Multidimensional Scaling by Particle Swarm Optimization

Víctor Bazán & Javier Trejos

School of Mathematics – CIMPA
University of Costa Rica

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Outline

Storage of Chemical Products

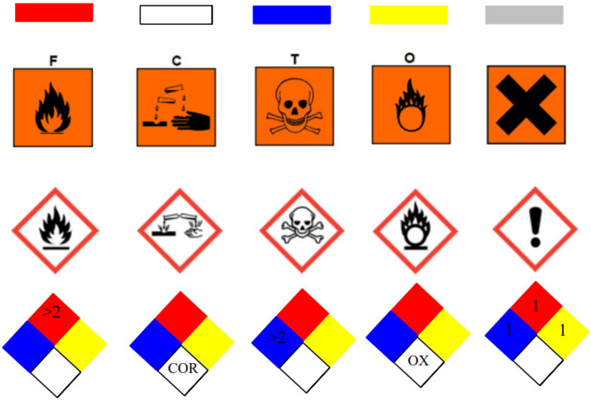
Motivation

Storage of Chemical Products

Restrictions on storage

- Some chemicals cannot be stored together or nearby
- Some have have specific risks, and some have pairwise risks

Flammable Corrosive Toxic Oxidant Other



Storage of Chemical Products

Restrictions on storage

- Restrictions are made by pairs of products
- For instance, at the University of Costa Rica we use the following table of incompatibilty:

green	can be stored together
yellow	check sections 1–7 of the Security Sheet
red	cannot be stored together or nearby

	1A	1B	2	3	4A	4B	5	6A	6B	7A	7B	8A	8B	9	10	11A	11B
1A	green	red	red	red	red	red	red	red	red	red	red	red	red	yellow	yellow	red	green
1B	red	green	red	yellow	red	red	red	red	red	red	red	red	red	yellow	yellow	yellow	red
2	red	red	green	red	red	red	red	red	red	red	red	red	red	yellow	yellow	yellow	yellow
3	red	yellow	red	green	red	red	red	red	red	yellow	yellow	yellow	yellow	yellow	yellow	yellow	yellow
4A	red	red	red	red	yellow	red	red	red	red	red	red	red	red	yellow	yellow	red	yellow
4B	red	red	red	red	red	yellow	red	red	red	red	red	red	red	yellow	yellow	yellow	red
5	red	red	red	red	red	red	yellow	red	red	red	red	red	red	yellow	yellow	yellow	yellow
6A	red	red	red	red	red	yellow	yellow	yellow	red	yellow	red	yellow	red	yellow	yellow	yellow	red
6B	yellow	red	yellow	yellow	yellow	red	yellow	red	yellow	red	yellow	red	yellow	yellow	yellow	red	yellow
7A	red	yellow	yellow	yellow	red	yellow	yellow	yellow	red	green	red	green	red	green	yellow	green	red
7B	red	red	yellow	yellow	yellow	red	yellow	red	yellow	red	green	red	green	green	yellow	red	green
8A	red	yellow	yellow	yellow	red	yellow	yellow	yellow	red	green	red	green	red	green	yellow	green	red
8B	red	red	yellow	yellow	yellow	red	yellow	red	yellow	red	green	red	green	green	yellow	red	green
9	green	yellow	yellow	yellow	yellow	yellow	yellow	yellow	yellow	green	green	green	green	green	yellow	green	green
10	yellow	yellow	yellow	yellow	yellow	yellow	yellow	yellow	yellow	yellow	yellow	yellow	yellow	yellow	yellow	yellow	yellow
11A	red	yellow	yellow	yellow	red	yellow	yellow	yellow	red	green	red	green	red	green	yellow	green	red
11B	green	red	yellow	yellow	yellow	red	yellow	red	yellow	red	green	red	green	green	yellow	red	green

Chemical Organization of Products

- For storage of chemical products, one has to be very careful since there are incompatible products that cannot be stored near
- Without good care, explosions and fire may arise
- We constructed a **dissimilarity matrix**, where $\delta_{ij} = 1$ means that products i and j are incompatible

Chemical Organization of Products

Incompatible Chemicals

Chemical Compatibility Chart

1	Inorganic Acids	1																							
2	Organic acids	X	2																						
3	Caustics	X	X	3																					
4	Amines & Alkanolamines	X	X		4																				
5	Halogenated Compounds	X		X	X	5																			
6	Alcohols, Glycols & Glycol Ethers	X					6																		
7	Aldehydes	X	X	X	X		X	7																	
8	Ketone	X		X	X			X	8																
9	Saturated Hydrocarbons									9															
10	Aromatic Hydrocarbons	X									10														
11	Olefins	X				X						11													
12	Petrolum Oils												12												
13	Esters	X		X	X									13											
14	Monomers & Polymerizable Esters	X	X	X	X	X	X								14										
15	Phenols			X	X			X							X	15									
16	Alkylene Oxides	X	X	X	X		X	X							X	X	16								
17	Cyanohydrins	X	X	X	X	X		X									X	17							
18	Nitriles	X	X	X	X												X		18						
19	Ammonia	X	X					X	X					X	X	X	X	X		19					
20	Halogens			X			X	X	X	X	X	X	X	X	X	X				X	20				
21	Ethers	X													X						X	21			
22	Phosphorus, Elemental	X	X	X																	X		22		
23	Sulfur, Molten									X	X	X	X				X						X	23	
24	Acid Anhydrides	X		X	X		X	X							X		X	X	X	X					24

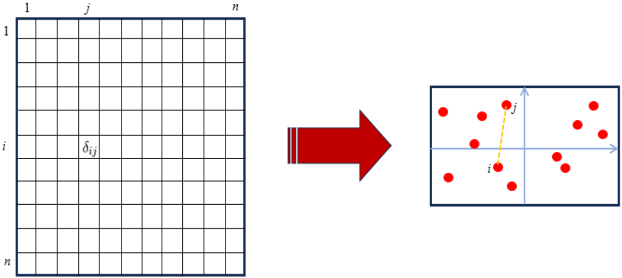
X Represents Unsafe Combinations

Represents Safe Combinations

Source: Utah State University, https://research.usu.edu/ehs/training-and-resources/incompatible-chemicals

Multidimensional Scaling

Multidimensional Scaling (MDS) is a set of dimension reduction data analysis techniques for plotting n points (representing n objects) in a small dimension space, such that distances in that space fit the best the dissimilarities between the n objects.



Multidimensional Scaling

Among the most well-known MDS approaches there are:

- **Classical MDS** (Torgerson): input dissimilarities are supposed Euclidean, there is a matrix decomposition that simplifies computations and there is a closed, unique, solution based on that matrix.
- **Metric MDS**: values of dissimilarities matter for the solutions.
- **Non-metric MDS**: rank of dissimilarities matter, rather than values themselves.
- **Unfolding**: for representation of the n objects in a line (one-dimensional space).
- **INDSCAL**: several dissimilarity tables between the n objects are analysed through a consensus plot.

Metric Multidimensional Scaling

Metric MDS

Input

Let $\Omega = \{1, 2, \ldots, n\}$ be the objects set and δ_{ij} the dissimilarities, w_{ij} are nonnegative weights.
Let p be the space dimension of representation for the n objects.

Output

$\mathbf{X}$ is the $n \times p$ matrix that contains the coordinates of the n points in $\mathbb{R}^p$.
Let $d_{ij}(\mathbf{X}) = d(\mathbf{x}_i, \mathbf{x}_j)$ be the Euclidean distances in $\mathbb{R}^p$.

Goal

We want to fit all $d_{ij}(\mathbf{X})$ to the original δ_{ij}:

$$\delta_{ij} \approx d_{ij}(\mathbf{X})$$

1. Raw Stress:

$$\sigma_r = \sigma_r(\mathbf{X}) = \sum_{i<j} w_{ij}[\delta_{ij} - d_{ij}(\mathbf{X})]^2.$$

2. Normalized Stress:

$$\sigma_1^2 = \sigma_1^2(\mathbf{X}) = \frac{\sum w_{ij}[\delta_{ij} - d_{ij}(\mathbf{X})]^2}{\sum w_{ij}[d_{ij}(\mathbf{X})]^2}.$$

3. Stress-1:

$$\sigma_1 = \sqrt{\sigma_1^2} = \sqrt{\frac{\sum w_{ij}[\delta_{ij} - d_{ij}(\mathbf{X})]^2}{\sum w_{ij}[d_{ij}(\mathbf{X})]^2}}.$$

4. S-Stress:

$$\sigma_{AL} = \sigma_{AL}(\mathbf{X}) = \sum_{i<j} w_{ij}[\delta_{ij}^2 - d_{ij}^2(\mathbf{X})]^2.$$

Issue: σ_1 in non convex and there is no closed solution for metric MDS when minimizing σ_1, therefore heuristic (iterative) approaches are needed; for instance:

- Gradient descent (Kruskal, 1964)
- SMACOF (De Leeuw, 1977; Groenen, 1993): based on a decomposition of σ_1^2 and the majorization optimization method (an easy to optimize function majorizes σ_1, and iterations are made, refining the solution)
- Tunneling (Groenen & Heiser, 1991)
- Distance smoothing (Pliner, 1996; Groenen, 1999)
- Optimization metaheuristics
  - Genetic algorithms (Mathar, 1997)
  - Simulated annealing (Trejos & Villalobos, 1999)
  - Tabu search (Villalobos & Trejos, 2000)

Particle Swarm Optimization

Particle Swarm Optimization (PSO) is a population-based optimization metaheuristic based on handling solutions in a numeric multidimensional space.

- It handles a population of solutions (called *particles*): feasible states of the problem
- Iteratively, states move to new positions
- PSO models social behavior: each individual tries to perform better according to its own experience and looking at his neighbors' experience
- Moves are based on:
  - Inertia: keep moving on the same direction.
  - Past experience: good experience of a particle should influence its new direction (conservative behavior)
  - Swarm (societal) experience, influence on:
    - what works for the others
    - what works for the neighbors
    - what works for the leader

Let $z_1(t), \ldots, z_m(t)$ be the positions of m particles in $\mathbb{R}^q$ in iteration t.
Then, position of particle z_s is updated according to:

$$z_s(t+1) = z_s(t) + v(t+1) \tag{1}$$

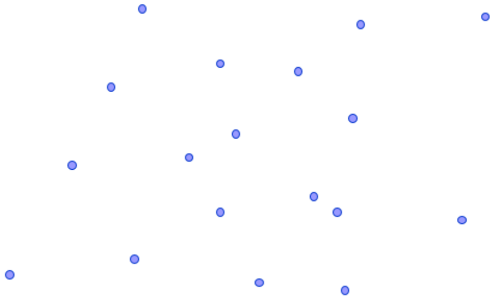
where

$$\begin{aligned} v(t+1) &= c_0 v(t) && \textit{inertia} \\ &\quad + c_1[p_s(t) - z_s(t)] && \textit{past experience} \\ &\quad + c_2[p_g(t) - z_s(t)] && \textit{imitate the leader} \\ &\quad + c_3[p_k(t) - z_s(t)] && \textit{neighbors' influence} \end{aligned} \tag{2}$$

with $c_l = \text{rand}(0, \varphi_l)$, $c_l \sim \mathcal{U}(0, \varphi_l)$, $\sum_{l=1}^{3} \varphi_l < 4$.

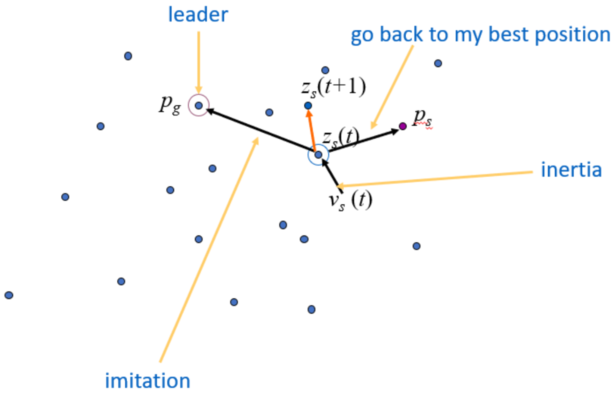
Particle Swarm Optimization

Illustration of PSO



Particle Swarm Optimization

Illustration of PSO



- **Clustering** numerical data for the minimization of variance (Trejos & Villalobos, 2007):
  particles are sets of K class centroids, that move in $\mathbb{R}^p$, where p is the dimension of the dataset. Centroids move according to PSO principles and objects are allocated to the nearest centroid for creating the clusters.
- **Nonlinear regression** for the minimization of the sum-of-squares (Quirós & Trejos, 2020):
  particles are sets of regression coefficients in nonlinear equations, that move in $\mathbb{R}^r$, where r is the number of parameters in the nonlinear equation.
  It was applied very successfully for the estimation of the zero-coupon yield curve in stocks market

PSO in MDS

Implementation

We have implemented a PSO approach for MDS with the following elements:

- Input: a dissimilarities matrix $[\delta_{ij}]_{n\times n}$; a dimension p
- Each particle z_s is a configuration $\mathbf{X}_s$ of n objects in $\mathbb{R}^p$
- We handle a set of m particles in each iteration
- Iterations are made according to equations (1) and (2)
- Combinations of influences:
  - Overall best solution
  - Best k neighbors
  - Both: best solution and neighbors
- Parameters tuning: c_0, c_1, c_2, c_3
- Output: best solution found $\mathbf{X}^*$
- Program in R

Toy Data Tables

- Points3 (triangle):

δ_{ij}	$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$
$\mathbf{x}_1$	0	1	1
$\mathbf{x}_2$	1	0	1
$\mathbf{x}_3$	1	1	0

- Square:

δ_{ij}	$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\mathbf{x}_4$
$\mathbf{x}_1$	0	1	$\sqrt{2}$	1
$\mathbf{x}_2$	1	0	1	$\sqrt{2}$
$\mathbf{x}_3$	$\sqrt{2}$	1	0	1
$\mathbf{x}_4$	1	$\sqrt{2}$	1	0

- Points4 (tetrahedre, 4×4), Points5 (5×5), Points6 (6×6), Points7 (7×7) and Points9 (9×9), defined by:

$$\delta_{ij} = \begin{cases} 1 & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}$$

Real Data Tables

- Colas (10×10)
- Countries (12×12)
- US Cities (31×31)
- Europe distances (20×20)
- Proteins (25×25)
- Costa Rica (10×10)
- Cuba (13×13)

Experiment Implementation

Parameters

- Dimension of representation: $p = 2$
- Number of particles: $m = 100$
- Intervals of representation defined by Torgerson solution ± 1.5 of its size in each direction
- Neighboring: we used 5 nearest neighbors
- Maximum number of iterations: 1000
- Bounds for c_l: $\varphi_0 = 0.729$, $\varphi_1 = \varphi_3 = 1.49$, $\varphi_2 = 0.75$
- $\lambda = 0.4$: bound for $v_s(t)$, such that $v_s(t+1) \leq \lambda v_s(t)$
- $v^{\max}$: bound for velocities, $v_{ij}^{\max} = \lambda(\mathbf{X}_{ij}^{\max} - \mathbf{X}_{ij}^{\min})$
- $\epsilon = 10^{-6}$: tolerance for convergence
- Stop criterion: when standard deviation of σ_1 in the population is less than ϵ, or the max nb of iterations is attained

Experimentation

- Multistart, with 105 starts (7 parallel kernels, 15 times each one)
- Initial configuration of each star:
  - with Torgerson solution as a particle in the population and the rest at random (`name.t`)
  - with all particles at random (`name.r`)

  Combination of factors:
  - Use of particles's best position and population best position (`gbest`).
  - Use of particles's best position and neighbors best position (`lbest`).
  - Use of particle's best position, `gbest` and `lbest` = `upso`.
- Comparison with SMACOF
- Report:
  - best value of stress-1 σ_1
  - attraction rate for the best solution
  - iteration when best value was obtained
  - time (in seconds)

Results for Toy Data Sets

Values of stress-1 σ_1 and attraction rates

Values of normalized stress σ_1

Table	upso.t	gbest.t	lbest.t	upso.r	gbest.r	lbest.r	Smacof.t	Smacof.r
Points3	**0.0000**	**0.0000**	**0.0000**	**0.0000**	**0.0000**	**0.0000**	**0.0000**	0.00029
Points4	**0.1691**	**0.1691**	**0.1691**	**0.1691**	**0.1691**	**0.1691**	**0.1691**	**0.1691**
Square	**0.0000**	**0.0000**	**0.0000**	**0.0000**	**0.0000**	0.00016	**0.0000**	0.00029
Points5	**0.0000**	**0.0000**	**0.0000**	**0.0000**	**0.0000**	0.00242	**0.0000**	0.00067
Points6	**0.2673**	**0.2673**	0.26993	**0.2673**	**0.2673**	0.26924	0.30653	**0.2673**
Points7	**0.29312**	**0.29312**	0.29556	**0.29312**	**0.29312**	0.29904	0.34381	0.29313
Points9	**0.0000**	**0.0000**	**0.0000**	0.00131	0.00433	0.16271	**0.0000**	0.00058

Attraction rates of σ_1 minima .

Table	upso.t	gbest.t	lbest.t	upso.r	gbest.r	lbest.r	Smacof.t	Smacof.r
Points3	1	1	1	1	0.990	0.152	1	0.019
Points4	1	1	0.01	1	1	0.029	1	0.990
Square	1	1	0.80	1	1	0.019	1	0.010
Points5	1	1	1	0.638	0.381	0.010	1	0.010
Points6	0.762	0.562	0.01	0.686	0.619	0.010	1	0.714
Points7	0.057	0.086	0.01	0.143	0.076	0.010	1	0.390
Points9	1	1	1	0.010	0.010	0.010	1	0.010

Results for Toy Data Sets

Number of iterations and time

Number of iterations needed for convergence .

Table	upso.t	gbest.t	lbest.t	upso.r	gbest.r	lbest.r	Smacof.t	Smacof.r
Points3	200	164	995	237	186	994	1	11
Points4	127	102	997	126	100	1001	17	16
Square	143	124	967	150	132	1001	1	15
Points5	154	132	995	147	123	1001	1	25
Points6	142	106	1001	144	109	1001	35	44
Points7	156	116	1001	157	117	1001	29	58
Points9	157	132	836	207	132	1001	1	36

Time (in seconds) .

Table	upso.t	gbest.t	lbest.t	upso.r	gbest.r	lbest.r	Smacof.t	Smacof.r
Points3	56.25	45.15	275.86	56.25	46.45	216.28	0.07	0.10
Points4	460.06	362.05	3417.47	460.06	339.17	3419.16	0.55	0.51
Square	496.33	427.44	3395.60	496.33	483.77	3295.67	0.04	0.10
Points5	609.86	518.45	4053.46	609.86	469.67	3767.07	0.05	0.17
Points6	681.48	468.33	4431.91	681.48	472.34	4273.16	0.14	0.18
Points7	806.85	577.39	4948.42	806.85	568.51	4739.78	0.16	0.28
Points9	960.00	770.29	5166.76	960.00	773.34	5663.70	0.06	0.20

Results for Real Data Sets

Values of stress-1 σ_1 and attraction rates

Values of normalized stress σ_1 .

Table	upso.t	gbest.t	lbest.t	upso.r	gbest.r	lbest.r	Smacof.t	Smacof.r
Colas	0.1962	0.2017	0.2105	0.1943	0.1936	0.2159	0.2022	**0.1918**
Costa Rica	**0.0044**	**0.0044**	0.0050	0.0100	0.0086	0.1182	0.0046	0.0048
Countries	0.2181	0.2181	0.2336	0.2207	0.2254	0.2927	0.2185	**0.2178**
US Cities	0.1017	0.1385	0.0905	0.1827	0.2841	0.4057	**0.0042**	**0.0042**
Cuba	0.0347	0.0317	0.0273	0.0311	0.0322	0.1053	0.0225	**0.0221**
Europe	0.0738	0.0735	0.0803	0.1674	0.2062	0.3395	**0.0722**	**0.0722**
Proteins	0.1172	0.1149	0.1290	0.2852	0.2879	0.6663	0.1117	**0.1108**

Attraction rates of σ_1 minima .

Table	upso.t	gbest.t	lbest.t	upso.r	gbest.r	lbest.r	Smacof.t	Smacof.r
Colas	0.01	0.01	0.01	0.01	0.02	0.01	1	0.03
Costa Rica	0.11	0.28	0.02	0.01	0.01	0.01	1	0.01
Countries	0.01	0.04	0.02	0.01	0.01	0.01	1	0.34
US Cities	0.01	0.02	0.01	0.01	0.01	0.01	1	0.02
Cuba	0.01	0.01	0.01	0.01	0.01	0.01	1	0.01
Europe	0.01	0.02	0.01	0.01	0.01	0.01	1	0.82
Proteins	0.01	0.01	0.01	0.01	0.01	0.01	1	0.03

Number of iterations needed for convergence .

Table	upso.t	gbest.t	lbest.t	upso.r	gbest.r	lbest.r	Smacof.t	Smacof.r
Colas	159	103	1001	166	111	1001	27	99
Costa Rica	157	115	996	198	123	1001	5	67
Countries	168	117	1001	188	118	1001	28	95
US Cities	1001	966	1001	200	118	1001	4	101
Cuba	160	113	1001	174	122	1001	44	83
Europe	169	118	1001	194	119	1001	17	77
Proteins	179	121	1001	207	130	1001	33	90

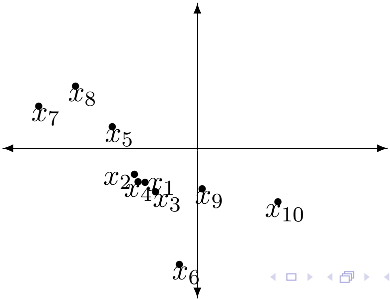
Time (in seconds) .

Table	upso.t	gbest.t	lbest.t	upso.r	gbest.r	lbest.r	Smacof.t	Smacof.r
Colas	1055.04	678.12	6853.13	1055.04	678.12	6853.13	0.63	0.63
Costa Rica	1052.95	763.16	6621.42	1052.95	763.16	6621.42	0.05	0.05
Countries	1262.06	887.63	7820.60	1262.06	887.63	7820.60	0.15	0.15
US Cities	16620.75	16381.56	16793.78	16620.75	16381.56	16793.78	0.11	0.11
Cuba	1250.05	936.75	7659.74	1250.05	936.75	7659.74	0.23	0.23
Europe	140.91	110.18	875.05	140.91	110.18	875.05	0.14	0.14
Proteins	176.36	128.98	990.24	176.36	128.98	990.24	0.22	0.22

Costa Rica data table

δ_{ij}	$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\mathbf{x}_4$	$\mathbf{x}_5$	$\mathbf{x}_6$	$\mathbf{x}_7$	$\mathbf{x}_8$	$\mathbf{x}_9$	$\mathbf{x}_{10}$
San José	0.00	18.00	18.00	9.00	82.5	114.00	168.00	151.5	73.5	172.5
Alajuela	18.00	0.00	36.00	10.5	67.5	127.5	150.00	135.00	90.00	184.5
Cartago	18.0	36.0	0.0	25.5	99.0	97.5	186.0	169.5	60.0	157.5
Heredia	9.0	10.5	25.5	0.0	78.0	118.5	160.5	145.5	82.5	181.5
Puntarenas	82.5	67.5	99.0	78.0	0.0	195.0	97.5	70.5	139.5	232.5
Limón	114.0	127.5	97.5	118.5	195.0	0.0	271.5	264.0	100.5	150.0
Liberia	168.0	150.0	186.0	160.5	97.5	271.5	0.0	54.0	234.0	330.0
Nicoya	151.5	135.0	169.5	145.5	70.5	264.0	54.0	0.0	208.5	300.0
PZ	073.5	90.0	60.0	82.5	139.5	100.5	234.0	208.5	0.0	99.0
Golfito	172.5	184.5	157.5	181.5	232.5	150.0	330.0	300.0	99.0	0.0

Solution for Costa Rica data table:



Application: Chemical Organization of Products

- Consider a set 24 chemical products that have to be stored in a warehouse
- A list of pairwise restrictions is given: products that cannot be stored side by side
- We defined a dissimilarity matrix:

$$\delta_{ij} = \begin{cases} 1 & \text{if products } i \text{ and } j \text{ are not compatible} \\ 0 & \text{if products } i \text{ and } j \text{ are compatible} \end{cases}$$

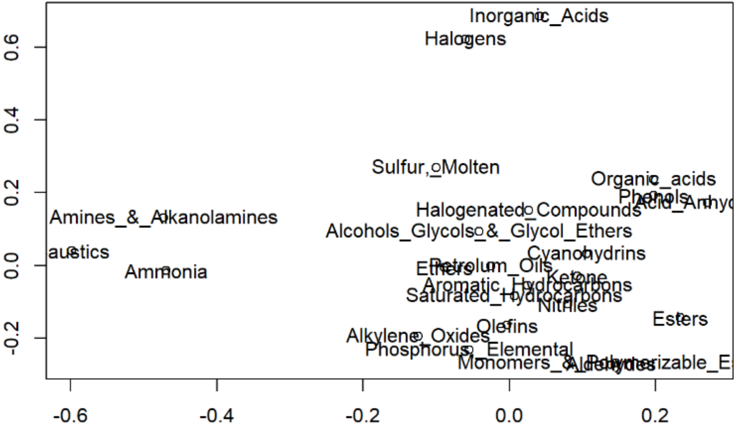
- It means that compatible products can be stored next to each other

Application: Chemical Organization of Products

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1. Inorganic acids	0	1	1	1	1	1	1	1	0	1	1	0	1	1	0	1	1	1	1	0	1	1	0	1
2. Organic acids	1	0	1	1	0	0	1	0	0	0	0	0	0	1	0	1	1	1	1	0	0	1	0	0
3. Caustics	1	1	0	0	1	0	1	1	0	0	0	0	1	1	1	1	1	1	0	1	0	1	0	1
4. Amines & alkanolamines	1	1	0	0	1	0	1	1	0	0	0	0	1	1	1	1	1	1	0	0	0	0	0	1
5. Halogenated compounds	1	0	1	1	0	0	0	0	0	0	1	0	0	1	0	0	1	0	0	0	0	0	0	0
6. Alcohols, Glycols & Glycol Ethers	1	0	0	0	0	0	1	0	0	0	0	0	0	1	0	1	0	0	0	1	0	0	0	1
7. Aldehydes	1	1	1	1	0	1	0	1	0	0	0	0	0	0	1	1	1	0	1	1	0	0	0	1
8. Ketone	1	0	1	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0
9. Saturated Hydrocarbons	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0
10. Aromatic Hydrocarbons	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0
11. Olefins	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0
12. Petroleum Oils	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0
13. Esters	1	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0
14. Monomers & Polymerizable Esters	1	1	1	1	1	1	0	0	0	0	0	0	0	0	1	1	0	0	1	1	1	0	0	1
15. Phenols	0	0	1	1	0	0	1	0	0	0	0	0	0	1	0	1	0	0	1	1	0	0	0	0
16. Alkylene Oxides	1	1	1	1	0	1	1	0	0	0	0	0	0	1	1	0	1	1	1	0	0	0	1	1
17. Cyanohydrins	1	1	1	1	1	0	1	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	1
18. Nitriles	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
19. Ammonia	1	1	0	0	0	0	1	1	0	0	0	0	1	1	1	1	1	0	0	1	0	0	0	1
20. Halogens	0	0	1	0	0	1	1	1	1	1	1	1	1	1	1	0	0	0	1	0	1	1	0	0
21. Ethers	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0
22. Phosphorus, Elemental	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0
23. Sulfur, Molten	0	0	0	0	0	0	0	0	1	1	1	1	0	0	0	1	0	0	0	0	0	1	0	0
24. Acid Anhydrides	1	0	1	1	0	1	1	0	0	0	0	0	0	1	0	1	1	1	1	0	0	0	0	0

Application: Chemical Organization of Products

MDS with PSO solution



Comments

- Further work has to be done:
  - Tuning the parameters: $\varphi_0, \varphi_2, \varphi_3, \varphi_4$
  - maximum number of iterations
  - initial configuration
  - better use of neighbors' information
- Consider larger and more complex data sets

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Thank you! **Questions?**

`victor.bazan@ucr.ac.cr`

`javier.trejos@ucr.ac.cr`

Forthcoming conferences in Costa Rica

See you in Costa Rica at the following conferences:

IFCS
Conference of the International Federation of Classification Societies
Costa Rica July 15-19th, 2024

VIII LACSC
VIII Latin American Conference on Statistical Computing
San José, Costa Rica July 15-19, 2024

https://ifcs.ucr.ac.cr/   https://lacsc.ucr.ac.cr/

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