

# Learning from (dis)similarity data

Nathalie Villa-Vialaneix

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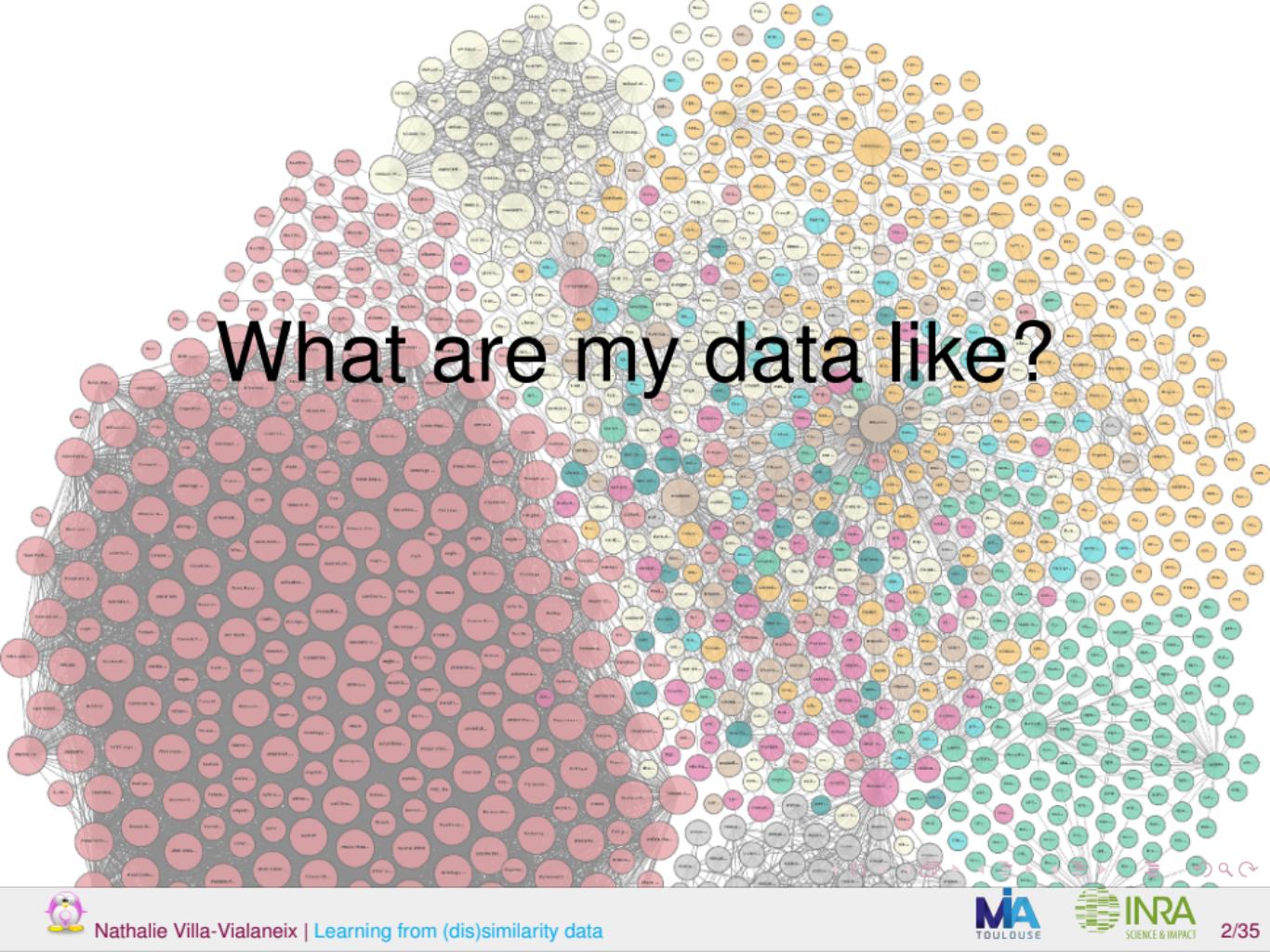
<http://www.nathalievilla.org>



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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

7.26. 1365. le  
mardi  
avant la  
pentecôte  
Ball a fief par mesme arnaud de roquefeul le dame  
Hélène de Castelnau son femme  
Bernarde de la Grailière sa femme fille de feu arnaud de la  
paroisse de St Jean de Cormes  
Dame mesme bethie a la grailière sonne de roquefeul  
une part auz latore de son de la grailière & la denre partie  
avec la rues publiques n° 2 l'anc de la grailière  
Ball son jardin tenu a la grailière auziorio de la  
grailière tenent une part avec le domme pectoral tendant  
la grailière vers castelnau d'autre part avec le jardin de  
jean de cahors d'autre part avec le jardin de guillaume de castel  
et a la grailière d'autre part avec le jardin de guillaume de castel  
Ball un autre jardin auziori tenent la grailière tenent  
de deux parts auz latore n° 2 l'anc de la grailière n° 3 l'anc de la grailière  
n° 4 l'anc de la grailière n° 5 l'anc de la grailière n° 6 l'anc de la grailière

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  
Ball a fief par mesme Arnaud de Roquefeul et Dame Hélène de Castelnau son épouse en faveur de Bernarde Cuirazès, fille de feu Arnaud de la paroisse de St Jean de Cormes, d'une maison située à la Grailière, paroisse de Cormes, tenant une partie avec la terre de Jean Cuirazès et de deux parts dit avec les rues publiques du dit lieu de La Grailière.

tenancier confront

1...7 autres transactions pour deux jardins un pré et 4 pièces de terre)  
sous la redevance de 6 d cabonc d'acarie à mutation de seigneur et de 3 (4 quartes) mesures  
davoine et 1 poule à notre Dame en septembre.

Jean de Combelcau, notaire et commissaire d'actes de monsieur l'officier de Cahors.

notaire  
seigneurs, acteurs de l'acte

# 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

26. 1363. le  
mardi  
avant la  
pentecôte  
Or il a fait par mesme arnaud de roquefeul le dame  
hélène de castelnau son femme  
en faveur de bernarde de cahuzac fille de feu arnaud de la  
paroisse de st jean de cornus  
bonne maistresse alagruliere mariee des roquefeul  
une part au château de son de cahuzac & une autre part à  
avec la rue publique n° 2 face de la boulangerie  
elle s'en servit telle eschise de la boulangerie au dessus de la  
grange dite tenant une part avec le château plus la boulangerie  
de la grange d'au château d'autre part avec le jardin de  
jean de cahuzac d'autre part avec le jardin de guillaume de castel  
et alquier d'autre part avec le jardin de guillaume de castel  
plus un autre jardin au dessus de la grange d'autre part avec  
la deux parts au château n° 2 face de la boulangerie tenant  
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AD 46 48 J6 page 37, acte 26 (analyse détaillée id\_acte=72, id\_transaction=142)  
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tenancier, acteur de l'acte  
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la Grulière, paroisse de Cornus, tenant d'une part avec la terre de Jean Cahuzac et de deux parts  
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... (7 autres transactions pour deux jardins un pré et 4 pièces de terre)  
sous la redevance de 6 d cabotin d'acarré à mutation de seigneur et de 3 (4 quartes) mesures  
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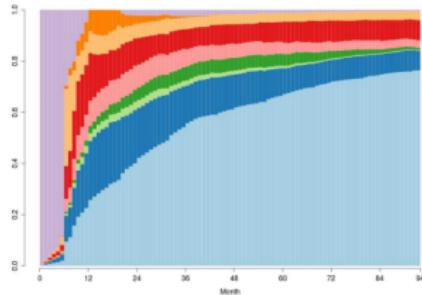
notaire  
seigneurs, acteurs de l'acte



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>



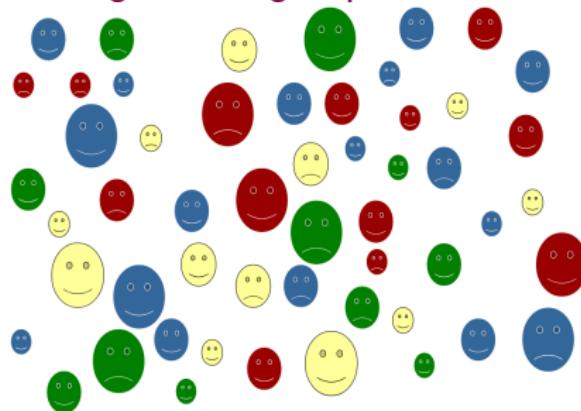
1. Available thanks to Génération 1998 à 7 ans - 2005, [producer] CERÉQ, [diffusion] Centre Maurice Halbwachs (CMH)



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How to cluster career paths into homogeneous groups?



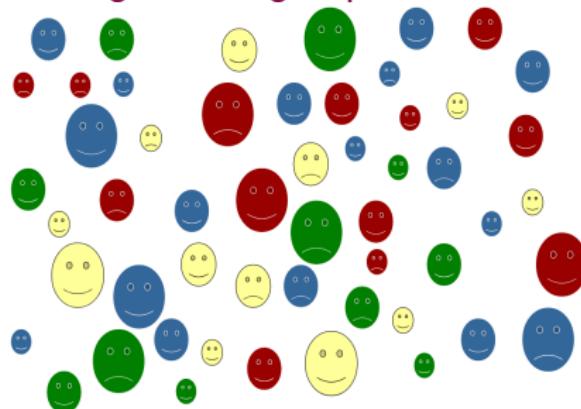
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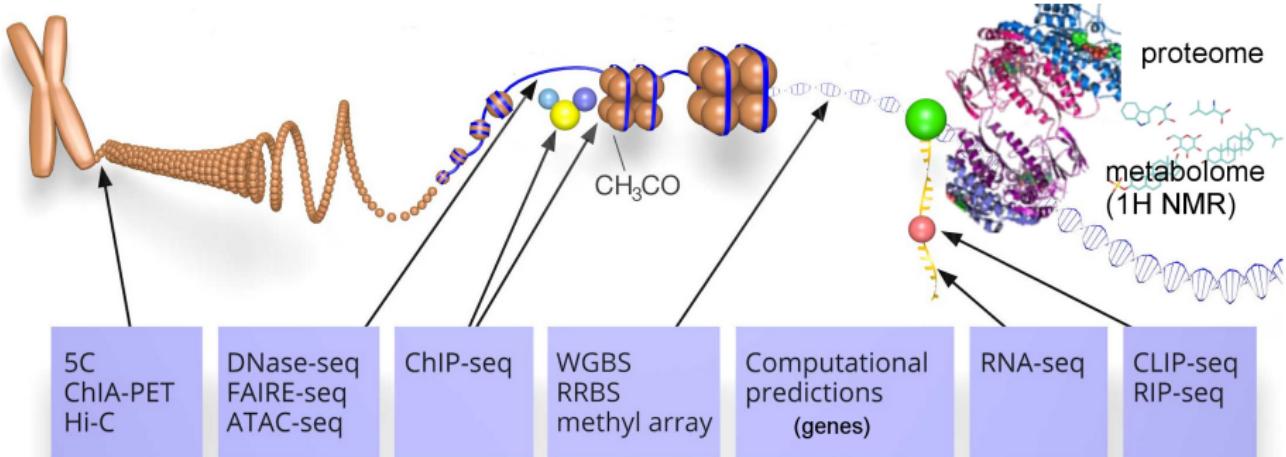
It is all about distance...

- $\chi^2$  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")

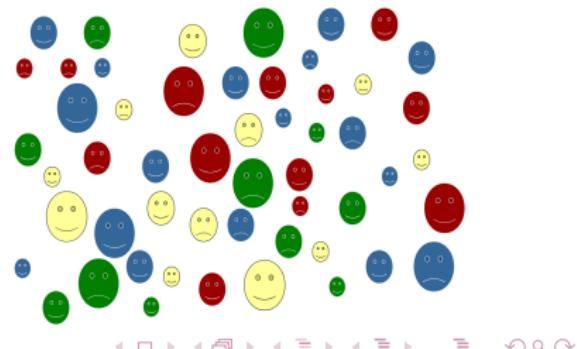
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# and then I went into NGS data...



and again...  
distances are everywhere



# a collection of NGS data...

## DNA barcoding

*Astraptes fulgerator*

optimal matching  
(edit) distances to  
differentiate species

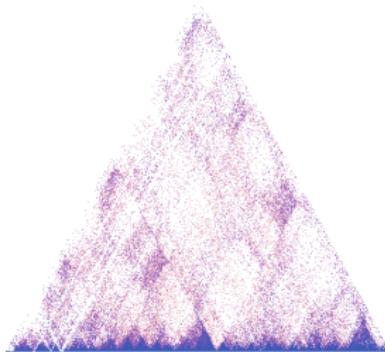
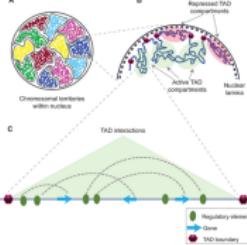


# a collection of NGS data...

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## Hi-C data



pairwise measure (similarity) related to  
the physical 3D distance between loci in  
the cell, at genome scale

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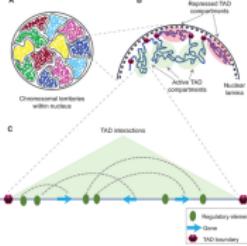
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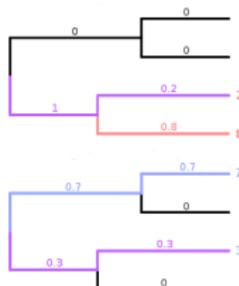
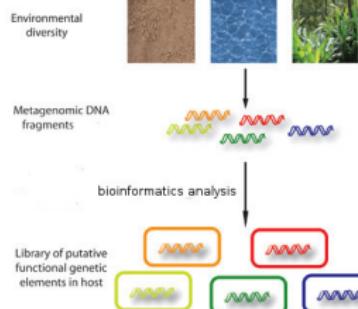
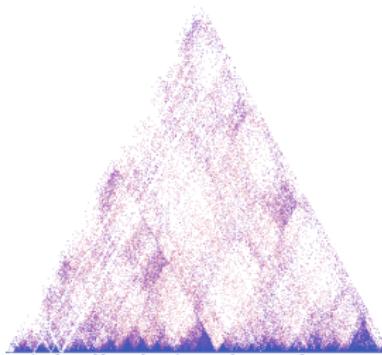
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## Hi-C data

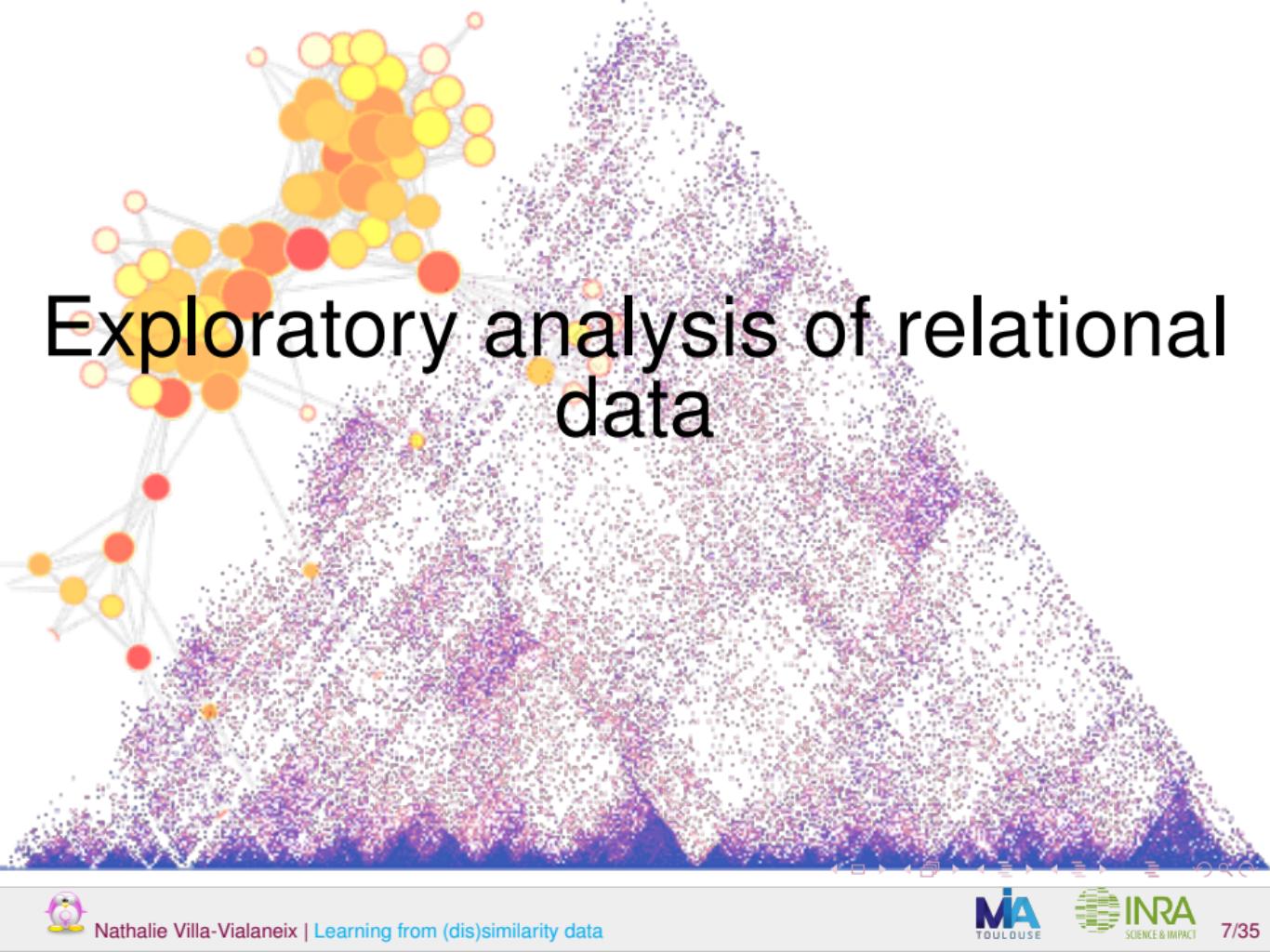


pairwise measure (similarity) related to the physical 3D distance between loci in the cell, at genome scale



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





# Exploratory analysis of relational data

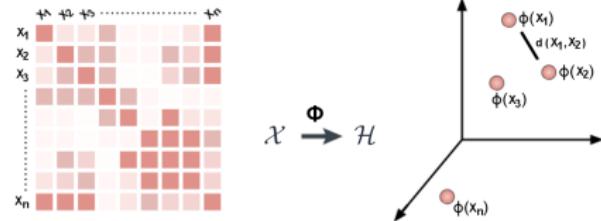
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Euclidean distances or (non Euclidean) dissimilarities between  $n$  entities: symmetric ( $n \times n$ )-matrix  $\mathbf{D}$  with positive entries and null diagonal

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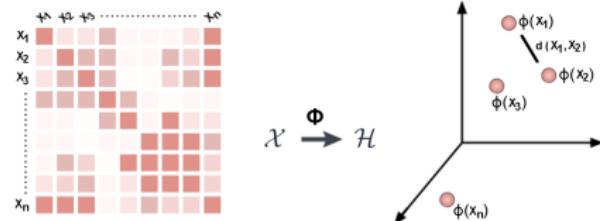
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networks/graphs: groups of  $n$  entities (nodes/vertices) linked by a (potentially weighted) relation (edges)

⇒ symmetric ( $n \times n$ )-matrix with positive entries and null diagonal  $\mathbf{W}$

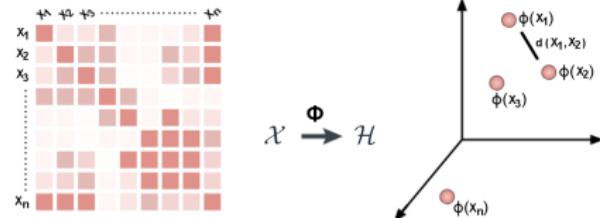


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Similarities between  $n$  entities: symmetric ( $n \times n$ )-matrix  $\mathbf{S}$  (with usually positive entries) but not necessarily definite positive

# 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]

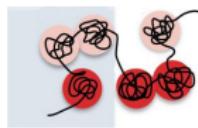
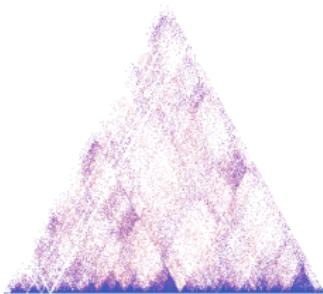
$\exists$  two Euclidean spaces  $\mathcal{E}_+$  and  $\mathcal{E}_-$  and two mappings  $\phi_+$  and  $\phi_-$  st:

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

# Application 1: Constrained Hierarchical Clustering



# Constrained clustering for genomic data



Hi-C data: **S**

- segmentation (or contiguous clustering) of the chromosome  
 $\Leftrightarrow$  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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- constrained hierarchical clustering for arbitrary similarities (or kernels) or dissimilarities (extends e.g., **rioja**)
- 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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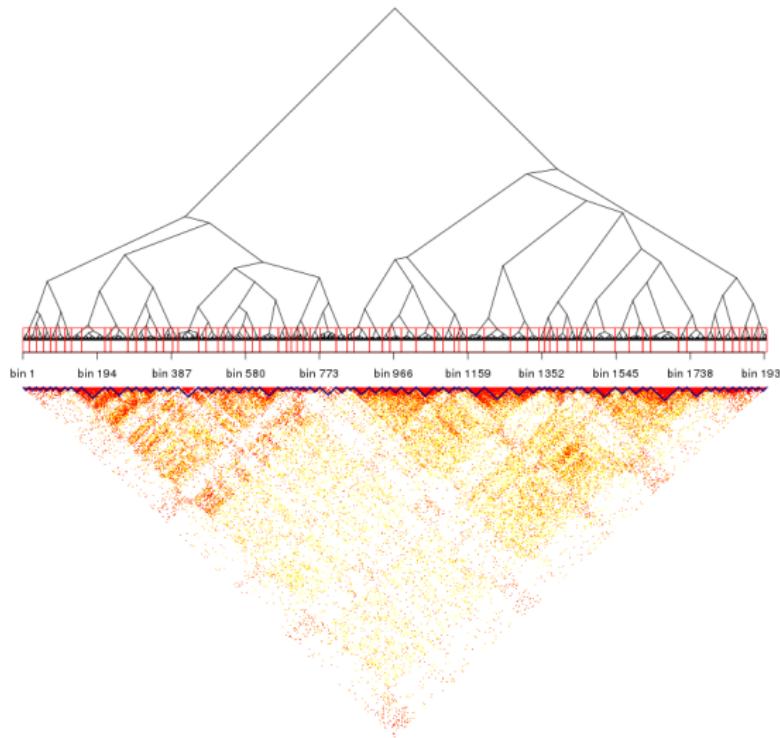
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## Icing on the cake:

- 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

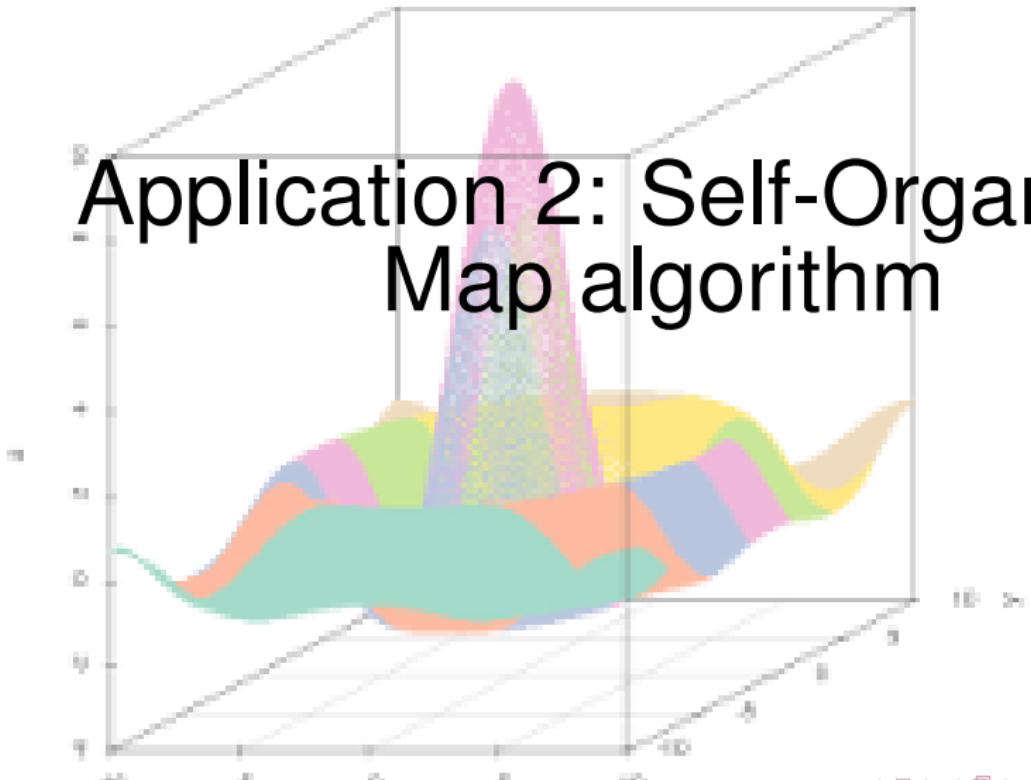
# Application to Hi-C data

with data from [Dixon et al., 2012]



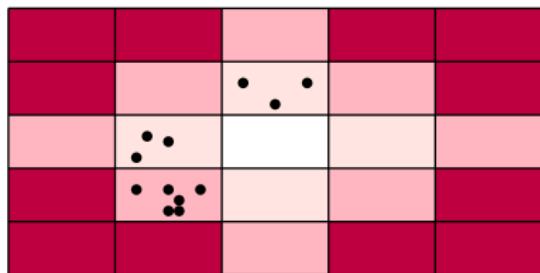
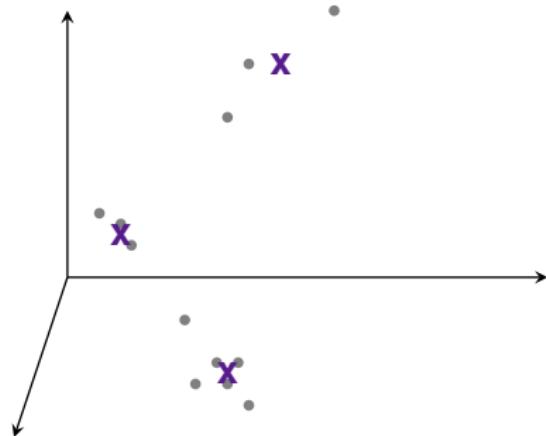
- constant average TAD size whatever the chromosome length
- similar results for broken stick and slope heuristic
- similar results for full and sparse (half - 1/10) versions

# Application 2: Self-Organizing Map algorithm



# Basics on (standard) stochastic SOM

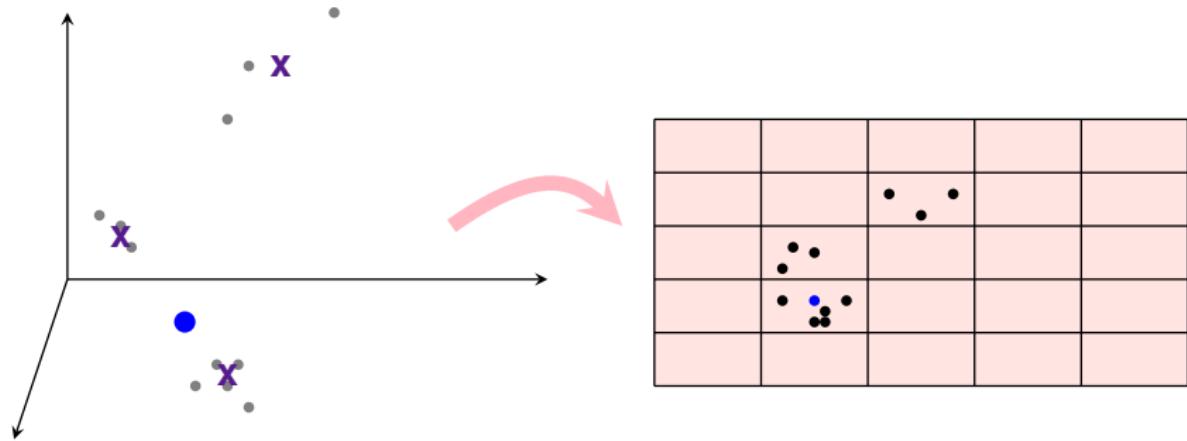
[Kohonen, 2001]



- $(x_i)_{i=1,\dots,n} \subset \mathbb{R}^d$  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

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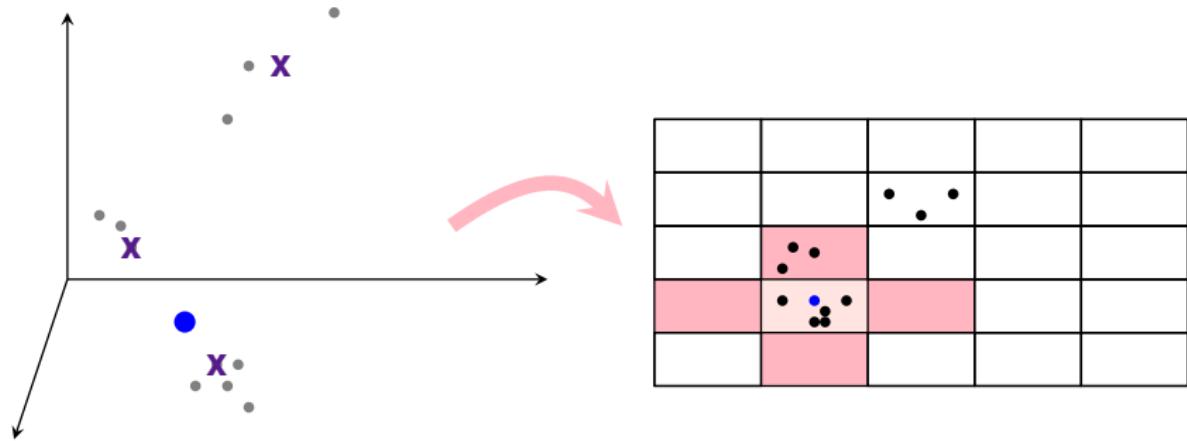


Iterative learning (assignment step):  $x_i$  is picked at random within  $(x_k)_k$  and affected to *best matching unit*:

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

# 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:

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7: **end for**

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

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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:

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

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

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

4:     Assignment

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

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**

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# 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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- 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!

SOMbrero Web User Interface (v0.1)

Select the data type: Numeric



Import Data Self-Organize Plot Map Superclasses Combine with external information Help

Third step: plot the self-organizing map

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.

Options

Plot what? Prototypes

Type of plot: polygon distances

Welcome to SOMbrero, the open-source on-line interface for self-organizing maps (SOM).



# Note on drawbacks of RSOM

Two main drawbacks:

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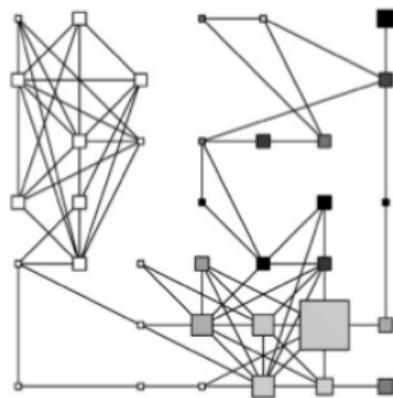
- For the non Euclidean case, the learning algorithm can be very unstable (saddle points)

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

# RSOM for mining a medieval social network

with the heat kernel

Individual  
Transaction



Graph induced by clusters:

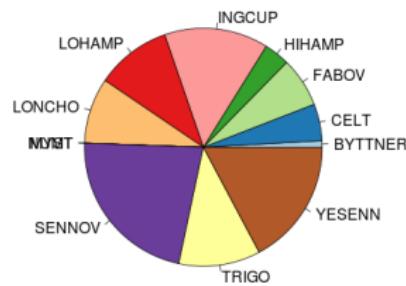
- has nice relations with space and time
- emphasizes leading people
- has helped to identify problems in the database (namesakes)

[Boulet et al., 2008]

But: biggest communities are still very complex

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

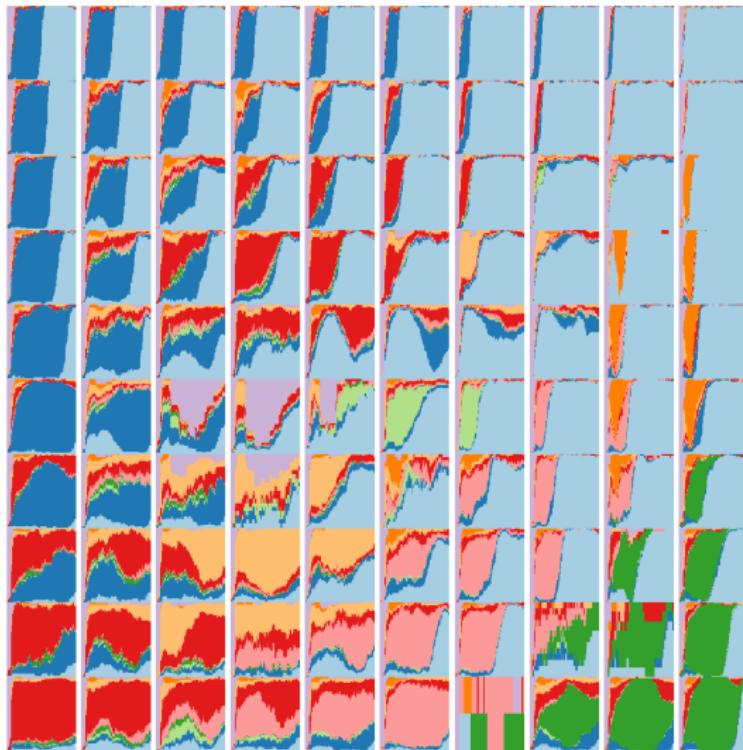
Edit distances between DNA sequences [Olteanu and Villa-Vialaneix, 2015a]



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

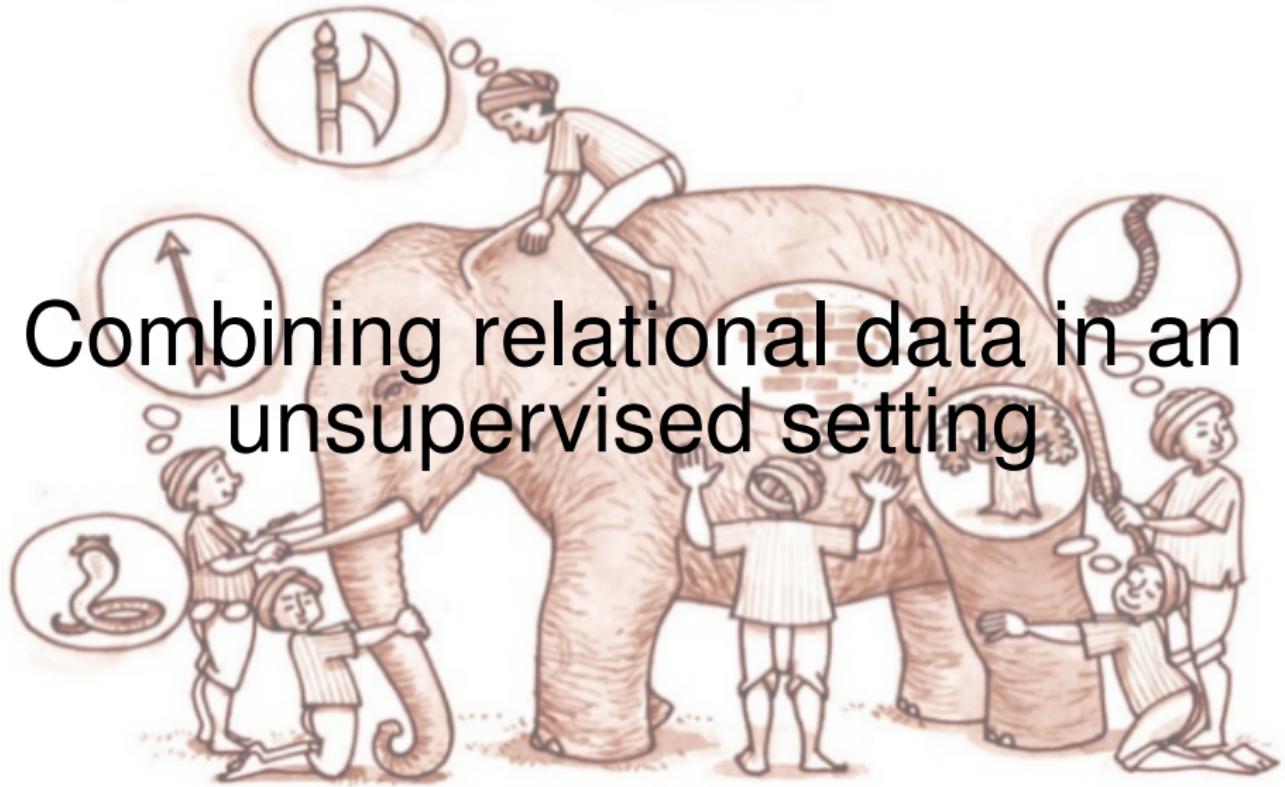
Edit distance between 12,000 categorical time series



- permanent-labor contract
- fixed-term contract
- apprenticeship contract
- public temporary-labor contract
- on-call contract
- unemployed
- inactive
- military service
- education



# Combining relational data in an unsupervised setting



# TARA Oceans datasets

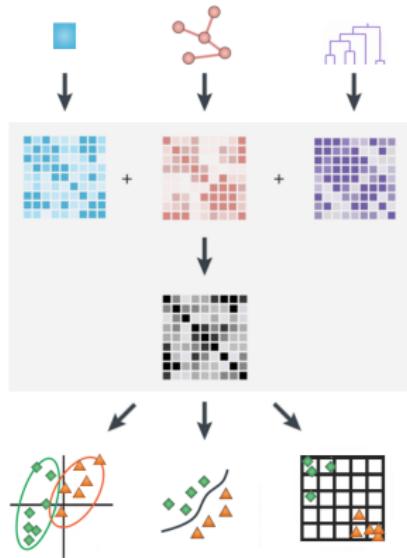


**TARA  
OCEANS**  
POLY  
EXPLORATION  
[www.tararesearch.org](http://tararesearch.org)

## 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 unifrac 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](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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$$\text{maximize}_{\mathbf{v}} \quad \sum_{m=1}^M \left\langle \mathbf{K}^*(\mathbf{v}), \frac{\mathbf{K}^m}{\|\mathbf{K}^m\|_F} \right\rangle_F = \mathbf{v}^\top \mathbf{C} \mathbf{v}$$

for  $\mathbf{K}^*(\mathbf{v}) = \sum_{m=1}^M v_m \mathbf{K}^m$  and  $\mathbf{v} \in \mathbb{R}^M$  such that  $\|\mathbf{v}\|_2 = 1$ .

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



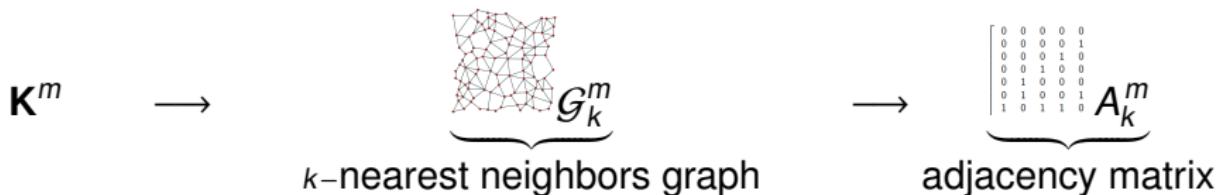
# A kernel preserving the original topology of the data I

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

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Proxy of the local geometry

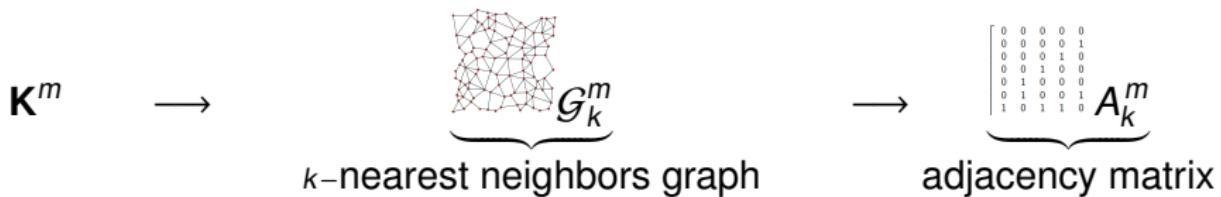


$$\Rightarrow W = \sum_m \mathbb{I}_{\{A_k^m > 0\}} \text{ or } W = \sum_m A_k^m$$

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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

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

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

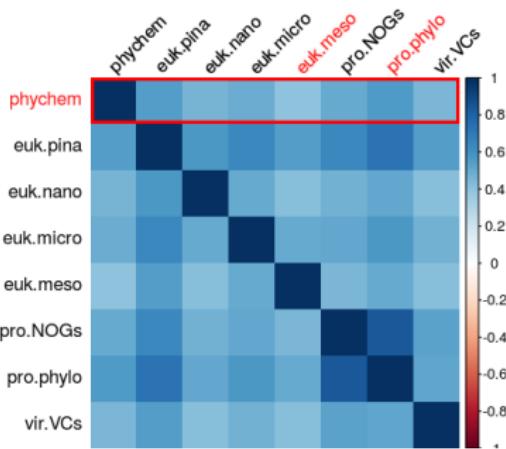
## Sparse version

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](#)])

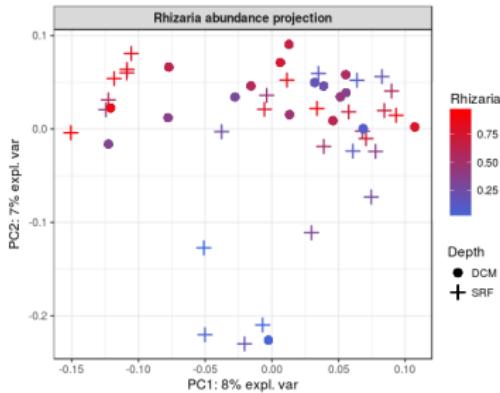
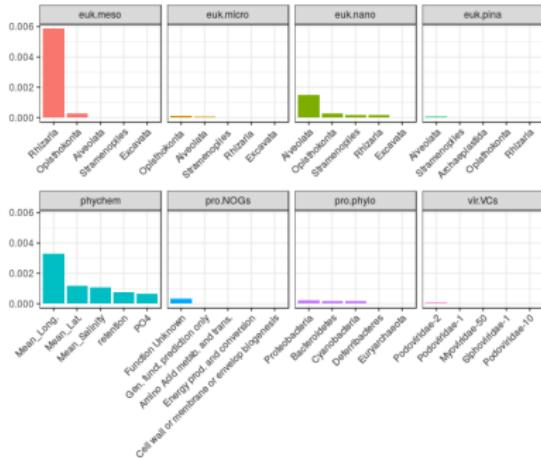
# Application to TARA oceans



## 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



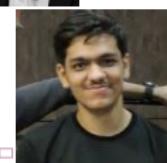
## SOMbrero and mixKernel



Jérôme Mariette

## adjclust

Pierre Neuville, Guillem Rigail, Christophe Ambroise and  
Shubham Chaturvedi





Toulouse  
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# Dendrogram corrections when reversals are detected

