, and alignment.

Integration of estimates (mainly, for composite systems) can be considered as summarization of the estimates by components (i.e., positions).

Let us consider vector-like proximity of two multiset estimates [386,392]. Let  $A_1$  and  $A_2$  be two alternatives with corresponding interval multiset estimates  $e(A_1)$ ,  $e(A_2)$ . Vector-like proximity for the alternatives above is:  $\delta(e(A_1), e(A_2)) = (\delta^-(A_1, A_2), \delta^+(A_1, A_2))$ , where vector components are: (i)  $\delta^-$  is the number of one-step changes: element of quality  $\iota + 1$  into element of quality  $\iota$  ( $\iota = \overline{1, l-1}$ ) (this corresponds to “improvement”); (ii)  $\delta^+$  is the number of one-step changes: element of quality  $\iota$  into element of quality  $\iota + 1$  ( $\iota = \overline{1, l-1}$ ) (this corresponds to “degradation”). It is assumed:  $|\delta(e(A_1), e(A_2))| = |\delta^-(A_1, A_2)| + |\delta^+(A_1, A_2)|$ .

Aggregation of multiset estimates can be defined as a median estimate for the specified set of initial estimates (traditional approach). Let  $E = \{e_1, \dots, e_\kappa, \dots, e_n\}$  be the set of specified estimates (or a corresponding set of specified alternatives), let  $D$  be the set of all possible estimates (or a corresponding set of possible alternatives) ( $E \subseteq D$ ). Thus, the median estimates (“generalized median”  $M^g$  and “set median”  $M^s$ ) are:  $M^g = \arg \min_{M \in D} \sum_{\kappa=1}^n |\delta(M, e_\kappa)|$ ;  $M^s = \arg \min_{M \in E} \sum_{\kappa=1}^n |\delta(M, e_\kappa)|$ .

**Multiple choice problem** with multiset estimates can be considered as follows [386,392]. Basic multiple choice problem is: (e.g., [218,325]):

$$\max \sum_{i=1}^m \sum_{j=1}^{q_i} c_{ij} x_{ij} \quad s.t. \quad \sum_{i=1}^m \sum_{j=1}^{q_i} a_{ij} x_{ij} \leq b; \quad \sum_{j=1}^{q_i} x_{ij} \leq 1, \quad i = \overline{1, m}; \quad x_{ij} \in \{0, 1\}.$$

In the case of multiset estimates of item “utility”  $e_i, i \in \{1, \dots, i, \dots, m\}$  (instead of  $c_i$ ), the following aggregated multiset estimate can be used for the objective function (“maximization” [386,392]): (a) an aggregated multiset estimate as the “generalized median”, (b) an aggregated multiset estimate as the “set median”, and (c) an integrated multiset estimate.

A special case of multiple choice problem is considered:

(1) multiset estimates of item “profit”/“utility”  $e_{i,j}, i \in \{1, \dots, i, \dots, m\}, j = \overline{1, q_i}$  (instead of  $c_{ij}$ ),

(2) an aggregated multiset estimate as the “generalized median” (or “set median”) is used for the objective function (“maximization”).

The item set is:  $A = \bigcup_{i=1}^m A_i, A_i = \{(i, 1), (i, 2), \dots, (i, q_i)\}$ .

Boolean variable  $x_{i,j}$  corresponds to selection of the item  $(i, j)$ . The solution is a subset of the initial item set:  $S = \{(i, j) | x_{i,j} = 1\}$ . The problem is:

$$\max e(S) = \max M = \arg \min_{M \in D} \sum_{(i,j) \in S = \{(i,j) | x_{i,j} = 1\}} |\delta(M, e_{i,j})|,$$

$$s.t. \quad \sum_{i=1}^m \sum_{j=1}^{q_i} a_{ij} x_{i,j} \leq b; \quad \sum_{j=1}^{q_i} x_{i,j} = 1; \quad x_{i,j} \in \{0, 1\}.$$

Here the following algorithms can be used (as for basic multiple choice problem) (e.g., [218,325,386,392]): (i) enumerative methods including dynamic programming approach, (ii) heuristics (e.g, greedy algorithms), (iii) approximation schemes (e.g., modifications of dynamic programming approach).

**Combinatorial synthesis** (Hierarchical Multicriteria Morphological Design - HMMD) with ordinal estimates of design alternatives is examined as follows ([374,376,385,386,392]). A composite (modular,

decomposable) system consists of components and their interconnection or compatibility (IC). Basic assumptions of HMMD are the following: (a) a tree-like structure of the system; (b) a composite estimate for system quality that integrates components (subsystems, parts) qualities and qualities of IC (compatibility) across subsystems; (c) monotonic criteria for the system and its components; (d) quality of system components and IC are evaluated on the basis of coordinated ordinal scales. The designations are: (1) design alternatives (DAs) for leaf nodes of the model; (2) priorities of DAs ( $\iota = \overline{1, l}$ ; 1 corresponds to the best one); (3) ordinal compatibility for each pair of DAs ( $w = \overline{1, \nu}$ ;  $\nu$  corresponds to the best one).

Let  $S$  be a system consisting of  $m$  parts (components):  $R(1), \dots, R(i), \dots, R(m)$ . A set of design alternatives is generated for each system part above. The problem is:

*Find a composite design alternative  $S = S(1) \star \dots \star S(i) \star \dots \star S(m)$  of DAs (one representative design alternative  $S(i)$  for each system component/part  $R(i)$ ,  $i = \overline{1, m}$ ) with non-zero compatibility between design alternatives.*

A discrete “space” of the system excellence (a poset) on the basis of the following vector is used:  $N(S) = (w(S); e(S))$ , where  $w(S)$  is the minimum of pairwise compatibility between DAs which correspond to different system components (i.e.,  $\forall R_{j_1}$  and  $R_{j_2}$ ,  $1 \leq j_1 \neq j_2 \leq m$ ) in  $S$ ,  $e(S) = (\eta_1, \dots, \eta_\iota, \dots, \eta_l)$ , where  $\eta_\iota$  is the number of DAs of the  $\iota$ th quality in  $S$ . Further, the problem is described as follows:

$$\max e(S), \quad \max w(S), \quad s.t. \quad w(S) \geq 1.$$

Here, composite solutions which are nondominated by  $N(S)$  (i.e., Pareto-efficient) are searched for. “Maximization” of  $e(S)$  is based on the corresponding poset. The considered combinatorial problem is NP-hard and an enumerative solving scheme is used.

Here, combinatorial synthesis is based on usage of multiset estimates of design alternatives for system parts. For the resultant system  $S = S(1) \star \dots \star S(i) \star \dots \star S(m)$  the same type of the multiset estimate is examined: an aggregated estimate (“generalized median”) of corresponding multiset estimates of its components (i.e., selected DAs). Thus,  $N(S) = (w(S); e(S))$ , where  $e(S)$  is the “generalized median” of estimates of the solution components. Finally, the modified problem is:

$$\max e(S) = M^g = \arg \min_{M \in D} \sum_{i=1}^m |\delta(M, e(S_i))|, \quad \max w(S), \quad s.t. \quad w(S) \geq 1.$$

Here enumeration methods or heuristics are used (e.g., [374,376,385,386,392]).

**Assignment problem** with multiset estimates is formulated as follows. Estimates of “profits”/“utilities” of local assignments (i.e., item-position)  $\{c_{ij}\}$  can be replaced by multiset estimates  $\{e_{ij}\}$ . Further, summarization in objective function can be implemented as summarization of multiset estimates or by searching for a median estimate ( $S$  is an assignment solution for all elements  $i = \overline{1, n}$ ):

$$\begin{aligned} \max e(S) = \max M = & \arg \min_{M \in D} \sum_{(i,j) \in S = \{(i,j) | x_{i,j}=1\}} |\delta(M, e_{i,j})|, \\ s.t. \quad \sum_{i=1}^m x_{i,j} \leq 1, j = \overline{1, n}; & \quad \sum_{j=1}^n x_{i,j} \leq 1, i = \overline{1, m}; \quad x_{i,j} \in \{0, 1\}, i = \overline{1, m}, j = \overline{1, n}. \end{aligned}$$

In the case of generalized problem (e.g., it is possible to assign several items to each position), the problem is (i.e., change of constraint for each position  $j$ ):

$$\begin{aligned} \max e(S) = \max M = & \arg \min_{M \in D} \sum_{(i,j) \in S = \{(i,j) | x_{i,j}=1\}} |\delta(M, e_{i,j})|, \\ s.t. \quad \sum_{i=1}^m x_{i,j} \leq b_j, j = \overline{1, n}; & \quad \sum_{j=1}^n x_{i,j} \leq 1, i = \overline{1, m}; \quad x_{i,j} \in \{0, 1\}, i = \overline{1, m}, j = \overline{1, n}, \end{aligned}$$

here  $b_j$  is constraint for number of assigned elements for each position  $j$ ). Clearly, other analogical constraints for each positions can be used as well (i.e., by other types of resources). It is reasonable to use heuristics as solving schemes.

#### 4.1.2. Towards Clustering with interval multiset estimates

In agglomerative algorithms, the basic methodological problem consists in selection/design of proximity measure for objects/clusters. Evidently, the measure is often based on many parameters and it is necessary to use vector proximity/distance. Here, it may be reasonable to simplify of the solving procedure via transformation of the vector proximity (proximities) into multiset estimate(s). Minimization of multiset estimates is a simple process (in some complex situations Pareto-efficient point(s) can be used).

Analogical approach can be used in k-means clustering method by the usage of interval multiset estimates instead of proximity/distance of objects to cluster centroids. In the case of assignment based clustering, the above-mentioned model based on multiset estimates can be used.

**Example 4.1.** A simplified numerical example is based on data from example 3.2: set of 9 end users ( $A = \{1, \dots, i, \dots, 9\}$ ) (Fig. 4.1) and their quantitative estimates (Table 3.15, vector estimate  $x_i, y_i, z_i$ ).

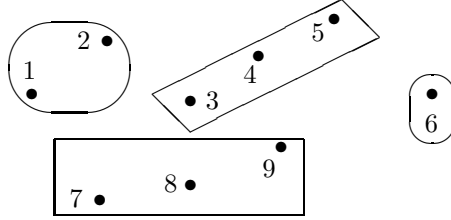


Fig. 4.1. Example: 9 items

Table 4.1 contains pair vector proximity estimates:  $\overline{D}(i_1, i_2) = (d_x(i_1, i_2), d_y(i_1, i_2), d_z(i_1, i_2))$ , where  $d_x(i_1, i_2) = |x_{i_1} - x_{i_2}|$ ,  $d_y(i_1, i_2) = |y_{i_1} - y_{i_2}|$ ,  $d_z(i_1, i_2) = |z_{i_1} - z_{i_2}|$ .

**Table 4.1.** Vector quantitative proximity between end users  $\overline{D}(i_1, i_2)$

| $i_1$ | $i_2 :$ | 2          | 3           | 4           | 5            | 6            | 7            | 8           | 9           |
|-------|---------|------------|-------------|-------------|--------------|--------------|--------------|-------------|-------------|
| 1     |         | (28, 9, 0) | (58, 9, 5)  | (80, 4, 0)  | (115, 16, 2) | (140, 4, 0)  | (22, 31, 0)  | (56, 31, 2) | (90, 25, 1) |
| 2     |         |            | (30, 18, 5) | (52, 5, 0)  | (107, 25, 3) | (112, 13, 0) | (6, 40, 0)   | (28, 40, 2) | (82, 34, 1) |
| 3     |         |            |             | (22, 13, 5) | (58, 25, 3)  | (82, 5, 5)   | (36, 22, 5)  | (2, 22, 3)  | (32, 16, 6) |
| 4     |         |            |             |             | (35, 12, 2)  | (60, 8, 0)   | (58, 35, 0)  | (24, 35, 2) | (10, 29, 1) |
| 5     |         |            |             |             |              | (25, 20, 2)  | (93, 48, 2)  | (59, 48, 0) | (25, 41, 1) |
| 6     |         |            |             |             |              |              | (118, 27, 0) | (84, 27, 2) | (50, 21, 1) |
| 7     |         |            |             |             |              |              |              | (34, 0, 2)  | (68, 6, 1)  |
| 8     |         |            |             |             |              |              |              |             | (34, 6, 3)  |

Table 4.2 contains corresponding vector ordinal proximity  $\overline{r}(i_1, i_2) = (r_x(i_1, i_2), r_y(i_1, i_2), r_z(i_1, i_2))$  (ordinal scale  $[1, 2, 3]$  is used, 1 corresponds to close values). Ordinal values are calculated as follows (for parameter  $x$ , for other parameters calculation is analogical):

$$r_x(i_1, i_2) = \begin{cases} 1, & \text{if } d_x^{min} \leq d_x(i_1, i_2) \leq d_x^{min} + \frac{\Delta_x}{3}, \\ 2, & \text{if } d_x^{min} + \frac{\Delta_x}{3} < d_x(i_1, i_2) \leq d_x^{min} + \frac{2\Delta_x}{3}, \\ 3, & \text{if } d_x^{min} + \frac{2\Delta_x}{3} < d_x(i_1, i_2) \leq d_x^{min} + \Delta_x, \end{cases}$$

where

$$\begin{aligned} d_x^{min} &= \min_{i \in A} d_i(x), & d_y^{min} &= \min_{i \in A} d_i(y), & d_z^{min} &= \min_{i \in A} d_i(z); \\ d_x^{max} &= \max_{i \in A} d_i(x), & d_y^{max} &= \max_{i \in A} d_i(y), & d_z^{max} &= \max_{i \in A} d_i(z); \\ \Delta_x &= d_x^{max} - d_x^{min}, & \Delta_y &= d_y^{max} - d_y^{min}, & \Delta_z &= d_z^{max} - d_z^{min}. \end{aligned}$$

Table 4.3 contains corresponding multiset estimates. The used multiset scale (poset) is shown in Fig. 4.2 (assessment over scale  $[1, 3]$  with three elements; analogue of poset in Fig. 2.16).



**Table 4.2.** Vector ordinal proximity between end users  $\bar{r}(i_1, i_2)$ 

| $i_1$ | $i_2 :$   | 2         | 3         | 4         | 5         | 6         | 7         | 8         | 9         |
|-------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 1     | (1, 1, 1) | (2, 1, 3) | (2, 1, 1) | (3, 1, 1) | (3, 1, 1) | (1, 2, 1) | (2, 2, 1) | (2, 2, 1) | (2, 2, 1) |
| 2     |           | (1, 2, 3) | (2, 1, 1) | (3, 2, 2) | (3, 1, 1) | (1, 3, 1) | (1, 3, 1) | (1, 3, 1) | (2, 3, 1) |
| 3     |           |           | (1, 1, 3) | (2, 2, 2) | (2, 1, 3) | (1, 2, 3) | (1, 2, 2) | (1, 2, 2) | (1, 1, 3) |
| 4     |           |           |           | (1, 1, 1) | (2, 3, 1) | (2, 3, 1) | (1, 3, 1) | (1, 3, 1) | (1, 2, 1) |
| 5     |           |           |           |           | (3, 2, 1) | (2, 3, 1) | (2, 3, 1) | (2, 3, 1) | (1, 3, 1) |
| 6     |           |           |           |           |           | (3, 2, 1) | (2, 2, 1) | (2, 2, 1) | (2, 2, 1) |
| 7     |           |           |           |           |           |           | (1, 1, 1) | (2, 1, 1) | (2, 1, 1) |
| 8     |           |           |           |           |           |           |           |           | (1, 1, 2) |

**Table 4.3.** Multiset proximity between end users  $e(i_1, i_2)$ 

| $i_1$ | $i_2 :$   | 2         | 3         | 4         | 5         | 6         | 7         | 8         | 9         |
|-------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 1     | (3, 0, 0) | (1, 1, 1) | (2, 1, 0) | (2, 0, 1) | (2, 0, 1) | (2, 1, 0) | (1, 2, 0) | (1, 2, 0) | (1, 2, 0) |
| 2     |           | (1, 1, 1) | (2, 1, 0) | (0, 2, 1) | (2, 0, 1) | (2, 0, 1) | (2, 0, 1) | (2, 0, 1) | (1, 1, 1) |
| 3     |           |           | (2, 0, 1) | (0, 3, 0) | (1, 1, 1) | (1, 1, 1) | (1, 1, 1) | (1, 2, 0) | (2, 0, 1) |
| 4     |           |           |           | (3, 0, 0) | (1, 1, 1) | (1, 1, 1) | (2, 0, 1) | (2, 0, 1) | (2, 1, 0) |
| 5     |           |           |           |           | (1, 1, 1) | (1, 1, 1) | (1, 1, 1) | (1, 1, 1) | (2, 0, 1) |
| 6     |           |           |           |           |           | (1, 1, 1) | (1, 2, 0) | (1, 2, 0) | (1, 2, 0) |
| 7     |           |           |           |           |           |           | (3, 0, 0) | (2, 1, 0) | (2, 1, 0) |
| 8     |           |           |           |           |           |           |           |           | (2, 1, 0) |

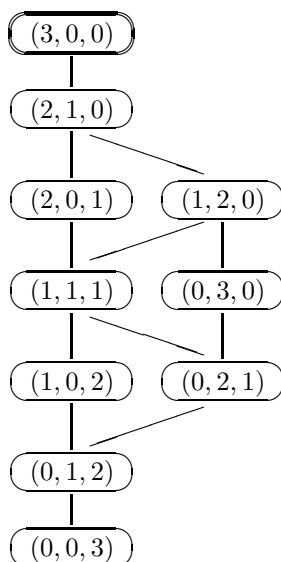


Fig. 4.2. Multiset scale

Application of hierarchical agglomerative balance by cluster size ( $\leq 3$ ) algorithm (while taking into account multiset proximity estimates) leads to the following results (integration of multiset estimates is implemented as searching for the median estimate).

*Iteration 1.* The smallest pair multiset proximity (3, 0, 0) correspond to the following item node pairs (with next integration of the pairs): (1, 2)  $\Rightarrow J_{1,2}$ , (4, 5)  $\Rightarrow J_{4,5}$ , and (7, 8)  $\Rightarrow J_{7,8}$  (concurrent elements integration).

*Iteration 2.* The smallest pair multiset proximity (2, 1, 0) correspond to the following item node pair (with next integration of the pairs): ( $J_{7,8}, 9$ )  $\Rightarrow J_{7,8,9}$ . Cluster  $X_1 = \{7, 8, 9\}$  is obtained.

*Iteration 3.* The smallest pair multiset proximity (2, 0, 1) correspond to the following item node pair (with next integration of the pairs): ( $J_{4,5}, 3$ )  $\Rightarrow J_{3,4,5}$ . Cluster  $X_2 = \{3, 4, 5\}$  is obtained.

Finally, the following clustering solution can be considered:

$$\widehat{X} = \{X_1, X_2, X_3, X_4, X_5\}, X_1 = \{7, 8, 9\}, X_2 = \{3, 4, 5\}, X_3 = \{1, 2\}, X_4 = \{6\}.$$

Note, a numerical example for assignment based clustering can be considered analogically (e.g., on the basis of data from example 3.2).

## 4.2. Restructuring in clustering

Restructuring approach in combinatorial optimization has been suggested by the author in [381,392]. In this section, restructuring approach for clustering problems is briefly described.

### 4.2.1. One-stage restructuring

Fig. 4.3 and Fig. 4.4 illustrate the restructuring process (one-stage framework) [381,392]. Restructuring in clustering problem is depicted in Fig. 4.5.

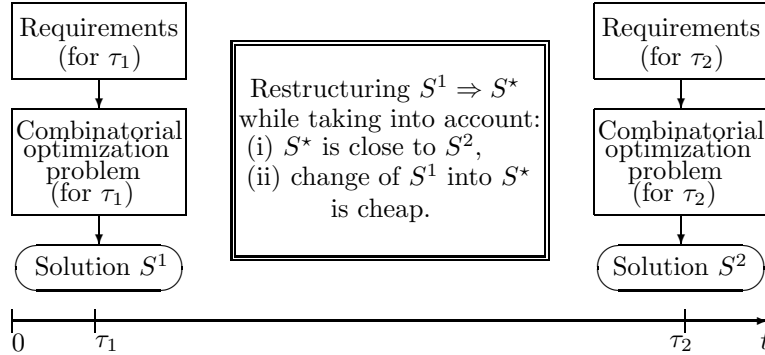


Fig. 4.3. Framework of restructuring process [381,392]

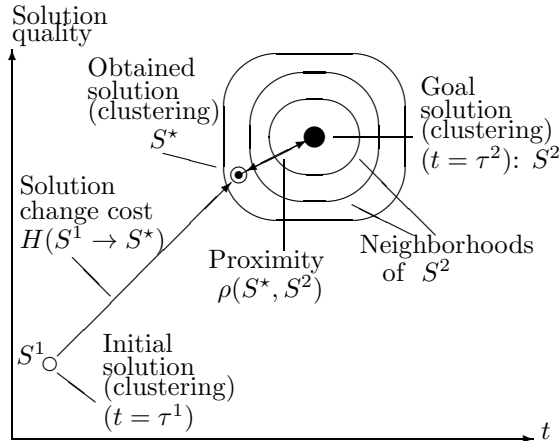


Fig. 4.4. Restructuring scheme [381,392]

Let  $P$  be a combinatorial optimization problem with a solution as structure  $S$  (i.e., subset, graph),  $\Omega$  be initial data (elements, element parameters, etc.),  $f(P)$  be objective function(s). Thus  $S(\Omega)$  be a solution for initial data  $\Omega$ ,  $f(S(\Omega))$  be the corresponding objective function. Let  $\Omega^1$  be initial data at an initial stage,  $f(S(\Omega^1))$  be the corresponding objective function.  $\Omega^2$  be initial data at next stage,  $f(S(\Omega^2))$  be the corresponding objective function. As a result, the following solutions can be considered: (a)  $S^1 = S(\Omega^1)$  with  $f(S(\Omega^1))$  and (b)  $S^2 = S(\Omega^2)$  with  $f(S(\Omega^2))$ .

In addition it is reasonable to examine a cost of changing a solution into another one:  $H(S^\alpha \rightarrow S^\beta)$ . Let  $\rho(S^\alpha, S^\beta)$  be a proximity between solutions  $S^\alpha$  and  $S^\beta$ , for example,  $\rho(S^\alpha, S^\beta) = |f(S^\alpha) - f(S^\beta)|$ . Clearly, function  $f(S)$  can be a vector function. Thus, the following version of restructuring problem is considered:

Find a solution  $S^*$  while taking into account the following:

- (i)  $H(S^1 \rightarrow S^*) \rightarrow \min$ , (ii)  $\rho(S^*, S^2) \rightarrow \min$  (or constraint).

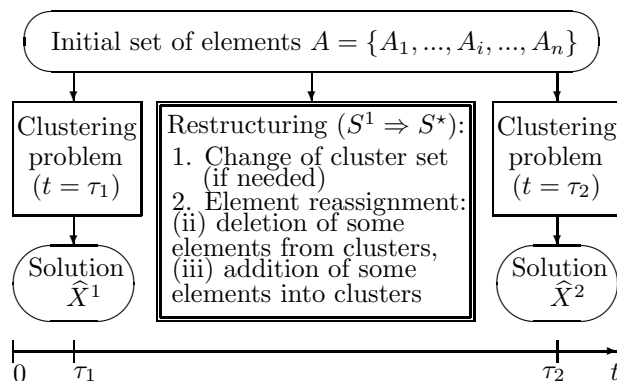


Fig. 4.5. Restructuring in clustering problem

The basic optimization model can be examined as the following:

$$\min \rho(S^*, S^2) \quad s.t. \quad H(S^1 \rightarrow S^*) \leq \hat{h},$$

where  $\hat{h}$  is a constraint for cost of the solution change. In a simple case, this problem can be formulated as knapsack problem for selection of a subset of change operations [381,392]:

$$\max \sum_{i=1}^n c_i^1 x_i \quad s.t. \quad \sum_{i=1}^n a_i^1 x_i \leq b^1, \quad x_i \in \{0, 1\}.$$

In the case of interconnections between change operations, it is reasonable to consider combinatorial synthesis problem (i.e., while taking into account compatibility between the operations).

**Example 4.2.** Initial information involves the following:

- (i) set of elements  $A = \{1, 2, 3, 4, 5, 6, 7, 8, 9\}$ ;
- (ii) initial solution 1 ( $t = \tau_1$ ):  $\hat{X}^1 \{X_1^1, X_2^1, X_3^1\}$ , clusters  $X_1^1 = \{1, 3, 8\}$ ,  $X_2^1 = \{2, 4, 7\}$ ,  $X_3^1 = \{5, 6, 9\}$ ;
- (iii) solution 2 ( $t = \tau_2$ ):  $\hat{X}^2 = \{X_1^2, X_2^2, X_3^2\}$ , clusters  $X_1^2 = \{2, 3\}$ ,  $X_2^2 = \{5, 7, 8\}$ ,  $X_3^2 = \{1, 4, 6, 9\}$ ;
- (v) general set of considered possible change operations (each element can be replaced, the number of solution clusters is not changed):

$O_{11}$ : none,  $O_{12}$ : deletion of element 1 from cluster  $X^1$ , addition of element 1 into cluster  $X^2$ ,  $O_{13}$ : deletion of element 1 from cluster  $X^1$ , addition of element 1 into cluster  $X^3$ ;

$O_{21}$ : none,  $O_{22}$ : deletion of element 2 from cluster  $X^2$ , addition of element 2 into cluster  $X^1$ ,  $O_{23}$ : deletion of element 2 from cluster  $X^2$ , addition of element 2 into cluster  $X^3$ ;

$O_{31}$ : none,  $O_{32}$ : deletion of element 3 from cluster  $X^1$ , addition of element 3 into cluster  $X^2$ ;  $O_{33}$ : deletion of element 3 from cluster  $X^1$ , addition of element 3 into cluster  $X^3$ ;

$O_{41}$ : none,  $O_{42}$ : deletion of element 4 from cluster  $X^2$ , addition of element 4 into cluster  $X^1$ ,  $O_{43}$ : deletion of element 4 from cluster  $X^2$ , addition of element 4 into cluster  $X^3$ ;

$O_{51}$ : none,  $O_{52}$ : deletion of element 5 from cluster  $X^3$ , addition of element 5 into cluster  $X^1$ ,  $O_{53}$ : deletion of element 5 from cluster  $X^3$ , addition of element 5 into cluster  $X^2$ ;

$O_{61}$ : none,  $O_{62}$ : deletion of element 6 from cluster  $X^3$ , addition of element 6 into cluster  $X^1$ ,  $O_{63}$ : deletion of element 6 from cluster  $X^3$ , addition of element 6 into cluster  $X^2$ ;

$O_{71}$ : none,  $O_{72}$ : deletion of element 7 from cluster  $X^2$ , addition of element 7 into cluster  $X^1$ ,  $O_{73}$ : deletion of element 7 from cluster  $X^2$ , addition of element 7 into cluster  $X^3$ ;

$O_{81}$ : none,  $O_{82}$ : deletion of element 8 from cluster  $X^1$ , addition of element 8 into cluster  $X^2$ ,  $O_{83}$ : deletion of element 8 from cluster  $X^1$ , addition of element 8 into cluster  $X^3$ ;

$O_{91}$ : none,  $O_{92}$ : deletion of element 9 from cluster  $X^3$ , addition of element 9 into cluster  $X^1$ ,  $O_{93}$ : deletion of element 9 from cluster  $X^3$ , addition of element 9 into cluster  $X^2$ .

In this case, optimization model (multiple choice problem) is:

$$\max \sum_{i=1}^n \sum_{j=1}^3 c(O_{ij}) x_{ij} \quad s.t. \quad \sum_{i=1}^n \sum_{j=1}^3 a(O_{ij}) x_{ij} \leq b, \quad x_{ij} \in \{0, 1\},$$

where  $a(O_{ij})$  is the cost of operation  $O_{ij}$ ,  $c(O_{ij})$  is a “local” profit of operation  $O_{ij}$  as influence on closeness of obtained solution  $X^*$  to clustering solution  $X^2$ . Generally, it is necessary to examine quality parameters of clustering solution as basis for objective function(s).

Evidently, the compressed set of change operations can be analyzed:

- $O_1$ : deletion of element 1 from cluster  $X^1$ , addition of element 1 into cluster  $X^3$ ;
- $O_2$ : deletion of element 2 from cluster  $X^2$ , addition of element 2 into cluster  $X^1$ ;
- $O_3$ : deletion of element 4 from cluster  $X^2$ , addition of element 4 into cluster  $X^3$ ;
- $O_4$ : deletion of element 5 from cluster  $X^3$ , addition of element 5 into cluster  $X^2$ ;
- $O_5$ : deletion of element 8 from cluster  $X^1$ , addition of element 8 into cluster  $X^2$ .

In this case, optimization model is knapsack problem:

$$\max \sum_{j=1}^9 c(O_j)x_j \quad s.t. \quad \sum_{j=1}^9 a(O_j)x_j \leq b, \quad x_j \in \{0,1\},$$

where  $a(O_j)$  is the cost of operation  $O_j$ ,  $c(O_j)$  is a “local” profit of operation  $O_j$  as influence on closeness of obtained solution  $X^*$  to clustering solution  $X^2$ .

Finally, let us point out an illustrative example of clustering solution (Fig. 4.6):

$\hat{X}^* = \{X_1^*, X_2^*, X_3^*\}$ , clusters  $X_1^* = \{1, 2, 3\}$ ,  $X_2^* = \{7, 8\}$ ,  $X_3^* = \{4, 5, 6, 9\}$ .

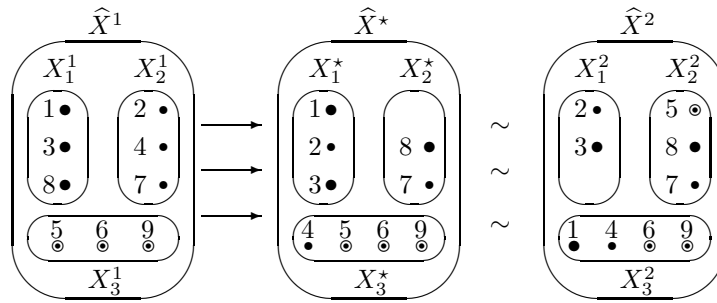


Fig. 4.6. Example: restructuring of clustering solution

#### 4.2.2. Multistage restructuring, cluster/element trajectories

This kind of clustering (or classification) model/problem is close to multistage system design [206,286, 389,391,392]. Fig. 4.7 and Fig. 4.8 illustrate multistage classification and multistage clustering problems:

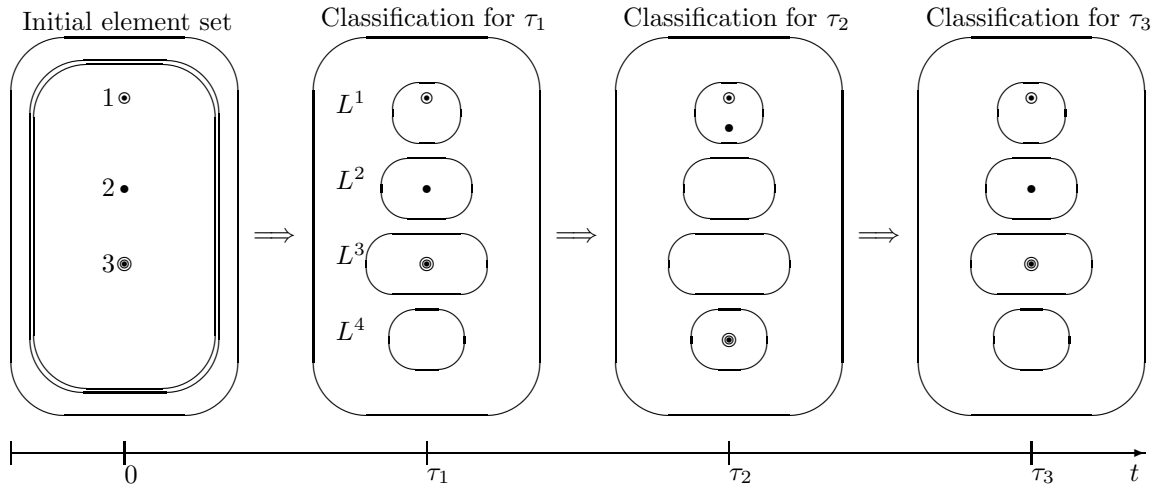


Fig. 4.7. Illustration of multistage classification

1. Multistage classification (Fig. 4.7): the same set of classes at each time stage (here: four classes  $L^1, L^2, L^3, L^4$ ), elements can belong to different classes at each stage. Here: elements 1, 2, 3; trajectory for

element 1:  $J(1) = \langle L^1, L^1, L^1 \rangle$ , trajectory for element 2:  $J(2) = \langle L^2, L^1, L^2 \rangle$ , trajectory for element 3:  $J(3) = \langle L^3, L^4, L^3 \rangle$ .

2. Multistage clustering (Fig. 4.8): different set of clusters at each time stage can be examined, elements can belong to different clusters at each stage. Here: elements 1, 2, 3; trajectory for element 1:  $J(1) = \langle L_1^1, L_2^1, L_3^1 \rangle$ , trajectory for element 2:  $J(2) = \langle L_1^2, L_2^2, L_3^2 \rangle$ , trajectory for element 3:  $J(3) = \langle L_1^3, L_2^4, L_3^5 \rangle$ .

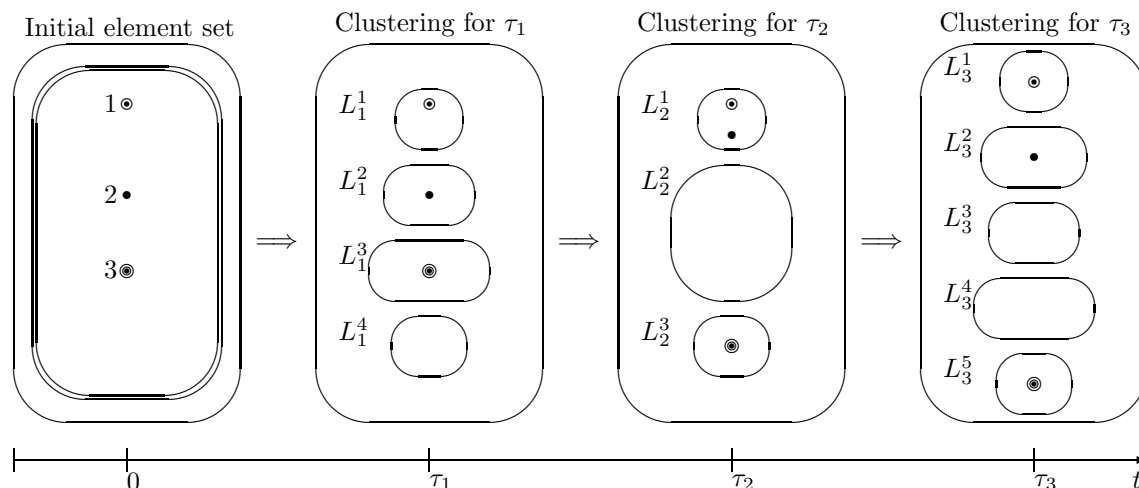


Fig. 4.8. Illustration of multistage clustering

In this problem, it is necessary to examine a set of change trajectories for each element. As a result, multi-stage restructuring problem has to be based on multiple choice model. Generally, this problem is very prospective.

#### 4.2.3. Restructuring in sorting

One-stage restructuring for sorting problem can be considered as well. Let  $A = \{A_1, \dots, A_i, \dots, A_n\}$  be a initial element set. Solution is a result of dividing set  $\{A\}$  into  $k$  linear ordered subsets (ranking):  $\hat{R} = \{R_1, \dots, R_j, \dots, R_k\}$ ,  $R_j \subseteq A \forall j = \overline{1, k}$ ,  $|R_{j_1} \cap R_{j_2}| = 0 \forall j_1, j_2$ . Linear order is:  $R_1 \rightarrow \dots \rightarrow R_j \rightarrow \dots \rightarrow R_k$ ,  $A_{i_1} \rightarrow A_{i_2}$  if  $A_{i_1} \in R_{j_1}$ ,  $A_{i_2} \in R_{j_2}$ ,  $j_1 < j_2$ .

Generally, the sorting problem (or multicriteria ranking) consists in transformation of set  $A$  into ranking  $R$ :  $A \Rightarrow R$  while taking into account multicriteria estimates of elements and/or expert judgment (e.g., [518,666]). In Fig. 4.9, illustration for restructuring in sorting problem is depicted. The problem is:

$$\min \delta(\hat{R}^2, \hat{R}^*) \quad s.t. \quad a(\hat{R}^1 \rightarrow \hat{R}^*) < b,$$

where  $\hat{R}^*$  is solution,  $\hat{R}^1$  is initial (the “first”) ranking,  $\hat{R}^2$  is the “second” ranking,  $\delta(\hat{R}^*, \hat{R}^2)$  is proximity between solution  $\hat{R}^*$  and the “second” ranking  $\hat{R}^2$  (e.g., structural proximity or proximity by quality parameters for rankings),  $a(\hat{R}^1 \rightarrow \hat{R}^*)$  is the cost of transformation of the “first” ranking  $\hat{R}^1$  into solution  $\hat{R}^*$  (e.g., editing “distance”),  $b$  is constraint for the transformation cost. Evidently, multi-stage restructuring problems (with change trajectories of elements) are prospective as well.

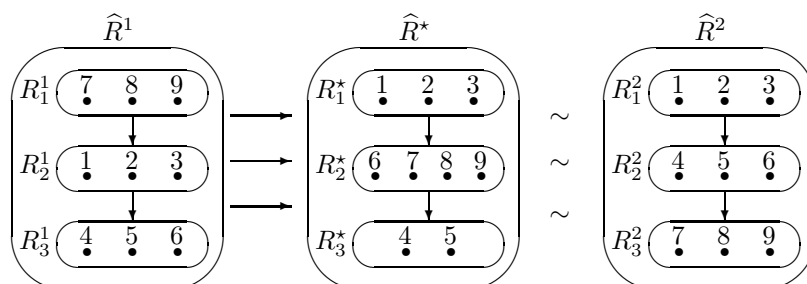


Fig. 4.9. Example: restructuring in sorting problem

### 4.3. Clustering with multi-type elements

#### 4.3.1. Basic problems

Our basic clustering problem can be considered as the follows: initial set of elements  $A$  consists of several subsets:  $A = \bigcup_{j=1}^n A^j$  where  $A^j = \{a_1^j, \dots, a_l^j, \dots, a_{n_j}^j\}$ ,  $j$  corresponds to a certain kind of element type, i.e., there is a set of the types:  $J = \{1, \dots, j, \dots, j_t\}$ . Special binary relation is defined over the set  $J$ :  $R_J$ .

The first clustering strategy is:

- (i) to group the initial set of elements  $A$  without analysis of the element types,
- (ii) to examine a connection of the elements of different types at the next stage (e.g., for each obtained cluster).

Here, the second clustering strategy is examined:

- (1) to obtain clustering for each subset  $A^j = \{A_1^j, \dots, A_l^j, \dots, A_{k_j}^j\}$ .
- (2) to find a correspondence between clusters of subset  $A^{j^1}$  and clusters of subset  $A^{j^2}$  (for the case  $R(j^1, j^2) = 1$ );
- (3) to find a correspondence between cluster elements of subsets  $A^{j^1}$  and cluster elements of subsets  $A^{j^2}$  (for the case  $R(j^1, j^2) = 1$ ).

Here, three new clustering problems with multi-type elements are suggested and examined: (i) clustering with two-type elements, (ii) clustering with three-type elements, and (iii) clustering with four-type elements. Examples of the special binary relation(s) over the element types are depicted in Fig. 4.10.

Fig. 4.11 and Fig. 4.12 illustrate the above-mentioned second clustering strategy (three-type elements):

(i) clustering of subsets:

$$G = G_1 \cup G_2 \cup G_3 \text{ where } G_1 = \{g_1^1, g_2^1, g_3^1\}, G_2 = \{g_1^2, g_2^2, g_3^2\}, G_3 = \{g_1^3, g_2^3, g_3^3\};$$

$$B = B_1 \cup B_2 \cup B_3 \text{ where } B_1 = \{b_1^1, b_2^1, b_3^1\}, B_2 = \{b_1^2, b_2^2, b_3^2\}, B_3 = \{b_1^3, b_2^3, b_3^3\};$$

$$H = H_1 \cup H_2 \cup H_3 \text{ where } H_1 = \{h_1^1, h_2^1, h_3^1\}, H_2 = \{h_1^2, h_2^2, h_3^2\}, H_3 = \{h_1^3, h_2^3, h_3^3\};$$

(ii) three-matching of the obtained clusters:  $\langle B_1 \star G_3 \star H_2 \rangle$ ,  $\langle B_2 \star G_1 \star H_3 \rangle$ , and  $\langle B_3 \star G_2 \star H_1 \rangle$ .

(iii) three-matching of cluster elements:

$$\langle B_1 \star G_3 \star H_2 \rangle: \langle b_1^1 \star g_3^3 \star h_2^2 \rangle, \langle b_2^1 \star g_3^3 \star h_2^2 \rangle, \langle b_3^1 \star g_2^2 \star h_1^1 \rangle;$$

$$\langle B_2 \star G_1 \star H_3 \rangle: \langle b_1^2 \star g_1^1 \star h_3^3 \rangle, \langle b_2^2 \star g_1^1 \star h_3^3 \rangle, \langle b_3^2 \star g_2^1 \star h_3^3 \rangle;$$

$$\langle B_3 \star G_2 \star H_1 \rangle: \langle b_1^3 \star g_2^2 \star h_3^1 \rangle, \langle b_2^3 \star g_1^2 \star h_1^1 \rangle, \langle b_3^3 \star g_3^2 \star h_2^1 \rangle.$$

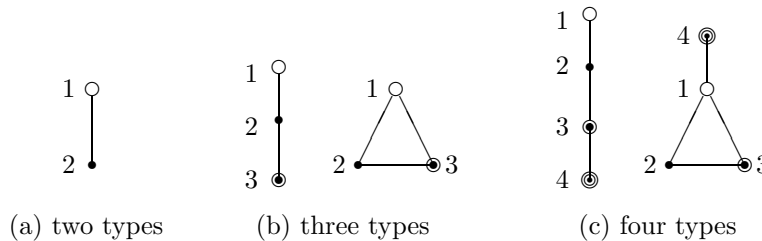


Fig. 4.10. Illustration for binary relation over element types

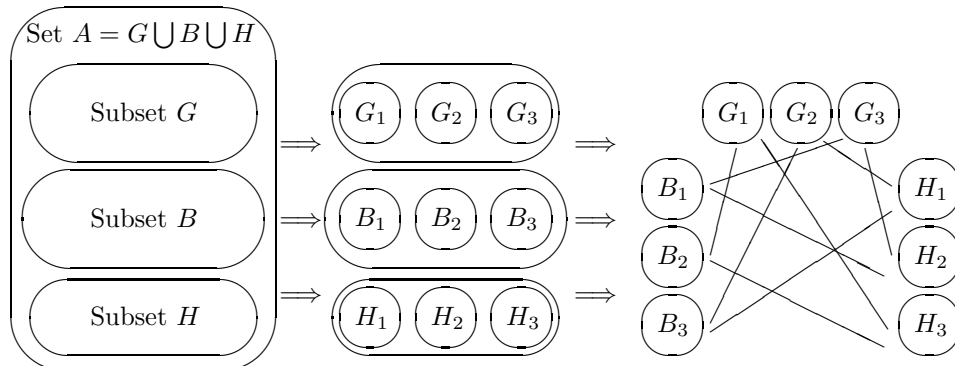


Fig. 4.11. Clustering strategy (three-type elements): clustering, three-matching

Problem solving frameworks are based on combinations of well-known combinatorial problems and cor-

responding algorithms: clustering (e.g., hierarchical clustering, k-means clustering), assignment/allocation, three-matching, for example:

- (a) clustering of elements for each element subset,
- (b) assignment of the obtained clusters (while taking into account the binary relation over element types),
- (c) assignment of cluster elements (while taking into account the binary relation over element types), and
- (d) analysis of the obtained solution and its correction/improvement.

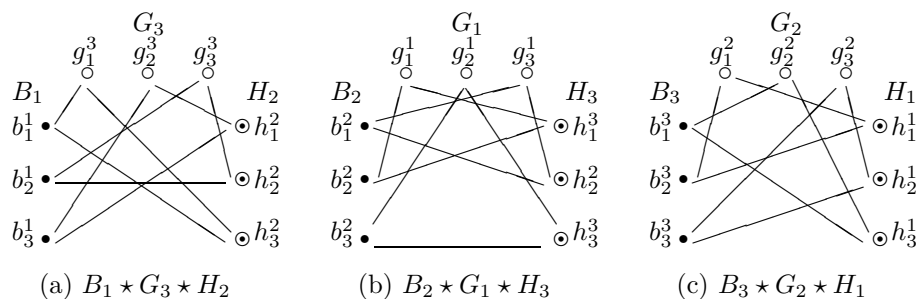


Fig. 4.12. Three-matching for elements

#### 4.3.2. Example of Team Design

The problems of analysis, modeling and design of teams are widely used in many domains (R&D, Start-Up companies, manufacturing, education, etc.). Some basic types of teams are briefly described in Table 4.4.

**Table 4.4.** Types of teams

| No. | Type  | Purpose(s)  | Domain(s)   | Source(s)     |
|-----|---|---|---|---------------|
| 1.  | R&D project team                                | Accomplishment of specific task   | R&D   | [204]         |
| 2.  | Multi-functional/<br>multi-disciplinary<br>team | Forming of multi-functional/<br>multi-disciplinary task(s)<br>(system life cycle) | R&D, design,<br>manufacturing,<br>logistics, marketing,<br>investment, etc. | [121,651]     |
| 3.  | Formal work group                               | To deliver a product or service   | R&D, design,<br>manufacturing,<br>logistics, etc.                           | [559]         |
| 4.  | Global virtual<br>teams                         | Forming and management of<br>distributed team(s)                                  | Integrated<br>distributed<br>technologies                                   | [403,497]     |
| 5.  | Informal group<br>(e.g., friends)               | To collect and pass on business<br>information                                    | Business  |               |
| 6.  | Community of<br>practice<br>(group of experts)  | Building and sharing/exchange<br>of knowledge, coordination                       | Professional<br>networks,<br>organizations                                  | [371,478,612] |
| 7.  | Start-Up team                                   | Design of new product/service   | Innovation  | [392]         |
| 8.  | Student team                                    | Joint educational work,<br>joint research project                                 | Education   | this paper    |
| 9.  | Professors/lecturers<br>teams                   | Design of/participation in<br>new educational program                             | Education   |               |

Some additional description for two special types of teams are:

(a) “communities of practice” are the groups of experts in applied domains (with interaction, exchange of knowledge and experience, etc.),

(b) global virtual (distributed) teams involves four major elements: (i) virtual team structure, (ii) strategic objectives, (iii) work characteristics, (iv) situational constraints [497].

The discipline of teams [322] contains several basic research problems, for example:

- (1) design of teams (e.g., structure, elements) (e.g., [392,403,497]),
- (2) selection/forming of multi-functional teams (e.g., [392,651]),
- (3) analysis of relationships between team design and team performance (e.g., [559]).
- (4) modeling of teams evolution and forecasting (e.g., [392]).

**Example 4.3.** A simplified numerical example for designing a multi-student teams for joint laboratory/project works is described. General solving framework consists of seven stages (Fig. 4.13):

- Stage 1.* Preliminary data analysis (expert judgment).  
*Stage 2.* Analysis and generation/processing of criteria (expert judgment, databases).  
*Stage 3.* Assessment of objects upon criteria, processing of estimates (expert judgment, computing).  
*Stage 4.* Grouping/classification of initial object set to obtain object subset for each type (filtering, classification/sorting).  
*Stage 5.* Evaluation of relationship between object pairs (e.g., “friendship”/compatibility) (expert judgment, databases).  
*Stage 6.* Design of object configurations (special composite structures) (e.g., morphological clique problem).  
*Stage 7.* Analysis of results.

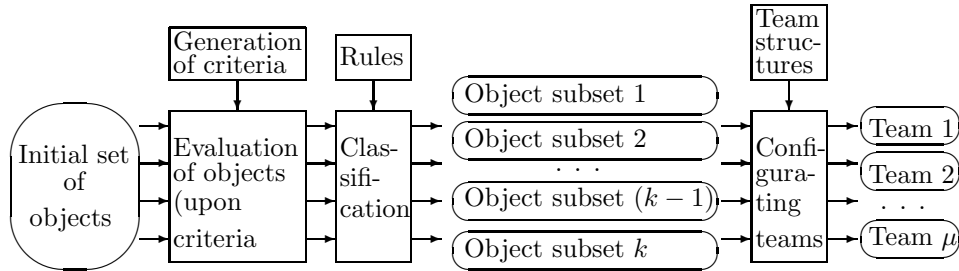


Fig. 4.13. Solving framework

Here example for 14 students (from Table 2.2) is considered: Table 4.5. The considered basic set of criteria (educational disciplines) is the following (ordinal scale [3, 4, 5], 5 corresponds to the best level): (1) mathematics  $C_1$ , (2) physics  $C_2$ , (3) computer systems  $C_3$ , (4) software engineering  $C_4$ , (5) antenna devices  $C_5$ , (6) signal processing  $C_6$ , (7) receiver and sender systems  $C_7$ , (8) information transmission  $C_8$ , (9) measurement in radio engineering  $C_9$ , (10) control systems  $C_{10}$ .

The following student types are examined (by professional inclination/skill):

- (1) formal methods ( $O_1$ ), support disciplines by criteria:  $C_1, C_5, C_6, C_8, C_{10}$ ;
- (2) physical processes ( $O_2$ ), support disciplines by criteria:  $C_2, C_9$ ;
- (3) system design ( $O_3$ ), support disciplines by criteria:  $C_3, C_6, C_8, C_{10}$ ;
- (4) software development ( $O_4$ ), support disciplines by criteria:  $C_3, C_4$ ;
- (5) simulation ( $O_5$ ), support disciplines by criteria:  $C_1, C_3, C_4$ ;
- (6) signal processing ( $O_6$ ), support disciplines by criteria:  $C_1, C_3, C_4, C_8, C_9$ ;
- (7) data transmission ( $O_7$ ), support disciplines by criteria:  $C_1, C_2, C_3, C_5, C_6, C_7, C_8$ .

Thus, it is necessary to transform initial estimates of students upon basic set of criteria (i.e.,  $C_1, \dots, C_5$ ) into estimates by inclination (i.e.,  $O_1, O_2, O_3, O_4$ ) with selection of “domain leader”/“quasi-domain leader” for each inclination type (i.e., by some rule(s), multicriteria ranking/sorting problem, expert judgment) (Table 4.6). Here, 1 corresponds to level of “domain leader”, 2 corresponds to level of “quasi-domain leader”.

In the example, the problem purpose is to form the following laboratory/project student teams (joint laboratory works, student joint projects):

- (1) monitoring system project  $T_1$ , support professional skills (as team structure):  $T_1 = O_1 \star O_3 \star O_4 \star O_5 \star O_7$ ;
- (2) medical systems (measurement and analysis)  $T_2$ , support professional skills (as team structure):  $T_2 = O_1 \star O_3 \star O_4 \star O_6$ ;



(3) GIS and seismic modeling  $T_3$ , support professional skills (as team structure):  $T_3 = O_1 \star O_2 \star O_3 \star O_4 \star O_5 \star O_6$ .

Ordinal estimates of student friendship is presented in Table 4.7 (expert judgment, ordinal scale  $[0, 1, 2, 3]$  is used, 3) corresponds to the best friendship).

The design process is based on morphological clique problem while taking into account ordinal quality of elements (Table 4.6) and elements compatibility (Table 4.7). Structures for configuration design of team  $T_1$ , team  $T_2$ , team  $T_3$  are depicted in Fig. 4.14, in Fig. 4.15, and in Fig. 4.16.

It is assumed that each student team consists of 2, 3, or 4 students. “Domain leader(s)” or “quasi-domain leader(s)” have to be contained into each team. In educational process, elements which are not “domain leaders”/“quasi-domain leaders” have to be added into some some student teams (composite solutions). Numerical examples of composite solutions are:

(a) for  $T_1$  (Fig. 4.14):

$$T_1^1 = A_6 \star A_9 \star A_2 \star A_{11}, T_1^2 = A_6 \star A_9 \star A_2 \star A_{11}, T_1^3 = A_6 \star A_9 \star A_2, T_1^4 = A_6 \star A_9 \star A_2;$$

(b) for  $T_2$  (Fig. 4.15):

$$T_2^1 = A_6 \star A_9 \star A_2 \star A_{11}, T_2^2 = A_6 \star A_9 \star A_2 \star A_{11}, T_2^3 = A_6 \star A_9 \star A_2, T_2^4 = A_6 \star A_9 \star A_2;$$

(c) for  $T_3$  (Fig. 4.16):

$$T_3^1 = A_6 \star A_9 \star A_2 \star A_{11}, T_3^2 = A_6 \star A_9 \star A_2 \star A_{11}, T_3^3 = A_6 \star A_9 \star A_2, T_3^4 = A_6 \star A_9 \star A_2.$$

**Table 4.5.** Students, estimates upon criteria

| Item (student) | $C_1$ | $C_2$ | $C_3$ | $C_4$ | $C_5$ | $C_6$ | $C_7$ | $C_8$ | $C_9$ | $C_{10}$ |
|----------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|----------|
| Student 1      | 3     | 3     | 4     | 4     | 4     | 4     | 5     | 5     | 5     | 4        |
| Student 2      | 3     | 3     | 3     | 3     | 3     | 4     | 4     | 3     | 4     | 3        |
| Student 3      | 4     | 4     | 4     | 4     | 4     | 4     | 4     | 4     | 4     | 4        |
| Student 4      | 5     | 5     | 4     | 4     | 4     | 4     | 4     | 5     | 3     | 4        |
| Student 5      | 3     | 3     | 3     | 4     | 3     | 4     | 4     | 3     | 4     | 3        |
| Student 6      | 5     | 4     | 5     | 4     | 5     | 5     | 5     | 5     | 5     | 4        |
| Student 7      | 3     | 3     | 3     | 4     | 3     | 4     | 4     | 3     | 4     | 3        |
| Student 8      | 4     | 4     | 4     | 4     | 3     | 4     | 4     | 4     | 5     | 4        |
| Student 9      | 5     | 5     | 5     | 5     | 5     | 5     | 5     | 5     | 5     | 5        |
| Student 10     | 5     | 5     | 5     | 4     | 5     | 5     | 5     | 5     | 5     | 5        |
| Student 11     | 3     | 3     | 3     | 3     | 3     | 3     | 4     | 3     | 5     | 3        |
| Student 12     | 3     | 4     | 4     | 4     | 4     | 4     | 4     | 4     | 5     | 4        |
| Student 13     | 5     | 5     | 5     | 5     | 5     | 4     | 4     | 5     | 4     | 5        |
| Student 14     | 3     | 4     | 4     | 4     | 4     | 4     | 4     | 4     | 4     | 4        |

**Table 4.6.** Students, evaluation by inclination types

| Item (student) | $O_1$ | $O_2$ | $O_3$ | $O_4$ | $O_5$ | $O_6$ | $O_7$ |
|----------------|-------|-------|-------|-------|-------|-------|-------|
| Student 1      |       |       |       | 2     |       |       |       |
| Student 2      |       |       |       |       |       |       |       |
| Student 3      | 2     |       |       |       |       | 2     | 2     |
| Student 4      | 2     | 2     |       |       |       | 2     | 2     |
| Student 5      |       |       |       |       |       |       |       |
| Student 6      | 1     | 2     | 1     | 2     | 2     | 1     | 1     |
| Student 7      |       |       |       |       |       |       |       |
| Student 8      |       | 2     | 2     |       |       | 2     |       |
| Student 9      | 1     | 1     | 1     | 1     | 1     | 1     | 1     |
| Student 10     | 1     | 1     | 1     | 2     | 2     | 1     | 1     |
| Student 11     |       |       |       |       |       |       |       |
| Student 12     |       | 2     | 2     | 2     |       |       |       |
| Student 13     | 1     | 2     | 1     | 1     | 1     | 1     | 2     |
| Student 14     |       |       |       | 2     |       |       |       |

**Table 4.7.** Ordinal estimates of student friendship (compatibility)

| Discipline | $A_2$ | $A_3$ | $A_4$ | $A_5$ | $A_6$ | $A_7$ | $A_8$ | $A_9$ | $A_{10}$ | $A_{11}$ | $A_{12}$ | $A_{13}$ | $A_{14}$ |
|------------|-------|-------|-------|-------|-------|-------|-------|-------|----------|----------|----------|----------|----------|
| $A_1$      | 0     | 3     | 1     | 3     | 3     | 1     | 1     | 2     | 2        | 3        | 3        | 1        | 1        |
| $A_2$      |       | 1     | 2     | 1     | 2     | 3     | 2     | 1     | 1        | 1        | 2        | 1        | 2        |
| $A_3$      |       |       | 3     | 3     | 3     | 1     | 1     | 2     | 3        | 3        | 3        | 1        | 1        |
| $A_4$      |       |       |       | 2     | 3     | 1     | 1     | 2     | 1        | 3        | 3        | 0        | 2        |
| $A_5$      |       |       |       |       | 3     | 1     | 1     | 3     | 2        | 2        | 3        | 1        | 0        |
| $A_6$      |       |       |       |       |       | 0     | 0     | 1     | 0        | 3        | 3        | 1        | 1        |
| $A_7$      |       |       |       |       |       |       | 3     | 2     | 3        | 1        | 2        | 1        | 2        |
| $A_8$      |       |       |       |       |       |       |       | 3     | 3        | 1        | 2        | 1        | 0        |
| $A_9$      |       |       |       |       |       |       |       |       | 3        | 2        | 3        | 2        | 1        |
| $A_{10}$   |       |       |       |       |       |       |       |       |          | 3        | 3        | 2        | 0        |
| $A_{11}$   |       |       |       |       |       |       |       |       |          |          | 3        | 2        | 2        |
| $A_{12}$   |       |       |       |       |       |       |       |       |          |          |          | 2        | 2        |
| $A_{13}$   |       |       |       |       |       |       |       |       |          |          |          |          | 2        |

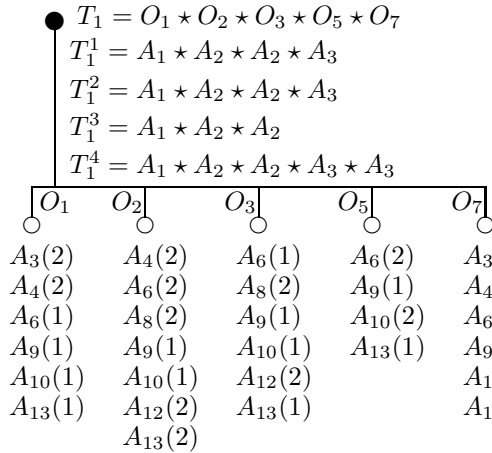


Fig. 4.14. 5-component team  $T_1$

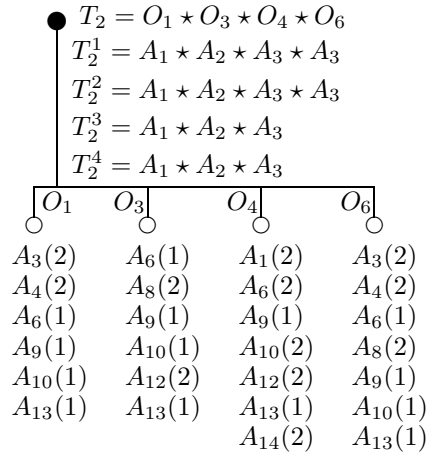


Fig. 4.15. 4-component team  $T_2$

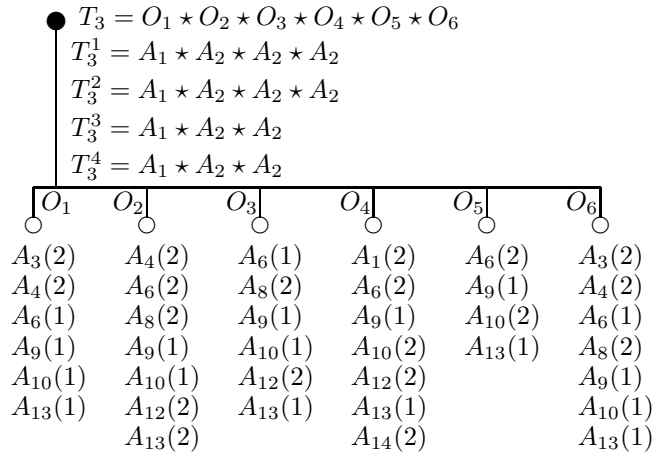


Fig. 4.16. 6-component team  $T_3$

Note, the system problem to design a trajectory of composite teams (or multistage team design) is very prospective one [392].

### 4.3.3. Analysis of Network

Multi-type clustering strategy can be applied for analysis in networks. The types of networks nodes can be obtained by analysis of their connections (the number and types of neighbors): (a) multi-connected nodes (type 1), (b) connected nodes (type 2), (c) outliers (type 3), (d) isolated nodes (type 4).

Let  $G = (A, E)$  be the examined network (graph), where  $A = \{A_1, \dots, A_i, \dots, A_n\}$  is the set of nodes,  $E$  is the set of edges ( $|E| = h$ ). The following clustering scheme can be considered:

*Stage 1.* Building the list of nodes (with info on neighbors)  $O(n)$

*Stage 2.* Selection of multi-neighbor nodes (type 1) (complexity estimate equals  $O(n)$ ). Result: subset  $B_1 \subset A$ .

*Stage 3.* Selection of outlier nodes (i.e., leaves, type 3) (complexity estimate equals  $O(n)$ ). Result: subset  $B_3 \subset \{A \setminus B_1\}$ .

*Stage 4.* Selection of other nodes (type 2) (complexity estimate equals  $O(n)$ ). Result: subset  $B_2 \subset A$ ,  $B_2 = \{A \setminus \{B_1 \cup B_3\}\}$ .

*Stage 5.* Clustering of multi-neighbor nodes  $B_1$  (complexity estimate equals about  $O(|B_1|^2)$  (about  $O((n/3)^2)$ ). Thus, a preliminary clustering solution is:  $\hat{X}^1 = \{X_1^1, \dots, X_l^1, \dots, X_{q_1}^1\}$ . Now, a macro-network can be built:  $G^1 = (\hat{X}^1, E^1)$ , where  $\hat{X}^1$  is the node set that corresponds to the obtained clustering solution (i.e., set of clusters),  $E^1$  is a built set of edges. (Note, the obtained clusters can be used as centroids in k-means clustering at the next step(s)).

*Stage 6.* Clustering of nodes of type 2, i.e., set  $B_2$  (if needed). The corresponding clustering solution is:  $\hat{X}^2 = \{X_1^2, \dots, X_l^2, \dots, X_{q_2}^2\}$ . Now, a macro-network can be built:  $G^2 = (\hat{X}^2, E^2)$ , where  $\hat{X}^2$  is the node set that corresponds to the obtained clustering solution (i.e., set of clusters),  $E^2$  is a built set of edges.

*Stage 7.* Matching of two graphs  $G^1 = (\hat{X}^1, E^1)$  and  $G^2 = (\hat{X}^2, E^2)$ . The matching process can be based on edges from initial network or on the usage of additional parameters (e.g., node coordinates). As a result, integrated clustering solution can be obtained  $\hat{X}^{12} = \{X_1^{12}, \dots, X_l^{12}, \dots, X_{q_{12}}^{12}\}$ .

*Stage 8.* Joining outliers ( $B_3$ ) to clusters of solution  $\hat{X}^{12}$ . As a result, integrated clustering solution can be obtained  $\hat{X}^{123}$ .

#### 4.4. Scheduling in multi-beam antenna communication system

There are the following initial information (Fig. 4.17):

- (a) multi-beam antenna system,
- (b) number of antenna beams:  $\mu$ ,
- (c) set of communication nodes  $A = \{A_1, \dots, A_i, \dots, A_n\}$ ,
- (d) volume of transmitted data is about the same for each  $A_i$ .

The problem is:

Design a schedule for connection of antenna system to communication nodes while taking into account the following: (i) minimization of total connection time, (ii) providing the best communication quality (by the minimum interference between neighbor (by angle) connections, i.e.,

$$\max_{i \in A} \min_{i_1, i_2 \in A} D^{angular}(A_{i_1}, A_{i_2}),$$

where  $D^{angular}(A_{i_1}, A_{i_2})$  is angular separation  $D^{angular}(A_{i_1}, A_{i_2})$  (section 2.2.4) (or angle between beams to the nodes).

The solving scheme is the following:

*Stage 1.* Linear ordering of communication nodes by their angle (Fig. 4.17, node 1 is the 1st).

*Stage 2.* Dividing of the obtain list of nodes into  $\mu$  equal by size groups (the last group can have less elements) and numeration as follows:

group 1:  $\{(1, 1), (1, 2), \dots, (1, k)\}$ ,

group 2:  $\{(2, 1), (2, 2), \dots, (2, k)\}$ ,

...

group  $\mu$ :  $\{(\mu, 1), (\mu, 2), \dots, (\mu, k)\}$ .

Here  $k = \lceil \frac{n}{\mu} \rceil$ .

*Stage 3.* Generation of scheduling by the rules: Slot  $j$  ( $j = \overline{1, k}$ ): the  $j$ -th element from each group ( $\zeta = 1, 2, \dots, \mu$ ), i.e., elements  $\{\zeta, j\}$  (Fig. 4.17).

*Stage 4.* Stop.

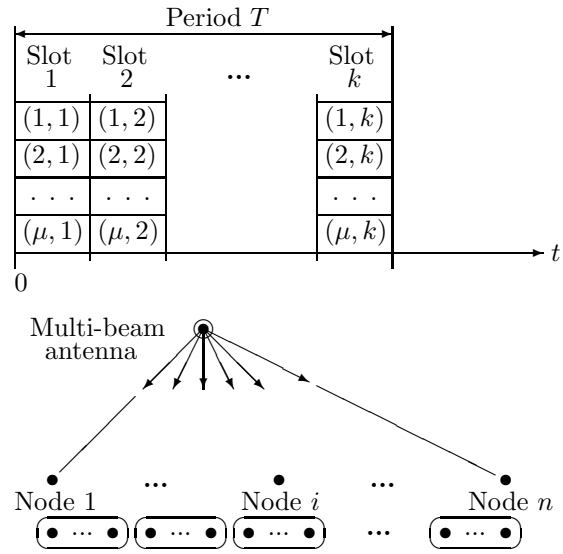


Fig. 4.17. Multi-beam antenna system

## 5. Conclusions

The paper addresses combinatorial modular viewpoints to clustering problems and procedures: (a) generalized modular clustering frameworks (i.e., typical combinatorial engineering frameworks); (b) main structural clustering models/methods (e.g., hierarchical clustering, minimum spanning tree based clustering, clustering as assignment, detection of clique/quasi-clique based clustering, correlation clustering, network communities based clustering); (c) main ideas for fast clustering schemes. Described problem solving frameworks are based on compositions of well-known combinatorial optimization problems and corresponding algorithms (e.g., assignment, partitioning, assignment, knapsack problem, multiple choice problem, morphological clique problem, searching for consensus/median for structures).

A set of numerical examples illustrate all stages of clustering processes (problem statement, assessment and evaluation, design of solving algorithms/schemes, analysis of results).

Future research directions can involve the following:

1. analysis and design of new composite problems and modular solving frameworks;
2. design of special decision support tools (modular solving environments) for structural clustering problems;
3. special study of dynamic structural clustering problems and very large applications;
4. applications of structural clustering problems in networking (design, covering, routing, etc.); and
5. application of the structural clustering problems in education and in educational data mining.

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