

# Learning from (dis)similarity data

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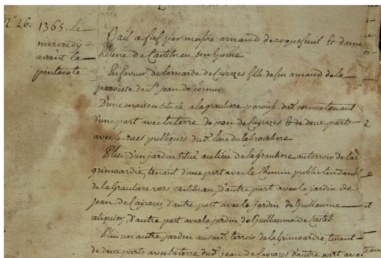
# What are my data like?



# A medieval social network [Boulet et al., 2008, Rossi et al., 2013]



corpus with more than 6,000 transactions, 3 centuries, all related to Castelnau Montratier



AD 46 48 J6 page 37, acte 26 (analyse détaillée id\_acte=72, id\_transaction=142)  
références documentaires

1365, le mercredi avant la Pentecôte date

paroisse

tenancier, acteur de l'acte

Bail à fief par messire Amaud de Roquefeuil et Dame Hélène de Castelnau son épouse en faveur de Bernarde Carazes, fille de feu Amaud de la paroisse de St Jean de Cornus, d'une maison située à La Graulière, paroisse de Cornus, tenant d'une part avec la terre de Jean Carazes et de deux parts avec les rues publiques du dit lieu de La Graulière.

tenancier confront

[...] (7 autres transactions pour deux jardins un pré et 4 pièces de terre)

sous la redevance de 6 d cahorsis d'acapte à mutation de seigneur et de 3 (4 quartes) mesures d'avoine et 1 poule à notre Dame en septembre.

notaire

Jean de Combeleau, notaire et commissaire d'actes de monsieur l'officiel de Cahors.

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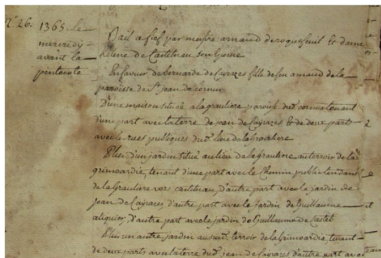


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corpus with more than 6,000 transactions, 3 centuries, all related to Castelnaud Montratier

Individual  
Transaction



AD 46 48 J6 page 37, acte 26 (analyse détaillée id\_acte=72, id\_transaction=142)

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lieu

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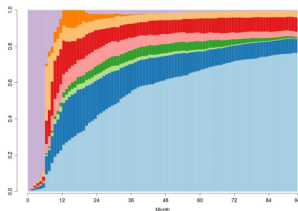
bipartite network with more than 17,000 nodes (~ 10,000 individuals)


What can we learn from the French medieval society?



# Career paths [Olteanu and Villa-Vialaneix, 2015a]

Survey “Génération 98”: labor market status (9 categories) on more than 16,000 people having graduated in 1998 during 94 months. <sup>1</sup>



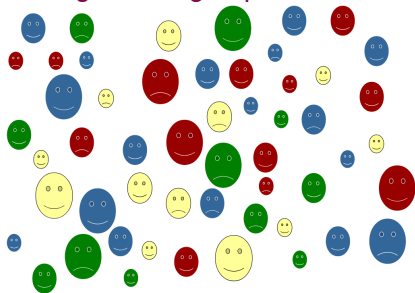
1. Available thanks to Génération 1998 à 7 ans - 2005, [producer] CEREQ, [diffusion] Centre Maurice Halbwachs (CMH) 



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How to cluster career paths into homogeneous groups?



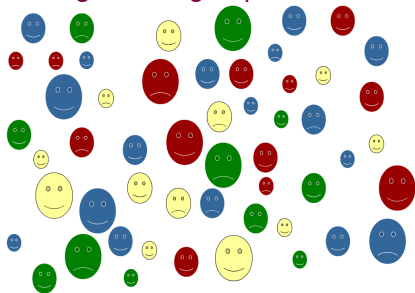
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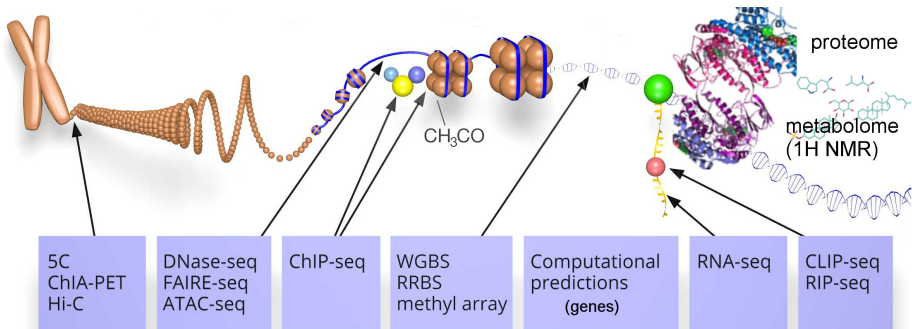
It is **all about distance...**

- $\chi^2$  dissimilarity emphasizes the contemporary identical situations
- Optimal-matching dissimilarities is more focused on the sequences similarities [Needleman and Wunsch, 1970] (or “edit distance”, “Levenshtein distance”)

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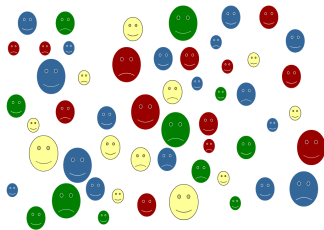


and then I went into NGS data...



and again...

distances are everywhere





# a collection of NGS data...

## DNA barcoding

*Astraptes fulgerator*

optimal matching  
(edit) distances to  
differentiate species



# a collection of NGS data...

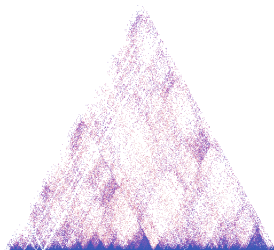
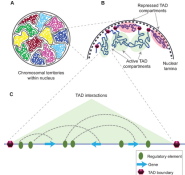
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## Hi-C data



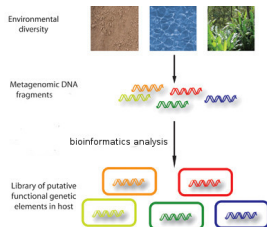
pairwise measure (similarity) related to  
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the cell, at genome scale

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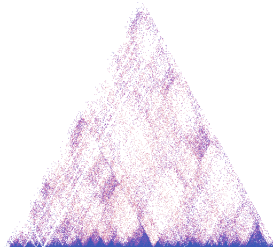
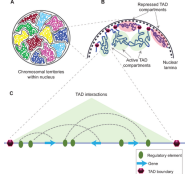
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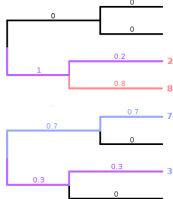
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## Metagenomics

dissemblance between  
samples is better  
captured when  
phylogeny between  
species is taken into  
account (unifrac  
distances)





# Exploratory analysis of relational data



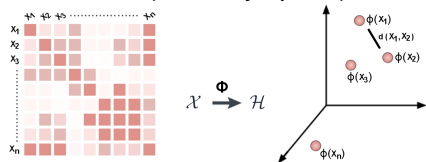
# Formally, relational data are:

Euclidean distances or (non  
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**kernels**: a symmetric and positive definite  $(n \times n)$ -matrix  $\mathbf{K}$  that measures a “relation” between  $n$  entities in  $\mathcal{X}$  (arbitrary space)

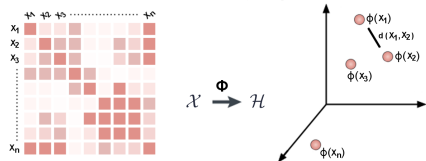


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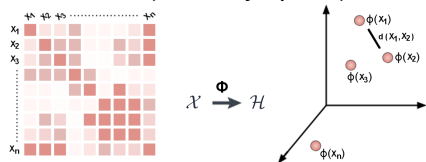
**networks/graphs**: groups of  $n$  entities (nodes/vertices) linked by a (potentially weighted) relation (edges)

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**Similarities** between  $n$  entities: symmetric  $(n \times n)$ -matrix  $\mathbf{S}$  (with usually positive entries) but not necessarily definite positive





# Different relational data types are related to each others

- a kernel is equivalent to an Euclidean distance:

$$\mathbf{D}(x, x') := \sqrt{\mathbf{K}(x, x) + \mathbf{K}(x', x') - 2\mathbf{K}(x, x')}$$

- from a dissimilarity, similarities can be computed:

$$\mathbf{S}(x, x) := a(x) \text{ (arbitrary)}, \mathbf{S}(x, x') = \frac{1}{2} (a(x) + a(x') - \mathbf{D}^2(x, x'))$$

- various kernels have been proposed for graphs (e.g., based on the graph Laplacian): [[Kondor and Lafferty, 2002](#)]



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### in summary

useful simplification: “is the framework Euclidean or not?” (e.g., kernel vs non Euclidean dissimilarity)

# Principles for learning from relational data

Euclidean case (kernel  $\mathbf{K}$ )  
rewrite all quantities using:

- $\mathbf{K}$  to compute distances and dot products
- linear or convex combinations of  $(\phi(x_i))_i$  to describe all unobserved elements (centers of gravity and so on...)

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Works for: PCA,  $k$ -means, linear regression, ...

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**non Euclidean case** (non Euclidean dissimilarity  $\mathbf{D}$ ): do almost the same using a pseudo-Euclidean framework

[Goldfarb, 1984]

$\exists$  two Euclidean spaces  $\mathcal{E}_+$  and  $\mathcal{E}_-$  and two mappings  $\phi_+$  and  $\phi_-$  st:

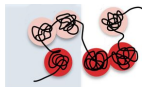
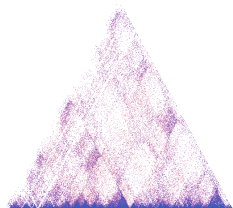
$$\mathbf{D}(x, x') = \|\phi_+(x) - \phi_+(x')\|_{\mathcal{E}_+}^2 - \|\phi_-(x) - \phi_-(x')\|_{\mathcal{E}_-}^2$$



# Application 1: Constrained Hierarchical Clustering



# Constrained clustering for genomic data



Hi-C data: **S**

- segmentation (or contiguous clustering) of the chromosome  
↔ functional domains (TAD)
- hierarchical clustering is relevant

Other similar problems in biology:  
Haplotypes based on LD between SNPs (groups of genomic positions inherited together)



# adjclust

<https://cran.r-project.org/package=adjclust>

## Features:

- constrained hierarchical clustering for arbitrary similarities (or kernels) or dissimilarities (extends *e.g.*, **rioja**)



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- can be used for large scale (*e.g.*, genomic) datasets: fast implementation based on sparsity of **S** [Dehman, 2015]  
complexity:
  - ▶ original method:  $O(n^2)$  (time) and  $O(n^2)$  (space)
  - ▶ **adjclust**:  $O(nh + n \log n)$  (time) and  $O(nh)$  (space) with  $h$  the non sparse band around the diagonal

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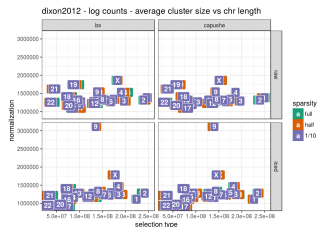
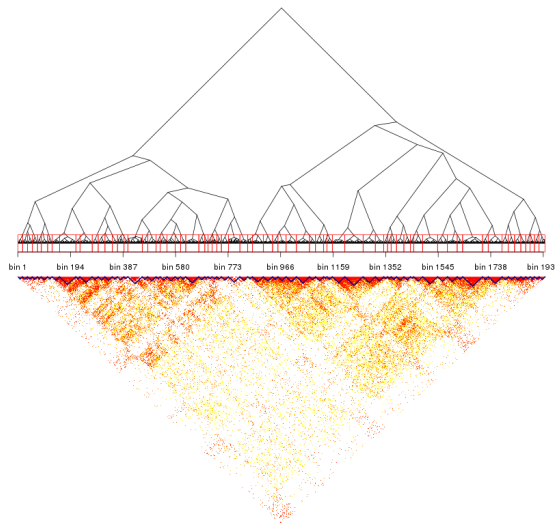
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## Icing on the cake:

- wrappers for Hi-C datasets and LD datasets
- model selection methods (broken stick and slope heuristic)
- corrected dendrogram to avoid reversals [Grimm, 1987]
- ... and other nice plots to compare data with clustering

# Application to Hi-C data

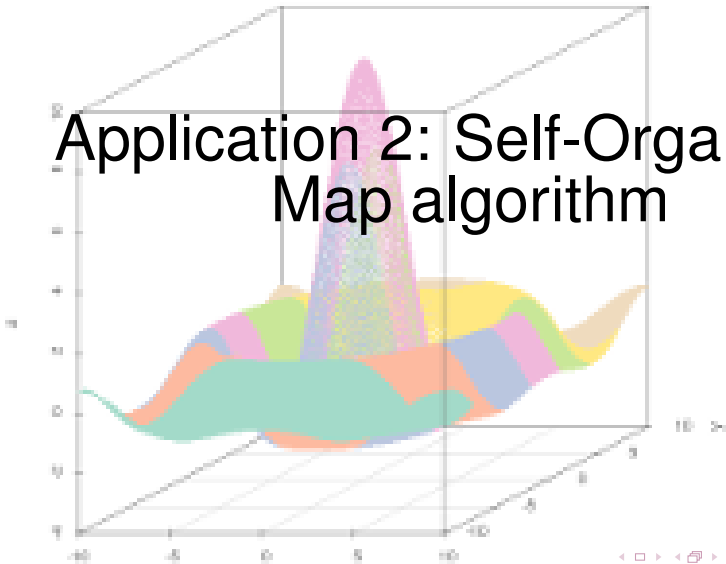
with data from [Dixon et al., 2012]



- constant average TAD size whatever the chromosome length
- similar results for broken stick and slope heuristic
- similar results for full and sparse (half - 1/10) versions

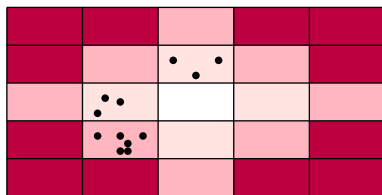
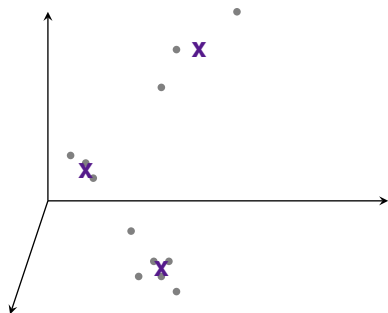


# Application 2: Self-Organizing Map algorithm



# Basics on (standard) stochastic SOM

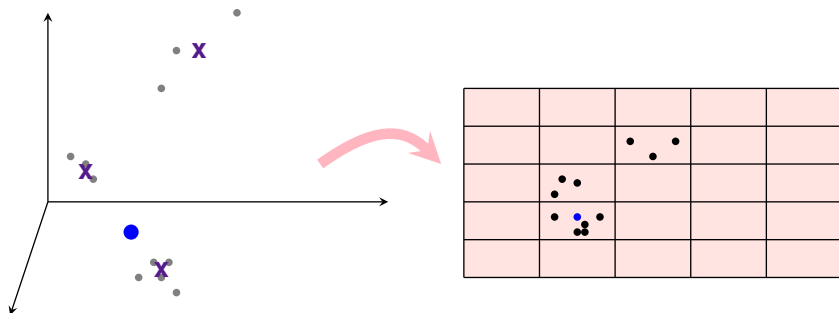
[Kohonen, 2001]



- $(x_i)_{i=1,\dots,n} \subset \mathbb{R}^d$  are affected to a unit  $f(x_i) \in \{1, \dots, U\}$
- the grid is equipped with a “distance” between units:  $d(u, u')$  and observations affected to close units are close in  $\mathbb{R}^d$
- every unit  $u$  corresponds to a **prototype**,  $p_u(\mathbf{x})$  in  $\mathbb{R}^d$

# Basics on (standard) stochastic SOM

[Kohonen, 2001]



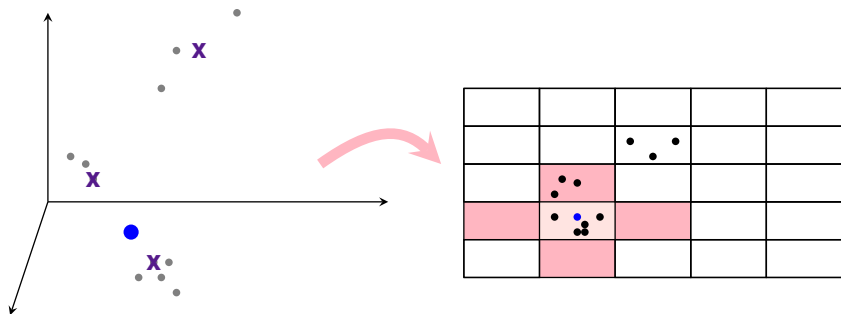
**Iterative learning (assignment step):**  $x_i$  is picked at random within  $(x_k)_k$  and affected to *best matching unit*:

$$f^t(x_i) = \arg \min_u \|x_i - p_u^t\|^2$$



# Basics on (standard) stochastic SOM

[Kohonen, 2001]



**Iterative learning (representation step):** all prototypes in neighboring units are updated with a gradient descent like step:

$$p_u^{t+1} \leftarrow p_u^t + \mu(t) H^t(d(f(x_i), u))(x_i - p_u^t)$$

# Extension of SOM to data described by a kernel or a dissimilarity

[Olteanu and Villa-Vialaneix, 2015a]

Data:  $(x_i)_{i=1,\dots,n} \in \mathbb{R}^d$

1: Initialization:

randomly set  $p_1^0, \dots, p_U^0$  in  $\mathbb{R}^d$

2: **for**  $t = 1 \rightarrow T$  **do**

3: pick at random  $i \in \{1, \dots, n\}$

4: **Assignment**

$$f^t(x_i) = \arg \min_{u=1,\dots,U} \|x_i - p_u^t\|^2$$

5: **for all**  $u = 1 \rightarrow U$  **do Representation**

6:

$$p_u^{t+1} = p_u^t + \mu(t)H^t(d(f^t(x_i), u))(x_i - p_u^t)$$

7: **end for**

8: **end for**



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# Extension of SOM to data described by a kernel or a dissimilarity

[Olteanu and Villa-Vialaneix, 2015a]

Data:  $(x_i)_{i=1,\dots,n} \in \mathcal{X}$

1: Initialization:

$$p_u^0 \sim \sum_{i=1}^n \beta_{ui}^0 x_i \text{ (convex combination)}$$

2: **for**  $t = 1 \rightarrow T$  **do**

3: pick at random  $i \in \{1, \dots, n\}$

4: **Assignment**

$$f^t(x_i) = \arg \min_{u=1,\dots,U} (\beta_u^t)^\top \mathbf{D}(\cdot, x_i) - \frac{1}{2} (\beta_u^t)^\top \mathbf{D} \beta_u^t$$

5: **for all**  $u = 1 \rightarrow U$  **do Representation**

6:

$$\beta_u^{t+1} = \beta_u^t + \mu(t) H^t(d(f^t(x_i), u)) (\mathbf{1}_i - \beta_u^t)$$

7: **end for**

8: **end for**



# SOMbrero

[Villa-Vialaneix, 2017], <https://cran.r-project.org/package=SOMbrero>

- stochastic variants of SOM (standard, KORRESP and relational) with a large number of diagnostic plots
- specific functions to **use with graphs** and obtain simplified representations  
[Olteanu and Villa-Vialaneix, 2015b]



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- specific functions to **use with graphs** and obtain simplified representations [Olteanu and Villa-Vialaneix, 2015b]
- contains comprehensive **vignettes** illustrated on **3 datasets** corresponding to the three algorithms (iris, presidentielles2002 and lesmis, a graph from “Les Misérables”)

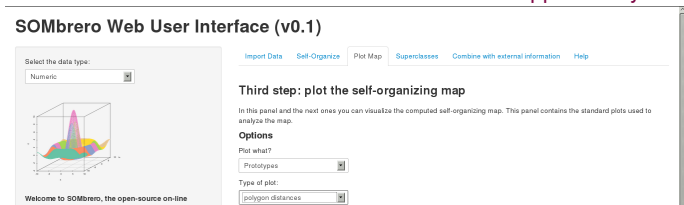


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- contains comprehensive **vignettes** illustrated on **3 datasets** corresponding to the three algorithms (iris, presidentielles2002 and lesmis, a graph from “Les Misérables”)
- **Web User Interface** (made with **shiny**) with `sombreroGUI()`

Tested on and approved by an historian!



The screenshot displays the SOMbrero Web User Interface (v0.1) in a browser window. The interface is titled "SOMbrero Web User Interface (v0.1)" and features a navigation bar with links for "Import Data", "Self-Organize", "Plot Map", "Superclasses", "Combine with external information", and "Help".

On the left, there is a panel titled "Select the data type:" with a dropdown menu set to "Numeric". Below this is a 3D plot showing a self-organizing map with a colorful surface and a vertical axis. At the bottom of this panel, it says "Welcome to SOMbrero, the open-source on-line interface for self-organizing maps (SOM)." and "https://www.sombrero.org/".

The main content area is titled "Third step: plot the self-organizing map" and contains the text: "In this panel and the next ones you can visualize the computed self-organizing map. This panel contains the standard plots used to analyze the map." Below this, there is an "Options" section with the following controls:

- "Plot what?" dropdown menu set to "Prototypes"
- "Type of plot:" dropdown menu set to "polygon distances"

At the bottom right of the interface, there are icons for a menu, search, and refresh.



# Note on drawbacks of RSOM

Two main drawbacks:

- For  $T \sim \gamma n$  iterations, complexity of RSOM is  $O(\gamma n^3 U)$  (compared to  $O(\gamma U d n)$  for numeric) [Rossi, 2014]

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Exact solution proposed in [Mariette et al., 2017] to reduce the complexity to  $O(\gamma n^2 U)$  with additional storage memory of  $O(Un)$  (implemented in **SOMbrero**)

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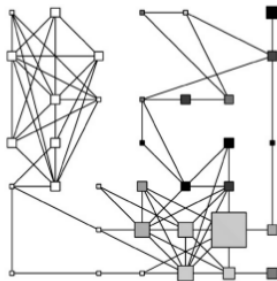
- For the non Euclidean case, the learning algorithm can be very unstable (saddle points)

clip or flip? [Chen et al., 2009]

# RSOM for mining a medieval social network

with the heat kernel

● Individual  
■ Transaction



Graph induced by clusters:

- has nice relations with space and time
- emphasizes leading people
- has helped to identify problems in the database (namesakes)

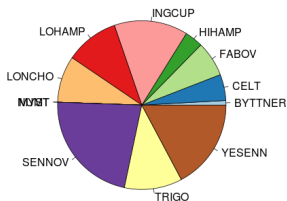
But: biggest communities are still very complex

[Boulet et al., 2008]



# RSOM for typology of *Astrartes fulgerator* from DNA barcoding

Edit distances between DNA sequences [Olteanu and Villa-Vialaneix, 2015a]



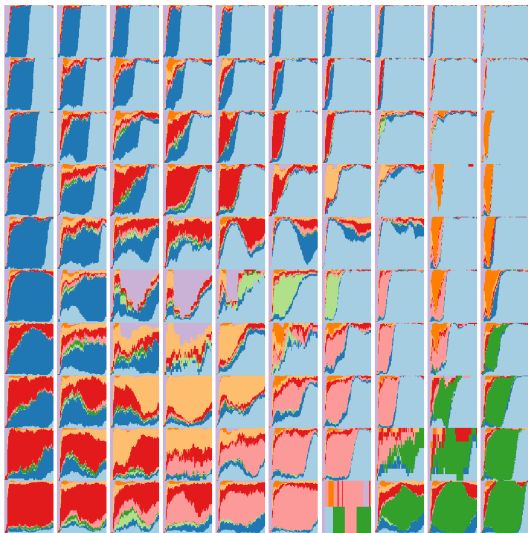
Almost perfect clustering (identifying a possible label error on one sample) with (in addition) **information on relations between species.**



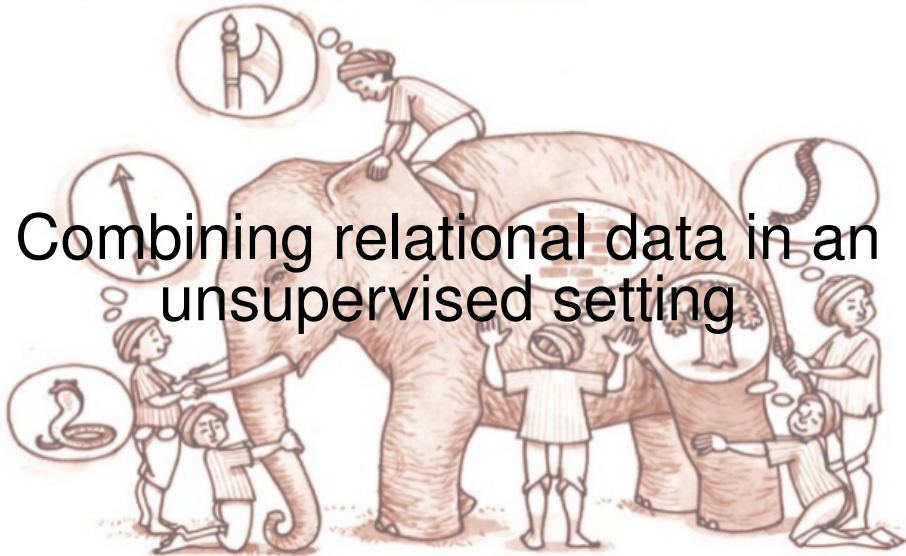


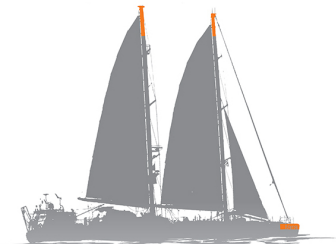
# RSOM for typology of school-to-time transitions

Edit distance between 12,000 categorical time series



# Combining relational data in an unsupervised setting





**TARA  
OCEANS**

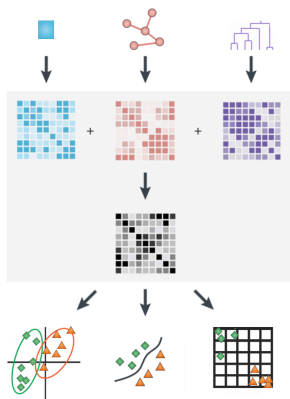


## The 2009-2013 expedition

- Co-directed by Étienne Bourgois and Éric Karsenti
  - **7,012 datasets** collected from **35,000 samples** of plankton and water (**11,535 Gb** of data)
  - Study the **plankton**: bacteria, protists, metazoans and viruses (more than 90% of the biomass in the ocean)
- Metagenomic datasets** similarity is well captured by unifracs distances



# Multi-kernel/distances integration



How to “optimally” combine several relational datasets in an unsupervised setting?

for kernels  $\mathbf{K}^1, \dots, \mathbf{K}^M$  obtained on the same  $n$  objects, search:  $\mathbf{K}_\beta = \sum_{m=1}^M \beta_m \mathbf{K}^m$  with  $\beta_m \geq 0$  and  $\sum_m \beta_m = 1$

- [Mariette and Villa-Vialaneix, 2018]
- Package R **mixKernel**  
<https://cran.r-project.org/package=mixKernel>

# STATIS like framework

[L'Hermier des Plantes, 1976, Lavit et al., 1994]

Similarities between kernels:

$$C_{mm'} = \frac{\langle \mathbf{K}^m, \mathbf{K}^{m'} \rangle_F}{\|\mathbf{K}^m\|_F \|\mathbf{K}^{m'}\|_F} = \frac{\text{Trace}(\mathbf{K}^m \mathbf{K}^{m'})}{\sqrt{\text{Trace}((\mathbf{K}^m)^2) \text{Trace}((\mathbf{K}^{m'})^2)}}.$$

( $C_{mm'}$  is an extension of the RV-coefficient [Robert and Escoufier, 1976] to the kernel framework)

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$$\begin{aligned} \text{maximize}_{\mathbf{v}} \quad & \sum_{m=1}^M \left\langle \mathbf{K}^*(\mathbf{v}), \frac{\mathbf{K}^m}{\|\mathbf{K}^m\|_F} \right\rangle_F = \mathbf{v}^\top \mathbf{C} \mathbf{v} \\ \text{for } \mathbf{K}^*(\mathbf{v}) = & \sum_{m=1}^M v_m \mathbf{K}^m \text{ and } \mathbf{v} \in \mathbb{R}^M \text{ such that } \|\mathbf{v}\|_2 = 1. \end{aligned}$$

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**Solution:** first eigenvector of  $\mathbf{C} \Rightarrow \text{Set } \beta = \frac{\mathbf{v}}{\sum_{m=1}^M v_m}$  (consensual kernel).



# A kernel preserving the original topology of the data I

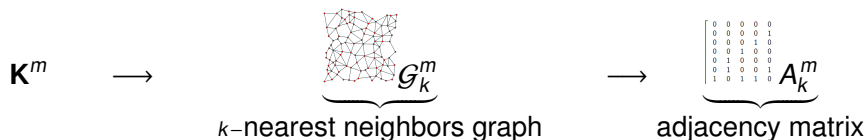
Similarly to [Lin et al., 2010], preserve the local geometry of the data in the feature space.



# A kernel preserving the original topology of the data I

Similarly to [Lin et al., 2010], preserve the local geometry of the data in the feature space.

Proxy of the local geometry



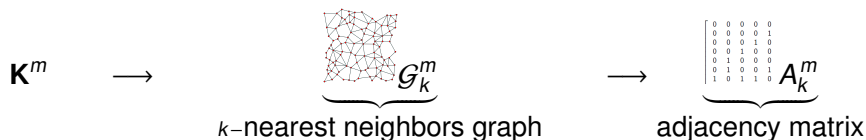
$$\Rightarrow W = \sum_m \mathbb{I}_{\{A_k^m > 0\}} \text{ or } W = \sum_m A_k^m$$



# A kernel preserving the original topology of the data I

Similarly to [Lin et al., 2010], preserve the local geometry of the data in the feature space.

## Proxy of the local geometry



$$\Rightarrow \mathbf{W} = \sum_m \mathbb{I}_{\{A_k^m > 0\}} \text{ or } \mathbf{W} = \sum_m \mathbf{A}_k^m$$

Feature space geometry measured by

$$\Delta_i(\beta) = \left\langle \phi_\beta^*(x_i), \begin{pmatrix} \phi_\beta^*(x_1) \\ \vdots \\ \phi_\beta^*(x_n) \end{pmatrix} \right\rangle = \begin{pmatrix} \mathbf{K}_\beta^*(x_i, x_1) \\ \vdots \\ \mathbf{K}_\beta^*(x_i, x_n) \end{pmatrix}$$

# A kernel preserving the original topology of the data II

## Sparse version

$$\text{minimize}_{\beta} \sum_{i,j=1}^N w_{ij} \|\Delta_i(\beta) - \Delta_j(\beta)\|^2$$

for  $\mathbf{K}_{\beta}^* = \sum_{m=1}^M \beta_m \mathbf{K}^m$  and  $\beta \in \mathbb{R}^M$  st  $\beta_m \geq 0$  and  $\sum_{m=1}^M \beta_m = 1$ .

## Non sparse version

$$\text{minimize}_{\mathbf{v}} \sum_{i,j=1}^N w_{ij} \|\Delta_i(\beta) - \Delta_j(\beta)\|^2$$

for  $\mathbf{K}_{\mathbf{v}}^* = \sum_{m=1}^M v_m \mathbf{K}^m$  and  $\mathbf{v} \in \mathbb{R}^M$  st  $v_m \geq 0$  and  $\|\mathbf{v}\|_2 = 1$ .

# A kernel preserving the original topology of the data II

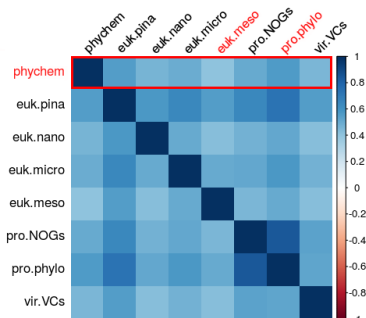
## Sparse version

equivalent to a standard QP problem with linear constraints (ex: package **quadprog** in R)

## Non sparse version

equivalent to a QPQC problem (harder to solve) solved with “Alternating Direction Method of Multipliers” (ADMM [[Boyd et al., 2011](#)])

# Application to TARA oceans

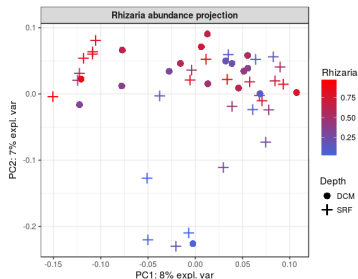
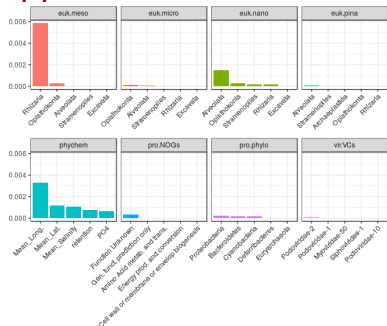


## Similarity between datasets (STATIS)

- **phychem** and small size organisms are the most similar (confirmed by [de Vargas et al., 2015] et [Sunagawa et al., 2015]).



# Application to TARA oceans



## Important variables

- *Rhizaria* abundance strongly structure the differences between samples (analyses restricted to some organisms found differences mostly based on water depths)
- and waters from Arctic Oceans and Pacific Oceans differ in terms of *Rhizaria* abundance





## SOMbrero

Madalina Olteanu,

Fabrice Rossi, Marie Cottrell,

Laura Bendhaïba and

Julien Boelaert



## SOMbrero and mixKernel



Jérôme Mariette

## adjclust

Pierre Neuvial, Guillem Rigail, Christophe Ambroise and

Shubham Chaturvedi



Google  
Summer of Code





Toulouse  
2019  
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[user2019.r-project.org](http://user2019.r-project.org)





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# Dendrogram corrections when reversals are detected

