Genie: A New, Fast, and Outlier-Resistant Hierarchical Clustering Algorithm and Its R Interface

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Outline

- Hierarchical Agglomerative Clustering – Issues
- The Genie Algorithm
- Implementation
- A Possible Generalization

Inputs

- Let $\mathfrak{d}$ be a pairwise dissimilarity measure over $\mathcal{X}$ (**distance**, see Deza and Deza, 2014), i.e., $\mathfrak{d} : \mathcal{X} \times \mathcal{X} \to [0, \infty]$ *at least* such that:
  - $\mathfrak{d}(\mathbf{x}', \mathbf{x}'') = \mathfrak{d}(\mathbf{x}'', \mathbf{x}')$ for all $\mathbf{x}', \mathbf{x}'' \in \mathcal{X}$,
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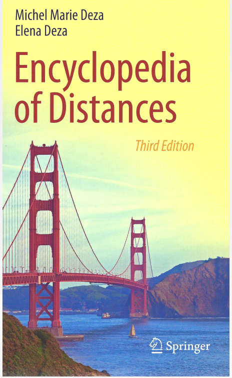

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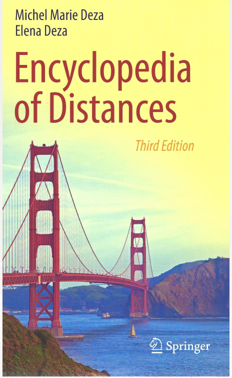
- Some examples:
    - $\mathbb{R}^d$ with the Euclidean or Manhattan metric,
    - $\{A, C, T, G\}^*$ with the Levenshtein or Dinu rank distance,
    - a chain with the natural distance,
    - raster images with RMSE of brightness values,
    - a Cartesian product of the above spaces with a convex combination of different distances.



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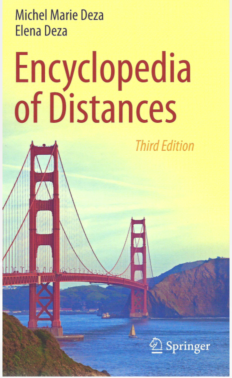
- Let $\{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)}\} \subseteq \mathcal{X}$ be a set of n objects.



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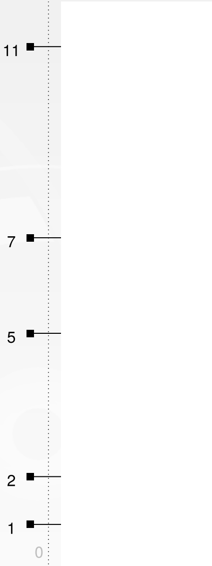

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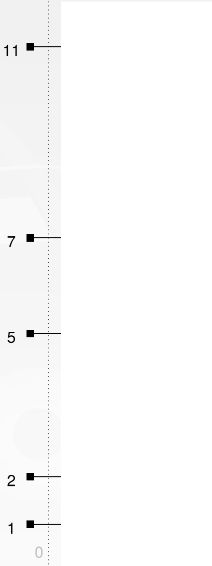

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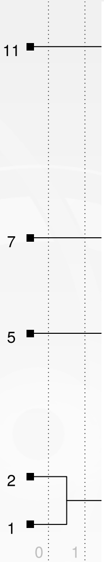

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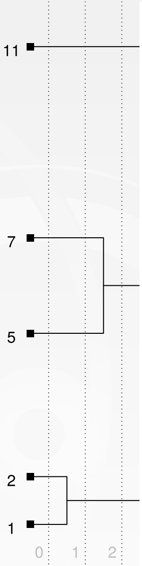

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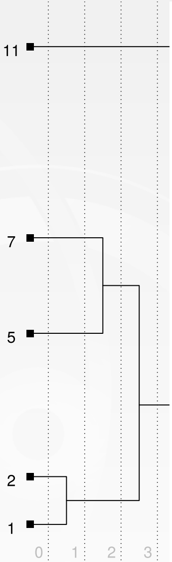

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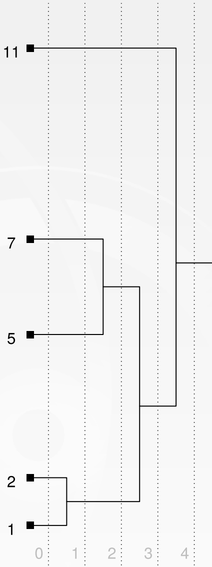

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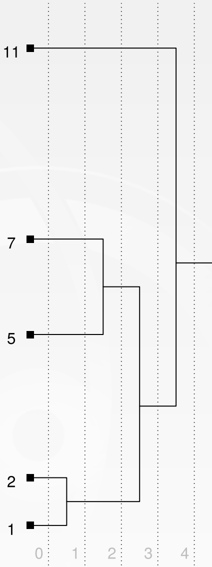
- Classical linkage criterion – for some *extension* $\tilde{\mathfrak{d}}$ of $\mathfrak{d}$ to $2^{\mathcal{X}}$:

$$\arg\min_{(u,v), u<v} \tilde{\mathfrak{d}}(C_u^{(j-1)}, C_v^{(j-1)}).$$



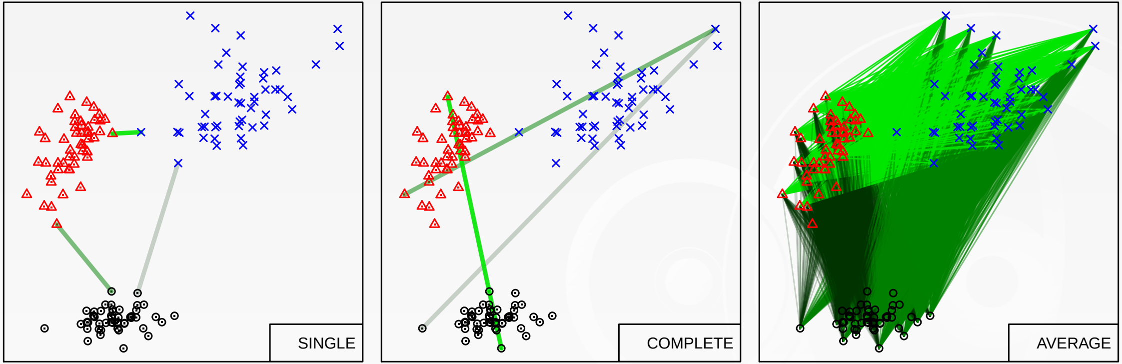
Hierarchical Agglomerative Clustering

$$\tilde{\mathfrak{d}}(C_u, C_v) = \ldots$$

$$\min_{\mathbf{a}\in C_u, \mathbf{b}\in C_v} \mathfrak{d}(\mathbf{a}, \mathbf{b})$$

$$\max_{\mathbf{a}\in C_u, \mathbf{b}\in C_v} \mathfrak{d}(\mathbf{a}, \mathbf{b})$$

$$\frac{1}{|C_u||C_v|} \sum_{\mathbf{a}\in C_u, \mathbf{b}\in C_v} \mathfrak{d}(\mathbf{a}, \mathbf{b})$$



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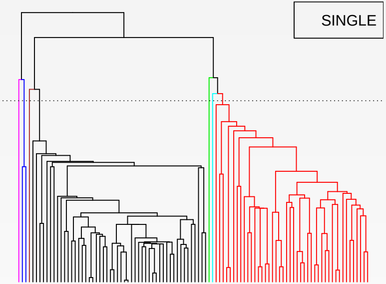

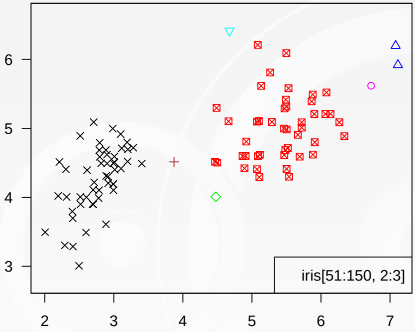

Is it a clustering or an outlier detection algorithm?

Hierarchical Agglomerative Clustering
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Definition.

$\mathsf{F} : \mathcal{G} \to [0, 1]$ is an **inequity measure** (see Aristondo, García-Lapresta, Lasso de la Vega, Marques Pereira, 2013; Beliakov, Gagolewski, James, 2016), whenever:

- $\inf_{\mathbf{x}\in\mathcal{G}} \mathsf{F}(\mathbf{x}) = 0$ and $\sup_{\mathbf{x}\in\mathcal{G}} \mathsf{F}(\mathbf{x}) = 1$,
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Examples: the normalized Gini, Bonferroni, de Vergottini indices.

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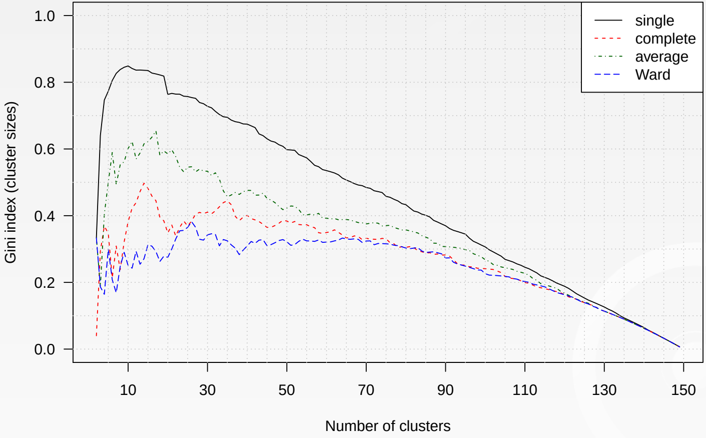

The Gini indices for the cluster size distributions – *Iris* dataset

$$\mathsf{G}(\mathbf{c}) = \frac{\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}|c_i - c_j|}{(n-1)\sum_{i=1}^{n} c_i},$$

$$\mathbf{c} = \left(|C_1^{(j)}|, \ldots, |C_{n-j}^{(j)}|\right)$$

The Genie Algorithm

Gagolewski M., Bartoszuk M., Cena A., Genie: A new, fast, and outlier-resistant hierarchical clustering algorithm, *Information Sciences* 363, 2016, 8–23;
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(b) If $\mathsf{F}(c_{(n-j)}, \dots, c_{(1)}) > g$,

$$\arg \min_{\substack{(u,v), u<v, \\ c_u = c_{(1)} \text{ or } \\ c_v = c_{(1)}}} \left(\min_{\mathbf{a} \in C_u^{(j)}, \mathbf{b} \in C_v^{(j)}} \mathfrak{d}(\mathbf{a}, \mathbf{b}) \right),$$

(search domain restricted to pairs of clusters s.t. one of them is of the smallest size)

The Genie Algorithm
Benchmark Data

21 Euclidean benchmarks datasets, see gagolewski.com/resources/data/clustering/: Sources:

- A. Gionis et al., Clustering aggregation, ACM Transactions on Knowledge Discovery from Data (TKDD), 2007, pp. 1-30.
- C.T. Zahn, Graph-theoretical methods for detecting and describing gestalt clusters, IEEE Transactions on Computers C-20(1), 1971, pp. 68-86.
- H. Chang, D.Y. Yeung, Robust path-based spectral clustering, Pattern Recognition 41(1), 2008, pp. 191-203.
- C.J. Veenman et al., A maximum variance cluster algorithm, IEEE Transactions on Pattern Analysis and Machine Intelligence 24(9), 2002, pp. 1273-1280.
- A. Jain, M. Law, Data clustering: A user's dilemma, Lecture Notes in Computer Science 3776, 2005, pp. 1-10.
- L. Fu, E. Medico, FLAME, a novel fuzzy clustering method for the analysis of DNA microarray data, BMC bioinformatics 8, 2007, p. 3.
- P. Fränti, O. Virmajoki, Iterative shrinking method for clustering problems, Pattern Recognition, 39(5), 2006, pp. 761-765.
- I. Kärkkäinen, P. Fränti, Dynamic local search algorithm for the clustering problem, Research Report A-2002-6.

Each dataset comes with a sequence of reference labels.

The Genie Algorithm
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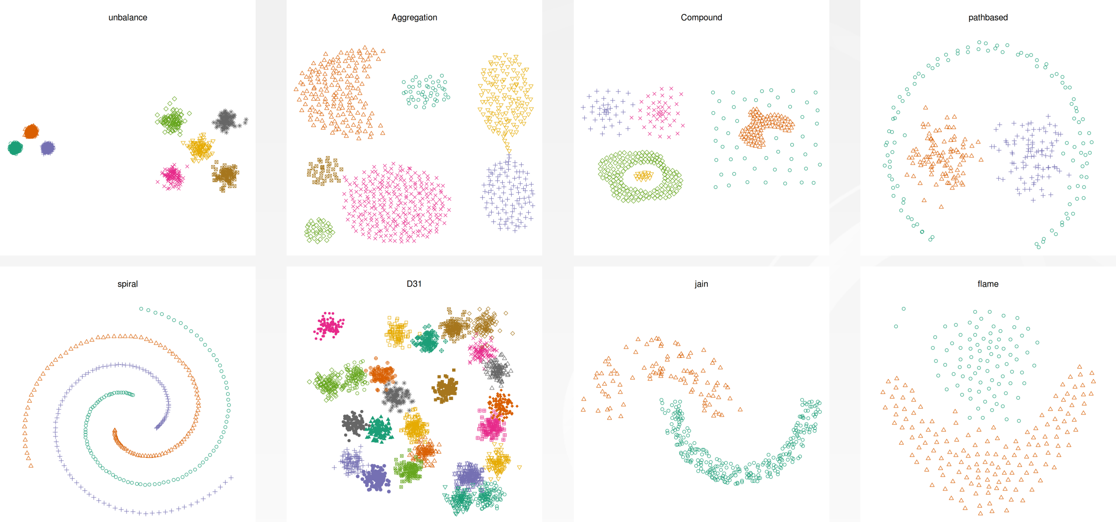

...and many more

The Genie Algorithm

Basic summary statistics of the FM-index distribution over the 21 Euclidean benchmark sets.

	single	complete	ward	average	gini_0.2	gini_0.3	gini_0.4	gini_0.5	gini_0.6	BIRCH	k-means
Min	0.257	0.339	0.337	0.357	0.582	**0.602**	0.563	0.529	0.482	0.350	0.327
Q1	0.480	0.623	0.674	0.707	0.723	0.697	**0.751**	0.742	0.695	0.653	0.701
Median	0.691	0.833	0.842	0.862	**0.923**	0.905	0.828	0.843	0.754	0.894	0.821
Q3	0.764	0.920	0.924	0.936	**0.987**	**0.987**	**0.987**	0.923	0.911	0.924	0.969
Max	**1.000**	**1.000**	**1.000**	**1.000**	**1.000**	**1.000**	**1.000**	**1.000**	**1.000**	**1.000**	**1.000**
Mean	0.629	0.777	0.803	0.812	**0.850**	0.841	0.833	0.828	0.789	0.801	0.816
St.Dev.	0.224	0.187	0.177	0.172	0.150	0.146	0.145	**0.138**	0.156	0.183	0.177

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- A modified Prim's algorithm (Olson, 1995):
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  - between $\sim 1\%$ and (curse of dimensionality) $\sim 120\%$ calls to $\mathfrak{d}$ (empirically).

Implementation

Calls to $\mathfrak{d}$ (relative to $(n^2 - n)/2$); $\mathbb{R}^d$; $\mathcal{N}$(random μs, σ)

σ	d	n	gini_0.3	gini_1.0 (single)	complete	Ward	average
0,50	2	10000	$*$4.8%	†100%	476%	204%	484%
0,50	5	10000	$*$22.0%	†100%	493%	221%	496%
1,50	10	10000	$*$30.3%	†100%	496%	240%	499%
1,50	15	10000	$*$58.3%	†100%	497%	253%	498%
1,50	20	10000	$*$84.9%	†100%	497%	261%	498%
3,50	100	10000	$*$101.8%	†100%	498%	299%	499%
5,00	250	10000	$*$100.9%	†100%	498%	312%	499%

$*$ – modified Kruskal, † – modified Prim

complete, Ward, average – `fastcluster` package for R; see Müllner, 2013; NN-chains etc.

Implementation

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Example.
$n = 100{,}000 \longrightarrow (n^2 - n)/2 = 4{,}999{,}950{,}000$ floats $\simeq 40$ GB.

See also: `fastcluster::hclust.vector()`

Implementation

A few technical details:

- 2.5k lines of C++ code;
- the Gini-index computed incrementally ($O(n)$ time per iteration);
- OpenMP for multi-threaded computations;
- a custom Union-Find data structure implementation (`disjoint_sets` in Boost are pretty slow);
- a number of tweaks in the VP-tree implementation (search for NNs of x_i only among x_js with $j > i$, make subtrees inactive if all elements are already in the same cluster, etc.).

Implementation

Exemplary run-times for different #threads, $n = 100{,}000$ [s].

			Thread count		
data	Algorithm	g	1	2	4
$d = 10$, $\sigma = 1.5$	Kruskal, VP-trees	0.3	46.5	33.4	28.2
	Prim	0.3	91.5	59.9	44.8
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Ward — `fastcluster::hclust.vector()`

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- Rcpp used to “glue” everything together (see below for discussion);
- Need for speed – R code reduced to:

```
> genie::hclust2
function (d=NULL, objects=NULL, thresholdGini=0.3, useVpTree=FALSE, ...)
{
    opts <- list(thresholdGini=thresholdGini, useVpTree=useVpTree, ...)
    result <- .hclust2_gini(d, objects, opts)  # a call to an Rcpp function
    result[["call"]] <- match.call()
    result[["method"]] <- "gini"
    if (any(result[["height"]] < 0)) {
        # ...
    }
    result
}
```

Implementation

R interface – An example:

```
> h <- genie::hclust2(objects=as.matrix(iris[,1:4]), d="euclidean")
> h
Call:
genie::hclust2(d = "euclidean", objects = as.matrix(iris[, 1:4]))

Cluster method   : gini
Distance         : euclidean
Number of objects: 150
> as.numeric(dendextend::FM_index(cutree(h, 3), iris[[5]]))
[1] 0.9234342
```

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Inputs:

- `objects` – `NULL` or a numeric matrix or a character vector or a list with integer vectors or . . . ;
- `d` – an object of "class" `dist` or a string: *euclidean, manhattan, minkowski, hamming, levenshtein, dinu, . . .*;
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  and elements:
  - `merge` – matrix with 2 columns and $n-1$ rows;
  - `height` – an integer vector with $n-1$ elements;
  - `order` – an integer vector with n elements;
  - `labels` – a character vector or NULL;

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Our C++ code is pretty **"R-independent"**.

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R Objects

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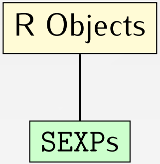

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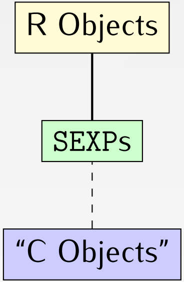

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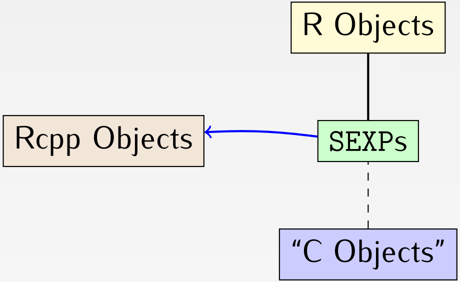

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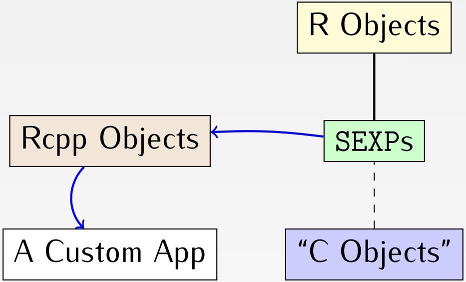

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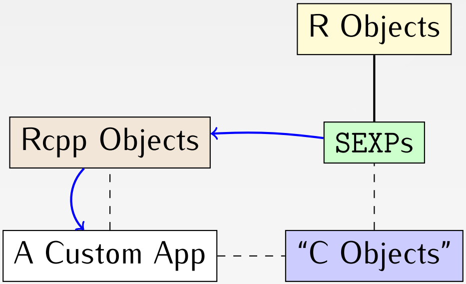

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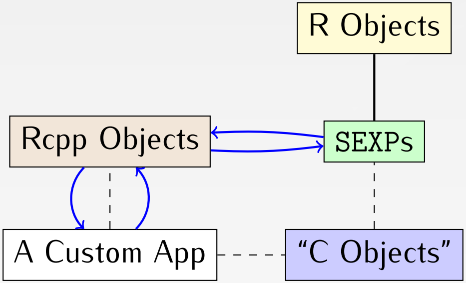

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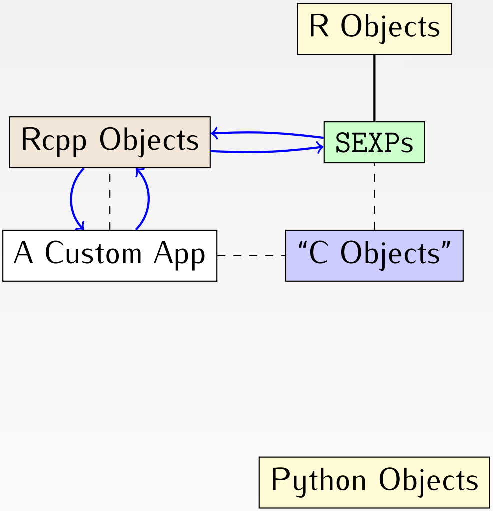

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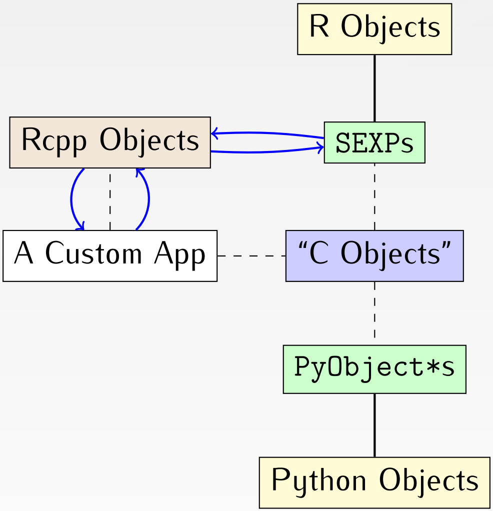

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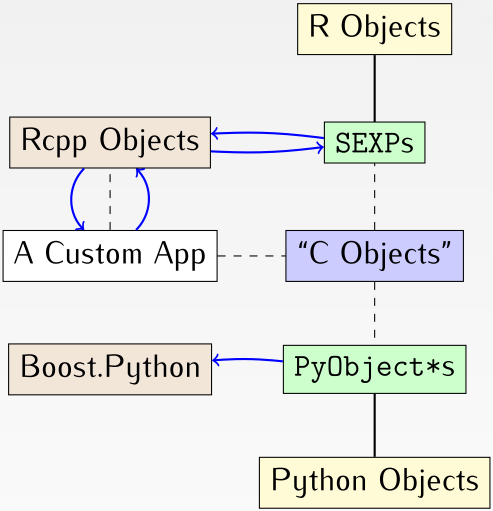

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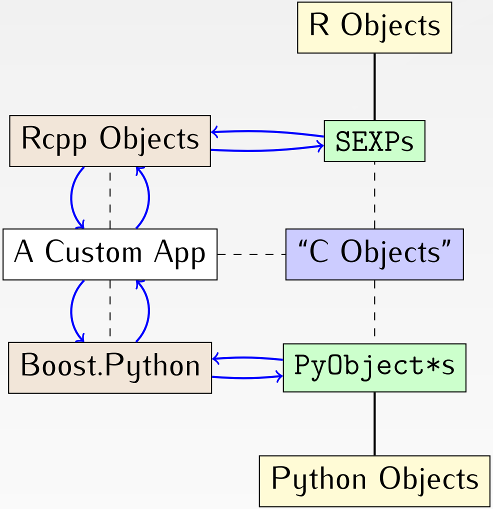

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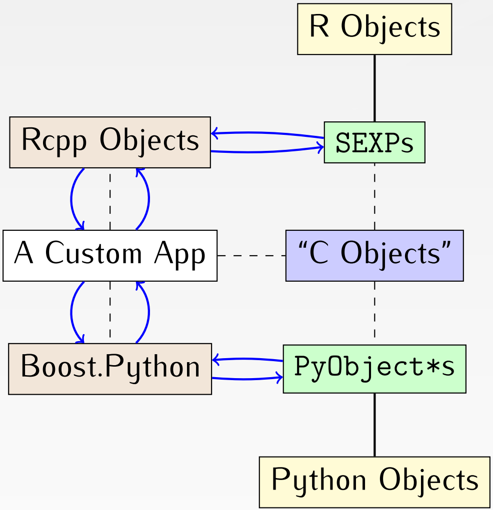

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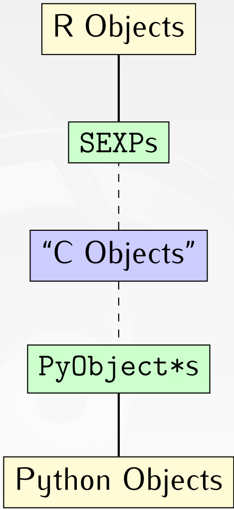

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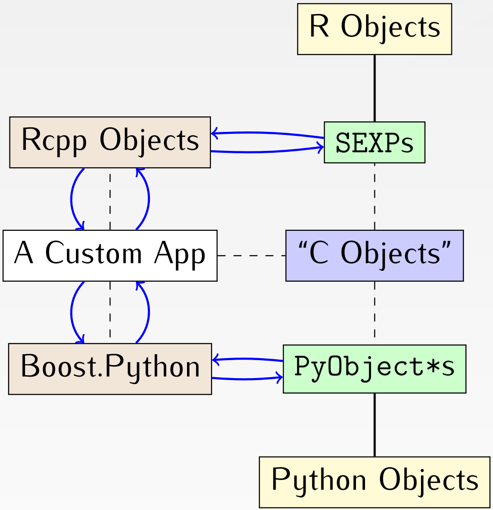

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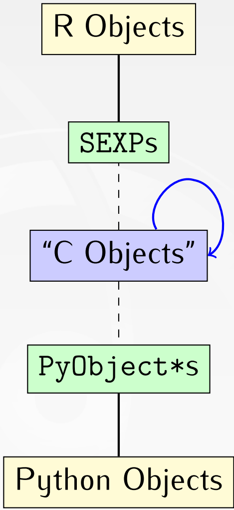

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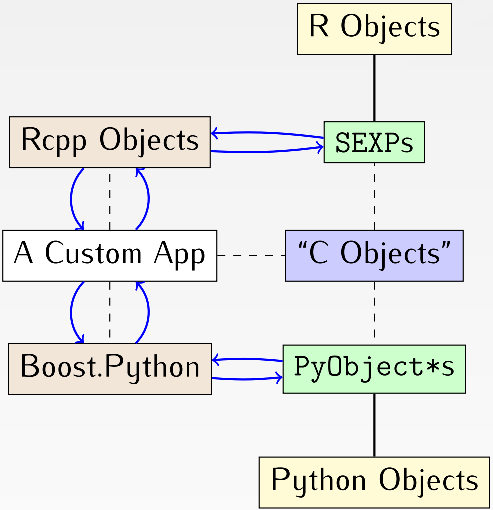

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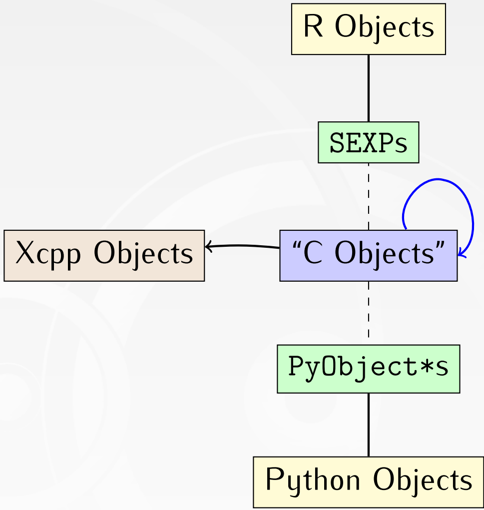

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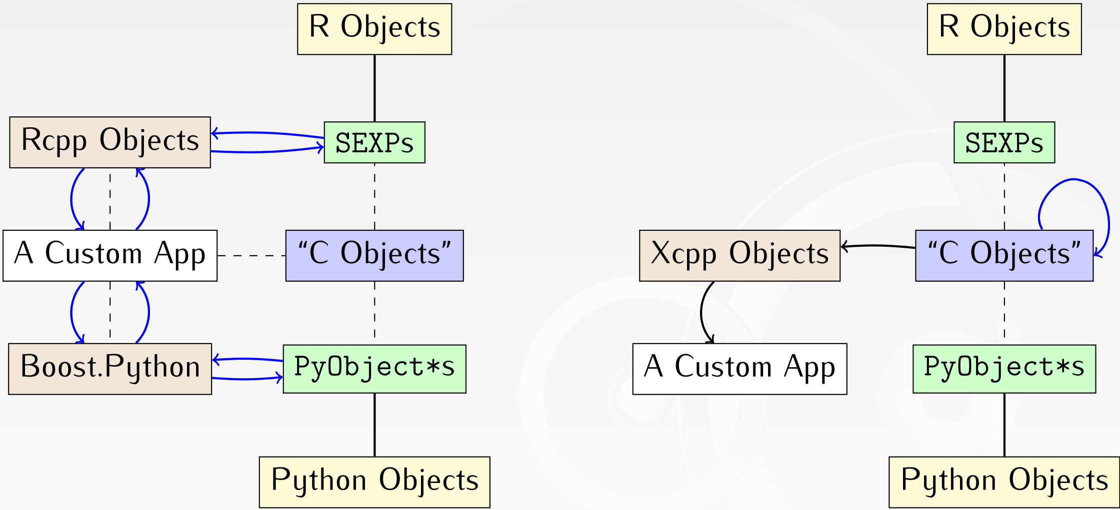

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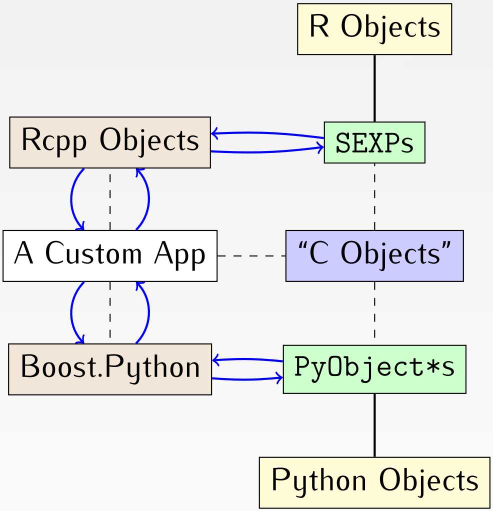

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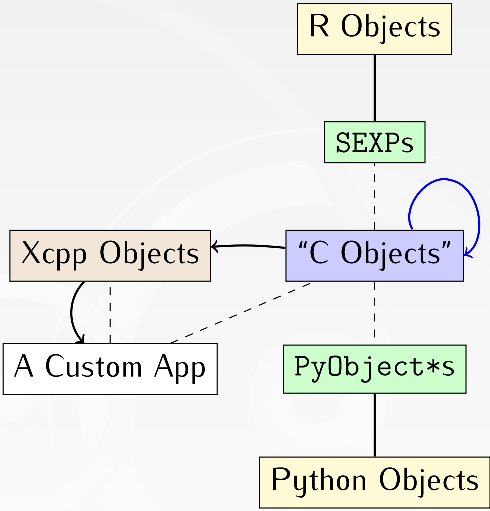

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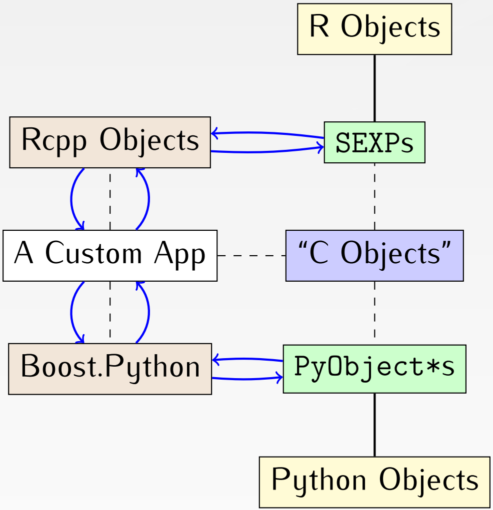

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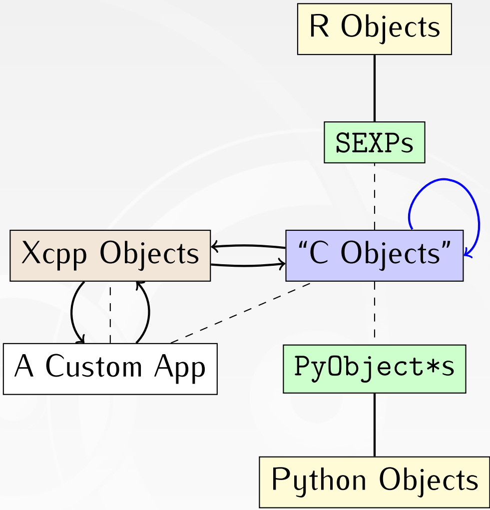

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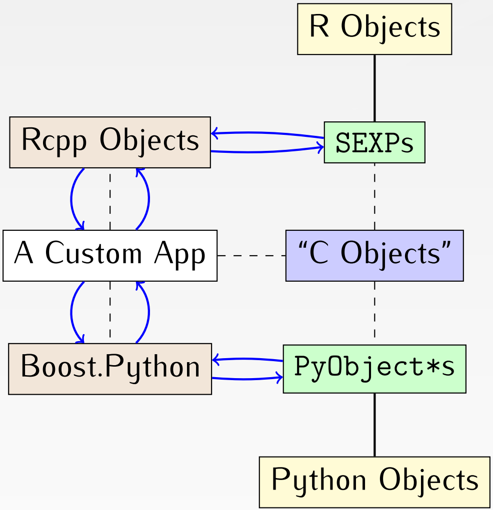

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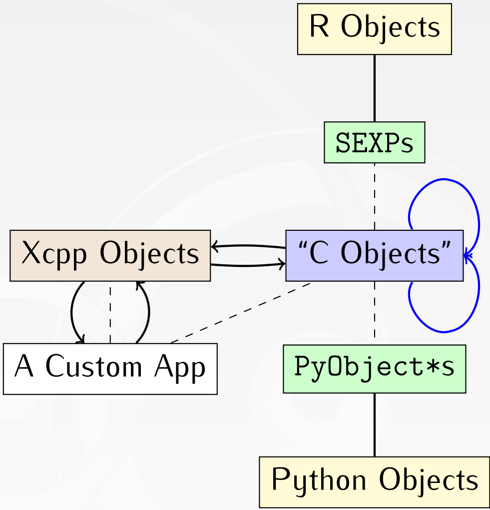

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  - “XPtrs” for auxiliary, “internal” data to be alive between function calls;

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  - "XPtrs" for auxiliary, "internal" data to be alive between function calls;
- Note that R/Pandas data frames are somewhere in-between matrices and dictionaries;

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New project (contributors needed!):

- Xcpp: Language-agnostic C++ bindings for scientific computing;
- Common, most useful objects:
  - bool, int, float, complex, string scalars
  - bool, int, float, complex, string vectors;
  - bool, int, float, complex, string matrices
    ("long" vectors with 2D indexing, C- or Fortran-order);
  - "lists" (sequences of arbitrarily-typed elements, integer-based indexing);
  - "dictionaries" (key-value pairs, string-based indexing)
    (in R – named lists, "objects", environments);
  - "XPtrs" for auxiliary, "internal" data to be alive between function calls;
- Note that R/Pandas data frames are somewhere in-between matrices and dictionaries;
- Of course, Rcpp-like "sugar" ops can be added (overloaded operators, etc.).

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- accessing/syncing RNG state;
- build & link – two possibilities:
  - independent builds for each language – not so efficient (time and space);
  - one "core" dynamically linked library, with separate language-specific interfaces that link to it – relying on C++-based libs may be hard (`extern "C"`, different compilers, etc. – e.g., R-tools gcc vs Anaconda MSVC).
- ...

Thank you!

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