CARAF: Complex Aggregates within RAndom Forests

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Relational Data

Relational Data

- Data represented across several tables: different kinds of objects.
- In this work, 2 tables:
 - main: objects we want to predict on,
 - secondary: objects in 1-to-many relationship with main table, composition for instance.
- Could be a star schema: one main table with several secondary tables directly related to the main.
- Task: build features of main objects using properties of secondary objects



Urban Blocks

Urban Blocks Dataset

- Urban blocks composed of several buildings.
- Learning task : predict of which kind is the urban block according to geometric properties.
- Data available from former project: 591 urban blocks from 4 areas of Strasbourg, composed of 7692 buildings.

• 6 class-problem.

Relational Two-Table Setting

Urban Blocks Example - Schema

| blo | ck_ | id | densit | cy convexit | y | elongatio | n | ar | ea | (| class |
|---------|-----------------------|---------|-----------|---------------|--------------|-----------|-------|-----|-------|-------|-------|
| 1 0.151 | | L 0.986 | 0.986 | | | 22925 | | h | indiv | | |
| 2 0.192 | | 0.832 | 0.832 | | | 15363 | | h | coll | | |
| | 3 0.204 | | 4 0.718 | 0.718 | | | 17329 | | h | mixed | |
| | | | | | | | | | | | |
| | 1 Main table - blocks | | | | | | | | | | |
| | | | | | | 0N | | | | | |
| | building id | | convexity | e | elongation a | | ea | blo | ck_ | id | |
| | 1 1 | | 1.000 | | 0.538 | 16 | 55 | 5 1 | | | |
| | 1 2 | | 0.798 | | 0.736 | 32 | 23 | | 1 | | |
| | 1_3 | | 1.000 | | 0.668 | | 4 | 1 | | | |
| | | | | | | | | | | | |
| | 2_1 | | 0.947 | | 0.925 2 | |)2 | 2 | | | |
| 2_2 | | 1.000 | | 0.676 147 | | 2 | | | | | |
| | | | | | | | | | | | |

Secondary table - buildings

State of the Art

Possible Approaches

- Tilde^a: logical decision tree induction, introduction of secondary objects through existential quantifier.
- RELAGGS^b: propositionalization through simple aggregation.

^aHendrik Blockeel and Luc De Raedt. "Top-Down Induction of First-Order Logical Decision Trees". In: Artif. Intell. 101.1-2 (1998), pp. 285–297. ^bM.-A. Krogel and S. Wrobel. "Facets of Aggregation Approaches to Propositionalization". In: Work-in-Progress Track at the Thirteenth International Conference on Inductive Logic Programming (ILP). 2003.

Our aim

- Introduce relevant secondary objects (like Tilde).
- Use aggregation to go further than the existential quantifier.
- \Rightarrow Complex Aggregation

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Complex Aggregates - Introduction

What is a Complex Aggregate

- Constructed feature of the objects of the main table.
- Aggregates the values of a feature of secondary objects that meet a certain condition.

Composition of Complex Aggregates

- Selection of secondary objects:
 - Link: Relationship between tables.
 - Filter: Conditions on secondary objects.
- Aggregation process:
 - Attribute to aggregate (not always).
 - Aggregation function.

Background on Complex Aggregates

Examples of Complex Aggregates



Examples

- Number of buildings in the block.
- Maximum area of buildings with elongation \geq 0.5.
- Average elongation of buildings with convexity < 0.9 and area ≥ 150 .

Example - Notation

avg(elongation, buildings, convexity $< 0.9 \land area \ge 150$)

Searching the Feature Space

Explosion of Search Space

- Problem: number of complex aggregates for a given problem is combinatorial, impossible to consider them all!
- Especially, the aggregation condition is a conjunction of several basic conditions.

ILP 2014

- RRHCCA¹: Random Restart Hill-Climbing of Complex Aggregates.
- In a single decision tree, find splits on complex aggregates.
- Given the aggregation process, find the best conjunction of conditions through random restart hill-climbing.

¹C. Charnay, N. Lachiche, and A. Braud. "Construction of Complex Aggregates with Random Restart Hill-Climbing". In: 24th International Conference on Inductive Logic Programming (ILP'14). 2014.

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Random Forests



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Random Forests for Complex Aggregates

Motivation

- Large Feature Space. ($\approx F \cdot A \cdot N^A$)
- Complex aggregates are specific, overfitting with a single decision tree.
- Relax the optimization method to search through the feature space.

Existing Methods

- Tilde extended to both complex aggregates and Random Forests, FORF^a.
- However, memory problems when language bias allows big conjunction for selection condition.
- Feature sampling is uniform \rightarrow may not create enough diversity.

^aAnneleen Van Assche et al. "First order random forests: Learning relational classifiers with complex aggregates". In: *Machine Learning* 64.1-3 (2006), pp. 149–182.

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Random Forests in CARAF

Complex Aggregate Feature Sampling

- Bootstrapping and recombination are classic.²
- Structural feature sampling: keep square root of aggregation processes and half of the attributes for conditions. (sampled feature space size \approx square root of the original feature space size)

| Attr Func | Area | Elong | Conv |
|--------------|------|-------|------|
| Average | x | | |
| Min | | | |
| Max | | | |
| Std Dev | | х | |
| Sum | x | | |

| Cond | Area | Elong | Conv |
|------|------|-------|------|
| | х | х | |

²Leo Breiman. "Random Forests". In: *Machine Learning* 45.1 (2001), pp. 5–32. Clément Charnay (ICube, UdS) CARAF ILP'15 14 / 19

Hill-Climbing of Aggregation Conditions

Hill-Climbing Strategies

- RRHCCA (ILP 2014): given the aggregation process, find the best conjunction by testing a neighborhood of refinements at each step.
- Random: given the aggregation process, try one random neighbor at each step.
- Global: try one random neighbor condition at each step, on every aggregation process at hand.

Refinements

From original condition area \geq 150, we can refine to:

- Empty condition.
- area \geq 150 \wedge elongation < 0.6
- area \geq 120
- area \geq 180

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Out-of-bag Accuracy Results

Out-of-bag Accuracy

- For each training instance, use sub-forest that did not see the instance at training to classify.
- Used to compare Random Forests.
- 33 trees in each forest.

| Dataset | RELAGGS | FORF | RRHCCA | Random | Global |
|------------|---------|--------|---------------|---------------|---------------|
| Auslan | 94.19% | ERR | 96.53% | 95.91% | 94.66% |
| Diterpenes | 89.09% | 90.49% | <u>92.95%</u> | 85.06% | <u>93.35%</u> |
| Jp-Vowels | 93.78% | 94.86% | 95.41% | 97.30% | 97.03% |
| Musk1 | 80.43% | 78.26% | <u>89.13%</u> | 84.78% | 80.43% |
| Musk2 | 76.47% | 75.49% | 81.37% | 85.29% | 82.35% |
| Opt-digits | 22.37% | 76.57% | <u>95.94%</u> | <u>94.60%</u> | <u>92.77%</u> |
| Urban | 83.42% | 75.81% | <u>84.94%</u> | <u>83.76%</u> | <u>84.60%</u> |
| | | | 7 - 6 | 6 - 5 | 6.5 - 6 |

Experimental Results and Conclusion

10-fold Cross Validation Results

| Dataset | Muta | Urban |
|-------------|--------|--------|
| RELAGGS-1 | 89.40% | 74.86% |
| RELAGGS-100 | 90.26% | 84.55% |
| RRHCCA-1 | 84.86% | 74.69% |
| RRHCCA-100 | 91.33% | 87.48% |
| Random-1 | 87.67% | 75.55% |
| Random-100 | 92.22% | 87.28% |
| Global-1 | 87.82% | 74.60% |
| Global-100 | 91.96% | 87.68% |



Conclusion and Future Work

Conclusion

- Random Forests improve over Decision Trees with Complex Aggregates.
- Our Hill-Climbing algorithms perform better than RELAGGS and FORF.
- Faster hill-climbing algorithms do not yield loss of accuracy.

Future Work

- Do Feature Selection with Random Forests: find most relevant families of aggregates.
- Handle Nested Relationships, especially complex aggregates as aggregated feature.