Learning from (dis)similarity data

Nathalie Vialaneix

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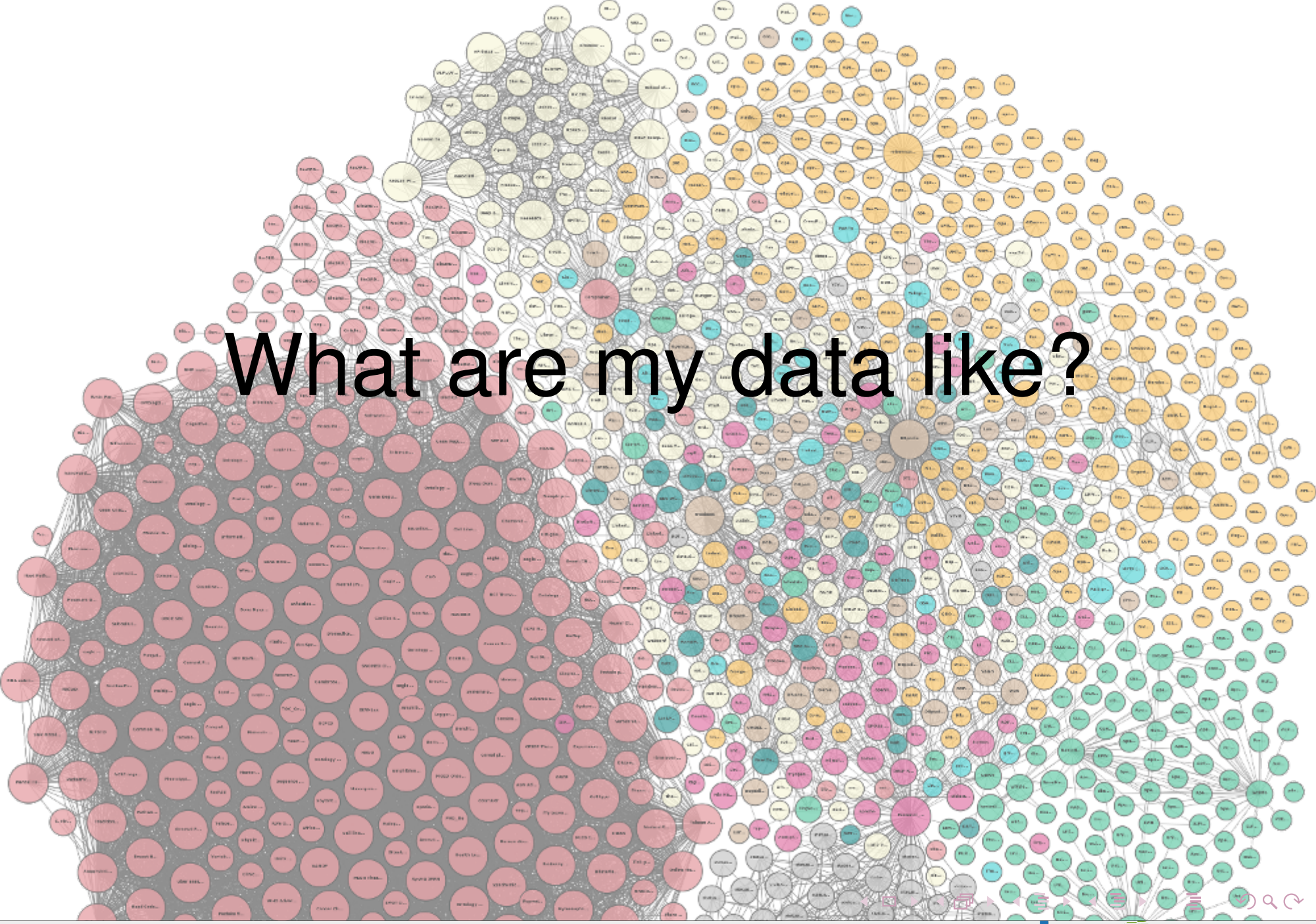
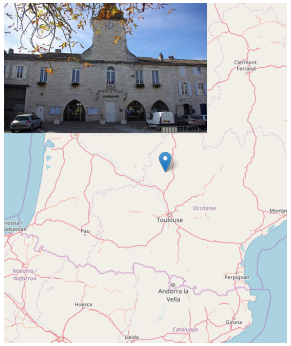
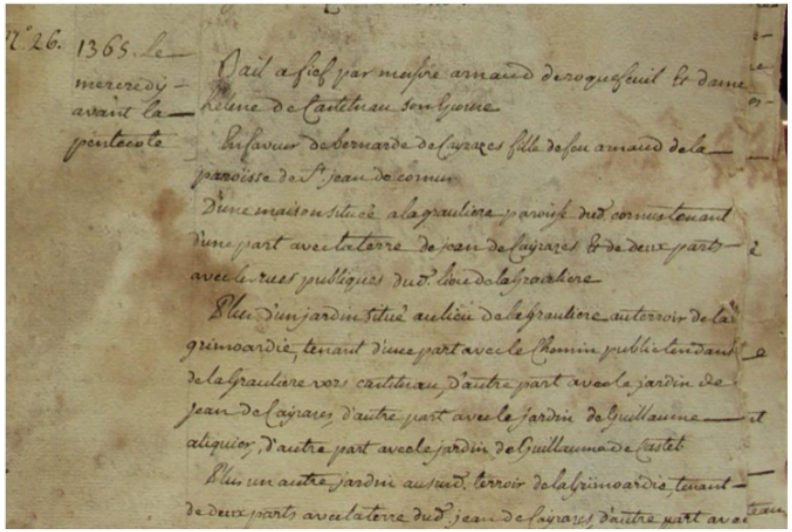


What are my data like?

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

tenancier, acteur de l'acte — paroisse

Bail à fief par messire Arnaud de Roquefeuil et Dame Hélène de Castelnau son épouse en faveur de Bernarde Cairazes, fille de feu Arnaud 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 Cairazes et de deux parts avec les rues publiques du dit lieu de La Graulière.

lieu dit — tenancier confront

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

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

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

notaire

seigneurs, acteurs de l'acte

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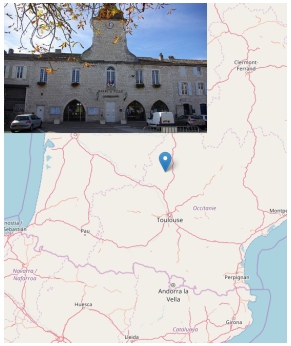

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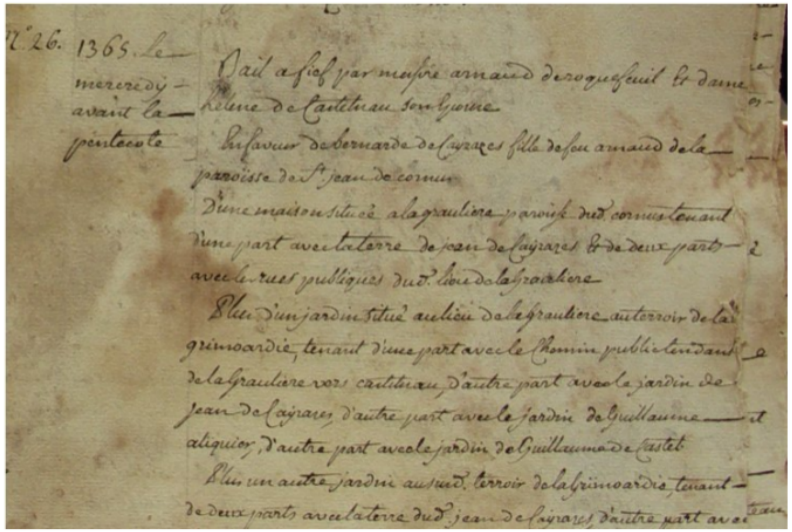

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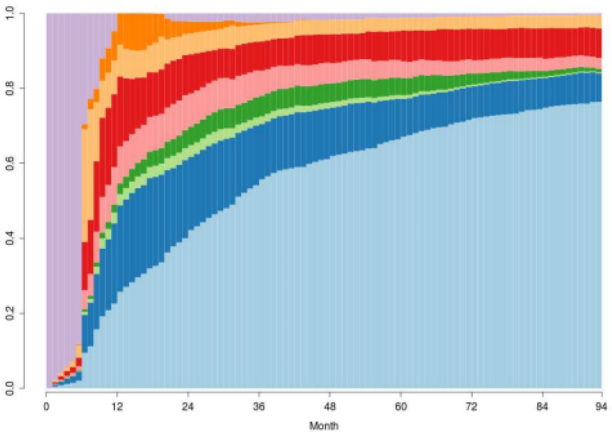
bipartite network with more than 17,000 nodes (∼ 10,000 individuals)

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. [1]



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

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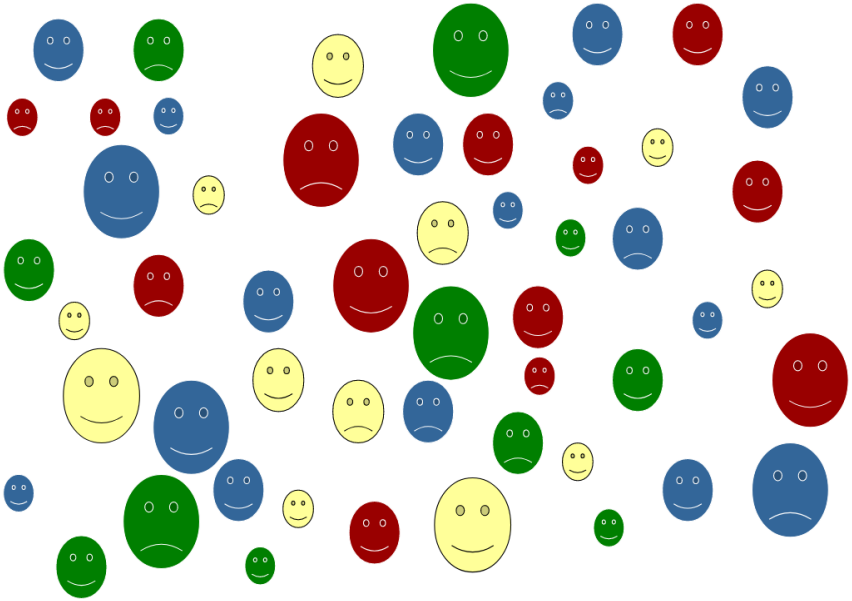

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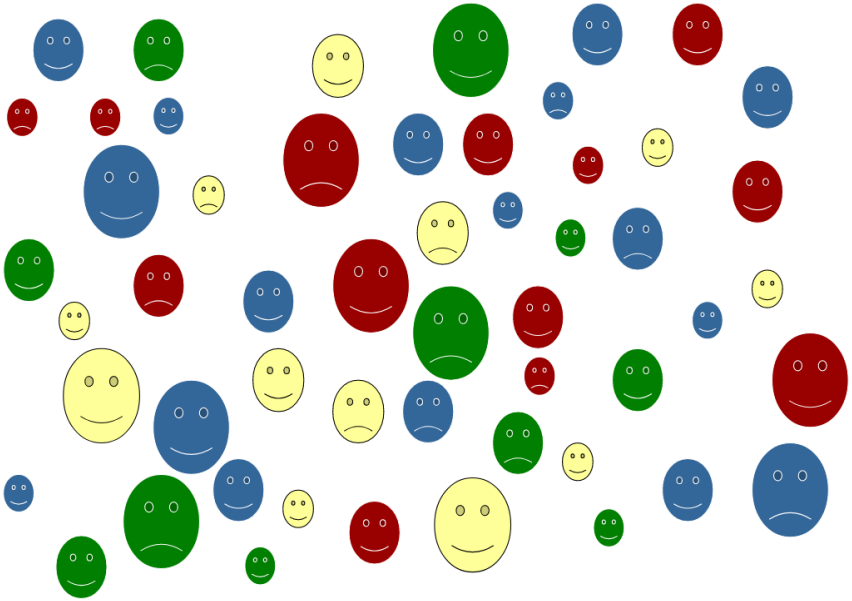

It is all about distance...

- χ^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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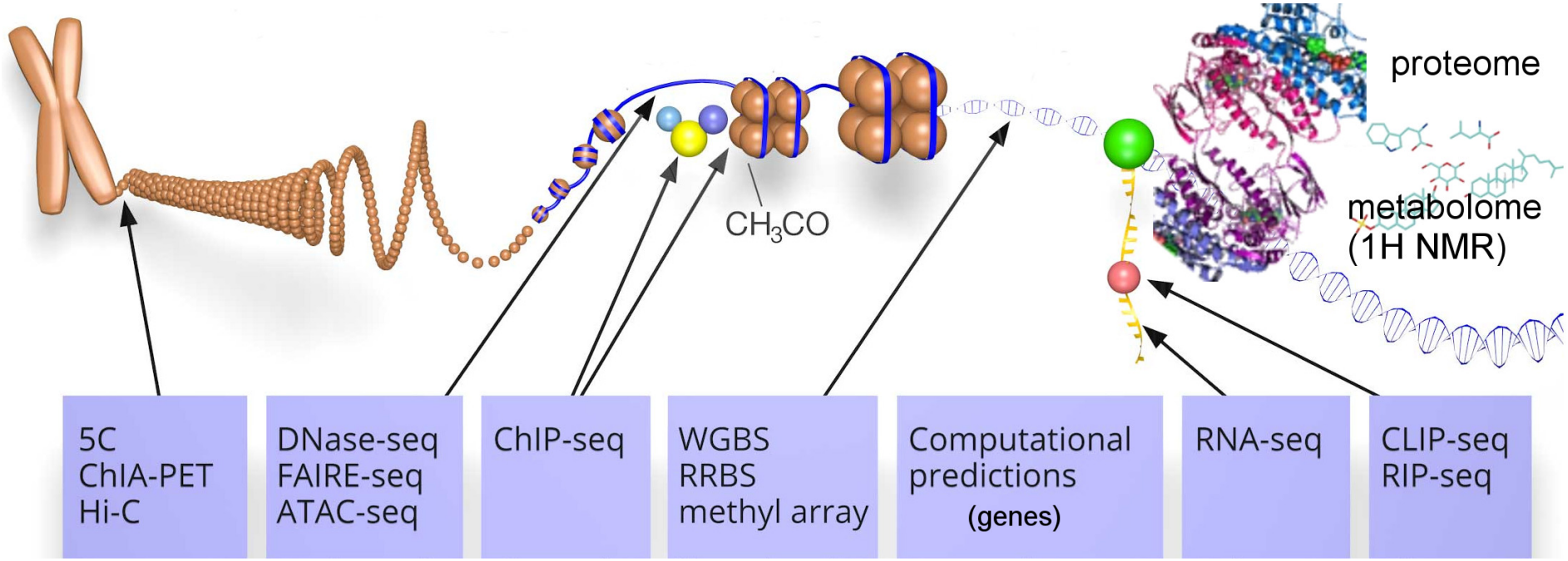
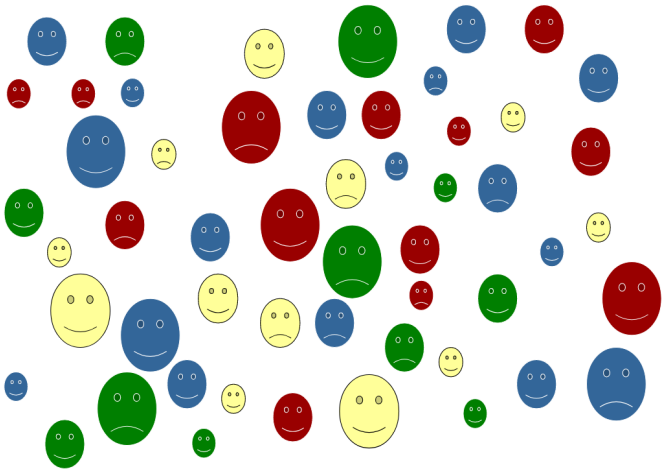
and then I went into NGS data...



and again...

distances are everywhere



a collection of NGS data...

DNA barcoding

Astraptes fulgerator

optimal matching (edit) distances to differentiate species

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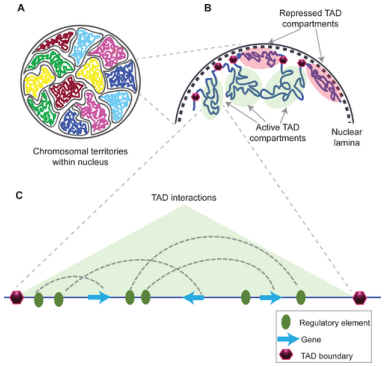
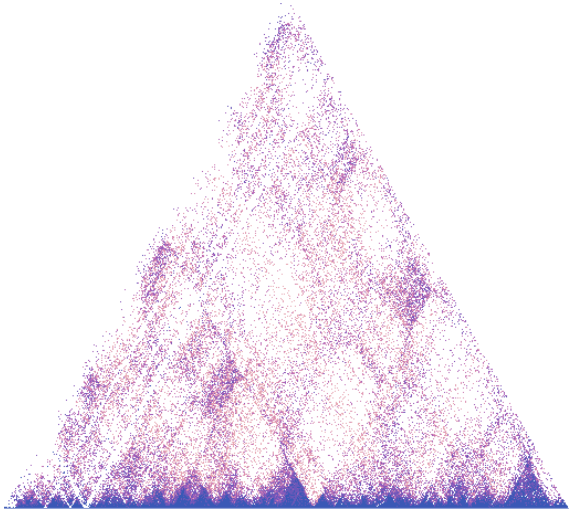
Hi-C data





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

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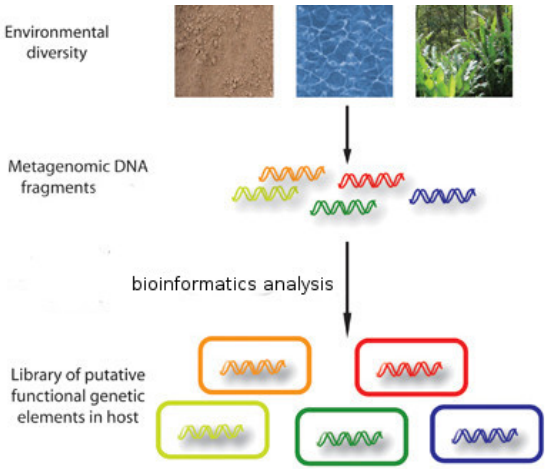

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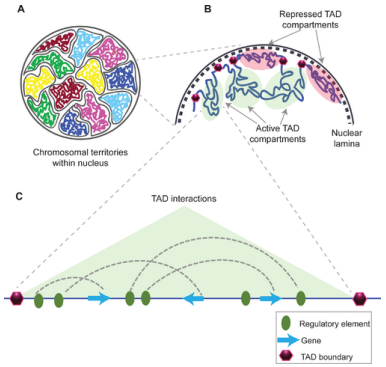

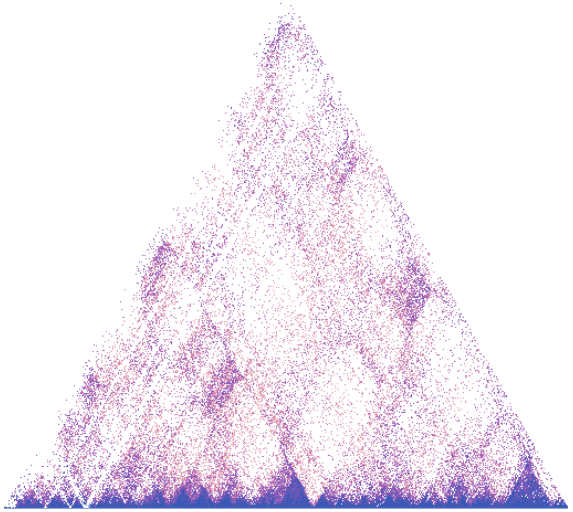

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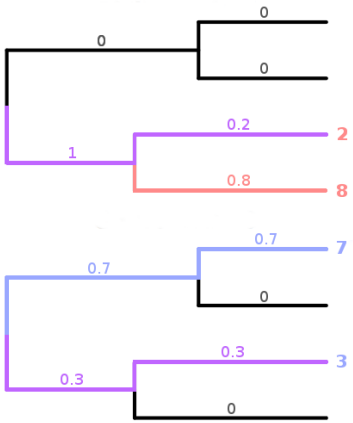

Metagenomics

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

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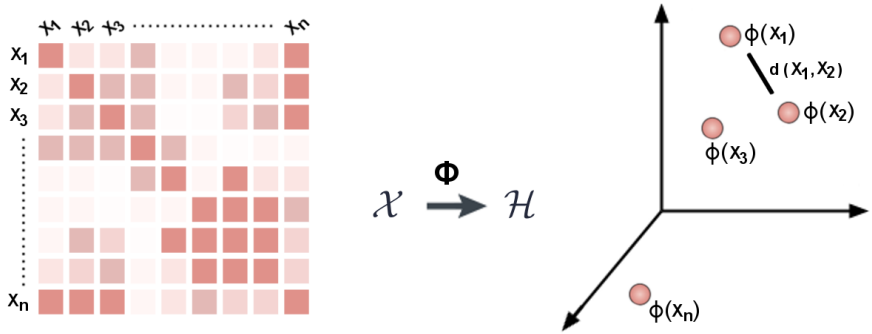
kernels: a symmetric and positive definite $(n \times n)$-matrix $\mathbf{K}$ that measures a "relation" between n entities in $\mathcal{X}$ (arbitrary space)



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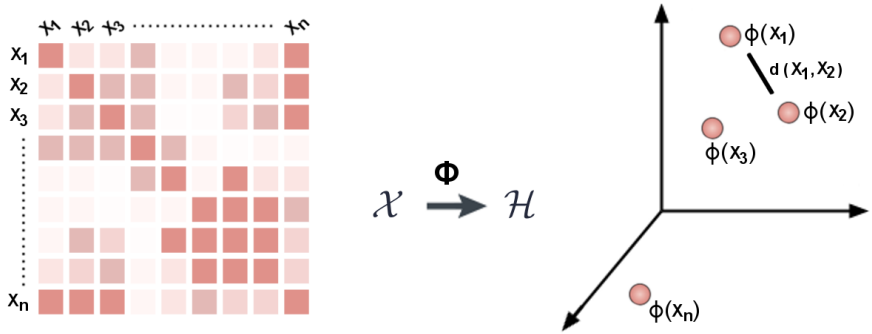

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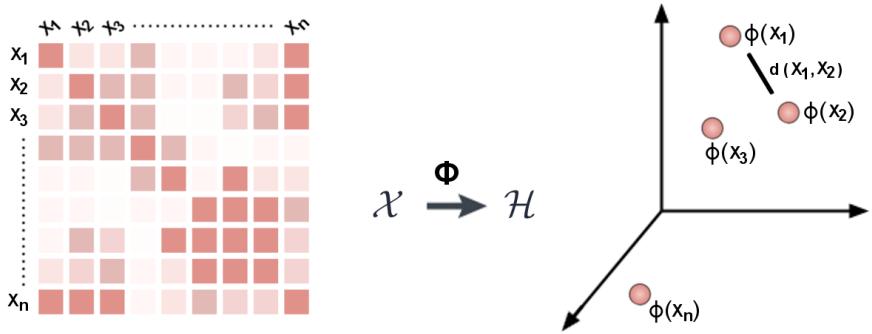

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Similarities between n entities: symmetric $(n \times n)$-matrix $\mathbf{S}$ (with usually positive entries) but not necessarily definite positive

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:

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

- 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 **K**)
rewrite all quantities using:

- **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...)

Principles for learning from relational data

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non Euclidean case (non Euclidean dissimilarity **D**): do almost the same using a pseudo-Euclidean framework

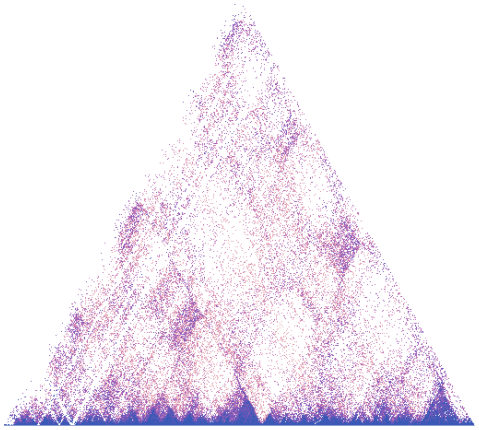
[Goldfarb, 1984]

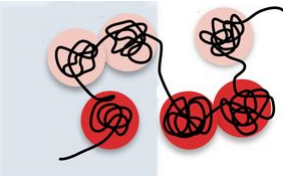
$\exists$ two Euclidean spaces $\mathcal{E}_+$ and $\mathcal{E}_-$ and two mappings ϕ_+ and ϕ_- st:

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

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

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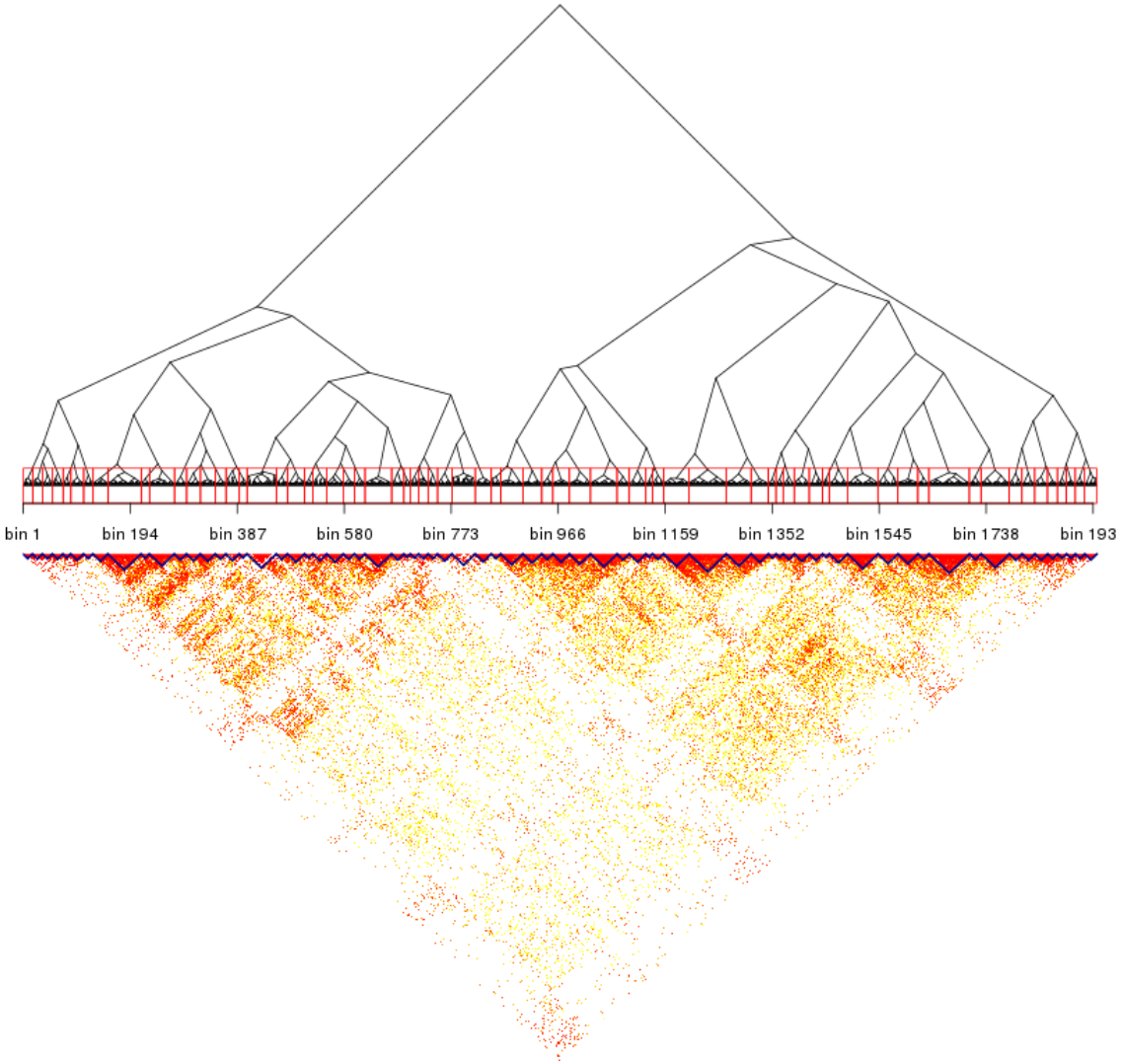
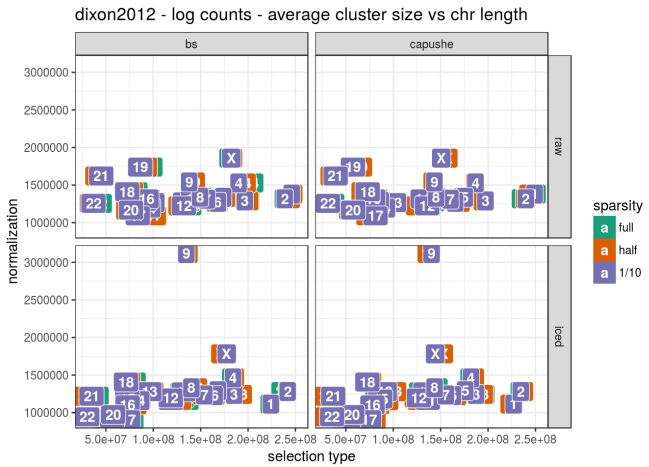
Icing on the cake:

- 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

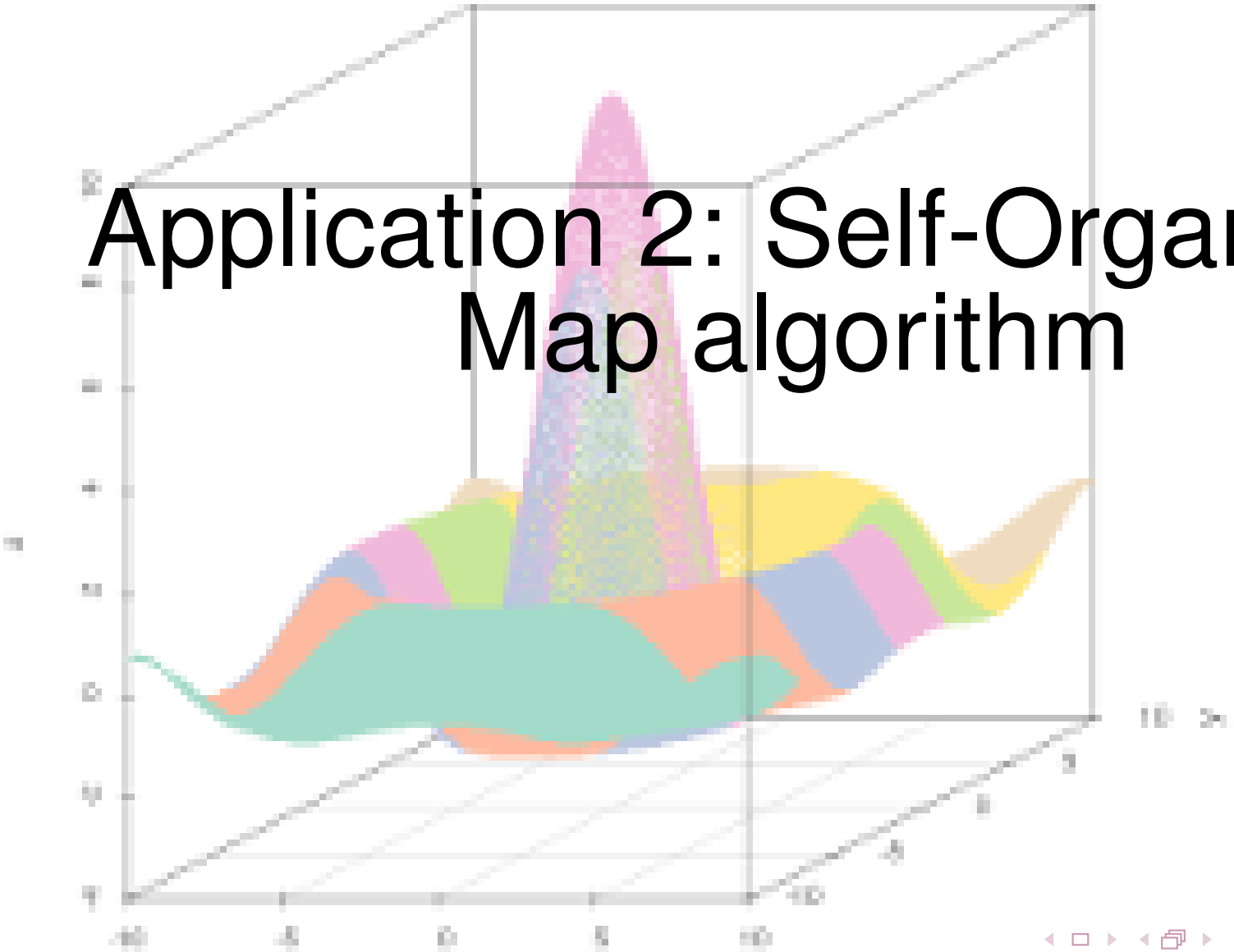
with data from **[Dixon et al., 2012]**





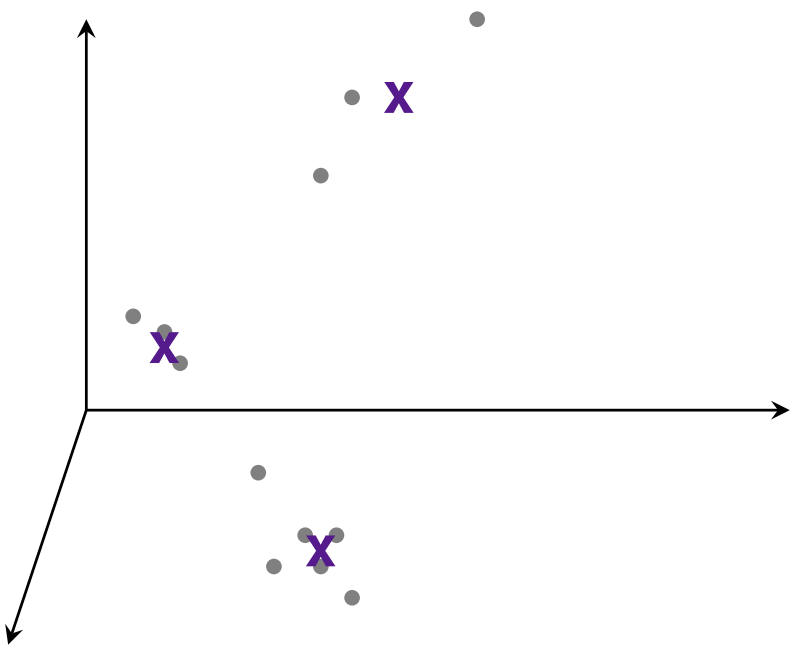
- constant average TAD size whatever the chromosome length
- similar results for broken stick and slope heuristic
- similar results for full and sparse (half - 1/10) versions

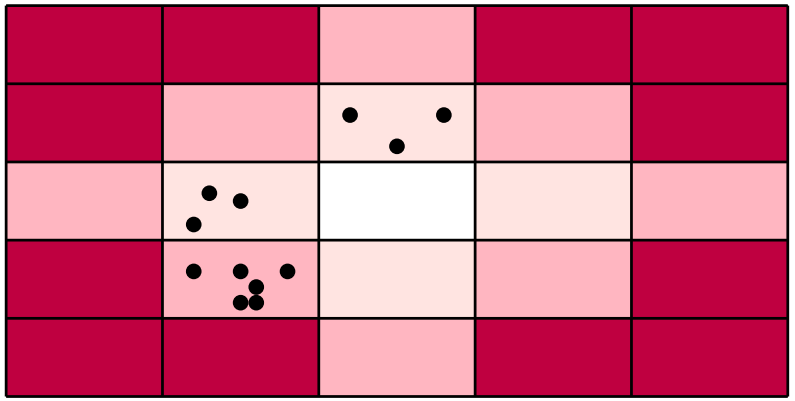
Application 2: Self-Organizing Map algorithm



Basics on (standard) stochastic SOM

[Kohonen, 2001]





- $(x_i)_{i=1,\ldots,n} \subset \mathbb{R}^d$ are affected to a unit $f(x_i) \in \{1, \ldots, U\}$
- 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 $\mathbb{R}^d$

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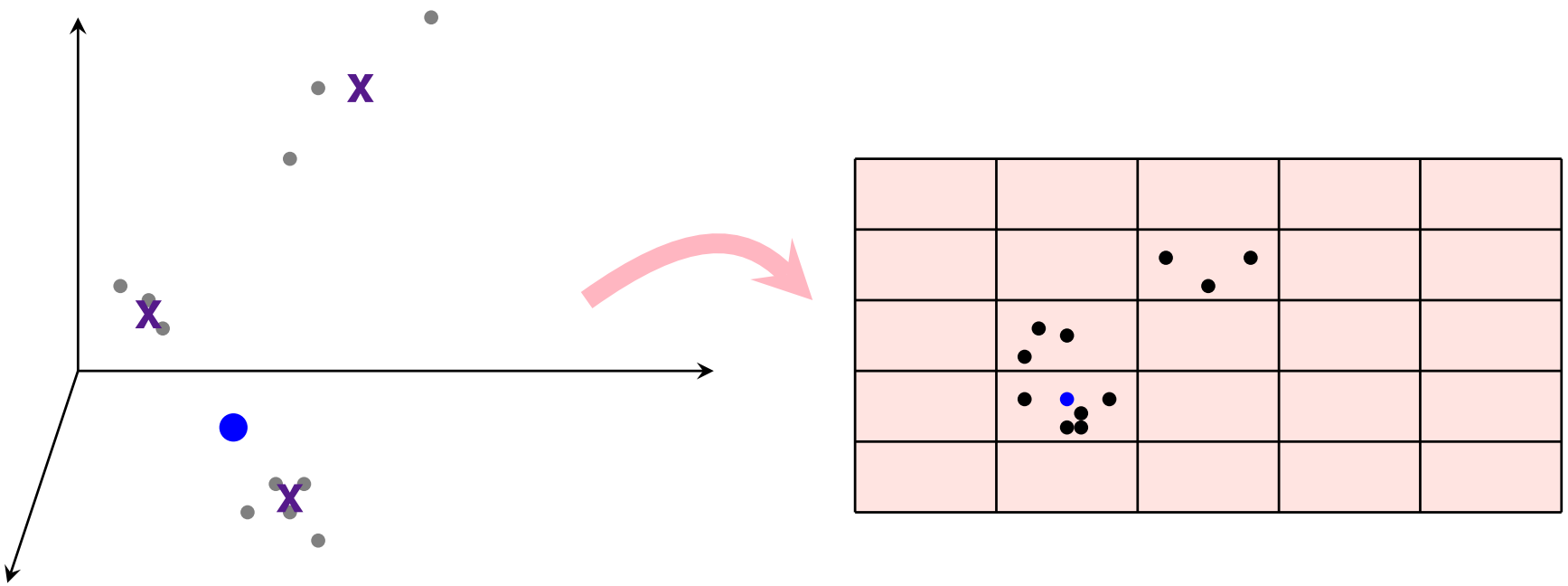

Iterative learning (assignment step): x_i is picked at random within $(x_k)_k$ and affected to *best matching unit*:

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

Basics on (standard) stochastic SOM

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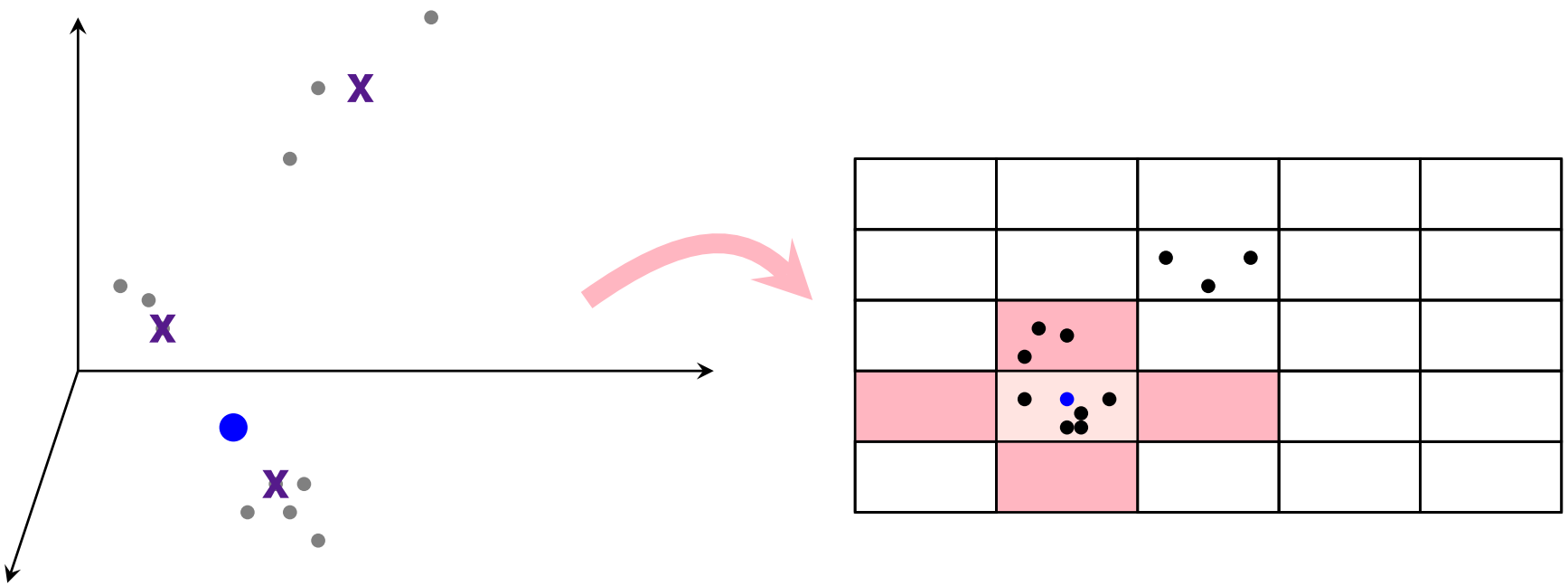

Iterative learning (representation step): all prototypes in neighboring units are updated with a gradient descent like step:

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

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, ..., 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:

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

7: **end for**
8: **end for**

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

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

6:

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

7: **end for**

8: **end for**

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** $t = 1 \to T$ **do**

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

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

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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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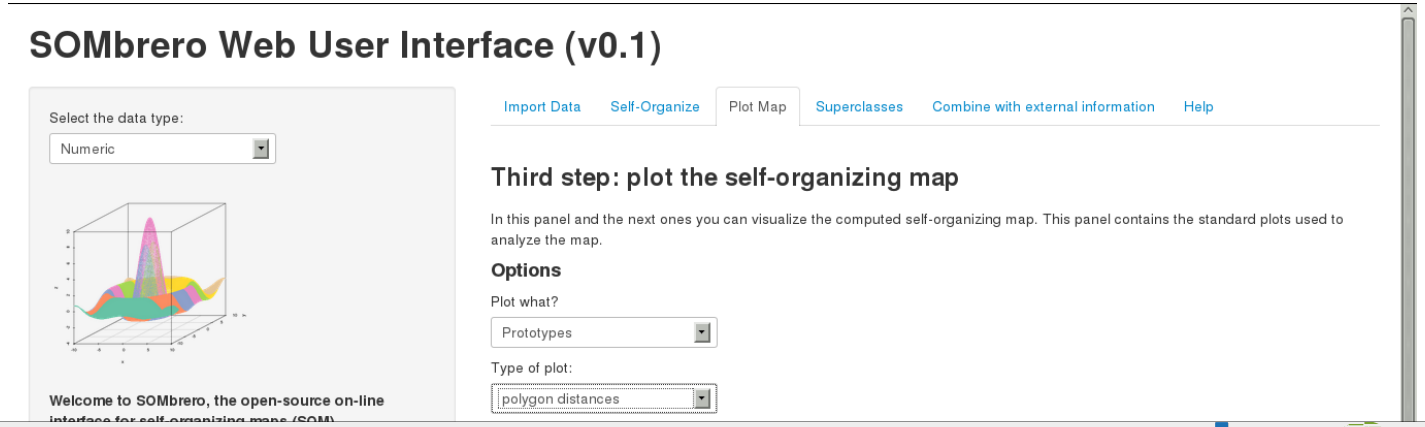
- Web User Interface (made with **shiny**) with `sombreroGUI()`

Tested on and approved by an historian!



Note on drawbacks of RSOM

Two main drawbacks:

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

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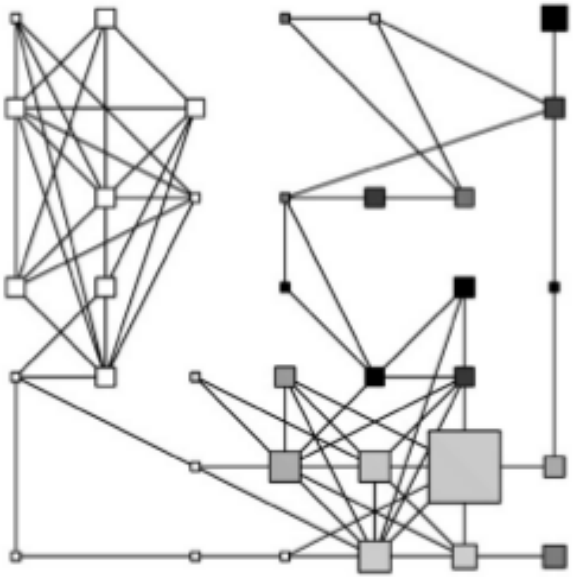
  clip or flip? **[Chen et al., 2009]**

RSOM for mining a medieval social network

with the heat kernel

[Boulet et al., 2008]



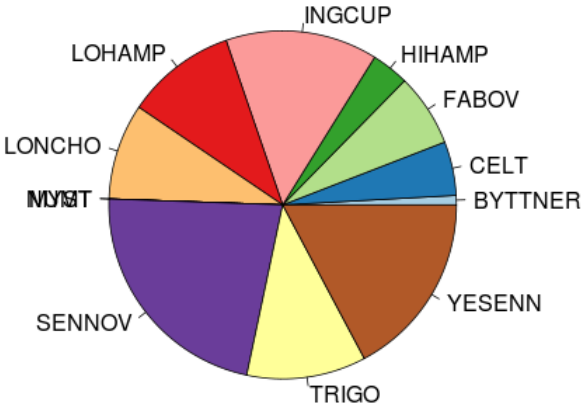
Graph induced by clusters:

- 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

RSOM for typology of *Astraptes fulgerator* from DNA barcoding

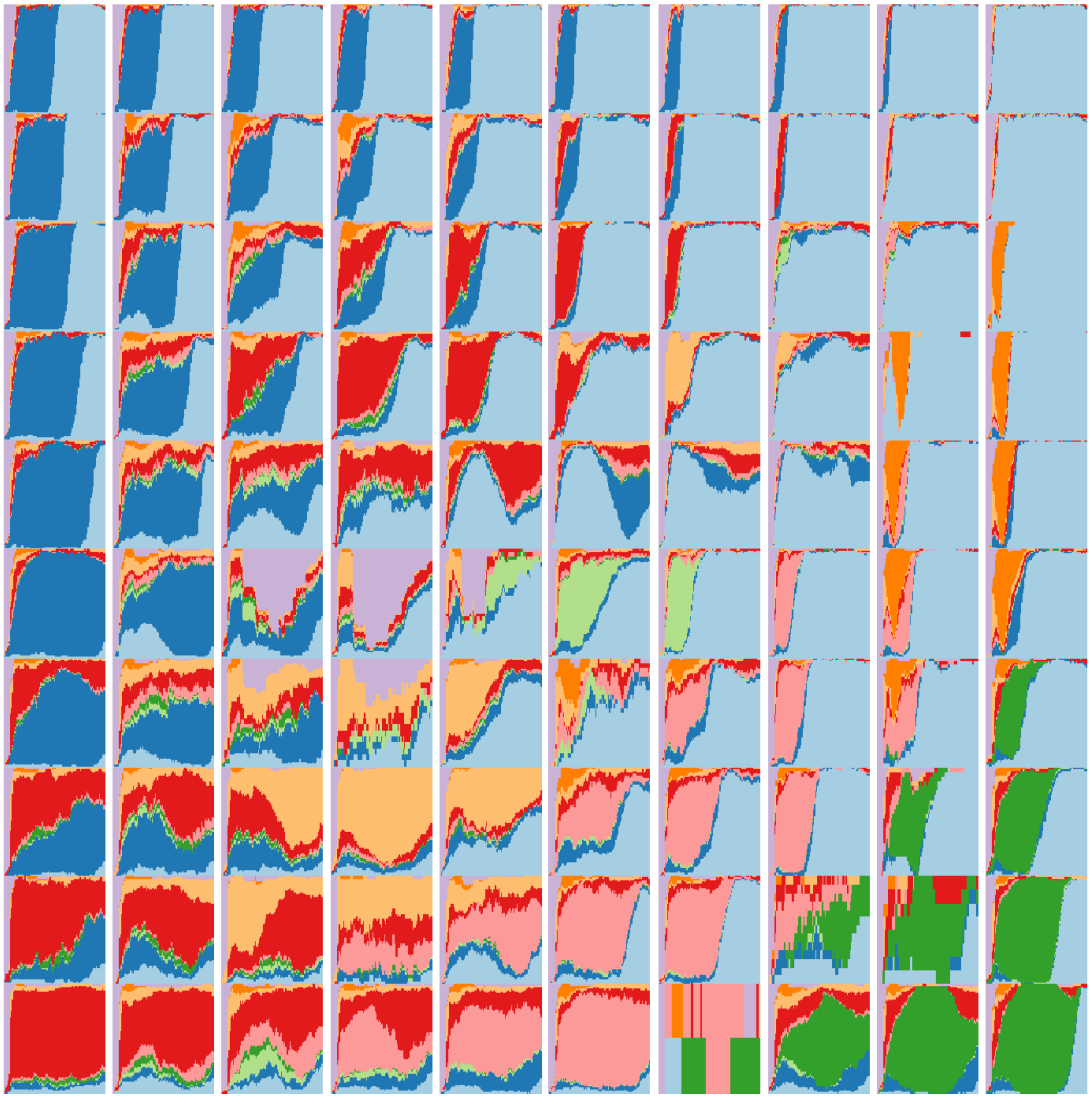
Edit distances between DNA sequences **[Olteanu and Villa-Vialaneix, 2015a]**



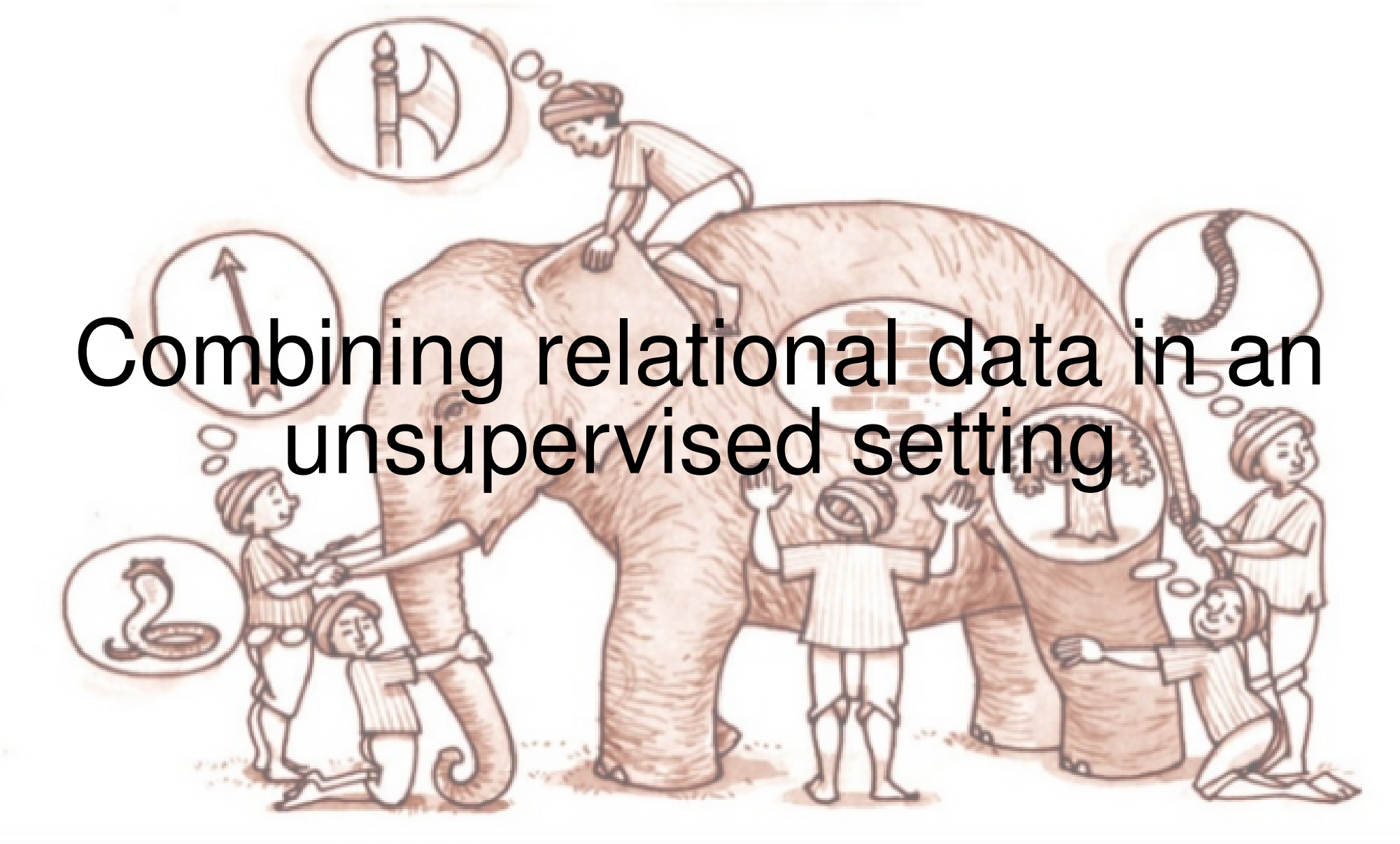
Almost perfect clustering (identifying a possible label error on one sample) with (in addition) information on relations between species.

RSOM for typology of school-to-time transitions

Edit distance between 12,000 categorical time series

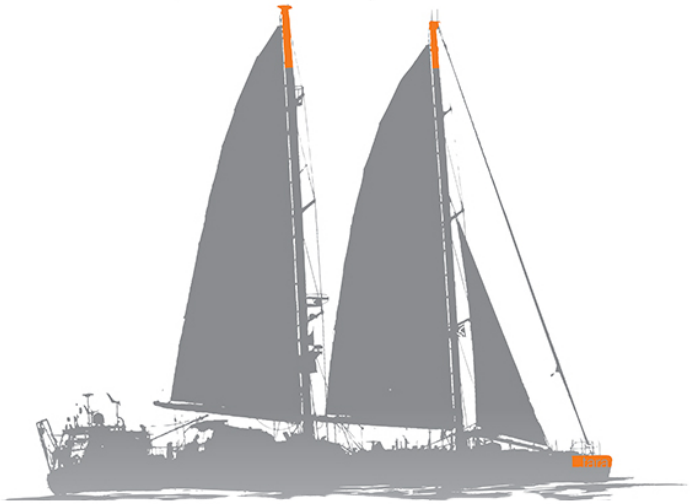


- permanent-labor contract
- fixed-term contract
- apprenticeship contract
- public temporary-labor contract
- on-call contract
- unemployed
- inactive
- military service
- education



Combining relational data in an unsupervised setting

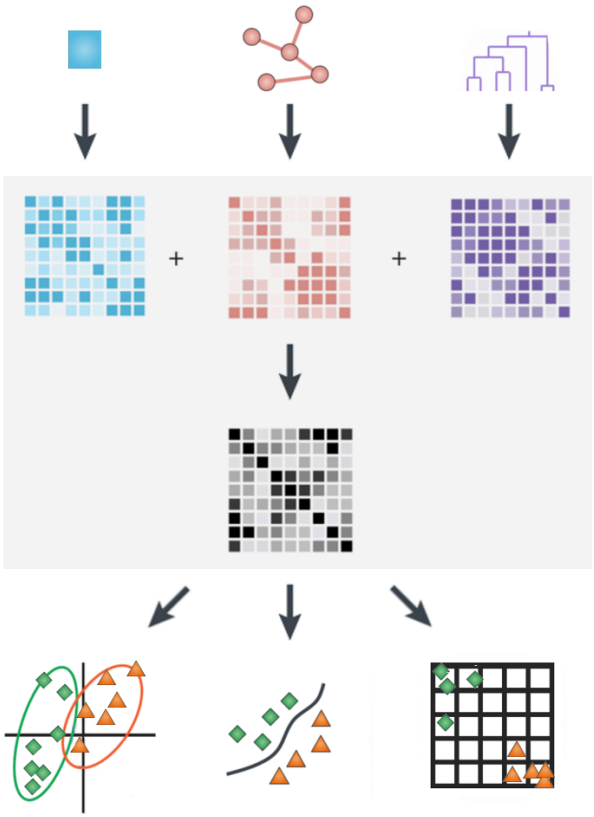
TARA Oceans datasets



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

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

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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

$$\mathbf{K}^m \longrightarrow \underbrace{\mathcal{G}_k^m}_{k-\text{nearest neighbors graph}} \longrightarrow \underbrace{A_k^m}_{\text{adjacency matrix}}$$

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

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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

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

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

Non sparse version

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

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A kernel preserving the original topology of the data II

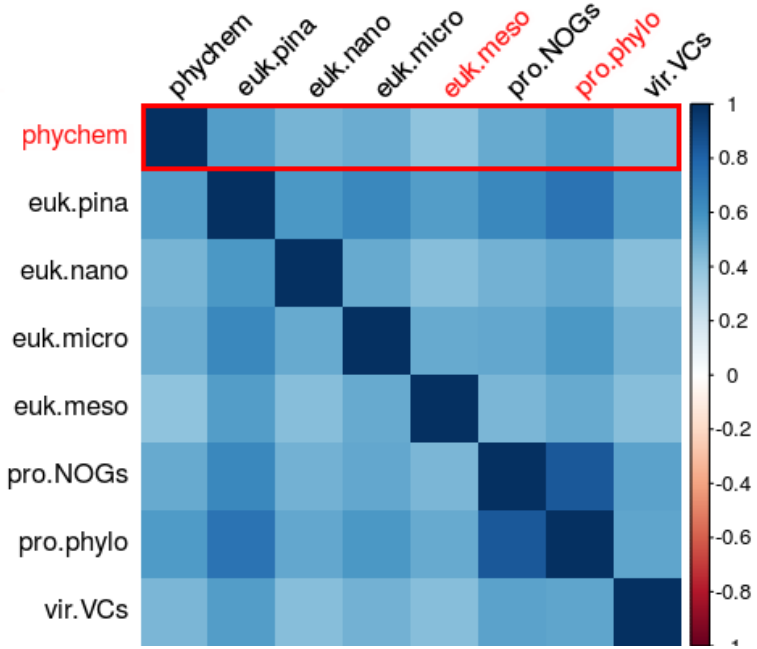
Sparse version

equivalent to a standard QP problem with linear constrains (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])

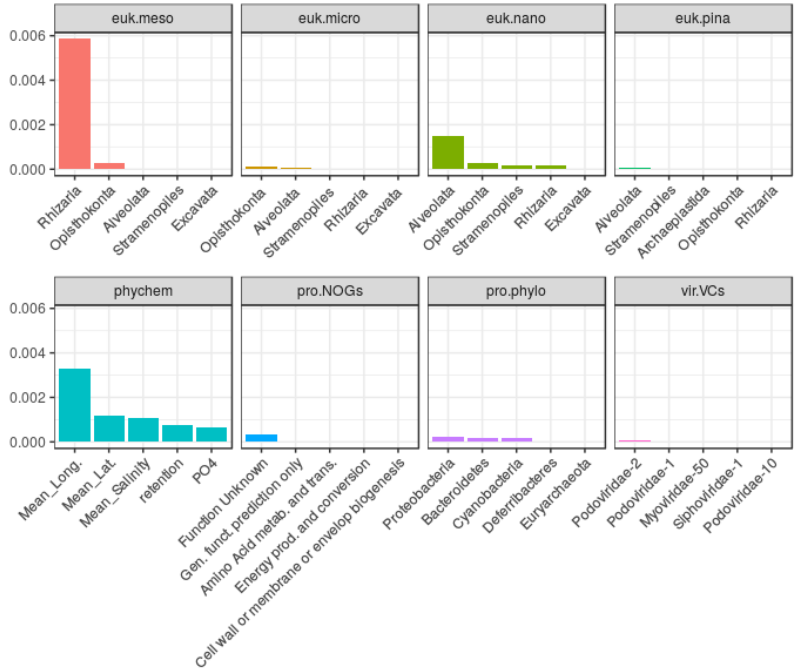
Application to *TARA* oceans

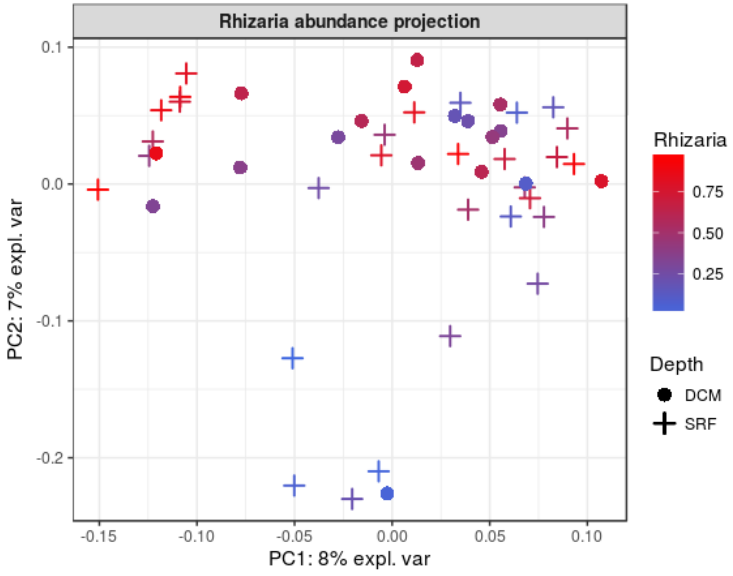


Similarity between datasets (STATIS)

- **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

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Credits for pictures

- Slide 2: Linking Open Data cloud diagram 2017, by Andrejs Abele, John P. McCrae, Paul Buitelaar, Anja Jentzsch and Richard Cyganiak. http://lod-cloud.net/
- Slide 3: Picture of Castelnau Montratier from https://commons.wikimedia.org/wiki/File:Place_Gambetta,_Castelnau-Montratier.JPG by Duch.seb CC BY-SA 3.0
- Slide 4: image based on ENCODE project, by Darryl Leja (NHGRI), Ian Dunham (EBI) and Michael Pazin (NHGRI)
- Slide 6: *Astraptes* picture is from https://www.flickr.com/photos/39139121@N00/2045403823/ by Anne Toal (CC BY-SA 2.0), Hi-C experiment is taken from the article Matharu *et al.*, 2015 DOI:10.1371/journal.pgen.1005640 (CC BY-SA 4.0) and metagenomics illustration is taken from the article Sommer *et al.*, 2010 DOI:10.1038/msb.2010.16 (CC BY-NC-SA 3.0)
- Slide 12: TADS picture is from the article Fraser *et al.*, 2015 DOI:10.15252/msb.20156492 (CC BY-SA 4.0)
- Slide 27: Adjacency matrix image from: By S. Mohammad H. Oloomi, CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=35313532

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Dendrogram corrections when reversals are detected