A dockerized string analysis workflow for Big Data

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Introduction

- **Data Science:** manipulation of data using mathematical and algorithmic methods to solve complex problems in an analytical way
- **Data of various types**: biological data, documents, energy consumption, etc.
  Big data + lack of generalized methods -> machine learning in large-scale infrastructures
- **Challenges**: high dimensionality, complexity and diversity of the data, limited resources, varying structures of the available analytic tools
- **Scientific workflows:** combine heterogeneous components to solve problems characterized by data diversity and high computational demands
- **Cloud computing:** a popular way of acquiring computing and storage resources on demand through virtualization technologies

Data Transformation into Strings

- Diversity of data
  - Need for expressing them in a common format
- We select to transform the input data into strings
  - Easy to handle them
  - Makes the whole process quicker
  - Lossy compression (in some cases)
    – controlled by the user
- Dockerization
  - Big data cannot fit in a single machine

Numeric Vectors

	Pos 1	Pos 2	..	Pos L
1	0.95	0.15	..	0.86
2	0.98	0.28	..	0.87
3	0.95	0.51	..	0.02
..	..	..	..	..
N	0.99	0.54	..	0.01

Character Vectors

	Pos 1	Pos 2	..	Pos L
1	A	R	..	F
2	A	R	..	F
3	A	K	..	Y
..	..	..	..	..
N	A	K	..	Y

Or

Strings

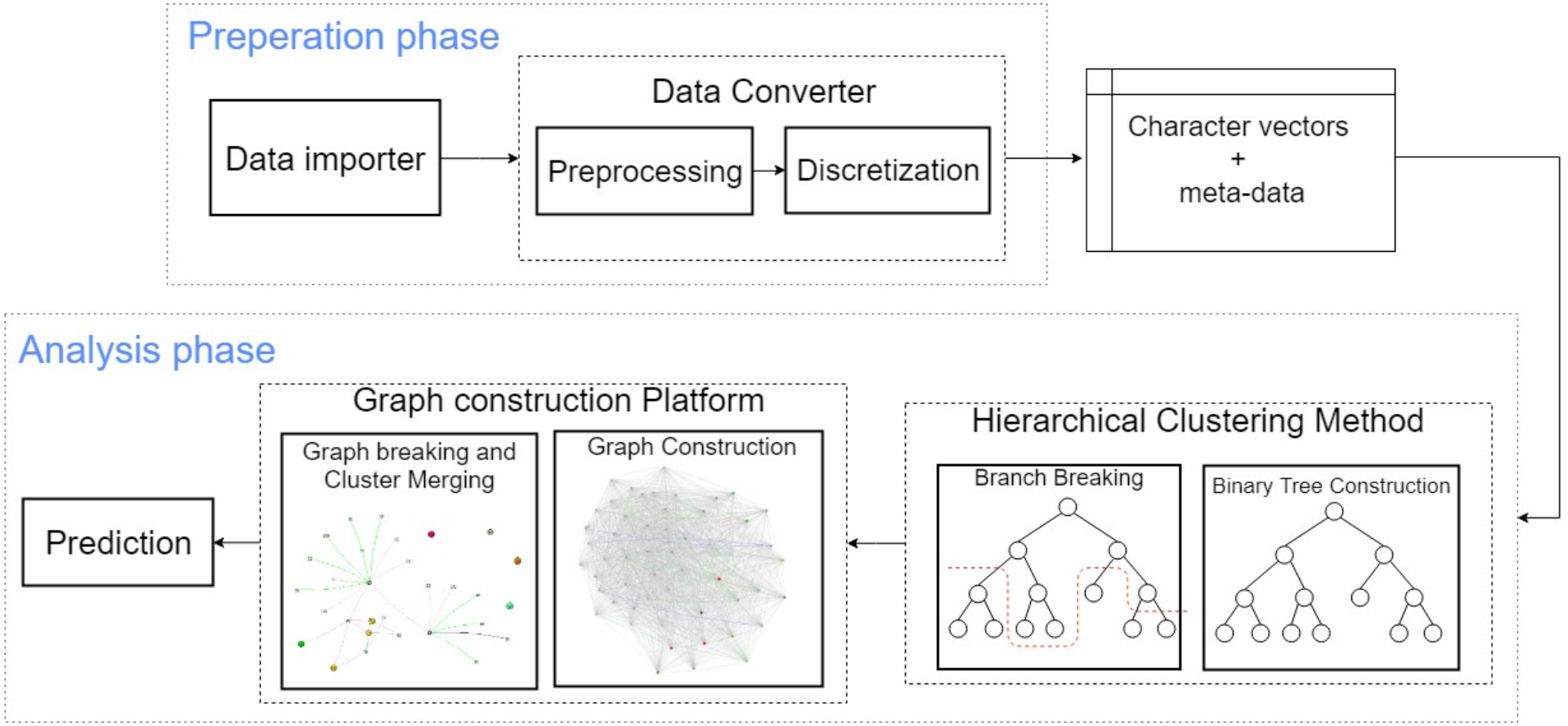
	Sequences
1	ARAYDFWSGYLF
2	ARVYDFWSGYLF
3	AKSGAIAAAGDY
..	..
N	AKSGTIAAAGDY

Dockerized String Analysis workflow (DSA)

The main objectives of DSA are:

1. **Transform** input data into internal format, considering domain specific features
2. Create **custom pipelines** based on the user preferences
3. Provide **analytics services** integrating new scalable tools
4. Provide **visualization services** that can support decision-making
5. Be available in both **script-based format** and in a **graphical interface**
6. Be suitable for **cloud infrastructures**

The DSA workflow architecture



docker

Takes into account: a) Domain-specific characteristics

b) User preferences

Preparation phase

The preparation phase includes **data importing** and **transformation**, in order for the input data to be reformatted as a set of

Character vectors + meta-data

Data importer: Acquire the data to be analyzed in specific supported formats based on their domain

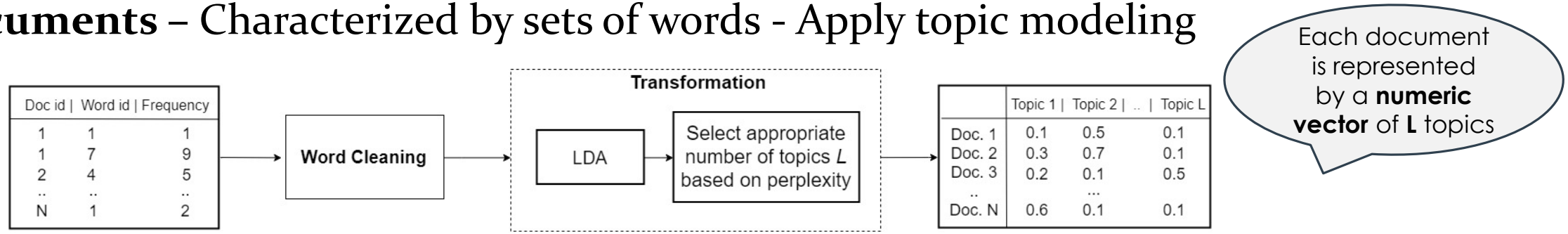
Preprocessing module: Clean the input data and transform them into a general format which is required by the analysis phase. Data are transformed into vectors of values accompanied with the appropriate meta-data depending on the domain.

Discretization module:

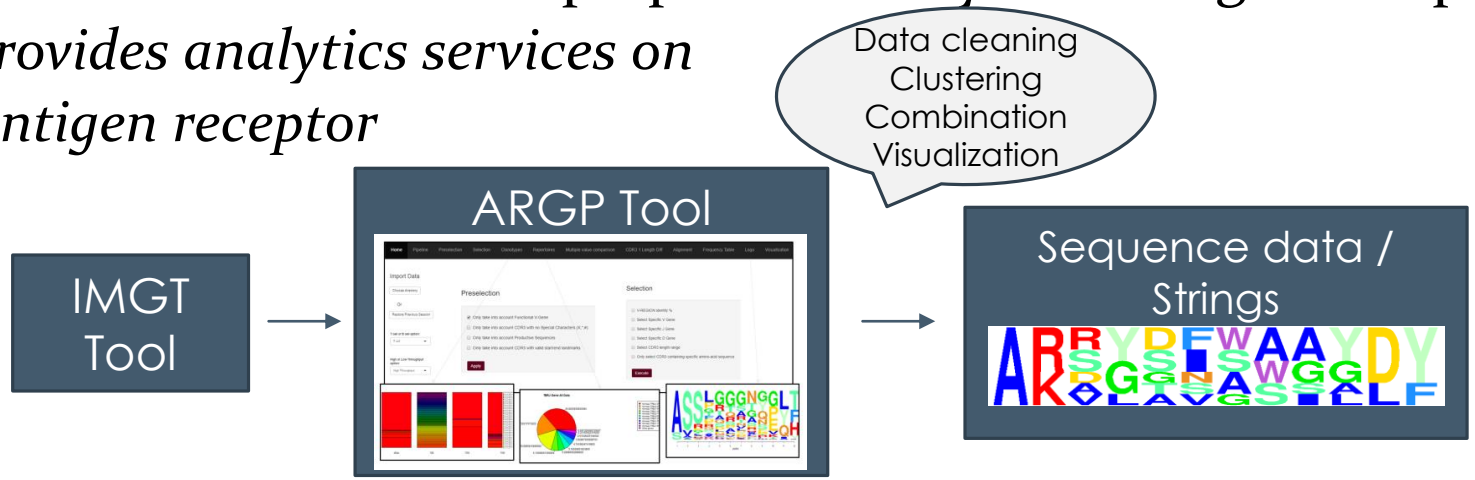
- The numeric vectors are discretized into partitions of **length *B*** by assigning each value into a **bin** based on the closed interval where it belongs to
- By making use of letters to represent the bins, the numeric vectors are converted into **strings**

Preprocessing module per domain

Documents – Characterized by sets of words - Apply topic modeling



Gene sequence data - Data are preprocessed by the Antigen receptor gene profiler (ARGP) - *Provides analytics services on antigen receptor*



Time series data - Data cleaning, normalization, missing value handling etc.

Analysis phase

Clustering module: A new scalable multi-metric algorithm for hierarchical clustering is applied. It is a Frequency Based Clustering (FBC) algorithm [1]

It consists of:

Binary Tree Construction + Branch Breaking

Algorithms

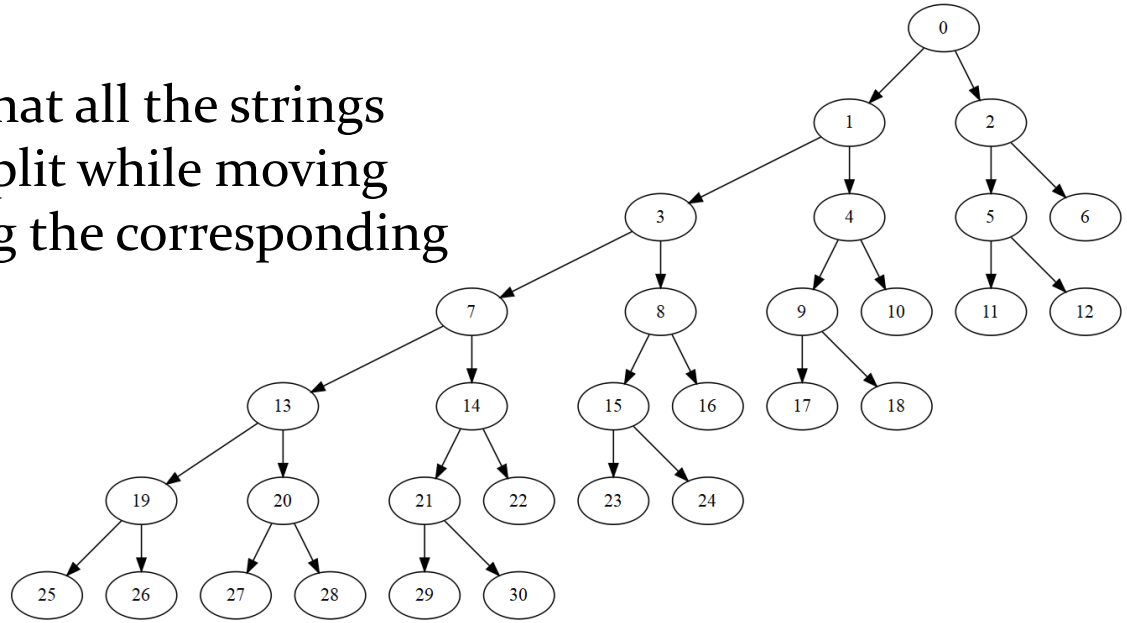
Graph mining module: Using clustering results in combination with graph construction techniques, we provide information about the data relationships in a graphical interactive environment. Graph mining metrics and graph clustering algorithms for sub-graph creation are also utilized.

Prediction module: Integrates the results from the previous modules to train a model that can make predictions for missing connections of data and classify new items.

[1] Kotouza, M., Vavliakis, K., Psomopoulos, F., & Mitkas, P. (2018, December). A hierarchical multi-metric framework for item clustering. In 2018 IEEE/ACM 5th International Conference on Big Data Computing Applications and Technologies (BDCAT) (pp. 191-197). IEEE.

Binary Tree Construction Algorithm (Overview)

- A top down hierarchical clustering method
- It is based on the usage of a matrix that contains the frequencies for each position of the target strings (FM)
- At the beginning of the process, it is assumed that all the strings belong to a single cluster, which is recursively split while moving along the different levels of the tree, by splitting the corresponding FM
- Metrics:
  - Identity
  - Entropy
  - Bin Similarity



Theoretical basis

- *Frequency Matrix:* $FM \rightarrow B \times L$

Each element (i,j) of the matrix corresponds to the number of times bin i is present in positions j for all the strings

- *Identity:* $I = \sum_{j=1}^{L} id_j / L \quad , \quad id_j = \begin{cases} 100\%, & if\ max(FM_{ij}) = 100\% \\ 0\%, & if\ max(FM_{ij}) \neq 100\% \end{cases}$

The percentage of sequences with an exact alignment

- *Entropy:* $H_j = -\sum p_i \log(p_i)$

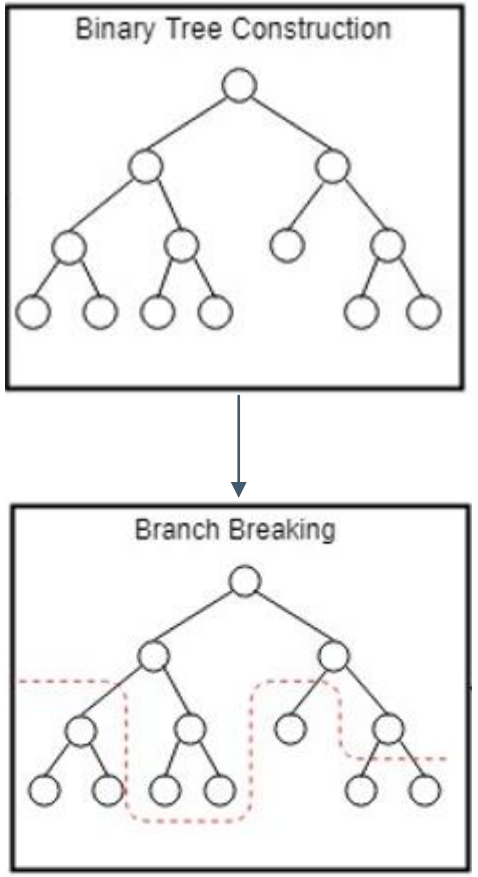
Represents the diversity of the column

- *Bin Similarity:* $BS = \sum_{j=1}^{L} BSM_j / L$, *BSM is a weighted version of FM*

Calculated using the similarities of the bins that participate in each topic

Branch Breaking Algorithm

- Asymmetric tree, the number of items that each cluster consists of varies
  -> the tree cannot be cut by selecting a unique level for the overall tree
  -> for each branch, the appropriate level to be cut is examined
- The parent cluster is compared to its two children clusters recursively as one goes down through the path of the tree branch
- The comparison is applied using the metrics that have been computed for each cluster C_i (I_i, H_i, BS_i) and user selected thresholds for each metric (*thrI*, *thrH*, *thrBS*)



Analysis phase (2)

Clustering module: A new scalable multi-metric algorithm for hierarchical clustering is applied.

It consists of the *Binary Tree Construction* and the *Branch Breaking* algorithms.

Graph mining module: Using clustering results in combination with graph construction techniques, we provide information about the data relationships in a graphical interactive environment. Graph mining metrics and graph clustering algorithms for sub-graph creation are also utilized.

Prediction module: Integrates the results from the previous modules to train a model that can make predictions for missing connections of data and classify new items.

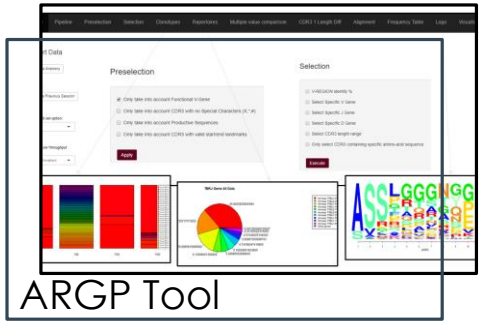
Network embedding – Application of Machine Learning techniques

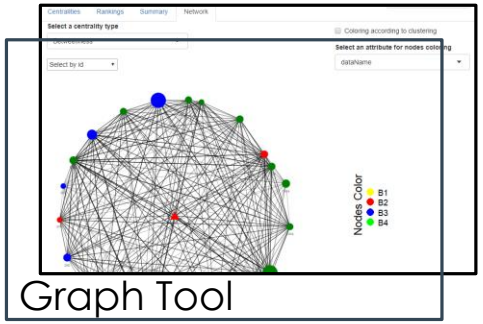
Software Implementation

- The modules are available in
  - **Script-based format**:
    - Command line interface
    - Faster execution
  - **Graphical user interface**:
    - For domain experts with limited technical experience

- The workflow components are dockerized
  -> able to run in cloud infrastructures

- All the modules are combined and described together using the Common Workflow Language (CWL)





Results

- *Case study 1*: Documents
- *Case study 2*: Gene sequence data
- *Case study 3*: Time series data -- in progress

Case study 1: Documents [1]

- We used benchmark data provided by the popular MovieLens 20M dataset:
  - 27,000 movies
- We created 20-length item vectors after applying LDA on the documents
- The item vectors were then discretized in 10 bins represented by alphabetic letters from A (90-100%) to J (0-10%)
- The groups of similar bins that were used are non-overlapping and are given by pairing bins in descending order i.e. <A,B>, <C,D>, <E,F>, <G,H>
- The results of the FBC algorithm were compared with those obtained by a Baseline Divisive Hierarchical Clustering (BHC) algorithm

#C	Algorithm	I	H	BS
23	BHC	13.696	0.167	85.769
	FBC	**74.783**	**0.081**	**93.264**
53	BHC	35.189	0.139	89.847
	FBC	**80.849**	**0.066**	**94.237**
125	BHC	53.080	0.120	92.886
	FBC	**90.600**	**0.038**	**96.981**

Performance results:
98% reduction in memory usage
99.4% reduction in computational time

[1] Kotouza, M., Vavliakis, K., Psomopoulos, F., & Mitkas, P. (2018, December). A hierarchical multi-metric framework for item clustering. In 2018 IEEE/ACM 5th International Conference on Big Data Computing Applications and Technologies (BDCAT) (pp. 191-197). IEEE.

Case study 2: Gene sequence data [2]

- We aimed to identify groups of patients based on a biologically important gene region of immunoglobulin
- Real-world dataset comprising 123 amino acid sequences of length 20, from patients with chronic lymphocytic leukemia
- The dataset was preprocessed using the ARGP tool
- FBC produced a binary tree with 19 levels
- The clustering results were assessed using the biological groups each sequence came from

Biological group	#Group seq/ #Cluster seq	Success rate	Level	Cluster
Subset #4	93/101	**92%**	4	13
Subset #4-34/20-1	2/2	**100%**	9	57
Subset #4-34-16	3/4	**75%**	5	31

[2] Tsarouchis, S. F., Kotouza, M. T., Psomopoulos, F. E., & Mitkas, P. A. (2018, May), A Multi-metric Algorithm for Hierarchical Clustering of Same-Length Protein Sequences, In IFIP International Conference on Artificial Intelligence Applications and Innovations (pp. 189-199). Springer, Cham.

Conclusion

- We present a workflow of **scalable algorithmic modules** that
  - Transforms the source data into strings, considering domain specific features
  - Provides big data analytic services
  - Provides fast execution of custom pipelines
  - Is dockerized

- Most of the modules of the workflow were applied on two practical case studies, showing promising results in terms of **efficiency** and **performance**

Future steps

- Adding further functionality on the graph mining module
- Development of the prediction module
- Further expansion of the work in more application fields, emphasizing in the source data transformation and the accurate representation of them
  - Time-series data
  - Data characterized by both numerical and verbal features

Thank you for your attention!

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