Grouping Games

Finding Clusters in Graphs, Digraphs and Hypergraphs

Marcello Pelillo European Centre for Living Technology Ca' Foscari University, Venice



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The "Classical" Clustering Problem

Given:

✓ a set of *n* "objects"

- k =an edge-weighted graph G
- ✓ an $n \times n$ matrix A of pairwise similarities

Goal: <u>*Partition*</u> the vertices of the *G* into maximally homogeneous groups (i.e., clusters).

Usual assumption: *symmetric* and *pairwise* similarities (*G* is an undirected graph)





Applications

Clustering problems abound in many areas of computer science and engineering.

A short list of applications domains:

Image processing and computer vision Computational biology and bioinformatics Information retrieval Document analysis Medical image analysis Data mining Signal processing

For a review see, e.g., A. K. Jain, "Data clustering: 50 years beyond K-means," *Pattern Recognition Letters* 31(8):651-666, 2010.



What is a Cluster?

No universally accepted (formal) definition of a "cluster" but, informally, a cluster should satisfy two criteria:

- Internal criterion: all "objects" *inside* a cluster should be highly similar to each other
- **External criterion**: all "objects" *outside* a cluster should be highly dissimilar to the ones inside





The Notion of "Gestalt"

«In most visual fields the contents of particular areas "belong together" as circumscribed units from which their surrounding are excluded.»

W. Köhler, Gestalt Psychology (1947)

«In gestalt theory the word "Gestalt" means any segregated whole.»







A Special Case: Binary Symmetric Similarities

Suppose the similarity matrix is a binary (0/1) matrix.

Given an unweighted undirected graph G=(V,E):



A *clique* is a subset of mutually adjacent vertices A *maximal clique* is a clique that is not contained in a larger one

In the 0/1 case, a meaningful (though strict) notion of a cluster is that of a *maximal clique* (Luce & Perry, 1949).



Advantages of the New Approach

- ✓ No need to know the number of clusters in advance (since we extract them sequentially)
- Leaves clutter elements unassigned (useful, e.g., in figure/ground separation or one-class clustering problems)
- ✓ Allows extracting overlapping clusters
- ✓ Works with asymmetric/negative/high-order similarities

Need a partition?

```
Partition_into_clusters(V,A)
repeat
Extract_a_cluster
remove it from V
until all vertices have been clustered
```



What is Game Theory?



"The central problem of game theory was posed by von Neumann as early as 1926 in Göttingen. It is the following: If *n* players, $P_1, ..., P_n$, play a given game Γ , how must the *i*th player, P_i , play to achieve the most favorable result for himself?"

> Harold W. Kuhn Lectures on the Theory of Games (1953)

A few cornerstones in game theory

- **1921–1928:** Emile Borel and John von Neumann give the first modern formulation of a mixed strategy along with the idea of finding minimax solutions of normal-form games.
- **1944, 1947:** John von Neumann and Oskar Morgenstern publish *Theory of Games and Economic Behavior*.
- **1950–1953:** In four papers John Nash made seminal contributions to both non-cooperative game theory and to bargaining theory.
- **1972–1982:** John Maynard Smith applies game theory to biological problems thereby founding "evolutionary game theory."

late 1990's -: Development of algorithmic game theory...



"Solving" a Game





Basics of (Two-Player, Symmetric) Game Theory

Assume:

- a (symmetric) game between two players
- complete knowledge
- a pre-existing set of **pure strategies** (actions) $O = \{o_1, ..., o_n\}$ available to the players.

Each player receives a payoff depending on the strategies selected by him and by the adversary. Players' goal is to maximize their own returns.

A mixed strategy is a probability distribution $\mathbf{x} = (x_1, \dots, x_n)^T$ over the strategies.

$$\Delta = \left\{ x \in \mathbb{R}^n : \forall i = 1...n : x_i \ge 0, \text{ and } \sum_{i=1}^n x_i = 1 \right\}$$

×3



Nash Equilibria

- Let A be an arbitrary **payoff** matrix: a_{ij} is the payoff obtained by playing i while the opponent plays j.
- ✓ The average payoff obtained by playing mixed strategy y while the opponent plays x, is:

$$\mathbf{y}'\mathbf{A}\mathbf{x} = \sum_{i} \sum_{j} a_{ij} y_{i} x_{j}$$

 \checkmark A mixed strategy **x** is a (symmetric) **Nash equilibrium** if

$\mathbf{x}'\mathbf{A}\mathbf{x} \ge \mathbf{y}'\mathbf{A}\mathbf{x}$

for all strategies **y**. (Best reply to itself.)

Theorem (Nash, 1951). Every finite normal-form game admits a mixed-strategy Nash equilibrium.



Evolution and the Theory of Games

"We repeat most emphatically that our theory is thoroughly static. A dynamic theory would unquestionably be more complete and therefore preferable.

But there is ample evidence from other branches of science that it is futile to try to build one as long as the static side is not thoroughly understood."

John von Neumann and Oskar Morgenstern Theory of Games and Economic Behavior (1944)





"Paradoxically, it has turned out that game theory is more readily applied to biology than to the field of economic behaviour for which it was originally designed."

> John Maynard Smith Evolution and the Theory of Games (1982)



Evolutionary Games and ESS's

Assumptions:

- ✓ A large population of individuals belonging to the same species which compete for a particular limited resource
- This kind of conflict is modeled as a symmetric two-player game, the players being pairs of randomly selected population members
- Players do not behave "rationally" but act according to a preprogrammed behavioral pattern (pure strategy)
- Reproduction is assumed to be asexual
- Utility is measured in terms of Darwinian fitness, or reproductive success

A Nash equilibrium **x** is an *Evolutionary Stable Strategy* (ESS) if, for all strategies y:

$$\mathbf{y}' A \mathbf{x} = \mathbf{x}' A \mathbf{x} \quad \Rightarrow \quad \mathbf{x}' A \mathbf{y} > \mathbf{y}' A \mathbf{y}$$



ESS's as Clusters

We claim that ESS's abstract well the main characteristics of a cluster:

- Internal coherency: High mutual support of all elements within the group.
- External incoherency: Low support from elements of the group to elements outside the group.



Basic Definitions

Let $S \subseteq V$ be a non-empty subset of vertices, and $i \in S$.

The (average) weighted degree of *i* w.r.t. *S* is defined as:

$$\operatorname{awdeg}_{S}(i) = \frac{1}{|S|} \sum_{j \in S} a_{ij}$$

Moreover, if $j \notin S$, we define:

$$\phi_{S}(i,j) = a_{ij} - \operatorname{awdeg}_{S}(i)$$



Intuitively, $\phi_{s}(i,j)$ measures the similarity between vertices *j* and *i*, with respect to the (average) similarity between vertex *i* and its neighbors in *S*.



Assigning Weights to Vertices

Let $S \subseteq V$ be a non-empty subset of vertices, and $i \in S$.

The **weight** of *i* w.r.t. *S* is defined as:

$$w_{S}(i) = \begin{cases} 1 & \text{if } |S| = 1\\ \sum_{j \in S - \{i\}} \phi_{S - \{i\}}(j, i) w_{S - \{i\}}(j) & \text{otherwise} \end{cases}$$

Further, the **total weight** of *S* is defined as:

$$W(S) = \sum_{i \in S} w_S(i)$$





Interpretation

Intuitively, $w_S(i)$ gives us a measure of the overall (relative) similarity between vertex *i* and the vertices of S-{*i*} with respect to the overall similarity among the vertices in S-{*i*}.



 $w_{\{1,2,3,4\}}(1) < 0$



 $w_{\{1,2,3,4\}}(1) > 0$



Dominant Sets

Definition (Pavan and Pelillo, 2003, 2007). A non-empty subset of vertices $S \subseteq V$ such that W(T) > 0 for any non-empty $T \subseteq S$, is said to be a **dominant set** if:

- 1. $w_{S}(i) > 0$, for all $i \in S$ (internal homogeneity)
- 2. $w_{S \cup \{i\}}(i) < 0$, for all $i \notin S$ (external homogeneity)



The set {1,2,3} is dominant.

Dominant sets \equiv clusters



The Clustering Game

Consider the following "clustering game."

- Assume a preexisting set of objects O and a (possibly asymmetric) matrix of affinities A between the elements of O.
- ✓ Two players play by simultaneously selecting an element of *O*.
- ✓ After both have shown their choice, each player receives a payoff proportional to the affinity that the chosen element has wrt the element chosen by the opponent.

Clearly, it is in each player's interest to pick an element that is strongly supported by the elements that the adversary is likely to choose.

Hence, in the (pairwise) clustering game:

- ✓ There are 2 players (because we have <u>pairwise</u> affinities)
- The objects to be clustered are the pure strategies
- ✓ The (null-diagonal) affinity matrix coincides with the similarity matrix



Dominant Sets are ESS's

Theorem (Torsello, Rota Bulò and Pelillo, 2006). Evolutionary stable strategies of the clustering game with affinity matrix *A* are in a one-to-one correspondence with dominant sets.

Note. Generalization of well-known Motzkin-Straus theorem from graph theory (1965).

Dominant-set clustering

- ✓ To get a single dominant-set cluster use, e.g., replicator dynamics (but see Rota Bulò, Pelillo and Bomze, CVIU 2011, for faster dynamics)
- ✓ To get a partition use a simple *peel-off* strategy: iteratively find a dominant set and remove it from the graph, until all vertices have been clustered
- To get overlapping clusters, enumerate dominant sets (see Bomze, 1992; Torsello, Rota Bulò and Pelillo, 2008)



Special Case: Symmetric Affinities

Given a symmetric real-valued matrix *A* (with null diagonal), consider the following Standard Quadratic Programming problem (StQP):

maximize $f(x) = x^T A x$ subject to $x \in \Delta$

Note. The function f(x) provides a measure of cohesiveness of a cluster (see Pavan and Pelillo, 2003, 2007; Sarkar and Boyer, 1998; Perona and Freeman, 1998).

ESS's are in one-to-one correspondence to (strict) local solutions of StQP

Note. In the 0/1 (symmetric) case, ESS's are in one-to-one correspondence to (strictly) **maximal cliques** (Motzkin-Straus theorem).



Replicator Dynamics

Let $x_i(t)$ the population share playing pure strategy *i* at *time t*. The **state** of the population at time *t* is: $x(t) = (x_1(t), \dots, x_n(t)) \in \Delta$.

Replicator dynamics (Taylor and Jonker, 1978) are motivated by Darwin's principle of natural selection:

$$\frac{\dot{x}_i}{x_i} \propto \text{payoff of pure strategy i} - \text{average population payoff}$$

which yields:

$$\dot{x}_i = x_i \Big[(Ax)_i - x^T Ax \Big]$$

Theorem (Nachbar, 1990; Taylor and Jonker, 1978). A point $x \in \Delta$ is a Nash equilibrium if and only if x is the limit point of a replicator dynamics trajectory starting from the interior of Δ .

Furthermore, if $x \in \Delta$ is an ESS, then it is an asymptotically stable equilibrium point for the replicator dynamics.



Doubly Symmetric Games

In a doubly symmetric (or partnership) game, the payoff matrix A is symmetric ($A = A^{T}$).

Fundamental Theorem of Natural Selection (Losert and Akin, 1983).

For any doubly symmetric game, the average population payoff $f(x) = x^{T}Ax$ is strictly increasing along any non-constant trajectory of replicator dynamics, namely, $d/dtf(x(t)) \ge 0$ for all $t \ge 0$, with equality if and only if x(t) is a stationary point.

Characterization of ESS's (Hofbauer and Sigmund, 1988)

For any doubly simmetric game with payoff matrix *A*, the following statements are equivalent:

a) $x \in \Delta^{ESS}$

- b) $x \in \Delta$ is a strict local maximizer of $f(x) = x^T A x$ over the standard simplex Δ
- c) $x \in \Delta$ is asymptotically stable in the replicator dynamics



Discrete-time Replicator Dynamics

A well-known discretization of replicator dynamics, which assumes nonoverlapping generations, is the following (assuming a non-negative *A*):

$$x_i(t+1) = x_i(t) \frac{A(x(t))_i}{x(t)^T A x(t)}$$

which inherits most of the dynamical properties of its continuous-time counterpart (e.g., the fundamental theorem of natural selection).

MATLAB implementation

distance=inf;
while distance>epsilon
old_x=x;
x = x.*(A*x);
x = x./sum(x);
distance=pdist([x,old_x]');
end



Measuring the Degree of Cluster Membership

The components of the converged vector give us a measure of the participation of the corresponding vertices in the cluster, while the value of the objective function provides of the cohesiveness of the cluster.





Application to Image Segmentation

An image is represented as an edge-weighted undirected graph, where vertices correspond to individual pixels and edge-weights reflect the "similarity" between pairs of vertices.

For the sake of comparison, in the experiments we used the same similarities used in Shi and Malik's normalized-cut paper (PAMI 2000).

To find a hard partition, the following *peel-off* strategy was used:

```
Partition_into_dominant_sets(G)
Repeat
   find a dominant set
   remove it from graph
until all vertices have been clustered
```

To find a single dominant set we used replicator dynamics (but see Rota Bulò, Pelillo and Bomze, *CVIU 2011*, for faster game dynamics).



Experimental Setup

The similarity between pixels i and j was measured by:

$$w(i,j) = \exp\left(\frac{-\|\mathbf{F}(i) - \mathbf{F}(j)\|_2^2}{\sigma^2}\right)$$

where σ is a positive real number which affects the decreasing rate of w, and:

- $\mathbf{F}(i) \equiv$ (normalized) intensity of pixel *i*, for intensity segmentation
- $\mathbf{F}(i) = [v, vs \sin(h), vs \cos(h)](i)$, where h, s, v are the HSV values of pixel *i*, for color segmentation
- $\mathbf{F}(i) = [|I * f_1|, \dots, |I * f_k|](i)$ is a vector based on texture information at pixel *i*, the f_i being DOOG filters at various scales and orientations, for texture segmentation



Intensity Segmentation Results





Dominant sets



Ncut



Intensity Segmentation Results





Dominant sets







Results on the Berkeley Dataset

Dominant sets

Ncut





GCE = 0.05, LCE = 0.04



GCE = 0.08, LCE = 0.05







GCE = 0.36, LCE = 0.27





GCE = 0.09, LCE = 0.08



GCE = 0.31, LCE = 0.22



Color Segmentation Results





Original image





Dominant sets





Ncut



Results on the Berkeley Dataset

Dominant sets

Ncut





GCE = 0.12, LCE = 0.12



GCE = 0.19, LCE = 0.13







GCE = 0.35, LCE = 0.29



GCE = 0.16, LCE = 0.16





GCE = 0.09, LCE = 0.09



Texture Segmentation Results



Dominant sets



Texture Segmentation Results



NCut



Other Applications of Dominant-Set Clustering

Bioinformatics

Identification of protein binding sites (*Zauhar and Bruist*, 2005) Clustering gene expression profiles (*Li et al*, 2005) Tag Single Nucleotide Polymorphism (SNPs) selection (*Frommlet*, 2010)

Security and video surveillance

Detection of anomalous activities in video streams (*Hamid et al.*, CVPR'05; Al'09) Detection of malicious activities in the internet (*Pouget et al.*, J. Inf. Ass. Sec. 2006) Detection of F-formations (Hung and Kröse, 2011)

Content-based image retrieval

Wang et al. (Sig. Proc. 2008); Giacinto and Roli (2007)

Analysis of fMRI data

Neumann et al (NeuroImage 2006); Muller et al (J. Mag Res Imag. 2007)

Video analysis, object tracking, human action recognition

Torsello et al. (EMMCVPR'05); Gualdi et al. (IWVS'08); Wei et al. (ICIP'07)

Feature selection

Hancock et al. (GbR'11; ICIAP'11; SIMBAD'11)

Image matching and registration

Torsello et al. (IJCV 2011, ICCV'09, CVPR'10, ECCV'10)



Extensions


Capturing Elongated Structures / 1







Capturing Elongated Structures / 2





Path-Based Distances (PDB's)

Path-based measure: Given a distance (dissimilarity) matrix **D**, the path-based distance measure between objects i and j is computed by [FB03]

$$\mathbf{D}_{ij}^{\text{path}} = \min_{\mathbf{p}\in\mathcal{P}_{ij}(\mathbf{O})} \left\{ \max_{1 \leq l \leq |\mathbf{p}|} \mathbf{D}_{\mathbf{p}(l)\mathbf{p}(l+1)} \right\},\tag{19}$$

where $\mathcal{P}_{ij}(\mathbf{O})$ is the set of all paths from i to j. Thereby, the effective distance between i and j is the largest gap of the path p^{*}, where p^{*} is the path with minimum largest gap among all admissible paths between i and j.

B. Fischer and J. M. Buhmann. Path-based clustering for grouping of smooth curves and texture segmentation. IEEE Trans. Pattern Anal. Mach. Intell., 25(4):513–518, 2003.



Example: Without PBD (\sigma = 2)



Figura 4.11: Cluster senza chiusura: $\sigma=2$



Example: Without PDB (\sigma = 4)



Figura 4.12: Cluster senza chiusura: $\sigma=4$



Example: Without PDB (\sigma = 8)



Figura 4.13: Cluster senza chiusura: $\sigma=8$



Example: With PDB ($\sigma = 0.5$)



Figura 4.14: Cluster mediante chiusura: $\sigma=0,5$







Finding Overlapping Classes

First idea: run replicator dynamics from different starting points in the simplex.

Problem: computationally expensive and no guarantee to find them all.



Finding Overlapping Classes: Intuition





Building a Hierarchy: A Family of Quadratic Programs

Consider the following family of StQP's:

maximize $f_{\alpha}(\mathbf{x}) = \mathbf{x}'(A - \alpha I)\mathbf{x}$ subject to $\mathbf{x} \in \Delta$

where $\alpha \ge 0$ is a parameter and *I* is the identity matrix.

The objective function f_{α} consists of:

- a data term (x'Ax) which favors solutions with high internal coherency
- a regularization term (-αx'x) which acts as an entropic factor: it is concave and, on the simplex Δ, it is maximized at the barycenter and it attains its minimum value at the vertices of Δ



The effects of *α*











The Landscape of f_{α}

Key observation: For any fixed α , the energy landscape of f_{α} is populated by two kinds of solutions:

- solutions which correspond to dominant sets for the original matrix A
- solutions which do not correspond to any dominant set for the original matrix A, although they are dominant for the scaled matrix A+α(ee' I)

The latter represent large subsets of points that are not sufficiently coherent to be dominant with respect to A, and hence they should be split.



Sketch of the Hierarchical Clustering Algorithm

Basic idea: start with a sufficiently large α and adaptively decrease it during the clustering process:

1) let α be a large positive value (e.g., $\alpha > |V| - 1$)

2) find a partition of the data into α -clusters

3) for all the α -clusters that are not 0-clusters recursively repeat step 2) with decreased α



Dealing with High-Order Similarities

A (weighted) hypergraph is a triplet H = (V, E, w), where

- V is a finite set of vertices
- $E \subseteq 2^{\vee}$ is the set of (hyper-)edges (where 2^{\vee} is the power set of V)
- $w : E \rightarrow R$ is a real-valued function assigning a weight to each edge

We will focus on a particular class of hypergraphs, called **k-graphs**, whose edges have fixed cardinality $k \ge 2$.



A hypergraph where the vertices are flag colors and the hyperedges are flags.



The Hypergraph Clustering Game

Given a weighted k-graph representing an instance of a hypergraph clustering problem, we cast it into a k-player (hypergraph) clustering game where:

- ✓ There are k players
- ✓ The objects to be clustered are the pure strategies
- ✓ The payoff function is proportional to the similarity of the objects/ strategies selected by the players

Definition (ESS-cluster). Given an instance of a hypergraph clustering problem H = (V, E, w), an ESS-cluster of H is an ESS of the corresponding hypergraph clustering game.

As in the k=2 case, ESS-clusters do incorporate both internal and external cluster criteria (see PAMI 2013)



ESS's and Polynomial Optimization

Theorem 3. Let $H = (V, E, \omega)$ be a hypergraph clustering problem, $\Gamma = (P, V, \pi)$ the corresponding clustering game, and $f(\mathbf{x})$ a function defined as

$$f(\mathbf{x}) = u\left(\mathbf{x}^{[k]}\right) = \sum_{e \in E} \omega(e) \prod_{j \in e} x_j.$$
(11)

Nash equilibria of Γ are in one-to-one correspondence with the critical points² of $f(\mathbf{x})$ over Δ , while ESSs of Γ are in one-to-one correspondence with strict local maximizers of $f(\mathbf{x})$ over Δ .



The Baum-Eagon Inequality

Theorem 4 (Baum-Eagon). Let $Q(\mathbf{x})$ be a homogeneous polynomial in the variables x_j with nonnegative coefficients, and let $\mathbf{x} \in \Delta$. Define the mapping $\mathbf{z} = \mathcal{M}(\mathbf{x})$ from Δ to itself as follows:

$$z_j = x_j \frac{\partial Q(\mathbf{x})}{\partial x_j} \Big/ \sum_{\ell=1}^n x_\ell \frac{\partial Q(\mathbf{x})}{\partial x_\ell}, \qquad j = 1, \dots, n.$$
(12)

Then, $Q(\mathcal{M}(\mathbf{x})) > Q(\mathbf{x})$, unless $\mathcal{M}(\mathbf{x}) = \mathbf{x}$.

Theorem 5. A point $\mathbf{x} \in \Delta$ is an ESS-cluster of an instance of a hypergraph clustering problem if and only if it is an asymptotically stable equilibrium point (and, hence, a local attractor) for the nonlinear dynamics (13).



An exampe: Line Clustering







In a nutshell...

The game-theoretic/dominant-set approach:

- makes no assumption on the structure of the affinity matrix, being it able to work with asymmetric and even negative similarity functions
- does not require *a priori* knowledge on the number of clusters (since it extracts them sequentially)
- leaves clutter elements unassigned (useful, e.g., in figure/ground separation or one-class clustering problems)
- ✓ allows principled ways of assigning out-of-sample items (*NIPS'04*)
- ✓ allows extracting overlapping clusters (*ICPR'08*)
- ✓ generalizes naturally to hypergraph clustering problems, i.e., in the presence of high-order affinities, in which case the clustering game is played by more than two players (*PAMI'13*)
- extends to hierarchical clustering (ICCV'03: EMMCVPR'09)
- ✓ allows using multiple affinity matrices using Pareto-Nash notion (SIMBAD'15)





Evolutionary game theory

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- J. Hofbauer and K. Sigmund. *Evolutionary Games and Population Dynamics*. Cambridge University Press (1998).

Dominant sets

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- S. Rota Bulò, M. Pelillo and I. M. Bomze. Graph-based quadratic optimization: A fast evolutionary approach. *CVIU 2011*.



The SIMBAD Project

- ✓ University of Venice (IT), *coordinator*
- ✓ University of York (UK)
- ✓ Technische Universität Delft (NL)
- ✓ Insituto Superior Técnico, Lisbon (PL)
- ✓ University of Verona (IT)
- ✓ ETH Zürich (CH)





The SIMBAD Book

M. Pelillo (Ed.) Similarity-Based Pattern Analysis and Recognition (2013)



