

An algorithm to recommend activities in scientific workflows:

An ontology, artificial intelligence and frequency-based approach

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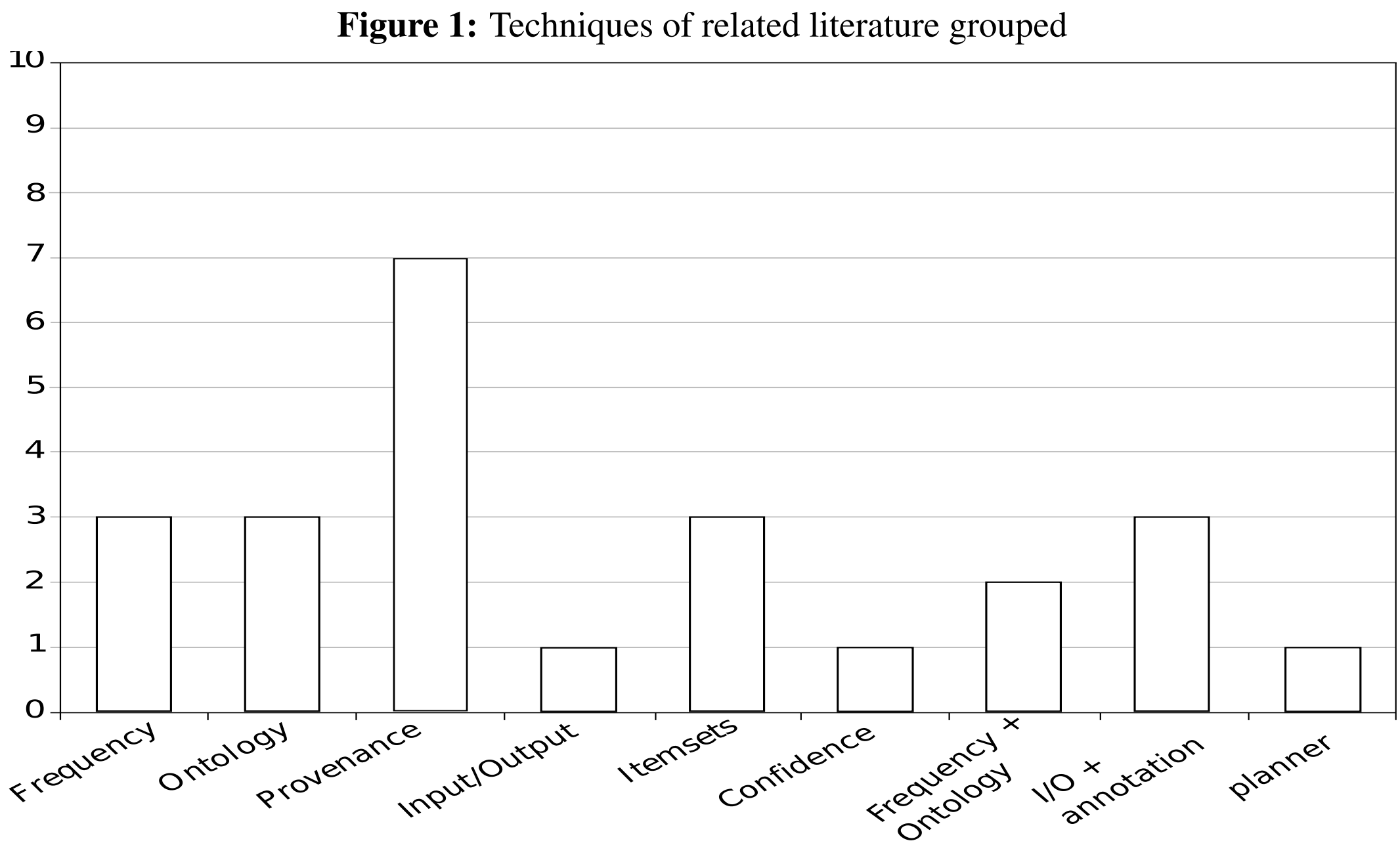
Introduction

The number of research projects using intensive computing has been growing in areas that lack advanced computer skills such as biology, physics, and astronomy. One of the tools to assist in the management and construction of intensive computing experiments are the workflows manager systems. *Scientific Workflows* represent structured and ordered processes, constructed manually, semi-automatically or automatically to solve scientific problems using activities, which can be: i) source code blocks; (ii) services; or iii) finished workflows. These systems facilitate the creation of new experiments, sharing of results and reuse of existing activities.

Nowadays, there are a large number of activities available in repositories such as *myExperiment* which stores more than 2,500 workflows and *BioCatalogue* Which provides more than 2,464 services. The large number of activities and the low reuse of some activities and workflows motivate the construction of techniques to recommend activities to the scientists during the composition of workflows.

In the workflow management systems, activities are typically represented as graphical icons with drag and drop functionality. Thus, it is possible to construct computational experiments by dragging icons and filling in input parameters. Most of these systems provide sets of basic activities that can be used in different domains, for example, an activity that calculates the average value of a set of data is applicable in biology, physics, astronomy, and other areas. However, there is a precondition for reusing and/or creating workflows: knowing the available activities.

In order to minimize the problem of knowing a large number of activities, several techniques were proposed to recommend activities or to compose workflows. In the first case, which aims to serve an expert user in these systems, during the construction of the workflow, activities are recommended to help to complete the workflow. In the second case, whose goal is to serve a less expert user on these systems, several workflows are built and the user should select which one most satisfies his/her need.



Main Contributions

Recommendation Algorithm

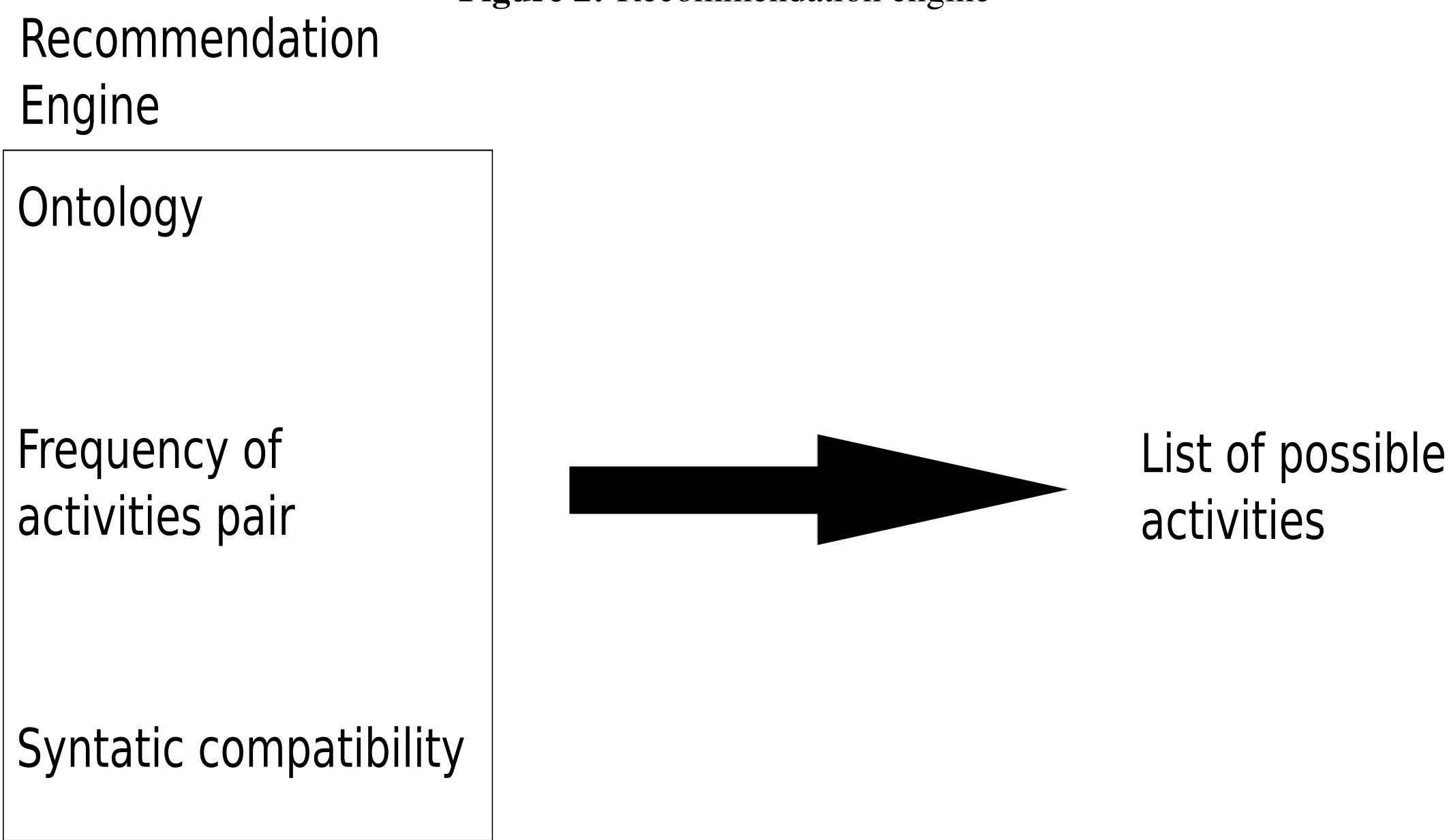
The proposed solution recommends activities using three concepts in the area of scientific workflows: i) frequency of activities; ii) compatibility between input and output; and iii) semantics of activities.

The proposed solution begins by calculating the frequency of occurrence of each pair of existing activities, which is the number of times that an activity W occurs immediately after another activity Z . By considering only activities that have already been connected (on the dataset of workflows), the output and input compatibility is guaranteed.

After calculating the frequency it is necessary to annotate all the workflows, using the concepts of the domain ontology, this step was performed manually (not automatically). Finally, the algorithm annotates all activities with the same annotations of their respective workflow; i.e., if the X activity is inside two workflows with distinct annotations, then this activity will be related to two different concepts from the ontology.

To understand the recommendation training mechanism, another example will be used to simulate a user interacting with the recommendation system. Let us assume that during the construction of the workflow a scientist inserts the Z activity and asks for a recommendation. The system will look at the list of activities after Z sorted by frequency and ontological concept and will return the recommendation list. The sorting considers the ontological concepts serves as a tiebreaker criterion when two activities have the same frequency.

Figure 2: Recommendation engine



Recommendation as a classification problem

The 73 bioinformatics' workflows together with their 280 activities were converted into a matrix $M_{i,j}$. In this matrix, each line corresponds to a workflow and each column to an activity. $M_{i,j} = 1$ means that the workflow i has the activity j . Otherwise, $M_{i,j} = 0$ means that the workflow i does not have the activity j . Table ?? presents an fictitious example of a matrix M . To perform the evaluation of the approach, an activity is removed from each row of the table ??, and a list of possible activities is recommended. The goal of the recommendation system is to correctly identify which activity is missing in the workflow (i.e., the one that was removed).

Figure 3: Matrix of scientific workflows

Workflow	Activ01	Activ02	...	Activ280
01	1	0	...	0
02	1	1	...	1
03	1	0	...	1
⋮	⋮	⋮	⋮	⋮
73	1	0	...	0

In order to use classification and regression techniques, some changes were proposed in the original dataset (exemplified in the table ??), which can be viewed in the table ??. Each workflow was replicated 118 times. 59 of these correspond to identical copies of the original workflow, while in the other 59 one activity was removed from original workflow and a new activity was added representing a possible recommendation. Thus, for each original workflow, there will be 59 correct instances and 59 incorrect instances and this type of information will be used to train the classifiers or regressors.

Figure 4: Adapted matrix of scientific workflows used in classification and regression problems

#	Workflow	Activ01	...	Activ280	Class
1	01	1	...	0	T
2	01	1	...	0	T
⋮	⋮	⋮	⋮	⋮	⋮
59	01	1	...	0	T
1	01	0 (removed)	...	0	F
2	01	0 (removed)	...	0	F
⋮	⋮	⋮	⋮	⋮	⋮
59	01	0 (removed)	...	1 (added)	F
⋮	⋮	⋮	⋮	⋮	⋮
1	73	1	...	0	T
2	73	1	...	0	T
⋮	⋮	⋮	⋮	⋮	⋮
59	73	1	...	0	T
1	73	1 (added)	...	0	F
2	73	1	...	0	F
⋮	⋮	⋮	⋮	⋮	⋮
59	73	1	...	1 (added)	F

Results

#	Approach	S@1	S@5	S@10	MRR
1	Random	0.0037	0.0260	0.0280	0.033
2	Apriori	0.0037	0.0385	0.0559	0.037
3	KNN _C	0.0037	0.0685	0.0959	0.040
4	Neural Network _C	0.0137	0.1507	0.1781	0.089
5	CART _C	0.0274	0.1233	0.3699	0.113
6	CART _R	0.1370	0.1370	0.2603	0.114
7	Naive Bayes _C	0.0274	0.1507	0.3425	0.114
8	Binomial _R	0.0822	0.1918	0.2055	0.136
9	Neural Network _R	0.1096	0.2603	0.2603	0.154
10	MARS _R	0.1233	0.2055	0.2192	0.167
11	FES	0.1474	0.2603	0.3699	0.196
12	SVM _R	0.1233	0.3151	0.4932	0.238
13	SVM _C	0.2425	0.4658	0.4932	0.244
14	composed SVM _C	0.2515	0.4458	0.5232	0.314
15	Rotation Forest _C	0.2925	0.4558	0.5432	0.324
16	FESO	0.3425	0.4658	0.5932	0.334

Figure 5: Figure caption

Conclusions

- This work developed a hybrid technique for recommending activities in scientific workflows, which uses syntactic compatibility, frequency, and domain ontologies to recommend activities, called FESO
- We have modeled the recommendation problem as a regression and classification problem in artificial intelligence
- As future works, we intend to investigate the use of data provenance to increase the accuracy of the recommendations..

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