Contribution à l'analyse de données non vectorielles

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Overview of the topics

data: non vectorial data,
high dimension...
methods: machine learning & data
mining, kernel methods, neuronal
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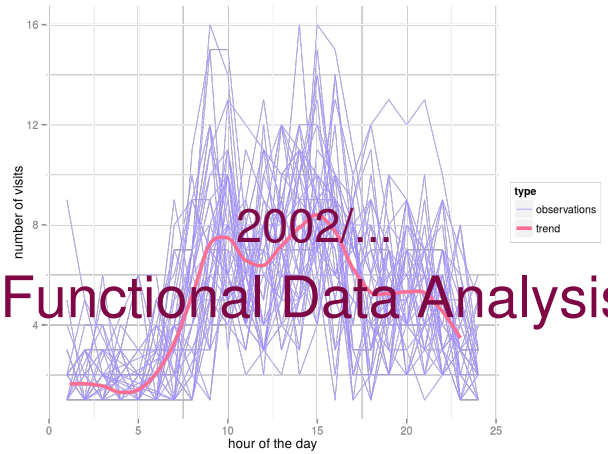
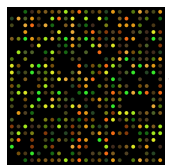


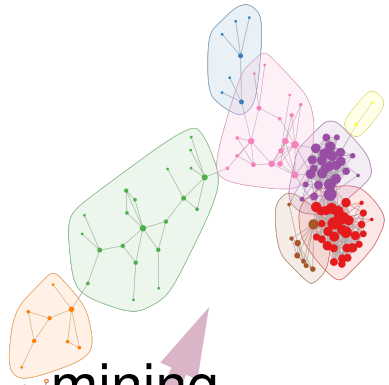
2002/...

Functional Data Analysis



inference

2012/...



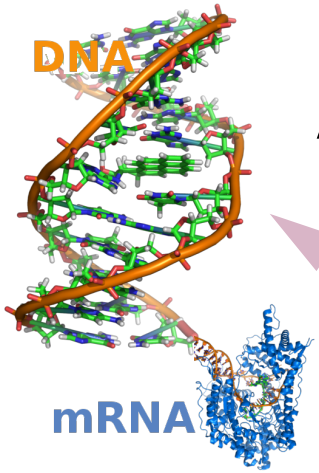
mining

visualization, clustering

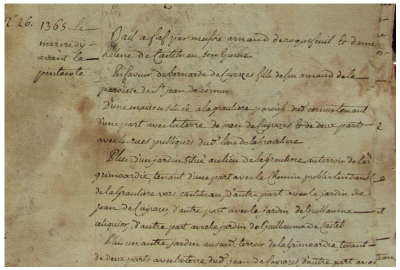
2006/...

Graph/Network

Overview of the topics



Applications in biology



Applications in human sciences

data: non vectorial data, high dimension...

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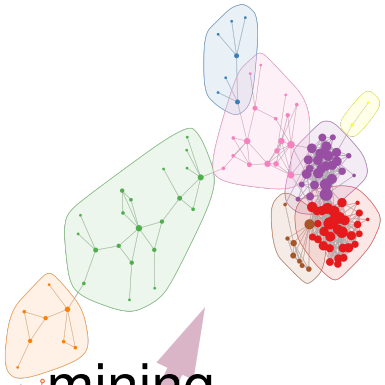

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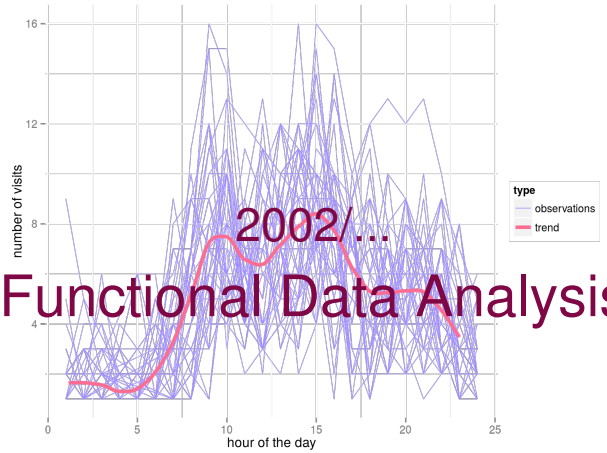

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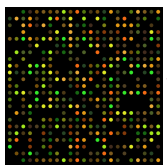

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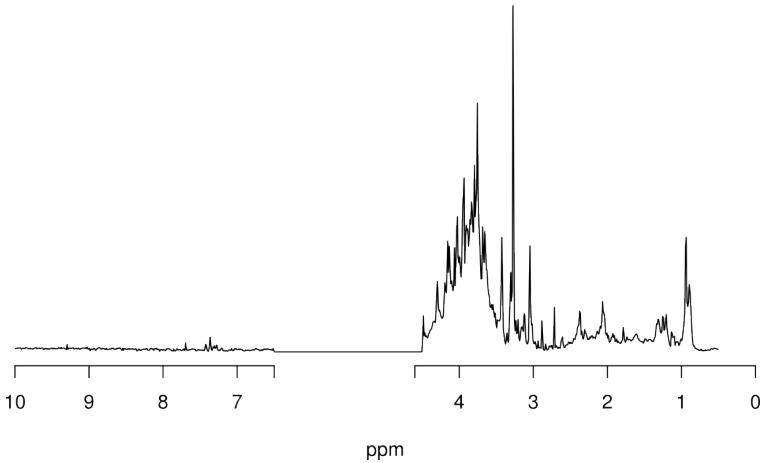
Functional Data Analysis

FDA framework and examples

Observations of a random variable X taking values in a space of functions $\mathcal{X}$ (typically, an infinite dimensional Hilbert space as L^2):
$x_1, \ldots, x_n$.
The function is observed at $t_{i1}, \ldots, t_{id_i}$.



Applications in: time series analysis, speech recognition, biochemistry (NIR spectra for instance), metabolomic data (NMR), weather data...

Typical issues in FDA

1. variance operator used in standard model does not have a continuous inverse: $\Gamma_X = \mathbb{E}(X \otimes X) - \mathbb{E}(X) \otimes \mathbb{E}(X)$ is a Hilbert Schmidt operator
   $\Rightarrow \Gamma_X^{-1}$ is not bounded.
   As a consequence, $\Gamma_X^n = \frac{1}{n} \sum_i x_i \otimes x_i - \overline{x} \otimes \overline{x}$ is ill-conditionned (and its inverse a bad estimate of Γ_X^{-1}).
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   $\Rightarrow$ regularization or penalization techniques are needed.
2. $(x_i)_i$ are never perfectly observed and only a digitized (sometimes noisy) estimation is available.
   $\Rightarrow$ reconstruction techniques are needed to provide a functional representation of the data, remove noise and measurement artefacts (translation, scaling, ..., of the functions).

Overview of my contributions

Supervised learning framework

(X, Y) st $X \in \mathcal{X}$, $Y \in \mathbb{R}$ (regression) or $Y \in \{-1, 1\}$ (binary classification).
Observations: $(x_i, y_i)_{i=1,\dots,n}$
Purpose: estimate $\hat{y}$ for a new x. $(x_i, y_i)_i$ is used to define a prediction function Φ^n.

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- Inverse methods use $\mathcal{L}(X|Y)$ to estimate $\mathcal{L}(Y|X)$
  - [2] (Ferré & Villa, *Scandinavian Journal of Statistics* , 2006) in the FIR (Functional Inverse Regression) model

$$Y = F\left(\langle X, \beta_1 \rangle, \dots, \langle X, \beta_d \rangle, \epsilon\right),$$

with F and $(\beta_j)_j$ to be estimated, smooth estimation of the $(\beta_j)_j$ combined with the estimation of F by multi-layer perceptron.

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  - [3] (Hernández, *et al.*, *Statistica Sinica*, 2014) calibration problem in chemiometry: under the assumption that $\mathcal{L}(X|Y)$ is Gaussian, estimation of

$$f(x|y) = \exp\left[\sum_{j\geq 1} \frac{r_j(y)}{\lambda_j}\left(x_j - \frac{r_j(y)}{2}\right)\right]$$

which is used in a plug-in estimate of $\mathbb{E}(Y|X = x)$.

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  - [3] (Hernández, *et al.*, *Statistica Sinica*, 2014)
- Kernel methods (less sensitive to high dimension, can include some functional pre-processing)
  - [6] (Rossi & Villa, *Neurocomputing*, 2006) SVM for functional data analysis
  - [8] (Rossi & Villa-Vialaneix, *Pattern Recognition Letter*, 2011) derivative-based kernel methods for functional classification and regression

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- [5, 12], (Rohart, *et al.*, *Journal of Animal Science*, 2012), (Villa-Vialaneix, *et al.*, *Communication in Statistics*, 2014) biomarker identification from metabolomic (NMR) data using functional approaches

Kernels for functional data

Given $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ st

- symmetry: $K(x, x') = K(x', x)$
- positivity: $\forall\, N \in \mathbb{N}, \forall\, (\alpha_i) \subset \mathbb{R}^N, \forall\, (x_i) \subset \mathcal{X}^N, \sum_{i,j} \alpha_i \alpha_j K(x_i, x_j) \geq 0.$

$\exists!\ (\mathcal{H}, \langle ., . \rangle_{\mathcal{H}})$ (RKHS) and $\Psi : \mathcal{X} \to \mathcal{H}$ st $K(x, x') = \langle \Psi(x), \Psi(x') \rangle_{\mathcal{H}}$

General form for FD

pre-processing: $\mathcal{P} : \mathcal{X} \to \mathcal{D}$

$$\forall\, x, x' \in \mathcal{X}, Q(x, x') = K(\mathcal{P}(x), \mathcal{P}(x')).$$

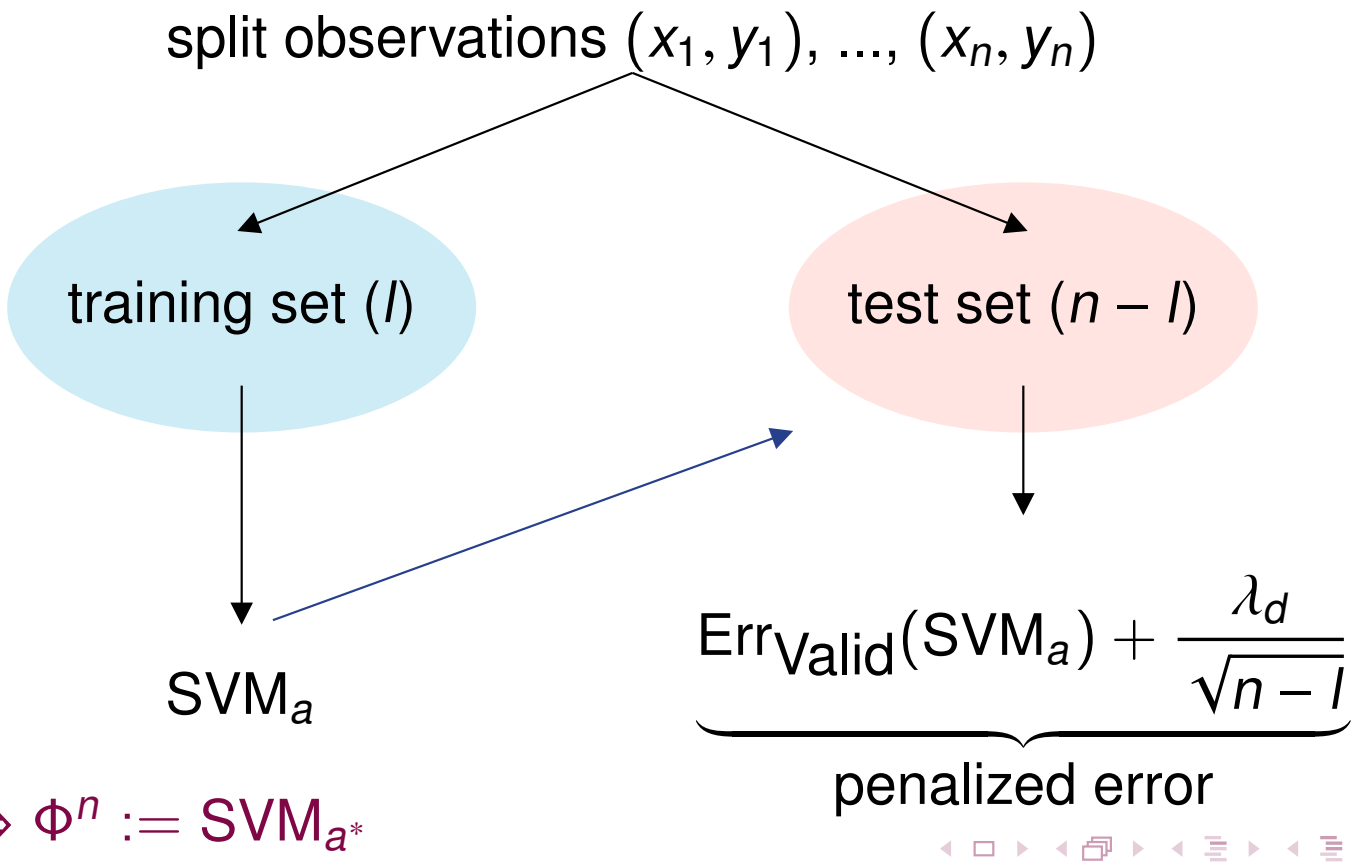
1. projections: for $V_d = \text{Vect}\{\psi_1, \ldots, \psi_d\}$, $\mathcal{P}(x) = \sum_{j=1}^{d} \langle x, \psi_j \rangle \psi_j$ (and $K = K_d$, standard kernel on $\mathbb{R}^d$).
2. functional transformation: $\mathcal{P}(x) = D^q x, \ldots$
3. FIR...

A consistent approach

[6] (Rossi & Villa, *Neurocomputing*, 2006)

SVM for functional data: $(X, Y) \in \mathcal{X} \times \{-1, 1\}$ with kernel $Q = K_d \circ \mathcal{P}_{V_d}$, K_d standard kernel on $\mathbb{R}^d$

selection of $a = (d, K_d, C) \in \mathbb{N} \times \mathcal{I}_d \times [0, C_d]$:



$\Rightarrow \Phi^n := \mathrm{SVM}_{a^*}$

Assumptions

[6] (Rossi & Villa, *Neurocomputing*, 2006)

Assumptions on the law of X

(A1) X takes its values in a bounded subspace of $\mathcal{X}$.

Assumptions on the parameters: $\forall\, d \geq 1$,

(A2) $\mathcal{J}_d$ is a finite set;
(A3) $\exists K_d \in \mathcal{J}_d$ (kernels on $\mathbb{R}^d$) st: K_d is universal and
$\exists \nu_d > 0 : \ \mathcal{N}(K_d, \epsilon) = \mathcal{O}(\epsilon^{-\nu_d})$;
(A4) $C_d > 1$;
(A5) $\sum_{d\geq 1} |\mathcal{J}_d| e^{-2\lambda_d^2} < +\infty$.

Assumptions on the training/validation sets

(A6) $\lim_{n\to+\infty} l = +\infty$;
(A7) $\lim_{n\to+\infty} n - l = +\infty$;
(A8) $\lim_{n\to+\infty} \frac{l \log(n-l)}{n-l} = 0$.

Convergence to the Bayes error

[6] (Rossi & Villa, *Neurocomputing*, 2006)

Theorem: universal consistency

Under the assumptions **(A1)-(A8)**,

$$L\Phi^n \xrightarrow{n\to+\infty} L^*,$$

where

- $L\Phi^n = \mathbb{P}(\Phi^n(X) \neq Y)$
- $L^* = \mathbb{P}(\Phi^*(X) \neq Y)$ with $\Phi^*(x) = \begin{cases} 1 & \text{if } \mathbb{P}(Y=1|X=x) > 1/2, \\ -1 & \text{otherwise.} \end{cases}$

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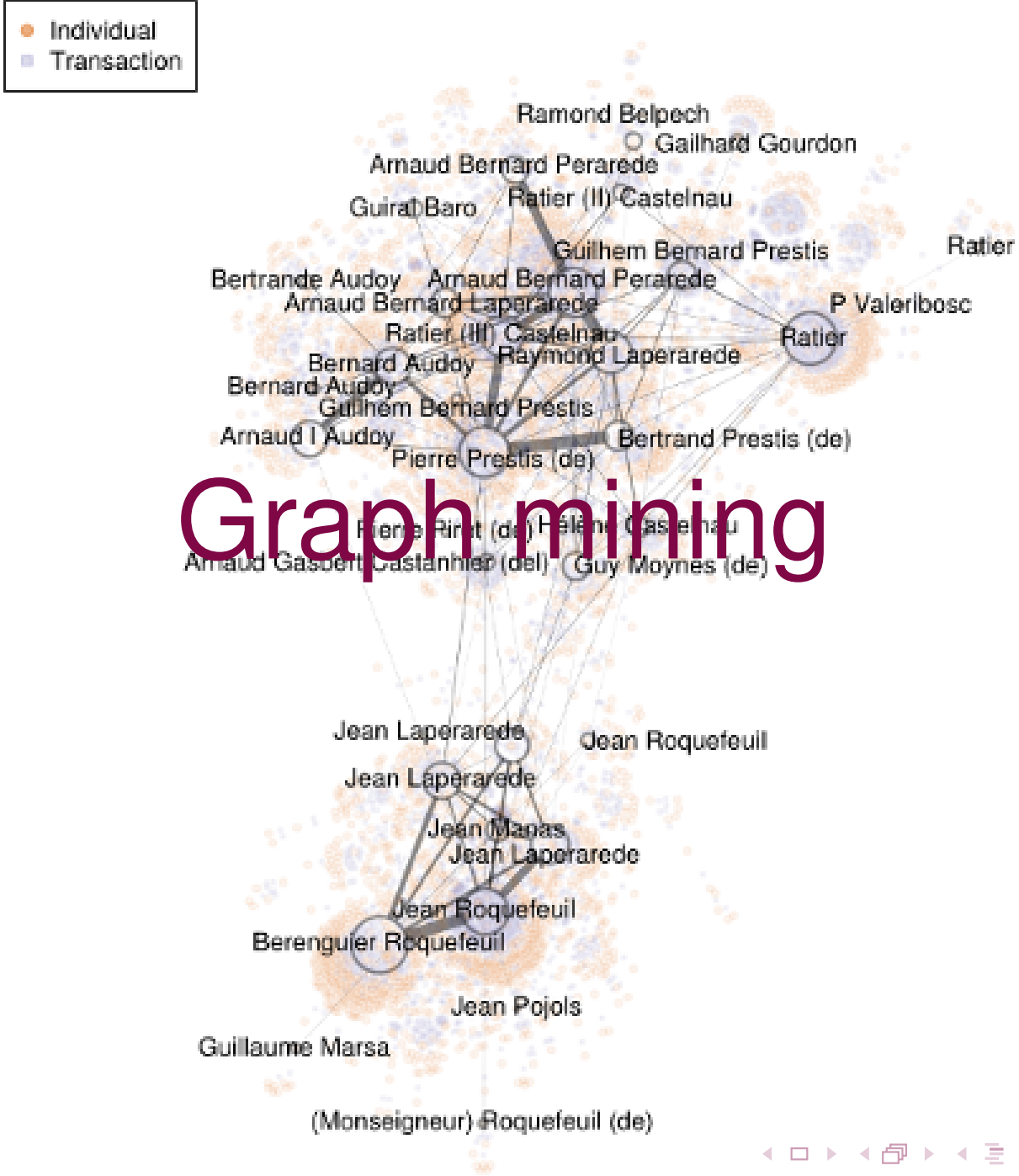
[8] (Rossi & Villa-Vialaneix, *Pattern Recognition Letter*, 2011) alternative kernel for:

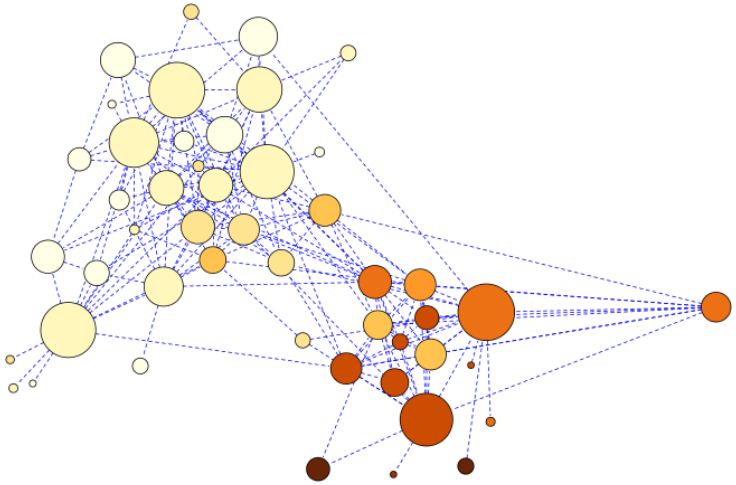
- digitized observations
- derivation preprocessing

with a general consistency result in regression and binary classification.



Graph mining

Framework of this section



A graph (network) $\mathcal{G} = (V, E, W)$ with

- n vertices $V = \{x_1, \ldots, x_n\}$;
- a set of edges, E, weighted by $W_{ij} = W_{ji} \geq 0$ ($W_{ii} = 0$).

Visualization: a tool for graph mining

Standard approach for graph visualization: force directed placement algorithms (FDP). Drawbacks:

- slow (impracticable for large graphs);
- based on aesthetic criteria rather than on interpretability:
  - *trend*: short and uniform length edges;
  - *negative consequence*: nodes with the largest degrees are grouped in the middle of the layout.

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A more natural way to explore a graph:

1. highlight the macroscopic structure: find “communities” and relations between them;
2. eventually focus on finer details in some communities.

Overview of my contributions

- topographic maps: combine clustering and visualization using a prior structure (*ie* a map):
  - batch kernel SOM [1] (Boulet, *et al.*, *Neurocomputing*, 2008) and on-line multiple relational SOM [4] (Olteanu & Villa-Vialaneix, *Neurocomputing*, 2015) (not restricted to graphs; can handle multiple graphs or labeled graphs)

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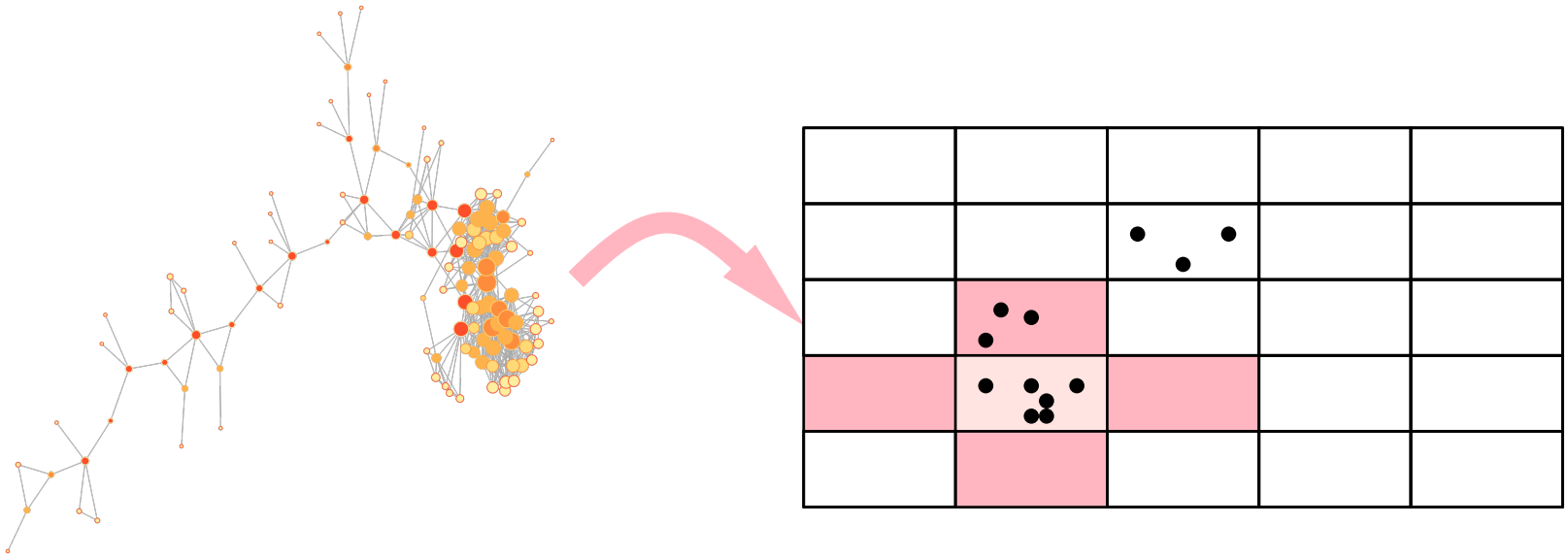
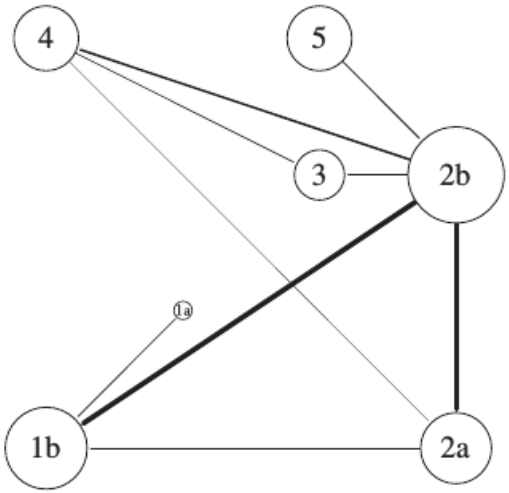
  - for mining a network extracted from a corpus of medieval documents [10] (Rossi, *et al.*, *Digital Medievalist*, 2013)
  - for co-expression network analysis [13] (Villa-Vialaneix, *et al.*, *PLoS ONE*, 2013) (clustering in co-expression network with ontology validation)

Using topographic maps to visualize a clustered graph



- vertices are clustered in U units
- units are arranged on a prior 2D-grid equipped with a topology
- prior positions of the units are used to produce a simplified representation



How to extend topographic maps to graph?

Generic approach using kernel/dissimilarity

[4] (Olteanu & Villa-Vialaneix, *Neurocomputing*, 2015), [1] (Boulet, *et al.*, *Neurocomputing*, 2008) graphs can be described by pairwise relations between nodes:

- with a kernel (ex: $K^\beta = e^{-\beta L}$, with L the graph Laplacian, heat kernel)
- with a dissimilarity (ex: shortest path length)

$\Rightarrow$ extension of SOM to kernel/dissimilarity data using prototypes of the form $p_u = \sum_{i=1}^{n} \gamma_{ui} x_i$.

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Graph specific approach

[7] (Rossi & Villa-Vialaneix, *Neurocomputing*, 2010) Extension of the modularity quality criterion to a criterion taking into account the prior topology

$$O = \frac{1}{2m} \sum_{ijk} M_{ik} S_{kl} M_{jk} B_{ij}$$

$B = \left(W_{ij} - \frac{d_i d_j}{2m}\right)$ modularity matrix ($d_i = \sum_j W_{ij}$ and $m = \frac{\sum_i d_i}{2}$); $M_{ik} = \mathbf{1}_{x_i \in k}$; S encodes the topology of the prior map (similarity)

Practical aspects of kernel/relational SOM

- this approach (and others) is implemented in the R package **SOMbrero** provided with a WUI based on **shiny**;
- it can also handle data described by multiple dissimilarities: the combination is optimized by including a gradient descent-like step in the relational SOM algorithm;

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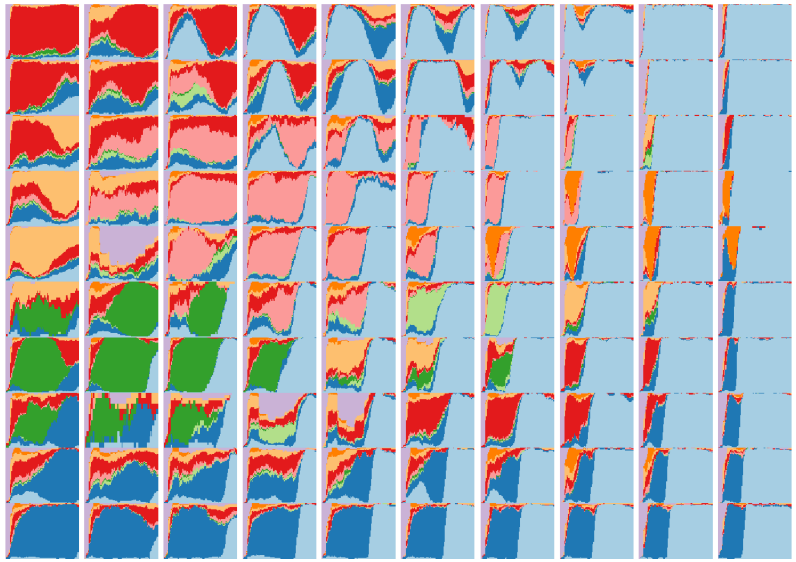
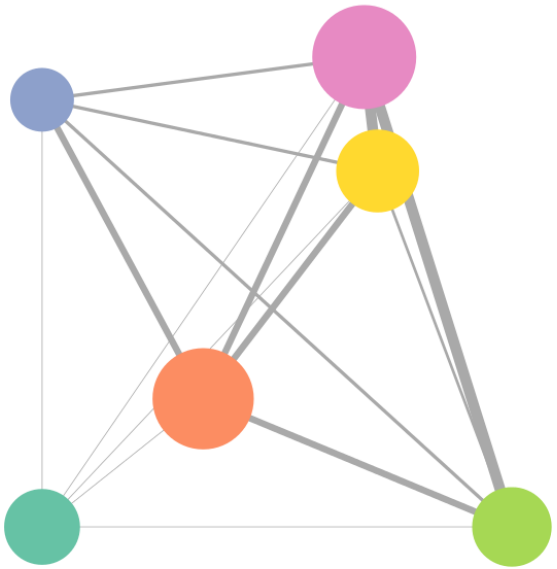
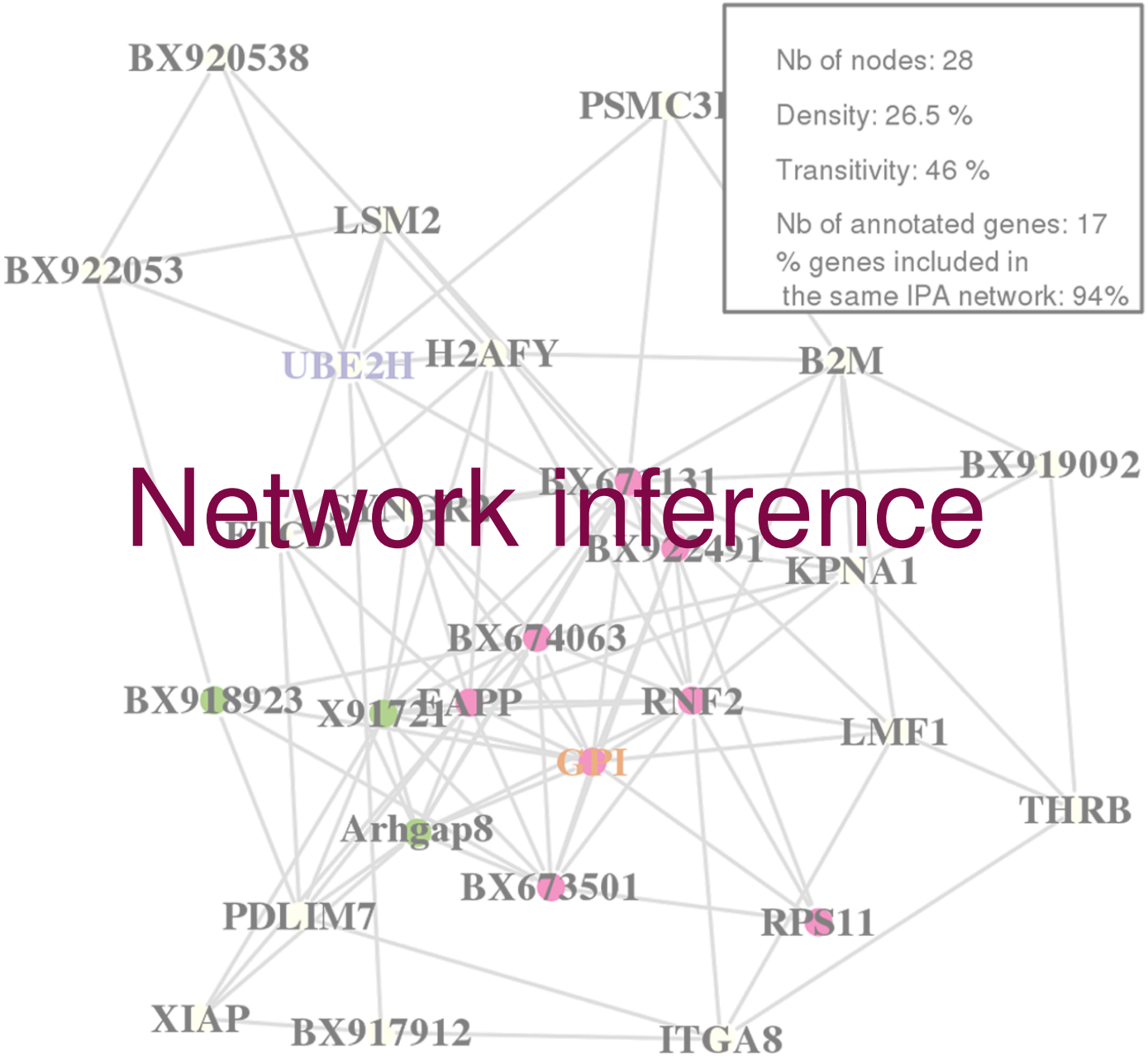
- it can also handle data described by multiple dissimilarities: the combination is optimized by including a gradient descent-like step in the relational SOM algorithm;
- it has been applied to graphs, labeled graphs and to other non vectorial data (school-to-work trajectories)







Network inference

Network inference

Data: large scale gene expression data

individuals
$n \simeq 30/50$

$$\underbrace{\left\{ X = \begin{pmatrix} . & . & . & . & . & . \\ . & . & X_i^j & . & . & . \\ . & . & . & . & . & . \end{pmatrix} \right.}_{\text{variables (genes expression), } p \simeq 10^4}$$

What we want to obtain: a graph/network with

- nodes: (selected) genes;
- edges: strong links between gene expressions.

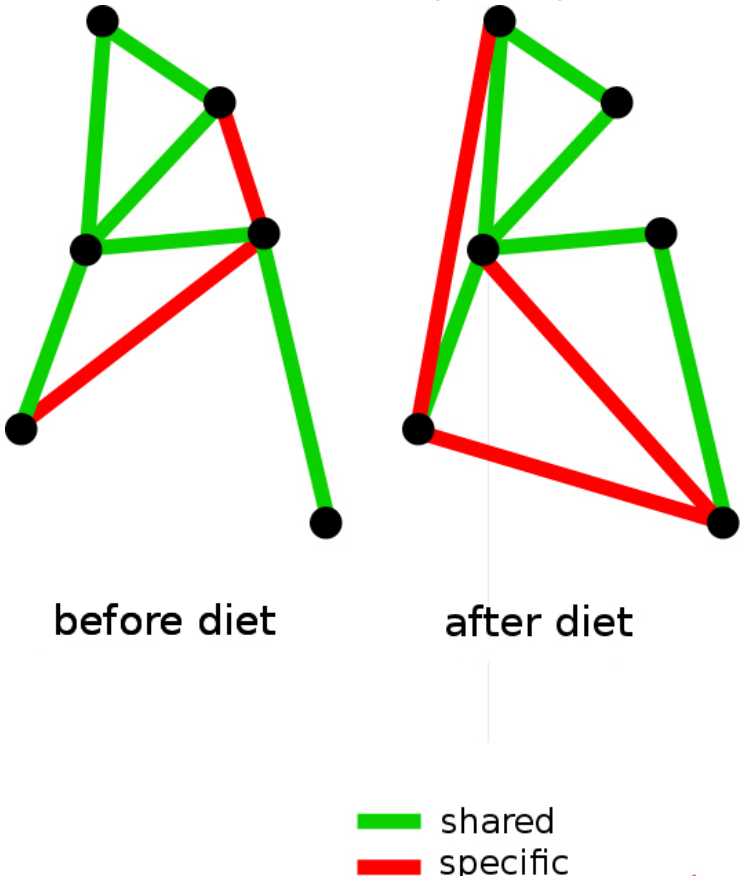
Overview of my contributions

- application of network inference for understanding the determinant of human adipose tissue gene expression [11] (Viguerie, *et al.*, *PLoS Genetics*, 2012)

- network inference with multiple samples [14] (Villa-Vialaneix, *et al.*, *Quality Technology and Quantitative Management*, 2014)

Motivation for multiple networks inference

Pan-European project Diogenes[1] (with Nathalie Viguerie, INSERM): gene expressions (lipid tissues) from 204 obese women before and after a low-calorie diet (LCD).



- Assumption: A common functioning exists regardless the condition;
- Which genes are linked independently from/depending on the condition?

[1] http://www.diogenes-eu.org

Consensus LASSO

GGM with L^1 penalty: one condition

$(X_i)_{i=1,\dots,n}$ are i.i.d. Gaussian random variables $\mathcal{N}(0,\Sigma)$

$$X^j = \beta_j^T X^{-j} + \epsilon \quad ; \quad \arg\min_{(\beta_{jj'})_{j'}} \sum_{i=1}^{n} \left(X_{ij} - \beta_j^T X_i^{-j}\right)^2 + \lambda \|\beta_j\|_{L^1}$$

$$j \longleftrightarrow j' \text{(genes } j \text{ and } j' \text{ are linked)} \Leftrightarrow \beta_{jj'} \neq 0$$

Consensus LASSO: multiple conditions

$$\frac{1}{2}\beta_j^T \widehat{\Sigma}_{\setminus j \setminus j} \beta_j + \beta_j^T \widehat{\Sigma}_{j \setminus j} + \lambda \|\beta_j\|_{L^1} + \mu \sum_c w_c \|\beta_j^c - \beta_j^{\text{cons}}\|_{L^2}^2$$

with $\widehat{\Sigma}_{\setminus j \setminus j}$: block diagonal matrix $\mathbb{D}\text{iag}\left(\widehat{\Sigma}^1_{\setminus j \setminus j}, \dots, \widehat{\Sigma}^k_{\setminus j \setminus j}\right)$ and similarly for $\widehat{\Sigma}_{j \setminus j}$:

- w_c: real number used to weight the conditions;
- μ regularization parameter;
- β_i^{cons} whatever you want...?

Choice of a consensus

Case 1: a priori consensus

Using a fixed β_j^{cons}, the optimization problem is equivalent to minimizing the p following standard quadratic problem in $\mathbb{R}^{k(p-1)}$ with L_1-penalty:

$$\frac{1}{2}\beta_j^T B^1(\mu)\beta_j + \beta_j^T B^2(\mu) + \lambda||\beta_j||_{L^1},$$

Case 2: learn the consensus

Using $\beta_j^{\text{cons}} = \sum_{c=1}^{k} \frac{n_c}{n}\beta_j^c$, the optimization problem is equivalent to minimizing the following standard quadratic problem with L_1-penalty:

$$\frac{1}{2}\beta_j^T S_j(\mu)\beta_j + \beta_j^T \widehat{\Sigma}_{j\backslash j} + \lambda||\beta_j||_{L^1}$$

Optimization by active set, combined with bootstrap approach (BOLASSO type). R package **therese**.

Future work

Research project: data mining and integration with SOM

On-going issues

- stabilize results, improve quality, speed-up training: aggregation, boosting...
- improve interpretability in a multi-kernel/dissimilarity context: visualization, prototype sparsity...
- targeted applications: multi-'omics integration and exploration; ncRNA typology

Collaborations

- methodological aspects: Jérôme Mariette (PhD, MIAT, INRA), Madalina Olteanu (SAMM, Université Paris 1)
- application to multi-'omics data: Nathalie Viguerie (INSERM, Diogenes project)
- application to ncRNA: Christine Gaspin (MIAT, INRA)

Research project: data mining and integration using graphical approaches

On-going issues

- integrating multi-'omics data in network inference and mining, possibly with different numbers of observations
- taking temporal aspects into account in network inference/clustering

Collaborations

- methodological aspects: Valérie Sautron (PhD, GenPhySE, INRA)
- applications: projects SusOStress & PigHeat (GenPhySE, INRA) on systems genetics in pigs (stress & heat resistance)
- application: Nathalie Viguerie (INSERM, Diogenes project) & Ignacio Gonzáles (MIAT, INRA)... *submitted article*

Thank you for your attention...

... questions?

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