A study of the manifold hypothesis for functional data by using spectral clustering

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Outline

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Functional Data (FD)

- In many applications, observations are realization of functional data (FD) (curves, time series, signals, images,...).
- Functional Data Analysis (FDA) extends multivariate data analysis techniques to FD or develops specific techniques for FD, see for e.g. [**?**, **?**].
- Objects under study are n real valued functions $\{x_i\}_{i=1,\dots,n}$ in $\mathbb{L}^2([0,T])$, where $T > 0$.
- However $\forall x_i$, we only have p measurements $\{y_{ij}\}_{j=1,\dots,p}$ at discrete time points $\{t_j\}_{j=1,\dots,p}$ in $[0,T]$ and these observations are assumed to be corrupted by noise ϵ_{ij} :

$$y_{ij} = x_i(t_j) + \epsilon_{ij}, \quad \forall i, \forall j$$

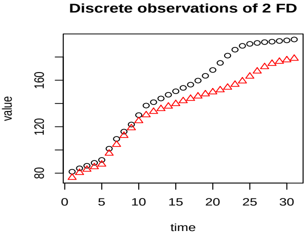
where ϵ_{ij} are assumed to be independent across i and j.

Functional Data Clustering (FDC)

- Given $\{y_{ij}\}_{i,j}$ find a partition of $\{x_i\}_i$ where FD in a class are more similar to each other than to FD in other classes (see for e.g. [**?**]).
- One possible workflow for FDC is the following one :
  - Represent the FD in a **low-dimensional space** using either :
    - Pre-defined finite set of basis functions such as bsplines.
    - Data-driven finite set of basis functions such as truncated Karhunen-Loeve expansion (a.k.a. functional PCA).
  - Apply **multivariate clustering techniques** either :
    - Assuming all FD belong to the whole low-dimensional representation space (e.g. k-means or hierarchical clustering).
    - Assuming that each cluster only belong to a subspace of the representation space (e.g. subspace clustering or model-based functional clustering techniques).

Example : Berkeley Growth data

- $\{y_{ij}\}_{j=1,\dots,p}$ = heights measured at different times t_j.



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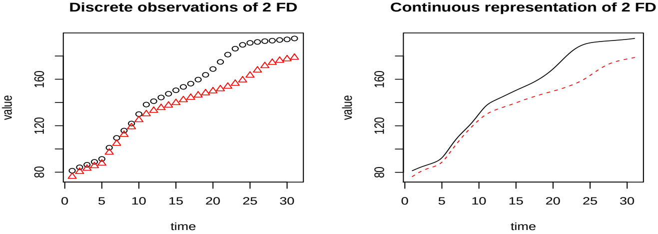

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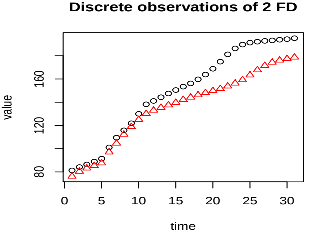

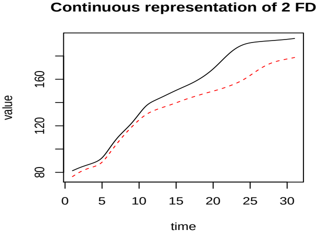

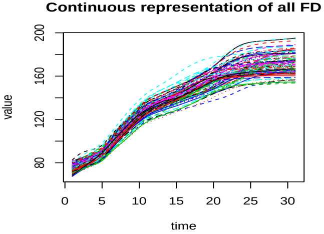

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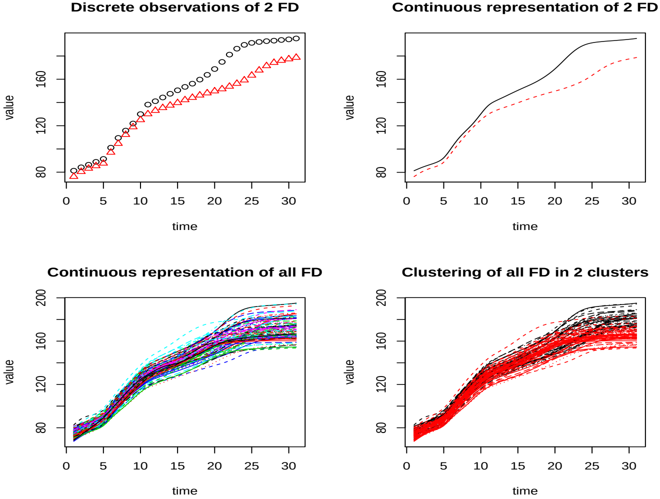

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$\Rightarrow$ We investigate these points **jointly** and from an **empirical viewpoint** using **20 benchmarks** and by using **spectral clustering (SC)**.

Outline

Spectral clustering (SC) in a nutshell

- Methods developed in the ML community since the early 2000's.
- Capture the intrinsic geometry of the data.
- Similarity, neighbor end Laplacian graphs are important concepts.
- Methodology : **use the spectral decomposition of the Laplacian matrix as an embedding** of the graph nodes in an Euclidean space then partition the nodes using k-means.
- Motivations : the eigenvalues and eigenvectors of the Laplacian encode information about the connected components (and more generally clusters) of the graph, they also provide solutions to (relaxed) graph cuts problems.
- See for e.g. [**?**] for an introduction.

Similarity and Neighbor graphs

- Similarities between objects as a **weighted undirected graph** $G = (\mathbb{V}, \mathbb{E})$:
  - $\mathbb{V} = \{x_1, \ldots, x_n\}$ is the set of nodes : objects to cluster.
  - $\mathbb{E}$ is the set of edges : pairs of objects that are similar to each other.
- Edges are weighted : if $(x_i, x_j) \in \mathbb{E}$ then $K(x_i, x_j) > 0$ is the **measure of the similarity**.
- G is represented by a **weighted adjacency matrix** denoted $\mathbf{W} = (w_{ij})_{i,j=1,\ldots,n}$ with :

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- K is a **kernel function** : objects belong to an RKHS.
- We can sparsify $\mathbf{W}$ and have a k **nearest neighbor graph** in order to strengthen the manifold hypothesis.

Laplacian matrix and its normalization

- Let $\mathbf{D} = (d_{ij})_{i,j=1,\dots,n}$ be the **degree matrix** defined by :

$$d_{ij} = \begin{cases} d_i & \text{if } i = j \\ 0 & \text{else} \end{cases}$$

  with $d_i = \sum_{j=1}^{n} w_{ij}$, $\forall i = 1, \dots, n$.

- The **Laplacian matrix** of G denoted $\mathbf{L}$ is given by :

$$\mathbf{L} = \mathbf{D} - \mathbf{W}$$

- Its **(symmetric) normalization** denoted $\mathbf{L}_{sym}$ is defined by :

$$\begin{aligned} \mathbf{L}_{sym} &= \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2} \\ &= \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2} \end{aligned}$$

  with $\mathbf{I}$ the identity matrix of order n.

Properties of the normalized Laplacian matrix

Property.

- $\mathbf{L}_{sym}$ *can be viewed as a quadratic form (that we aim at minimizing) :*

$$\mathbf{f}^\top \mathbf{L}_{sym}\mathbf{f} = \frac{1}{2}\sum_{i,j=1}^{n} w_{ij}\left(\frac{f_i}{\sqrt{d_i}} - \frac{f_j}{\sqrt{d_j}}\right)^2, \forall \mathbf{f} \in \mathbb{R}^n$$

- $\mathbf{L}_{sym}$ *is* **symmetric and psd** *:*

$$0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$$

- *The multiplicity order k of the* **null eigenvalue** *is the number of* **connected components** *of G. Let denote the latter subset of nodes as $C_1, \ldots, C_k$. The eigen subspace associated to λ_1 is spanned by* $\mathbf{D}^{1/2}\mathbf{1}_{C_1}, \ldots, \mathbf{D}^{1/2}\mathbf{1}_{C_k}$ *where $\mathbf{1}_{C_l}$ is the assignment vector of C_l.*

Illustration with a disconnected graph

- $\mathbb{V} = \{x_1, x_2, x_3, x_4, x_5\}$
- $\mathbb{E} = \{\underbrace{(x_1, x_2)}_{2}, \underbrace{(x_2, x_3)}_{3}, \underbrace{(x_4, x_5)}_{2}\}$

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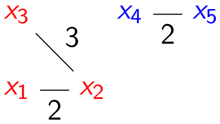

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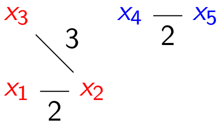

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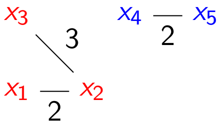

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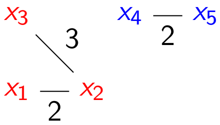

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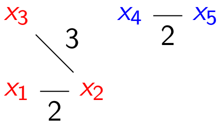

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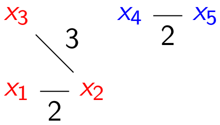

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$\rightarrow$ Spectra of $\mathbf{L}_{sym}$: $\{2, 2, 1, 0, 0\}$

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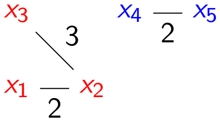

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$\rightarrow$ Spectra of $\mathbf{L}_{sym}$: $\{2,2,1,0,0\}$ $\rightarrow \underbrace{\mathbf{D}^{1/2}\mathbf{1}_{C_1}}_{\mathbf{f}_0^1} = \begin{pmatrix} 1.41 \\ 2.24 \\ 1.73 \\ 0 \\ 0 \end{pmatrix}$ and $\underbrace{\mathbf{D}^{1/2}\mathbf{1}_{C_2}}_{\mathbf{f}_0^2} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1.41 \\ 1.41 \end{pmatrix}$.

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Workflow

1. **Smoothing** : from $\{y_{ij}\}_{i,j}$ to $\{x_i\}_i$:
   - Basis functions are cubic bspline $\{\phi_k\}_{k=1,\dots,q}$ with $q = 4 + p$:

$$x_i(t) = \mathbf{c}_i^\top \phi(t) = \sum_{k=1}^{q} c_{ik}\phi_k(t)$$

     where $\mathbf{c}_i = \begin{pmatrix} c_{i1} & \dots & c_{iq} \end{pmatrix}^\top$ and $\phi(t) = \begin{pmatrix} \phi_1(t) & \dots & \phi_q(t) \end{pmatrix}^\top \in \mathbb{R}^q$.
   - We find $\mathbf{c}_i$ as follows :

$$\mathbf{c}_i = \arg\min_{\mathbf{c}\in\mathbb{R}^q} \sum_{j=1}^{p} (y_{ij} - x_i(t_j))^2 + \lambda \int_0^T D^2 x_i(t)dt$$

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4. Perform **clustering procedures**.
5. **Evaluate** clustering outputs and **compare** the results.

Kernel/Representation/Sparsification

- FD are centered : $\sum_{i=1}^{n} x_i(t) = 0, \forall t \in [0, T]$.

Kernel/Representation/Sparsification

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  - Linear kernel : $K_l(x_i, x_j) = \langle x_i, x_j \rangle_{\mathbb{L}^2} = \int_0^T x_i(t)x_j(t)dt$
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⇒ Main questions :
  - Does basis expansion and RKHS help ?
  - Does "fusing" both x_i and Dx_i and work in a Sobolev space help ?
  - Does sparsification (that emphasizes the manifold hypothesis) help ?

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- Baseline : kernel k-means with linear kernel $K_l(x_i, x_j) = \langle x_i, x_j \rangle_{\mathbb{L}^2}$.

List of the 18 clustering models

Acronym	Representation	Kernel	Clustering proc.	Sparsif.
`00_linear_K_km_`	$x_i \in \mathbb{L}^2([0, T])$	Linear	Ker. k-means	

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11_gaussian_K_km_	$Dx_i \in \mathbb{L}^2([0,T])$	Gaussian	Ker. k-means	
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01_gaussian_K_km_	$x_i \in \mathbb{W}^{1,2}([0,T])$	Gaussian	Ker. k-means	
00_linear_SC_km_0	$x_i \in \mathbb{L}^2([0,T])$	Linear	Spectral Clust.	Connected
00_gaussian_SC_km_0	$x_i \in \mathbb{L}^2([0,T])$	Gaussian	Spectral Clust.	Connected
11_linear_SC_km_0	$Dx_i \in \mathbb{L}^2([0,T])$	Linear	Spectral Clust.	Connected
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00_linear_SC_km_1	$x_i \in \mathbb{L}^2([0,T])$	Linear	Spectral Clust.	7 near. neig.
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20 datasets from fda, fda.usc and UCR_TS_Archive_2015

Source	Type	Name	Nb of FD	Nb of Class	Nb of obs.
fda		Growth	93	2	31
fda.usc		poblenou	115	2	24
fda.usc		tecator	215	2	100
fda.usc		phoneme	250	5	150
UCR_TS	Spectro	Beef	30	5	470
UCR_TS	Simulated	CBF	30	3	128
UCR_TS	Spectro	Coffee	28	2	286
UCR_TS	ECG	ECG200	100	2	96
UCR_TS	Image	FaceFour	24	4	350
UCR_TS	Image	Fish	175	7	463
UCR_TS	Motion	GunPoint	50	2	150
UCR_TS	Sensor	Lightning2	60	2	637
UCR_TS	Sensor	Lightning7	70	7	319
UCR_TS	Image	MedicalImages	381	10	99
UCR_TS	Spectro	OliveOil	30	4	570
UCR_TS	Image	OSULeaf	200	6	427
UCR_TS	Image	SwedishLeaf	500	15	128
UCR_TS	Image	Symbols	25	6	398
UCR_TS	Sensor	Trace	100	4	275
UCR_TS	Simulated	TwoPatterns	1000	4	128

Clustering assessment and comparison

- Clustering models assessment :
  - **External validation** : for each dataset we have the ground truth.
  - Compare a clustering output against the ground truth using the **Normalized Mutual Information (NMI)** criterion. This measure is between 0 and 1 and the bigger the better.

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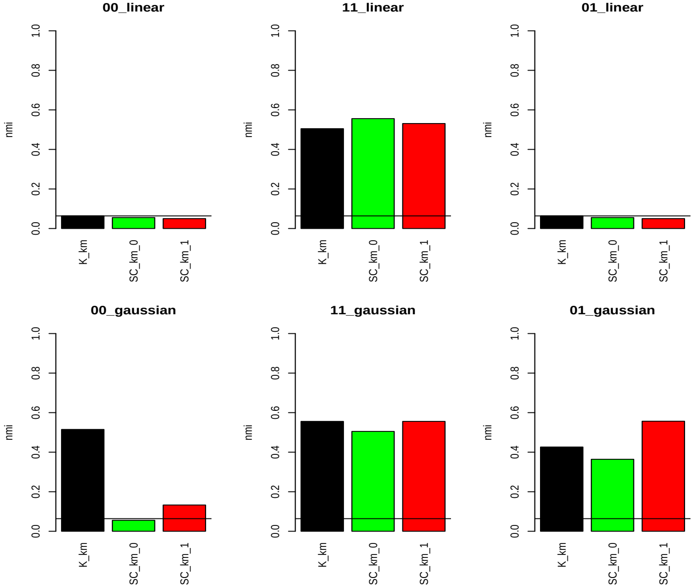
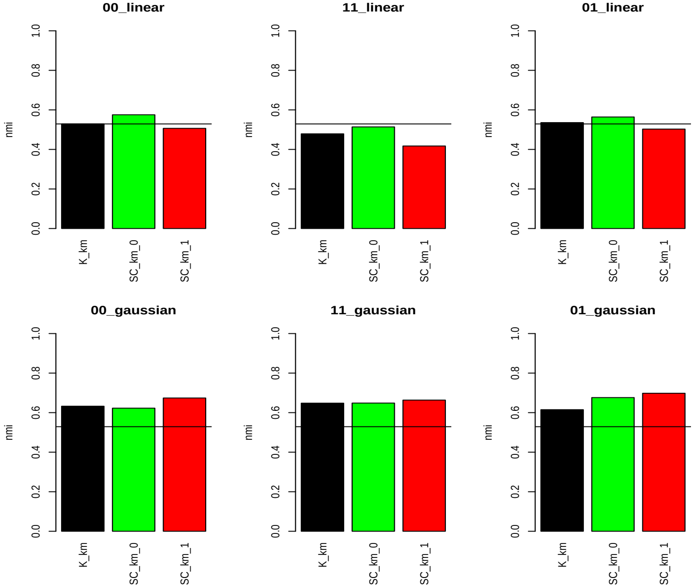
- Comparing the 18 clustering models :
  - For each pair of clustering models (i, j), we count the **nb of times** i **beats**[1] j among the 20 datasets (each dataset is seen as a "match").
  - For an overall ranking of the clustering models, we use **Borda's voting rule : we rank according to the total nb of wins**. Each clustering model "plays" in total $20 \times 17 = 340$ "matches".

1. i beats j for a given dataset, if NMI of $i >$ NMI of j

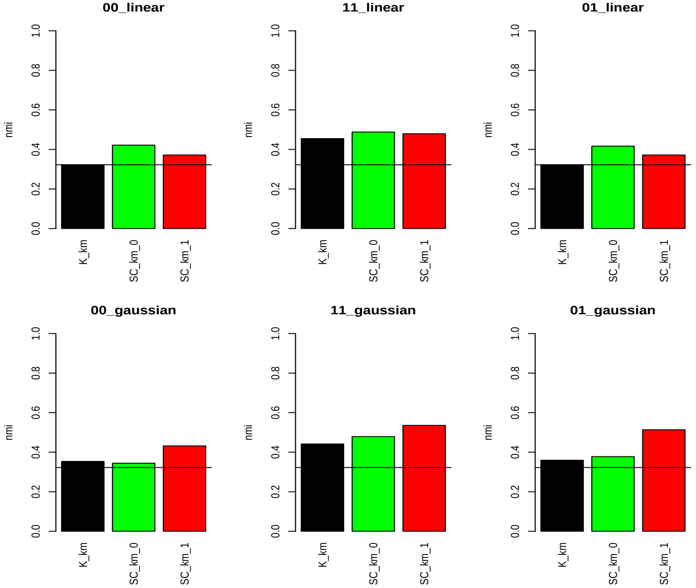
Examples of results : Growth data



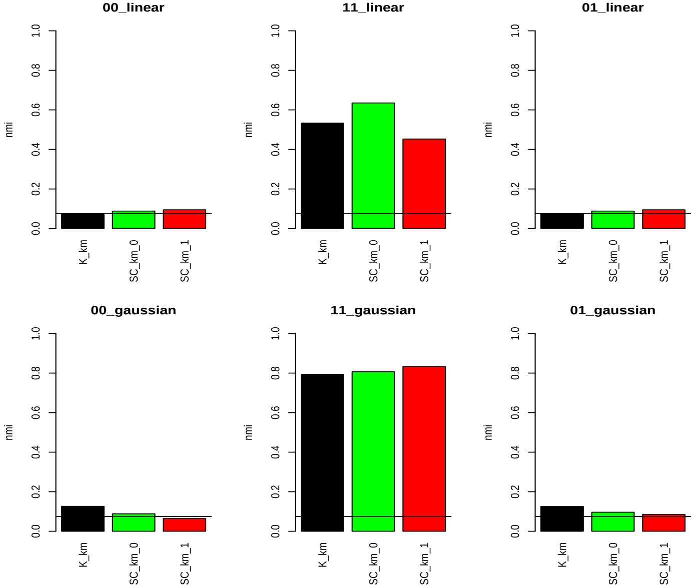
Examples of results : SwedishLeaf data



Examples of results : Fish data



Examples of results : Tecator data



Overall results : Borda's ranking

Rank	Clustering model	Nb of wins	Nb of losses
1	01_gaussian_SC_km_1	206	94
2	11_gaussian_K_km_	195	113
3	00_gaussian_K_km_	182	119
4	00_gaussian_SC_km_1	179	125
5	01_gaussian_SC_km_0	175	131
6	11_gaussian_SC_km_1	174	136
7	01_gaussian_K_km_	170	134
8	00_linear_SC_km_0	151	143
9	11_gaussian_SC_km_0	151	159
10	00_linear_SC_km_1	150	159
11	01_linear_SC_km_0	148	146
12	01_linear_SC_km_1	146	157
13	00_gaussian_SC_km_0	131	167
14	11_linear_SC_km_0	127	177
15	11_linear_K_km_	117	193
16	01_linear_K_km_	117	190
17	00_linear_K_km_	115	193
18	11_linear_SC_km_1	104	202

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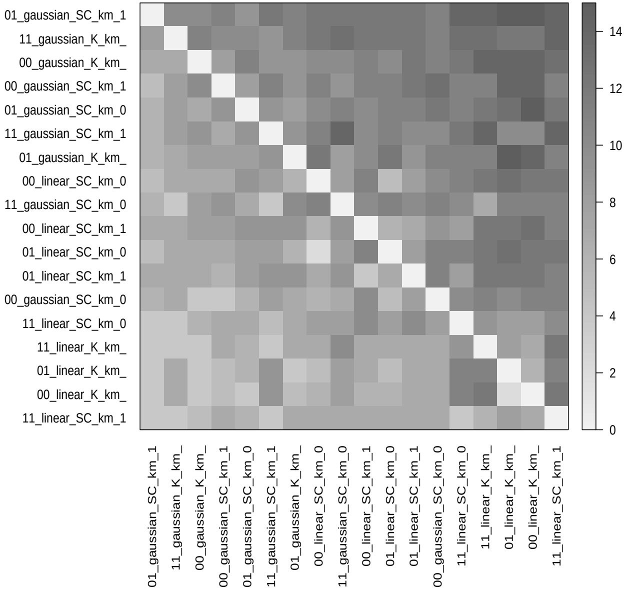
Borda's ranking visualization



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  $\Rightarrow$ Sparse clustering in Sobolev spaces : select discriminant features while performing the clustering.

Thank you for your attention !
Any question or comment ? :-)

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