Good Relations with R

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Rennes, useR! 2009

Motivation

Large scale benchmark analysis of performance of SVMs for classification and regression problems:

> *Meyer, Leisch & Hornik (2003), "The Support Vector Machine under test", Neurocomputing.*

Results: $\sim$ 1,000 figures ... Analysis and presentation?

> *Hothorn, Leisch, Zeileis & Hornik (2005), "The design and analysis of benchmark experiments", Journal of Computational and Graphical Statistics.*
>
> *Hornik & Meyer (2007), "Deriving consensus rankings from benchmarking experiments", Proceedings of GfKl 2006.*

In particular: how can the results on individual data sets be aggregated? More generally: how can possibly partial preference relations be aggregated?

Such issues are dealt with in social choice (going back to Borda and Condorcet), group choice, multi criteria decision making, ...

Consensus relations

Aggregation of individual relations amounts to determinining so-called *consensus relations*, e.g., as a *central relation* R which minimizes

$$\Phi(R) = \sum_{b=1}^{B} w_b d(R_b, R)$$

for a suitable dissimilarity measure d over a suitable class of relations R (e.g., preferences or linear orders).

Applications abound: rank proposals, candidates, journals, web pages, ..., based on possibly incomplete individual rankings.

Relations

Given k sets of objects $X_1, \ldots, X_k$, a k-ary relation R on $D(R) = (X_1, \ldots, X_k)$ is a subset $G(R)$ of the Cartesian product $X_1 \times \cdots \times X_k$.

So clearly,

- $D(R)$, the *domain* of R, is a k-tuple of sets
- $G(R)$, the *graph* of R, is a set of k-tuples

To provide a faithful computational model, we need *tuples* (where R vectors can serve reasonably well) and *sets*.

Sets in base R

A set is a collection of distinct objects.
Base R provides some functionality for set computations (`union`, `intersect`, `setdiff`, ...), but no data structures, and e.g.

```
> union(list(1), list("1"))

[[1]]
[1] 1

[[2]]
[1] "1"

> intersect(list(1), list("1"))

[[1]]
[1] "1"
```

(Part of the "problem" is that `match` is used for comparing elements.)

Package sets

Package `sets` provides data structures and basic operations for ordinary sets, and generalizations such as fuzzy sets, multisets, and fuzzy multisets (and tupels).

Operations include union, intersection, Cartesian product, etc., mostly also available as binary operators (`|`, `&`, `*`, etc.).

```
> A <- set(1)
> B <- set("1")
> A | B

{"1", 1}

> A & B

{}
```

Note that comparison is (by default) performed via `identical`.

Power sets and outer products

Power sets can be obtained via 2^.

Using `set_outer`, one can apply a function on all factorial combinations of the elements of two sets.

```
> S <- set(1, 2, 3)
> PS <- 2^S
> set_outer(PS, PS, FUN = set_is_subset)
```

```
           {}   {1}   {2}   {3} {1, 2} {1, 3} {2, 3} {1, 2, 3}
{}       TRUE  TRUE  TRUE  TRUE   TRUE   TRUE   TRUE      TRUE
{1}     FALSE  TRUE FALSE FALSE   TRUE   TRUE  FALSE      TRUE
{2}     FALSE FALSE  TRUE FALSE   TRUE  FALSE   TRUE      TRUE
{3}     FALSE FALSE FALSE  TRUE  FALSE   TRUE   TRUE      TRUE
{1, 2}  FALSE FALSE FALSE FALSE   TRUE  FALSE  FALSE      TRUE
{1, 3}  FALSE FALSE FALSE FALSE  FALSE   TRUE  FALSE      TRUE
{2, 3}  FALSE FALSE FALSE FALSE  FALSE  FALSE   TRUE      TRUE
{1, 2, 3} FALSE FALSE FALSE FALSE  FALSE  FALSE  FALSE      TRUE
```

Fuzzy sets

In emphFuzzy sets, elements have degrees of membership.

Introduced by Zadeh (1965) as an extension of the classical notion of a set, extending the basic set operations $\cap, \cup, \neg$ to the $\min, \max, 1-$ of the corresponding membership values.

Modern fuzzy set theory knows a variety of other extensions ("fuzzy logics") via t-norms, t-conorms, and negations.

Package `sets` supports the most popular fuzzy logic families (drastic, product, Lukasiewicz, Fodor, Frank, Hamacher, ...), and also offers a simple mechanism for fuzzy rules and fuzzy inference.

Food for thought

Implementing sets of *arbitrary* elements of the R language is surprisingly tricky.

Set elements should be "distinct", but how should they be compared? (Using ==, `all.equal`, `identical`, ...?) We provide "customizable" sets (class `cset`) where this can be changed.

Elements of sets have no position: hence, positional subscripting is disallowed. Iteration is used for accessing the elements, currently (rather low-level) via `lapply`/`as.list`. (Work on a general iteration mechanism for R has recently become available via the `iterators` package.)

Food for thought

Set operations involve checking and removal of duplicate elements, which can become costly. `unique()` is efficient, but currently ignores attributes . . . (Our implementation uses a two-pass procedure, based on hashed environments and `identical()`).

Because sets can be nested (sets of sets of . . .), we also need to enforce a canonical order of the elements. But sorting strings is locale-dependent, and Unicode allows different byte sequences for the same glyphs. Recursive objects are sorted according to their serialization.

Package relations

Package `relations` provides data structures and algorithms for k-ary relations with arbitrary domains, featuring relational algebra, predicate functions, and fitters for consensus relations.

Relations can be created via `relation` by giving the graph, characteristic function or incidences and possibly the domain, or via `as.relation` (e.g., unordered factors coerced to equivalence relations; ordered factors and numeric vectors to order relations, data frames taken as relation tables).

Characteristic function: membership function of the graph.

Incidences: array of memberships of the corresponding tuples in the graph.

Under the hood

The R universe features many "relational" data structures (cluster partitions correspond to equivalence relations; graphs, hypergraphs and networks; ...).

Relations are implemented as an S3 class which allows for a variety of internal representations ("Containers"). Currently, by default, we use a dense array representation of the incidences, and a more compact representation for "rankings" (weak orders).

Computations on relations are based on high-level generic getters for the basic constituents: `relation_domain`, `relation_graph`, `relation_charfun`, `relation_incidence`.

Example

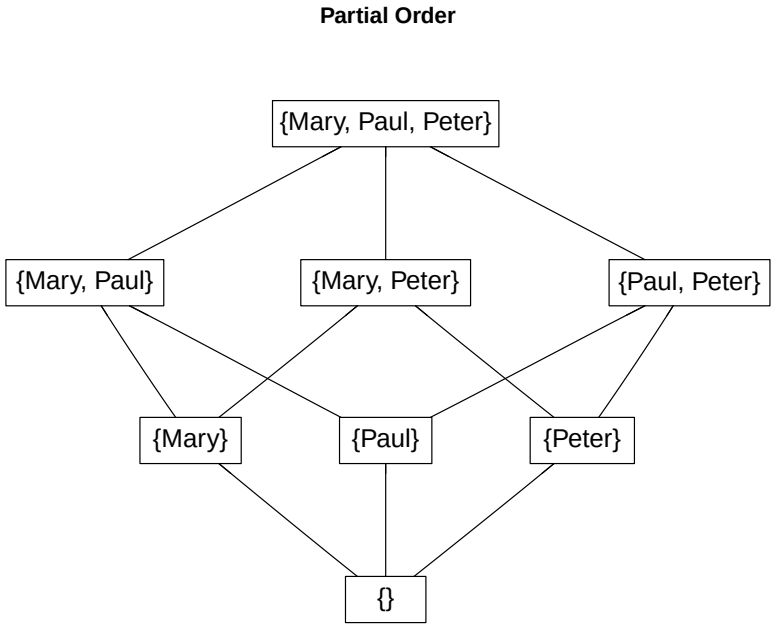
```
> R <- as.relation(c(1, 2))
> relation_domain(R)

Relation domain:
A pair with elements:
{1, 2}
{1, 2}

> relation_graph(R)

Relation graph:
A set with pairs:
(1, 1)
(1, 2)
(2, 2)

> relation_incidence(R)

Incidences:
  1 2
1 1 1
2 0 1
```

Example

```
> S <- set("Peter", "Paul", "Mary")
> R <- relation(incidence = set_outer(2^S, '<='))
> R
```

```
A binary relation of size 8 x 8.
```

```
> plot(R)
```



Endorelations and predicates

Endorelations are binary relations with domain $D = (X, X)$.
Such relations can be reflexive, symmetric, transitive, ...

Important combinations of the basic properties include

- **equivalance** reflexive, symmetric, and transitive
- **preference** complete, reflexive, and transitive (also known as "weak order")
- **linear order** antisymmetric preference

These properties can be tested for using `relation_is_`*`foo`* predicates.
The `summary` method for relations applies all available predicates.

Basic operations

Rich collection of basic operations, including

- Complement and dual
- Comparisons (using the natural ordering), meet and join
- Composition, union, intersection, difference
- Transitive reduction and closure, covering relation
- Plotting (via `Rgraphviz`) for certain endorelations (using Hasse diagrams)

Also implements relational algebra of Codd (1970) using convenient binary operators (e.g., inner/outer joins, projection, selection, ...).

Ensembles

Relation ensembles are collections of relations $R_b = (D_b, G_b), 1 \leq b \leq B$ with identical domains, i.e., $D_1 = \cdots = D_B$.

Implemented as suitably classed lists of relation objects, making it possible to use `lapply` for computations on the individual relations in the ensemble.

Available methods for relation ensembles include those for subscripting, `c`, `t`, `rep`, and `print`.

Dissimilarities

Several methods for computing dissimilarities between (ensembles of) relations, with default the symmetric difference distance (the cardinality of the symmetric difference of two relations, i.e., the number of tuples contained in exactly one of two relations).

Characterizable as the least element moves distance in the lattice of relations on the same domain under the natural (set inclusion of the graphs) order. For preference relations: Kemeny-Snell distance. In addition, Cook-Kress and Cook-Kress-Seiford distances.

Allows for dissimilarity based analysis of relation ensembles (clustering, scaling, ...).

Consensus relations

Several methods for obtaining consensus relations, including Borda, Condorcet and Copeland methods, but most importantly for finding central relations minimizing weighted average symmetric distance

$$\Phi(R) = \sum_{b=1}^{B} w_b d(R_b, R)$$

over suitable "families" of relation (e.g., equivalence, preferences and linear orders).

Accomplished by reformulating the consensus problem as a binary linear program

$$\sum_{i,j} c_{ij}(w_1, \ldots, w_B, R_1, \ldots, R_B) x_{ij} \rightarrow \max$$

for the 0/1 incidences x_{ij} of the consensus relation.

Consensus relations

Allows using solvers from packages `Rcplex`, `Rglpk`, `Rsymphony` and `lpSolve`.

(Encapsulates creation and solution of MILPs/MIQPs, to be spun off into an optimization infrastructure package eventually.)

Always possible to find *all* solutions via poor person's branch and cut (only `lp_solve` and `cplex` provide some solver support for this).

For equivalences and preferences, one can specify the desired number of equivalence classes. For this, the consensus problem is reformulated as a binary quadratic program.

Example: SVM Benchmarking

Results for benchmarking 17 classification methods on 21 data sets: relation ensemble of length 21 with encoding

$$l(R_b)_{i,j} = \begin{cases} 1 & \text{if method } i \text{ did not significantly outperform} \\ & \text{method } j \text{ on data set } b \\ 0 & \text{otherwise} \end{cases}$$

Load the data set:

```
> data("SVM_Benchmarking_Classification")
> SVM_Benchmarking_Classification

An ensemble of 21 relations of size 17 x 17.
```

Fit all consensus linear orders and preferences:

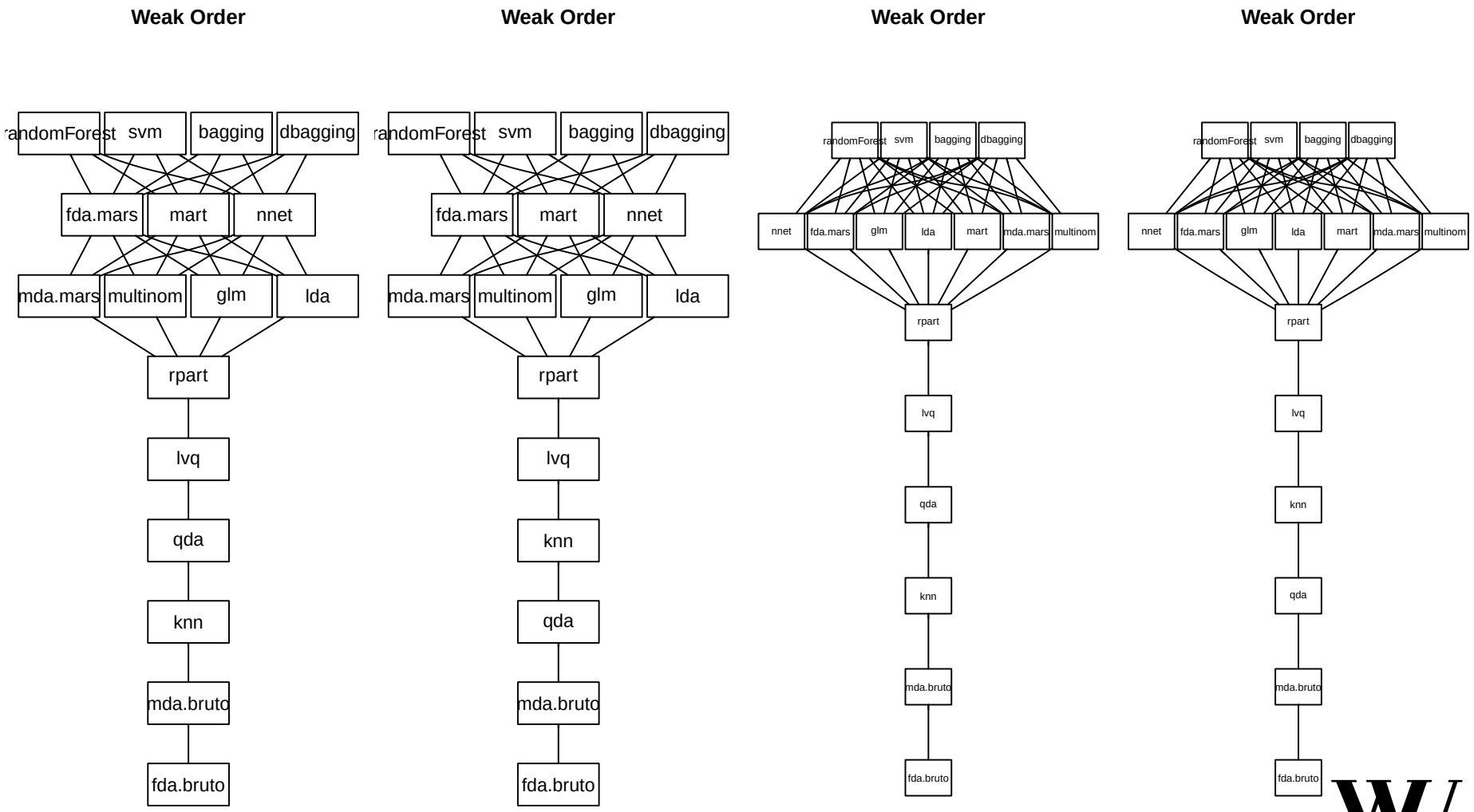
```
> cens_L <- relation_consensus(SVM_Benchmarking_Classification,
+     "SD/L", all = TRUE)
> cens_P <- relation_consensus(SVM_Benchmarking_Classification,
+     "SD/P", all = TRUE)
```

Consensus Relations: Linear Orders

```
> plot(c(cens_L, min(cens_L)), layout = c(1, 5))
```

Consensus Relations: Weak Orders

```
> plot(cens_W, layout = c(1, 4))
```



Extensions

The package also offers ...

- Fuzzy relations
- Prototype-based partitioning ("clustering") of relation ensembles
- Social choice (e.g., determine the/all "k-winners"):

```
> relation_choice(SVM_Benchmarking_Classification, k = 4)

Using the GLPK callable library version 4.37
{"bagging", "dbagging", "randomForest", "svm"}
```

- and much more.

Coordinates

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