

Find similarity in Galaxy tools and predict next tools in workflows

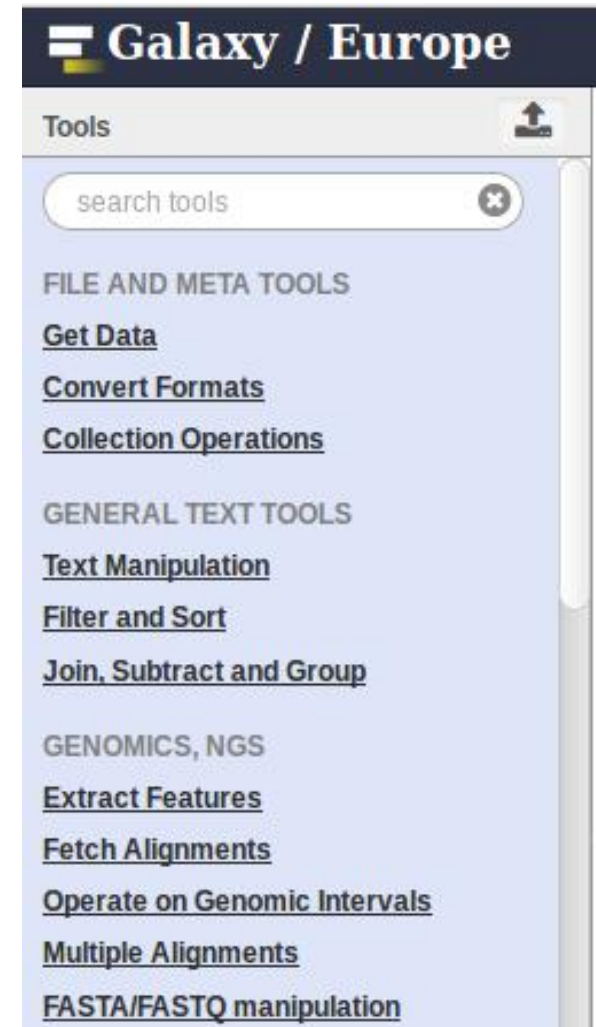
(Master's thesis)

Anup Kumar

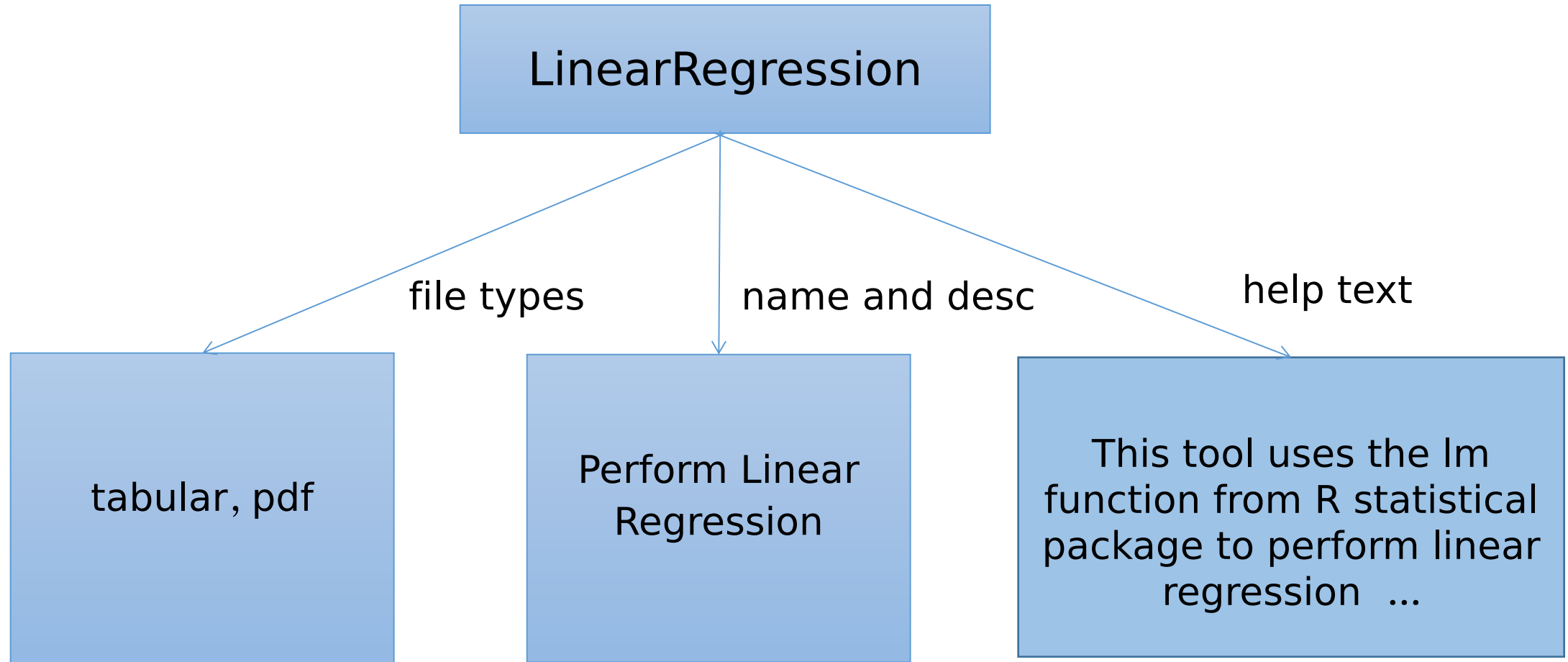
Find similarity in Galaxy tools

Machine learning (ML) and natural language processing (NLP) approaches

- Paragraph Vectors
- Gradient Descent



Tool's attributes



Approach

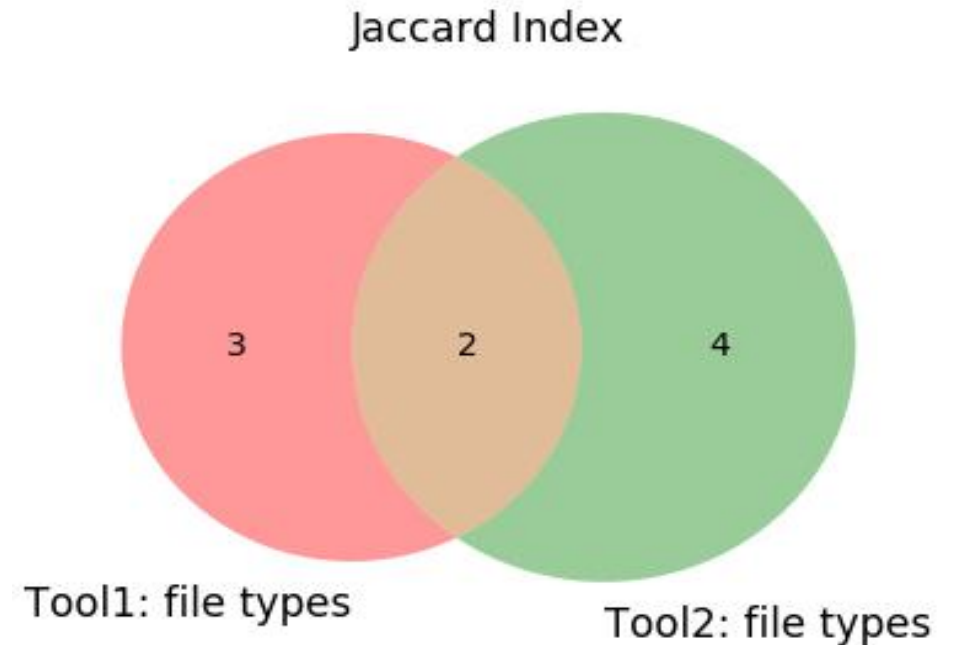
- Extract tool's attributes
- Clean text
- Create sets of tokens
- Learn similarities
- Combine optimally
- Visualize

Tokens

Attributes/ Tools	LinearRegression	LogisticRegression	Similarity
Input, output	'pdf' , 'tabular'	'tabular'	?
Name, description	'regress' , 'linear' , 'perform'	'logist' , 'regress' , 'perform'	?
Help text	'regress' , 'assumpt' , 'lm' , 'statist' , 'linear' ...	'vif' , 'regress' , 'glm' , 'car' , 'inflat' , 'function' , 'statist' , 'logist' ...	?

Compute similarity

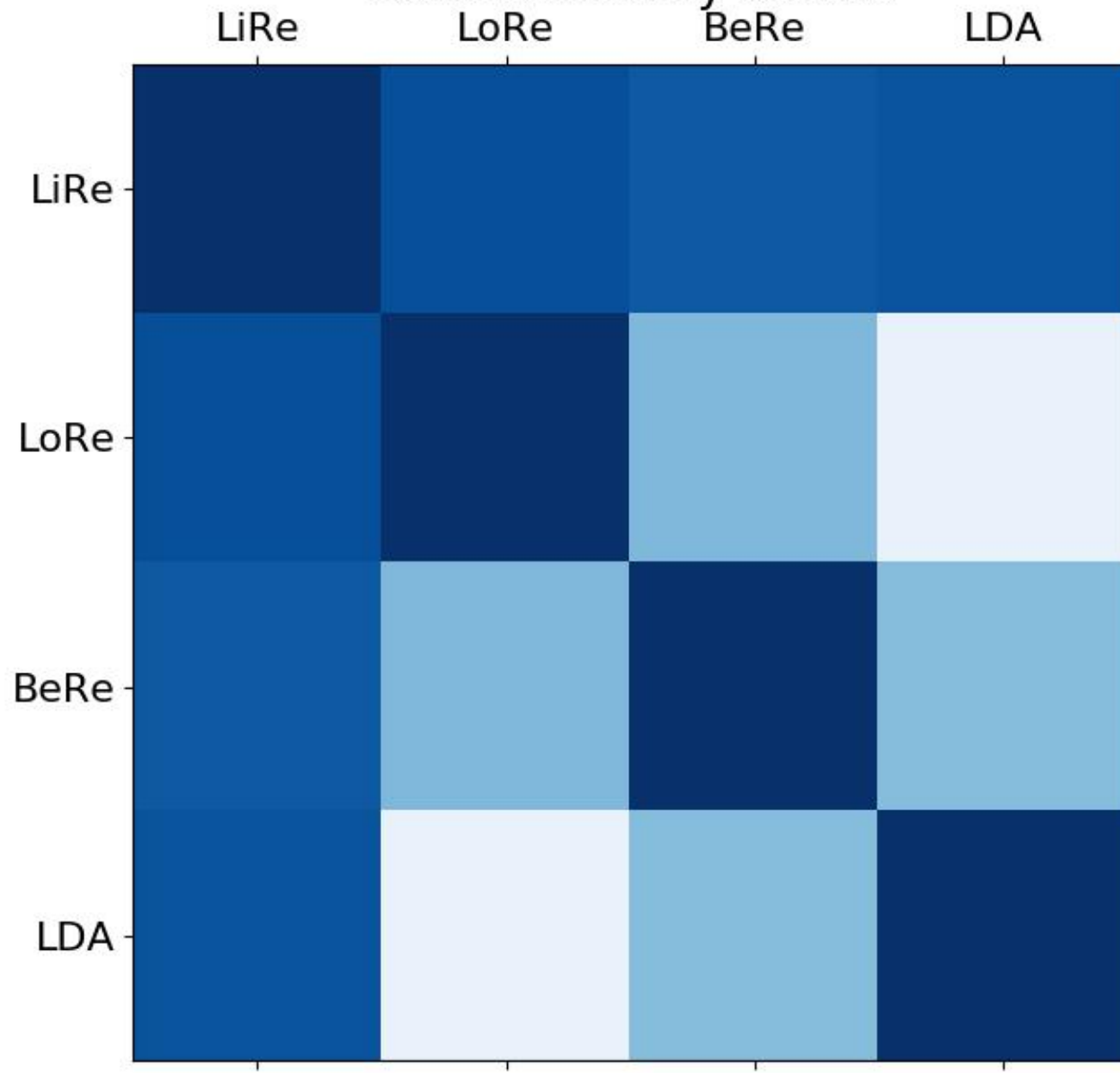
- Compute Jaccard Index for input/output



- Learn dense vectors for name, description and helptext*
- ['regress', 'linear', 'perform'] = [0.98, 0.07, ... , 0.12]
- Compute cosine distance between dense vectors

*[https://cs.stanford.edu/~quocle/paragraph_vector.pdf]

Tools similarity matrix



- LiRe - Linear Regression
- LoRe - Logistic Regression
- BeRe - BestSubsetsRegression
- LDA - LDA Analysis

How to combine ?

- 3 similarity matrices, one for each attribute
- How to combine them ? Take average ?
- Optimal combination, learn weights for each tool
- Similarity:

$$\arg \max_{(w_1, \dots, w_n)} \sum_{i=1}^N w_i \cdot s_i$$

Optimization

s1	Input, output				s2	Name, desc.				s3	Helptext			
↙	1	0.34	0.65	0.44	↙	1	0.76	0.63	0.85	↙	1	0.06	0.1	0.17
	0.34	1		0.76	1		0.06	1
	0.65	...	1	...		0.63	...	1	...		0.1	...	1	...
	0.44	1		0.85	1		0.17	1

$$\text{Minimize } ([1.0, 1.0, 1.0, \dots, 1.0] - [w1 \cdot s1 + w2 \cdot s2 + w3 \cdot s3])$$

$$\text{where } w1 + w2 + w3 = 1$$

Example

- Tool: LinearRegression
- Similarity for input/output: **s1** = [1.0, 0.34, 0.65, 0.44]
- Similarity for name, desc: **s2** = [1.0, 0.76, 0.63, 0.85]
- Similarity for helptext: **s3** = [1.0, 0.06, 0.1, 0.17]
- Optimal weights: **w1** = 0.3, **w2** = 0.6, **w3** = 0.1
- Similarity:

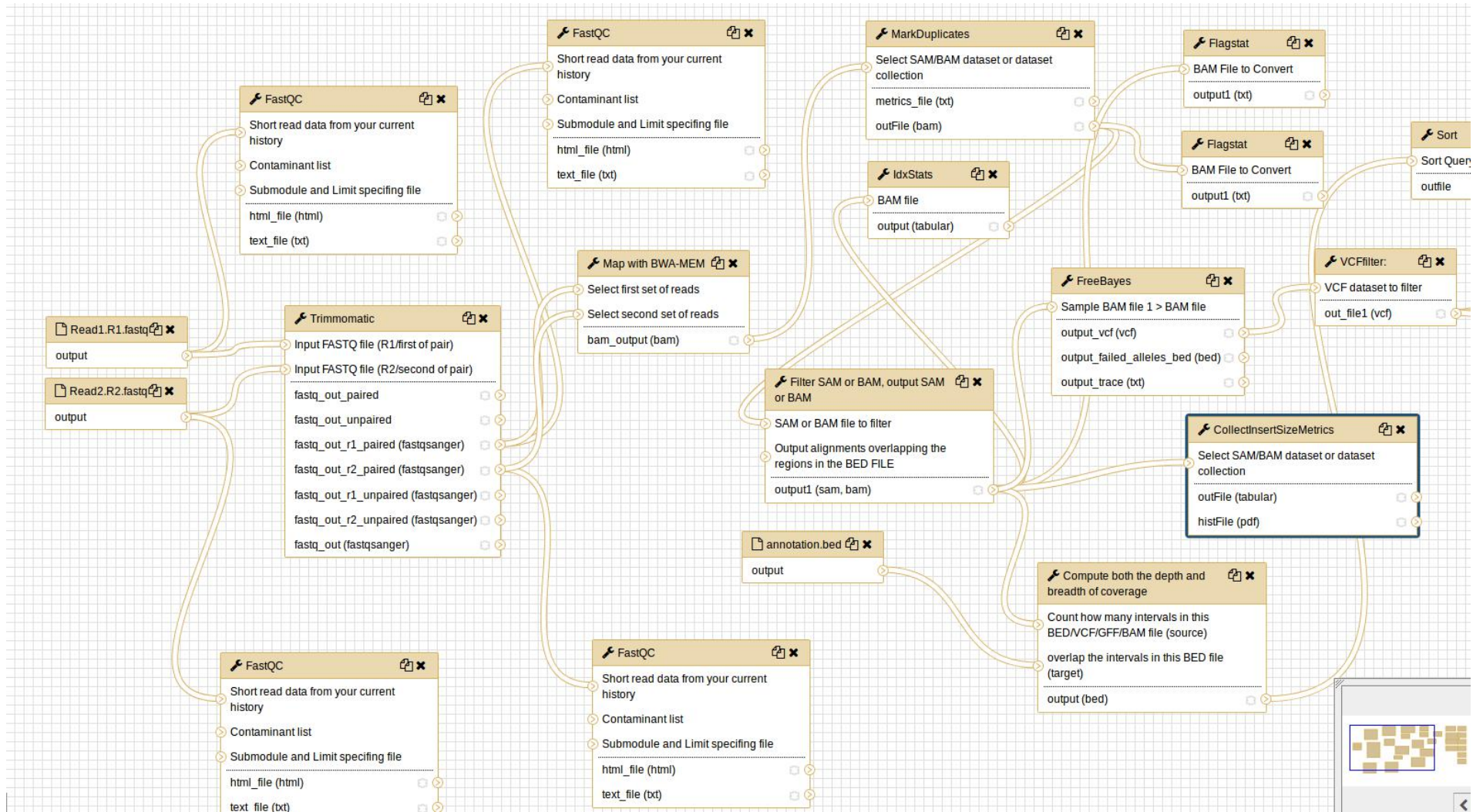
$$[w1 \cdot s1 + w2 \cdot s2 + w3 \cdot s3]$$

Visualizer and References

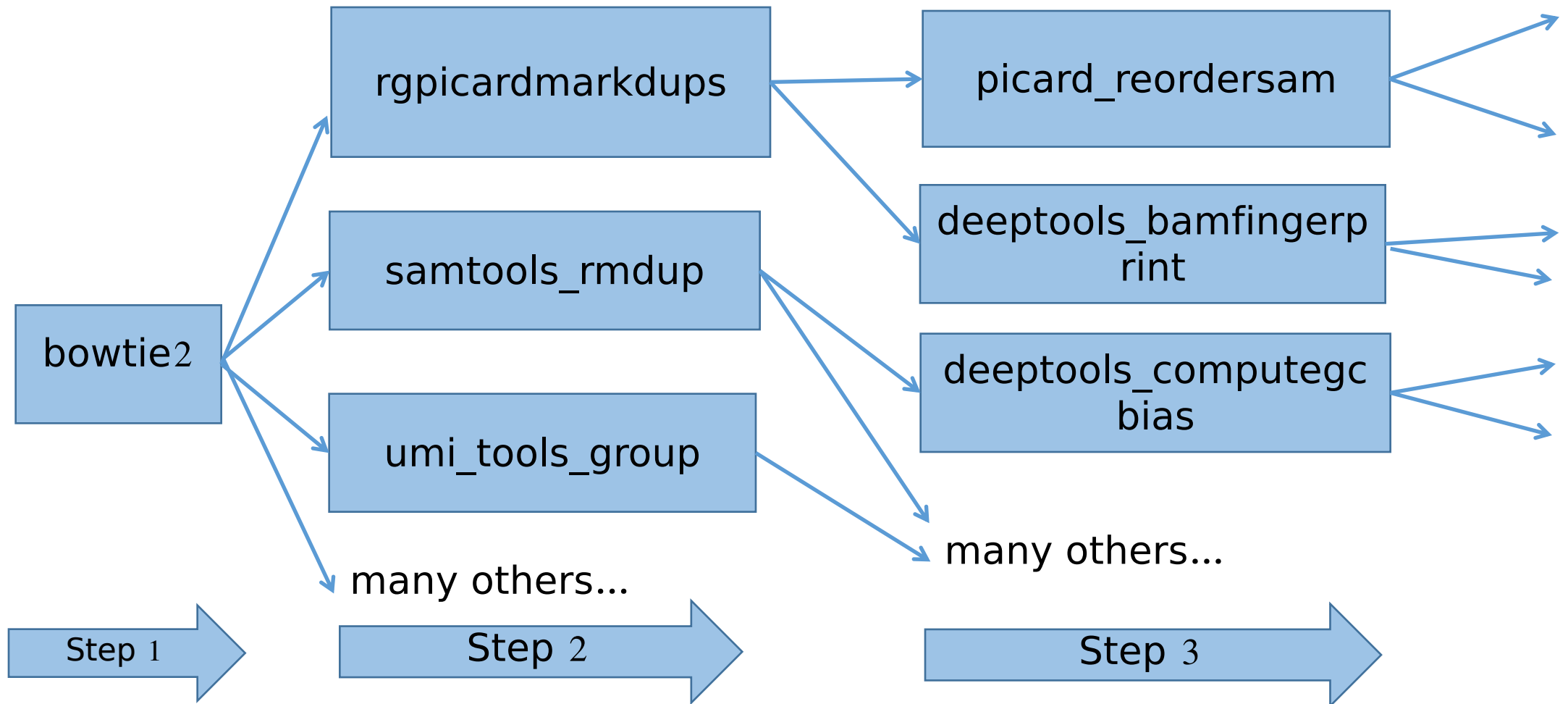
- Static website: results for ~ 1000 tools
- https://rawgit.com/anuprulez/similar_galaxy_tools/master/viz/similarity_viz.html
- https://github.com/anuprulez/similar_galaxy_tools
- https://cs.stanford.edu/%7Equocle/paragraph_vector.pdf
- <https://arxiv.org/pdf/1607.05368.pdf>

Predict next tools in Galaxy workflows

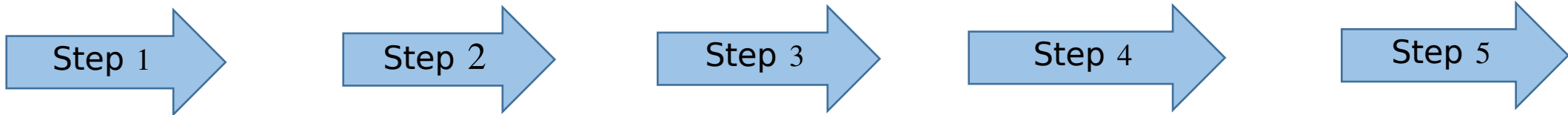
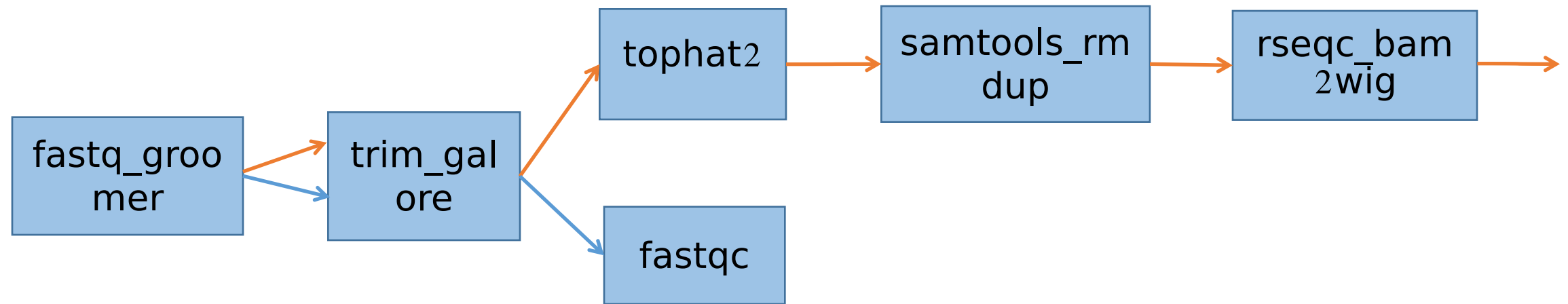
Galaxy workflow



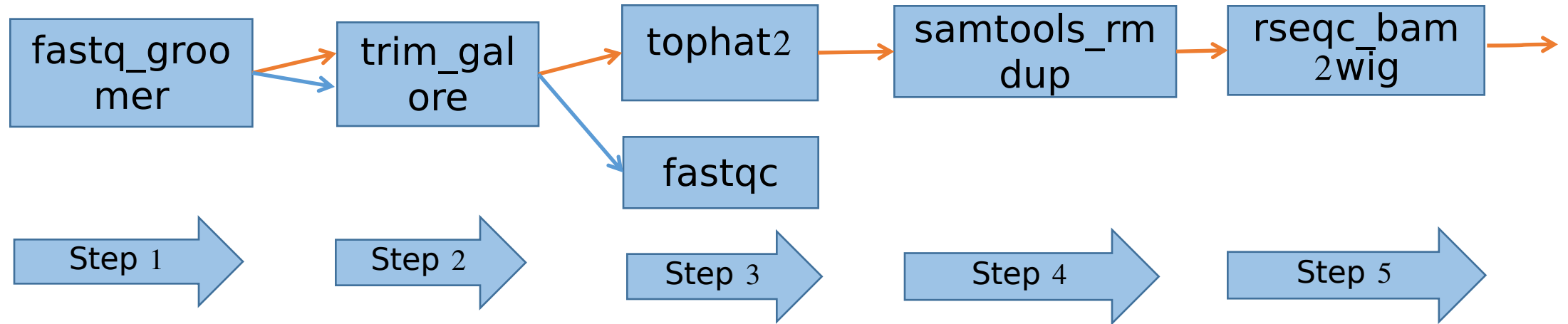
Next tools ?



Workflow as a sequence



Data preprocessing



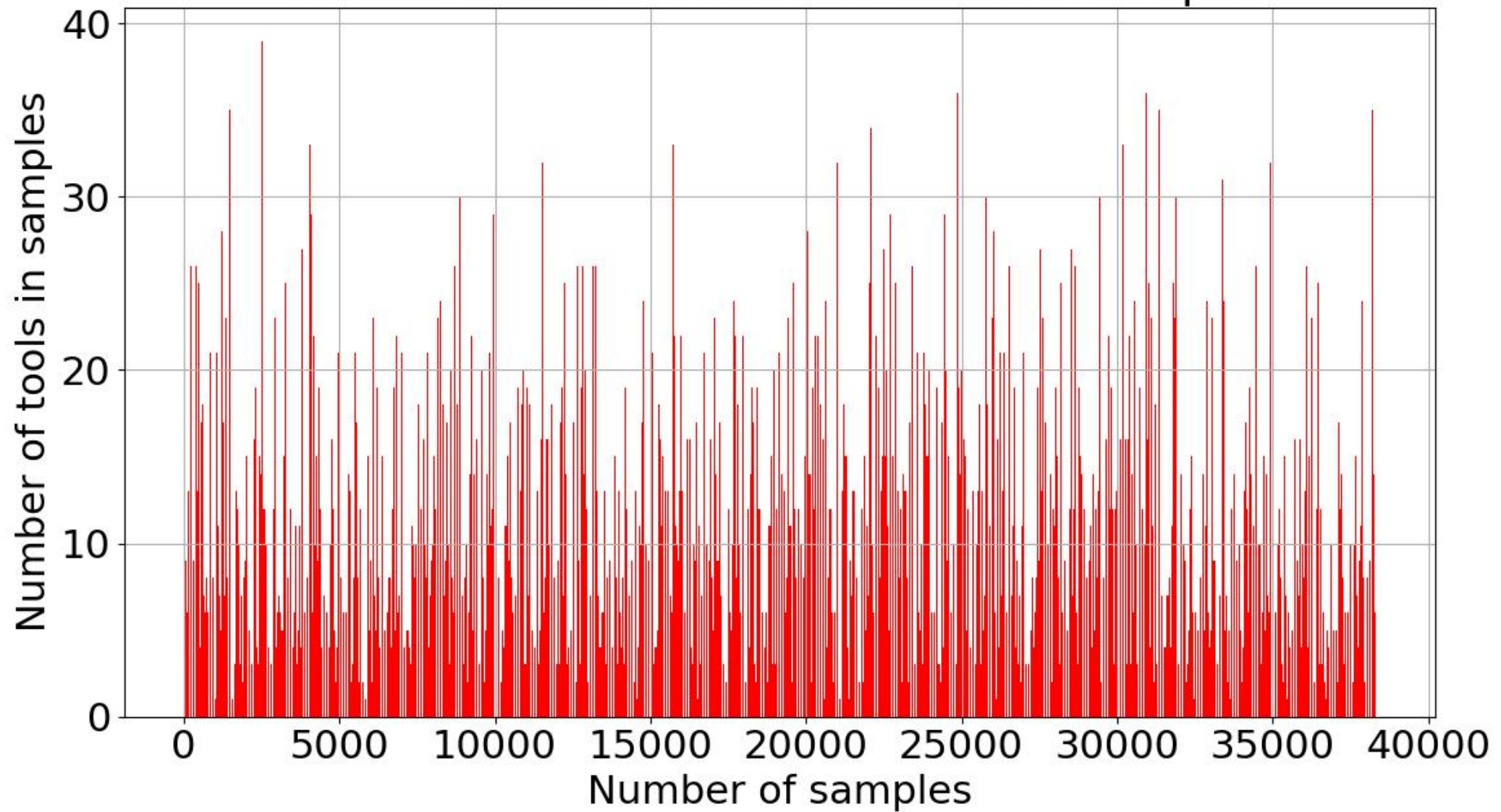
- fastq_groomer, trim_galore (Step 1)
- fastq_groomer, trim_galore, tophat2, fastqc (Step 2)
- fastq_groomer, trim_galore, tophat2, samtools_rmdup (Step 3)
- fastq_groomer, trim_galore, tophat2, samtools_rmdup, rseqc_bam2wig (Step 4)

Data preprocessing

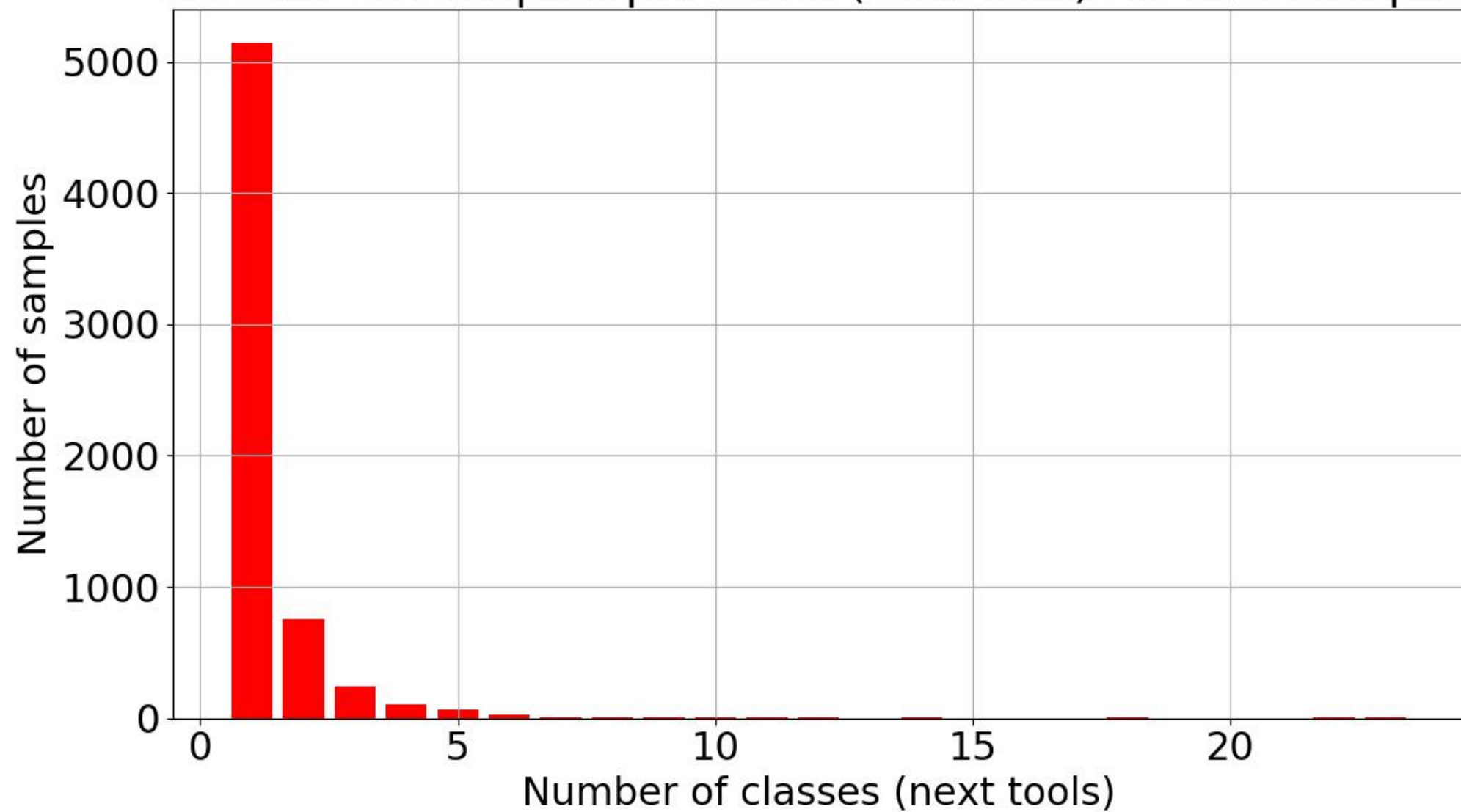
‘fastq_groomer’: 1, ‘trim_galore’: 2, ‘tophat2’: 3,
‘samtools_rmdup’: 4, ‘rseqc_bam2wig’: 5, ‘fastqc’: 6

Sample	Label (next tool(s)/classes)
1,2 (fastq_groomer, trim_galore)	3, 6 (tophat2, fastqc)
1,2,3	4
....
....

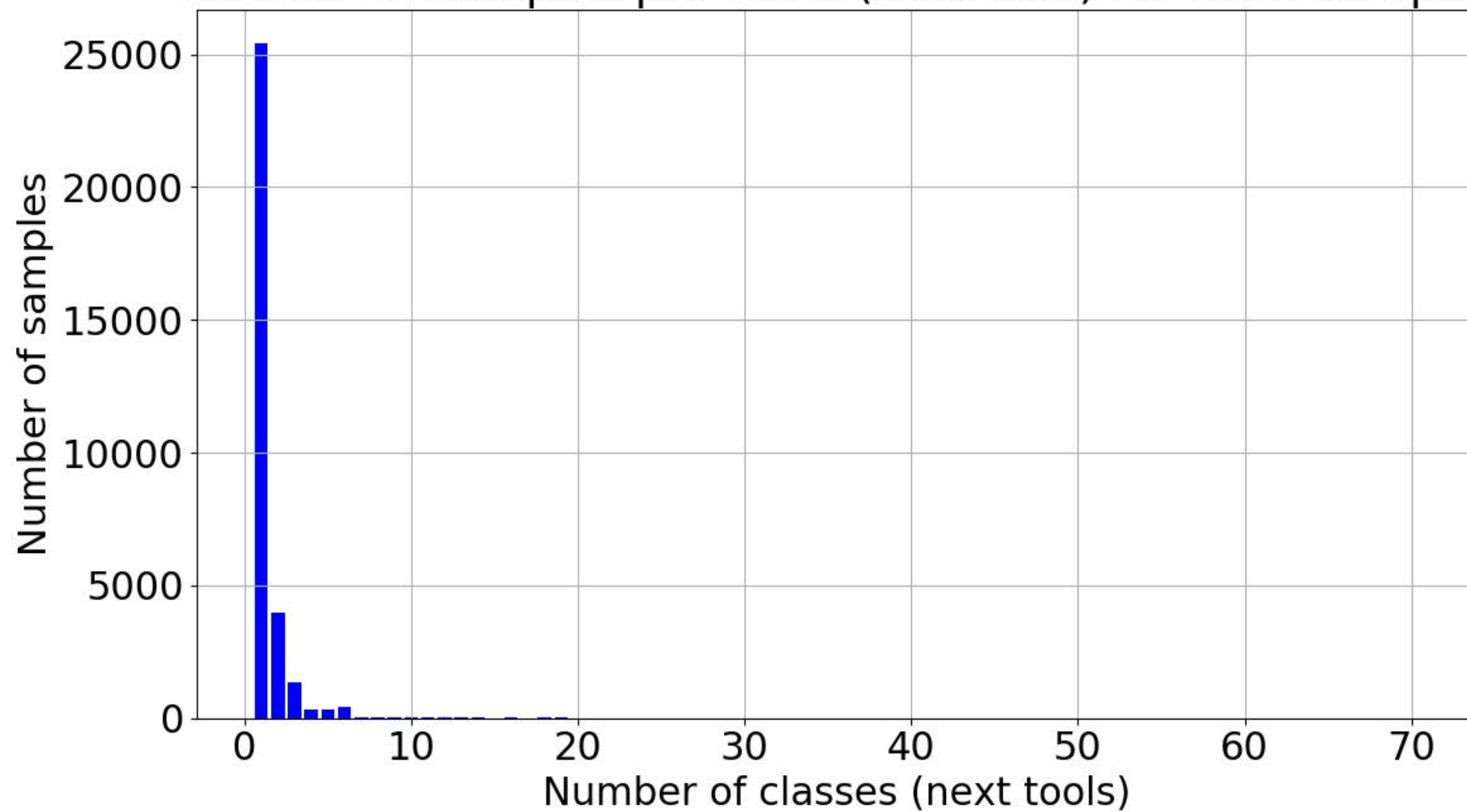
Distribution of number of tools in samples



Number of samples per class (next tool) for test samples

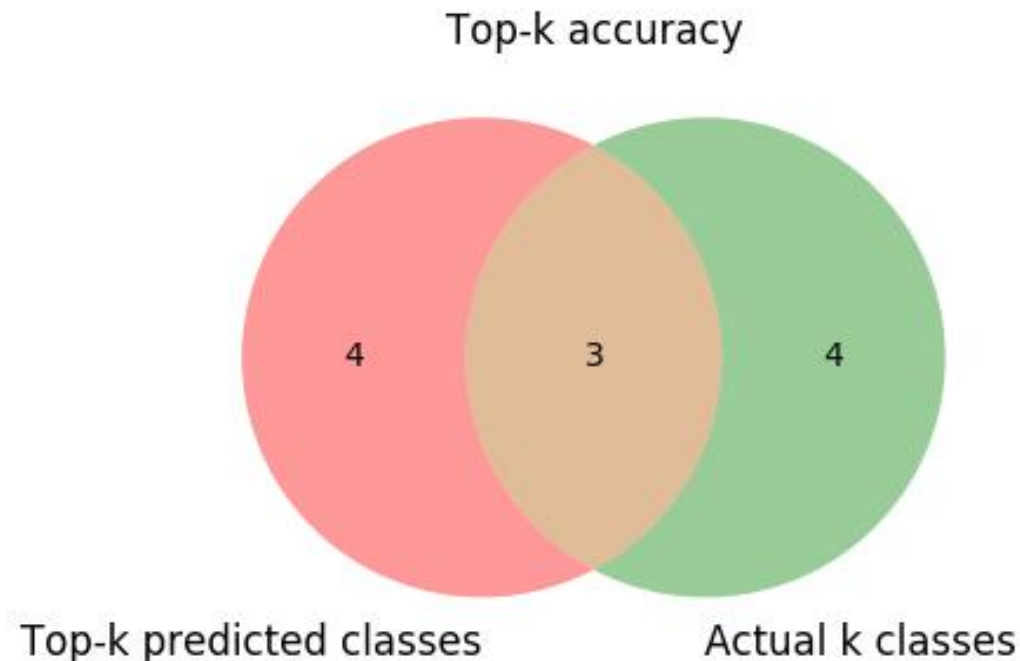


Number of samples per class (next tool) for train samples

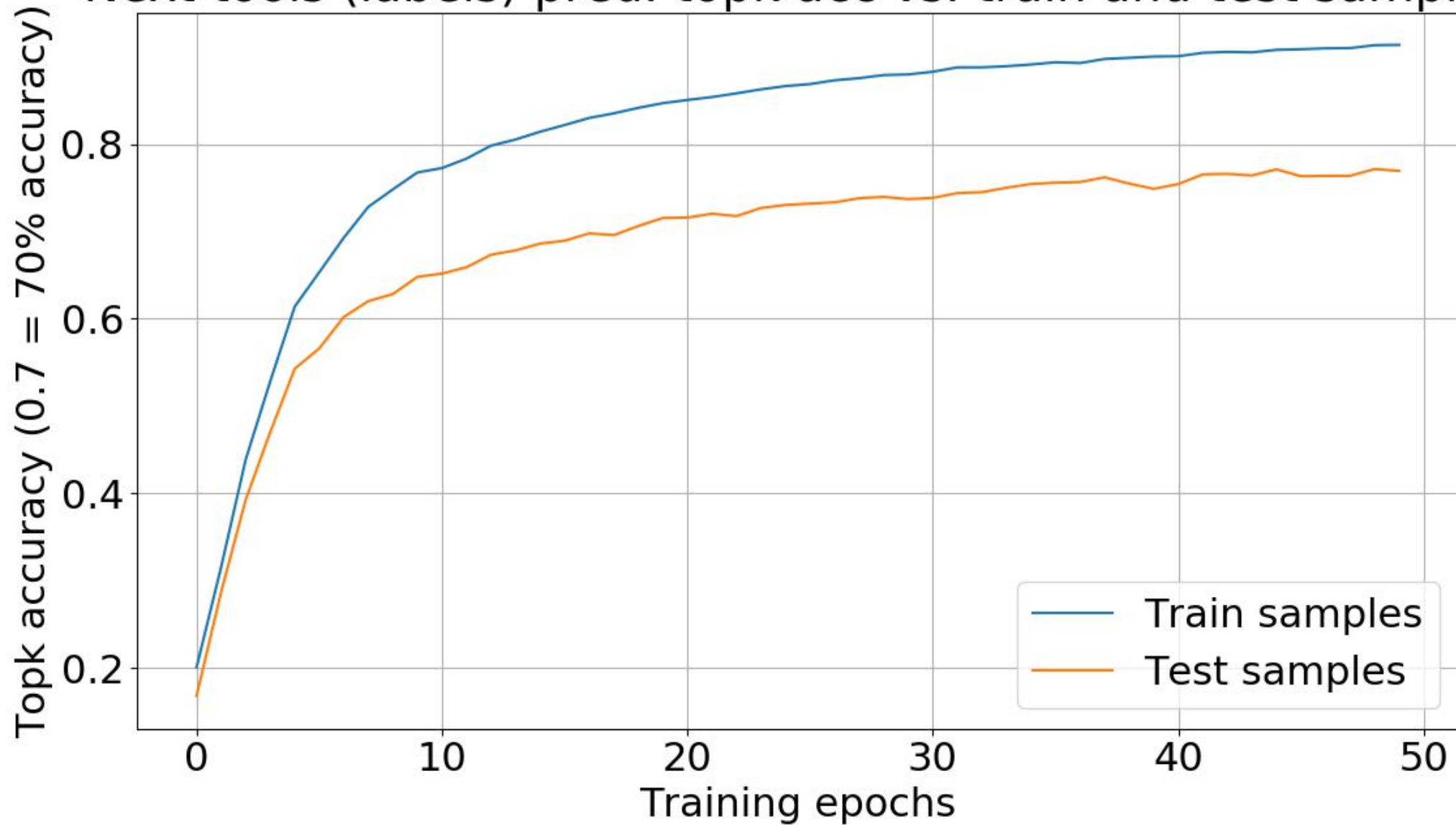


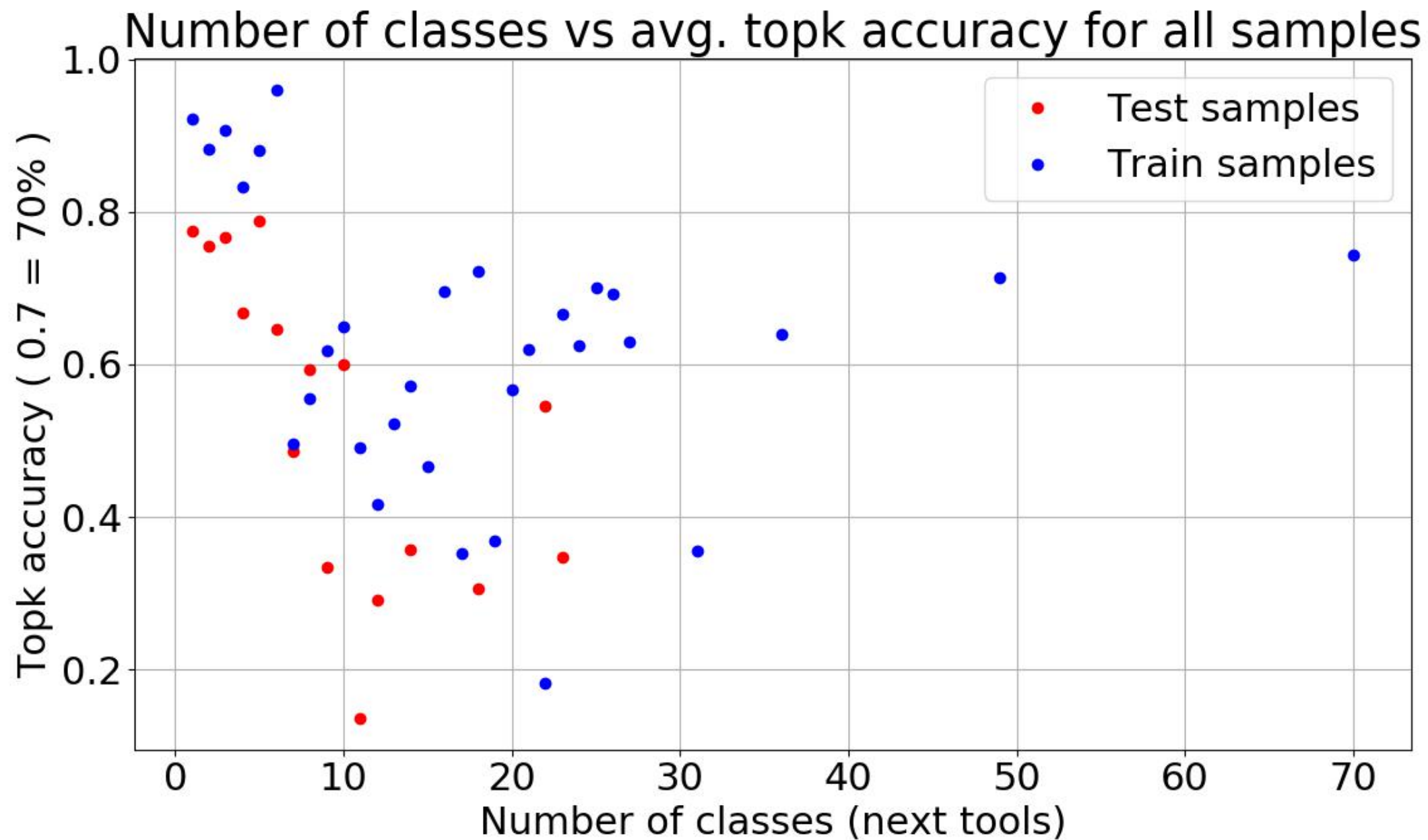
Classification

- Multi label, multi class classification
- Long short term memory (LSTM) networks
- Topk accuracy



Next tools (labels) pred. topk acc vs. train and test samples





References

- https://github.com/anuprulez/similar_galaxy_workflow
- <https://arxiv.org/pdf/1511.03677.pdf>
- <https://arxiv.org/pdf/1604.04573.pdf>
- <https://arxiv.org/pdf/1506.00019.pdf>

Thank you for your attention

Questions ?