Research on Event Search

towards Reproducible Experiment Platform

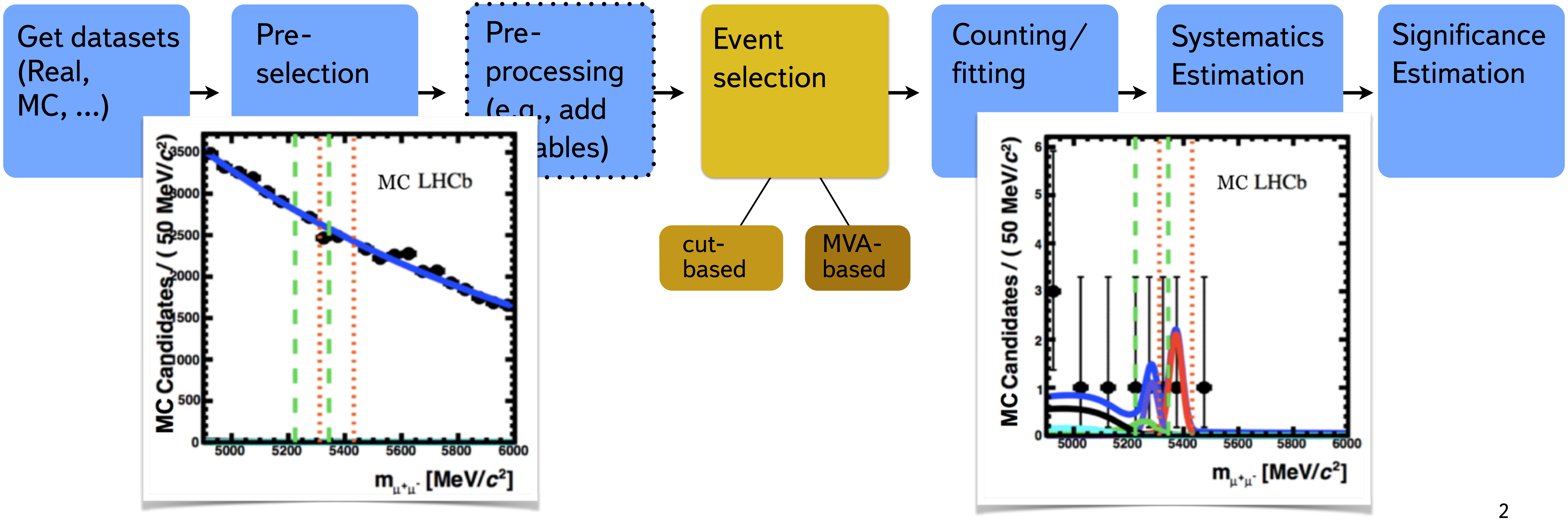
Andrey Ustyuzhanin

Yandex, NRC «Kurchatov Institute», Moscow

Imperial College, London

Quest for analysis sensitivity (LHCb)

Analysis Value Chain



Get datasets (Real, MC, …) → Pre-selection → Pre-processing (e.g., add ables) → Event selection → Counting / fitting → Systematics Estimation → Significance Estimation

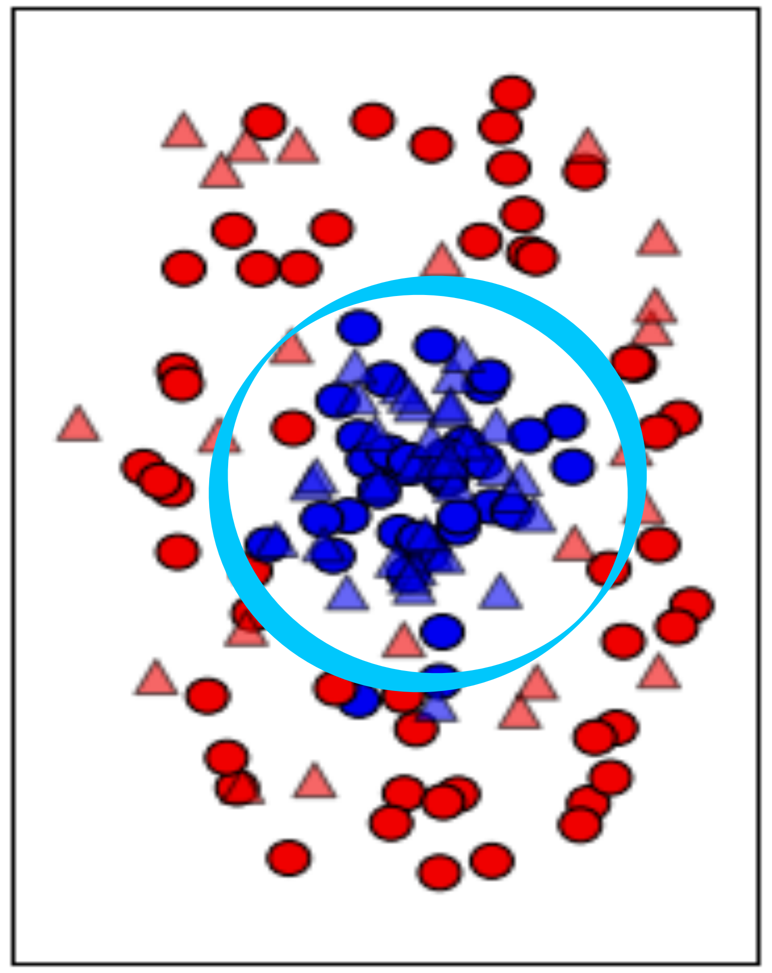
Event selection: cut-based, MVA-based

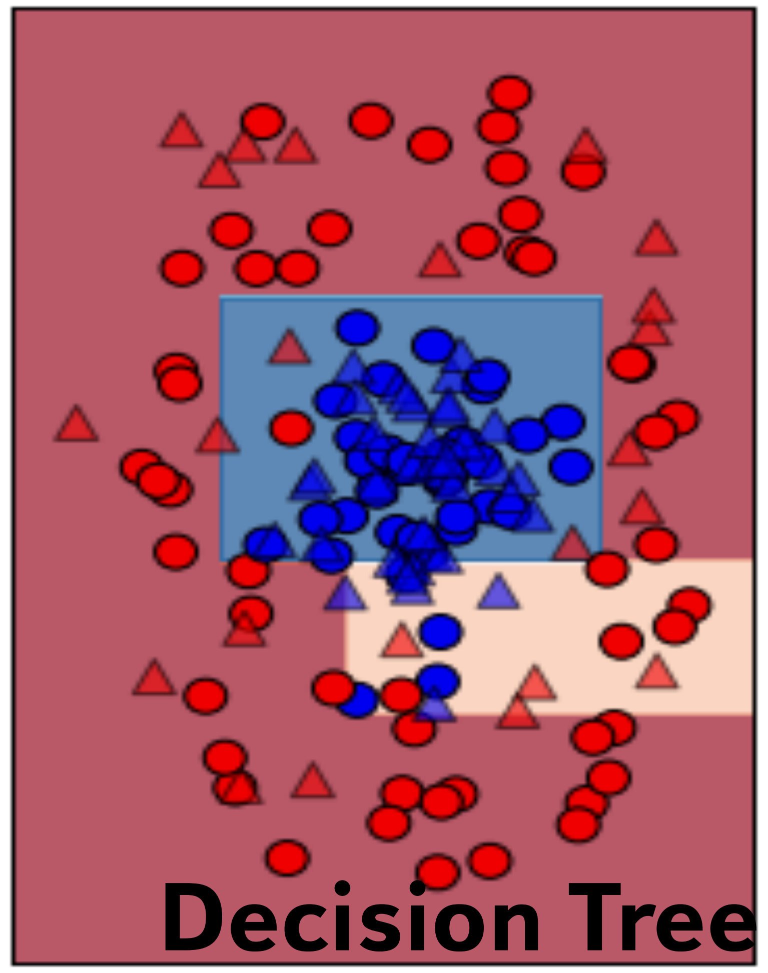
MC LHCb
MC Candidates / (50 MeV/c²)
3500
3000
2500
2000
1500
1000
500
0
5000
5200
5400
5600
5800
6000
$m_{\mu^+\mu^-}$ [MeV/c²]
MC LHCb
MC Candidates / (50 MeV/c²)
6
5
4
3
2
1
0
5000
5200
5400
5600
5800
6000
$m_{\mu^+\mu^-}$ [MeV/c²]

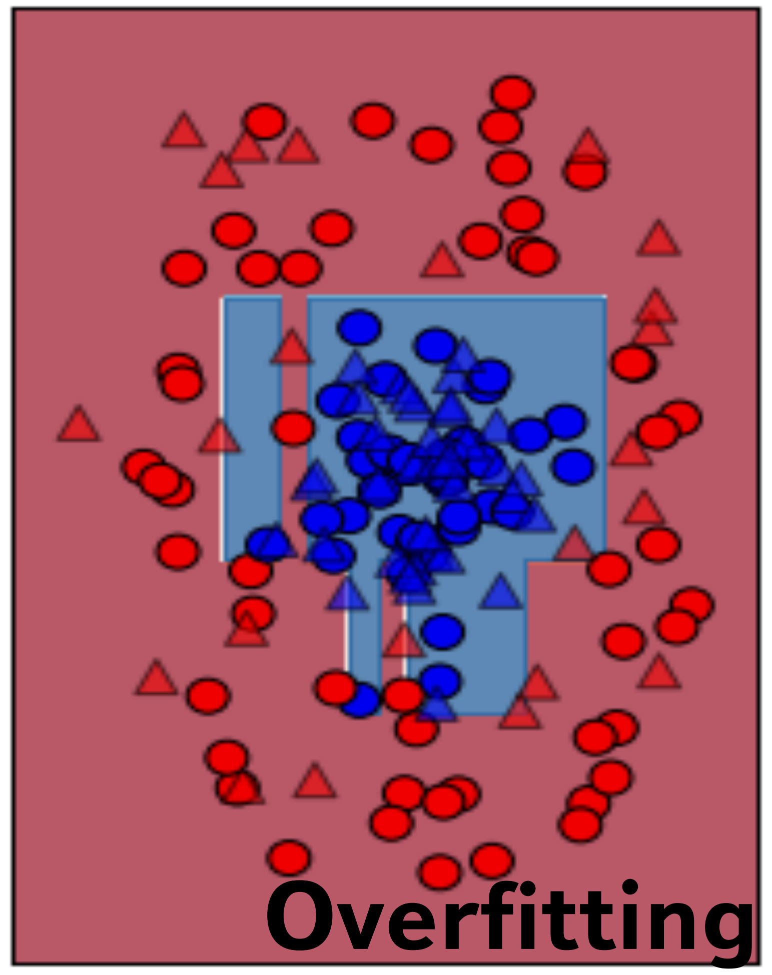
Sources of better sensitivity

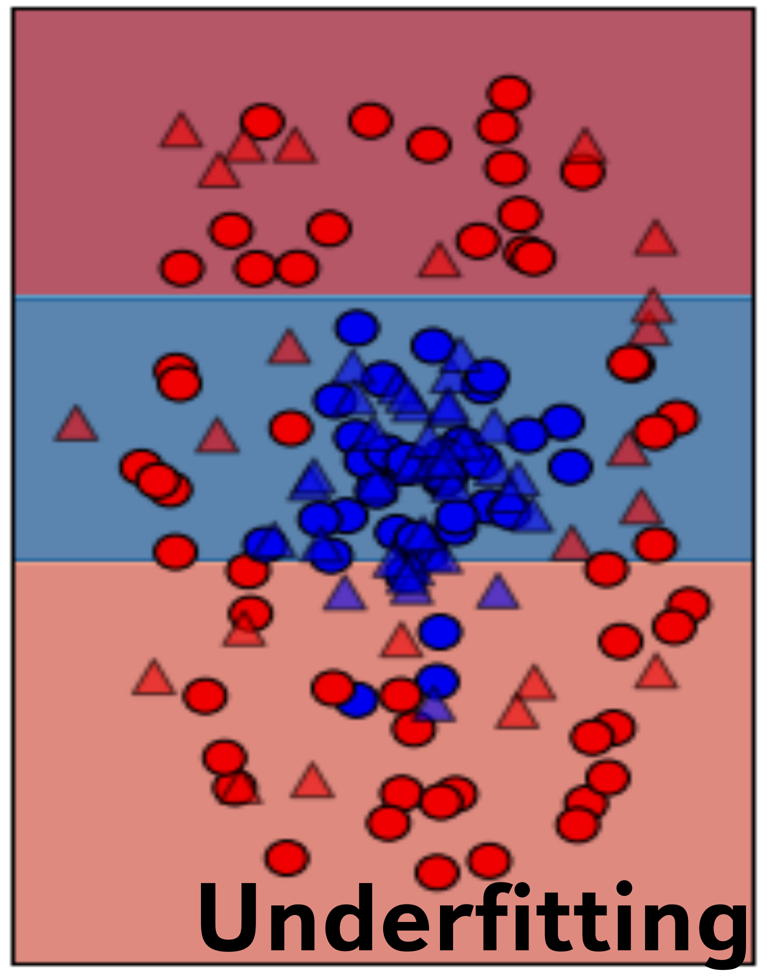
1. more powerful algorithms (e.g. BDT, Deep Neural Networks)
2. improved features (e.g. «isolation» variables or particle identification)
3. complex training scenarios (e.g. n-folding, ensembling, blending, cascading)

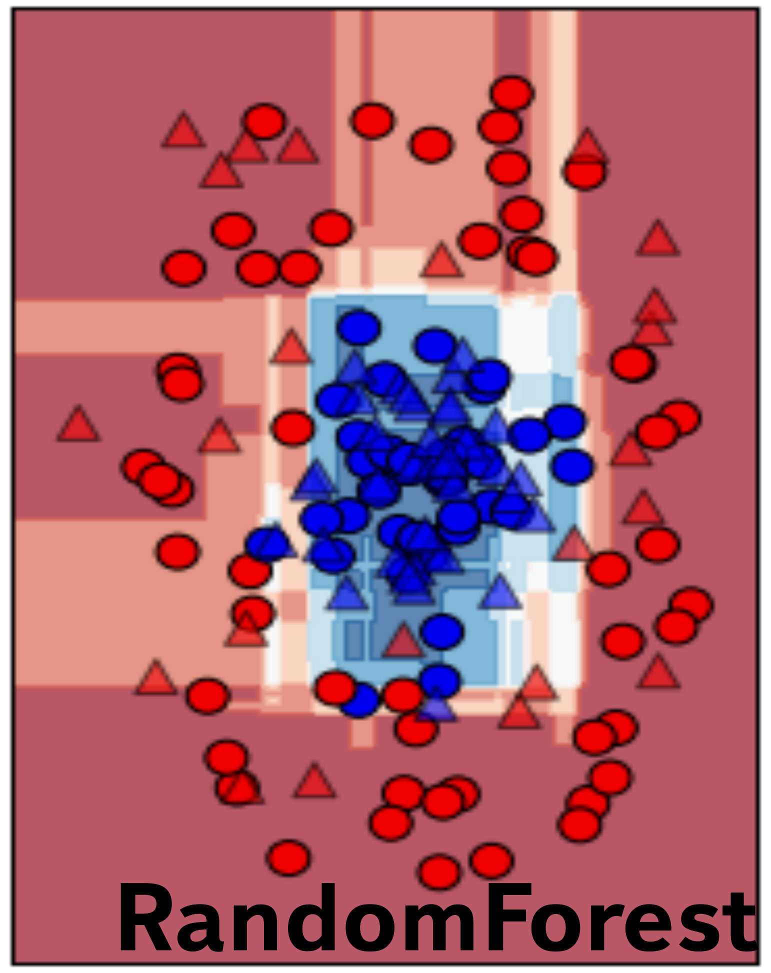
MVA Performance (ROC, Learning curve)

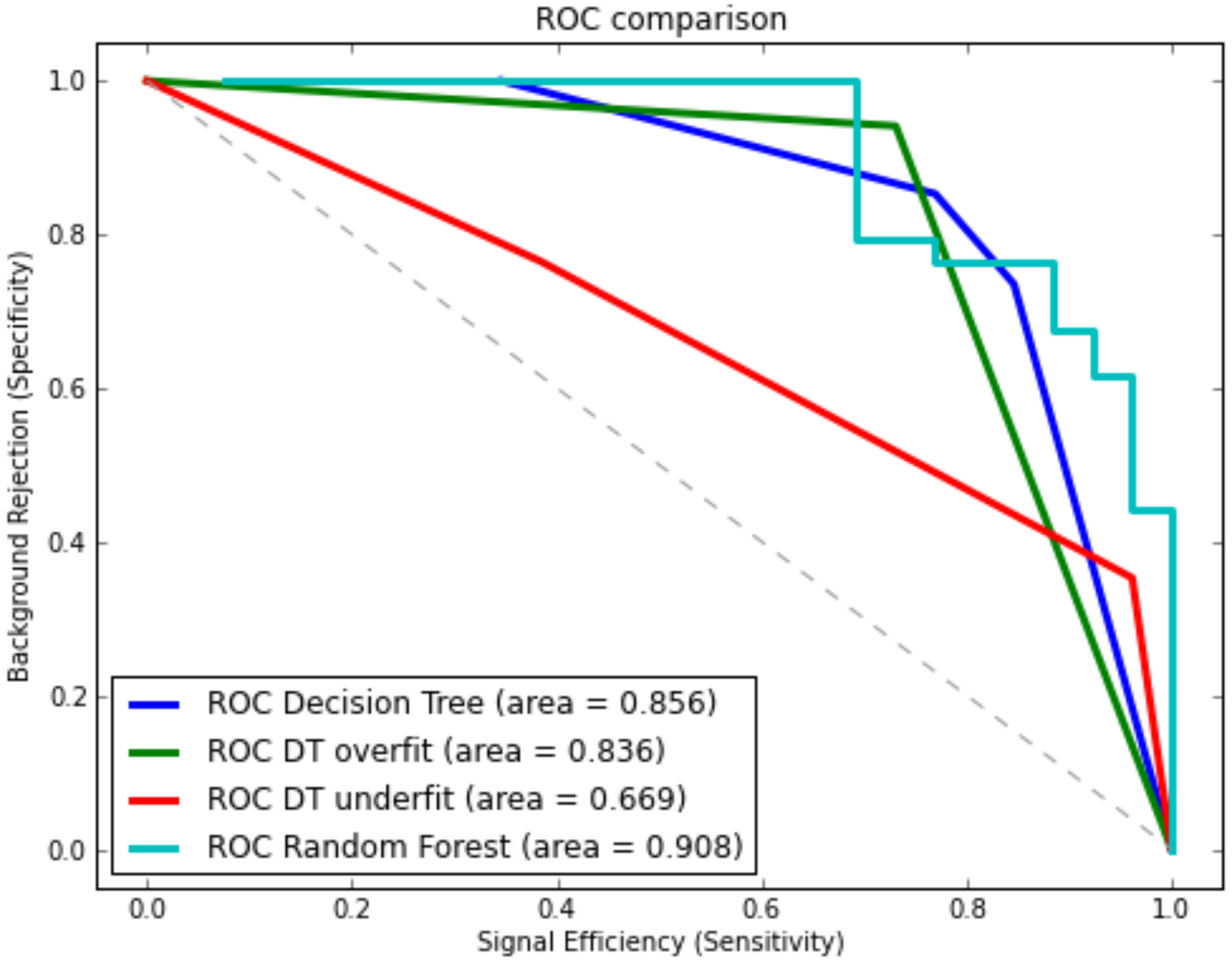


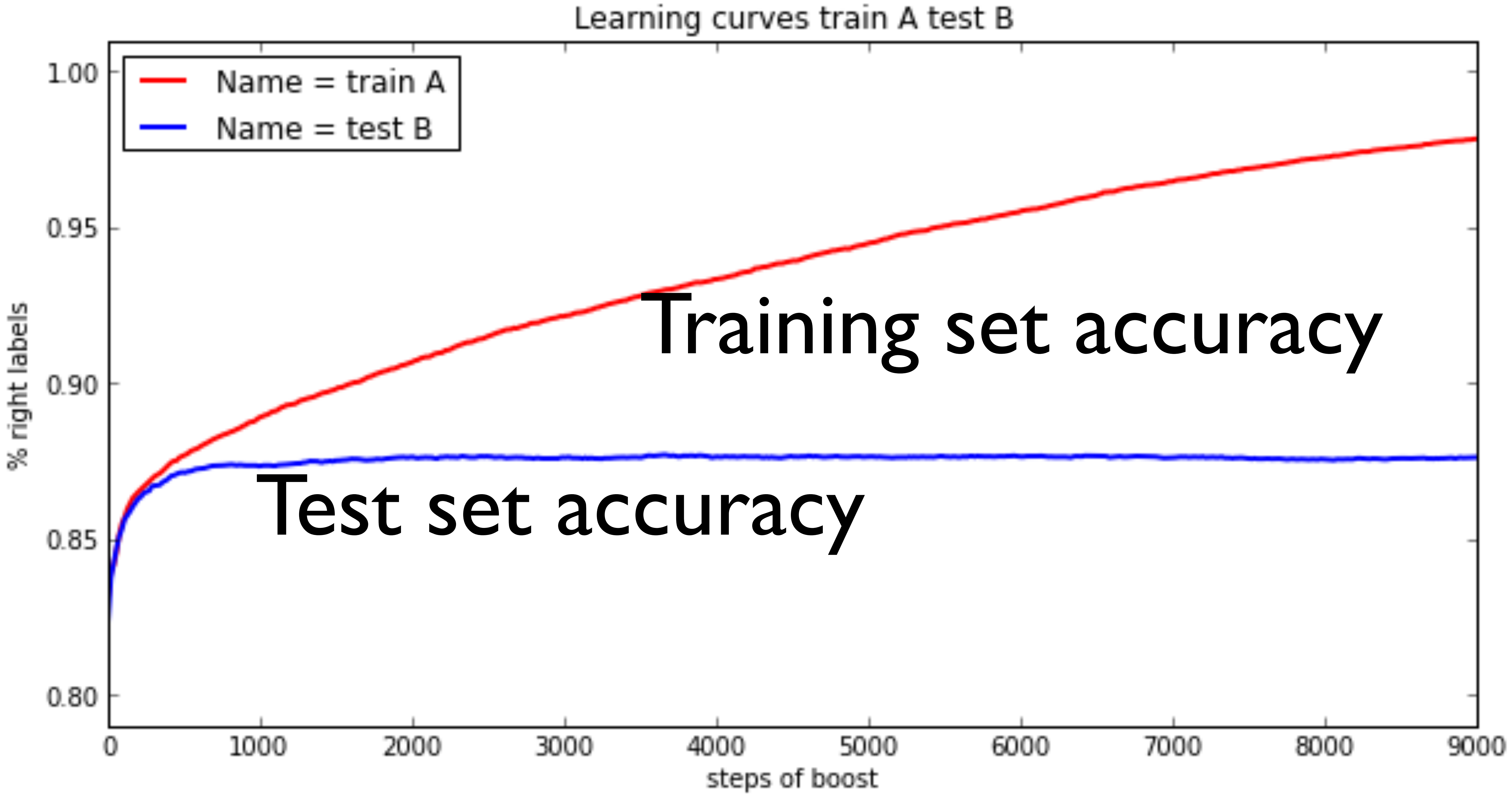












Training set accuracy

Test set accuracy

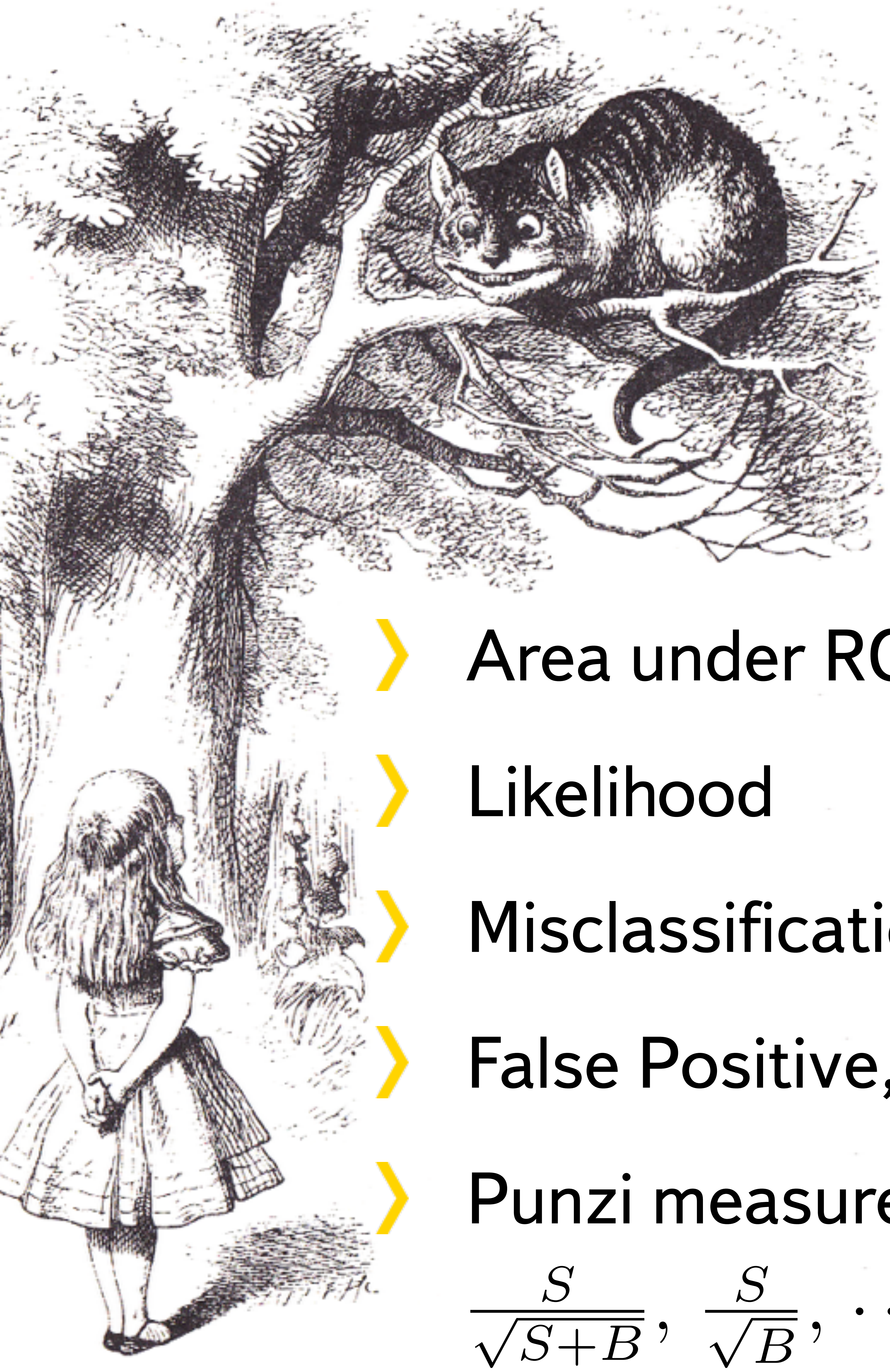
MVA algorithms: easy to find, hard to choose

- Families:
  - Boosted Decision Trees (BDT)
  - Artificial Neural Network (ANN)
  - Support Vector Machine (SVM)
  - Clustering, Bayesian Networks, …
- Implementations
  - TMVA (60+ algorithms)
  - NeuroBayes
  - python scikit-learn
  - R packages
  - Private (Matrixnet, predict.io)
  - XGBoost, …

Price for sensitivity

- **How do I check quality of event discriminating function?**
  - Overfitting?
  - Correlations?
  - Relevance of figure of merit to analysis significance?
- **How do I deal with complexity?**
  - Estimate influence of model parameters
  - Extra computation
  - Organization (cross-checks, collaboration)

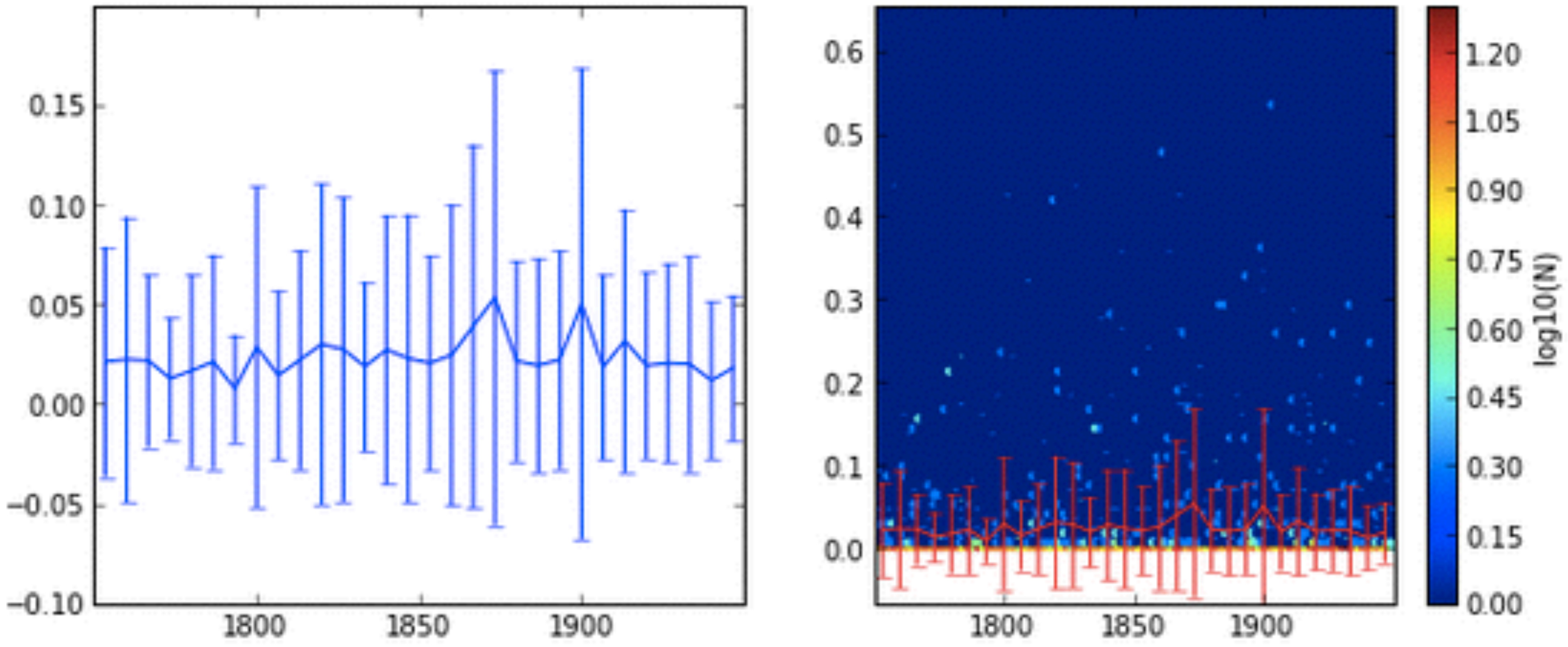
Figure-of-Merits Land



- Area under ROC
- Likelihood
- Misclassification
- False Positive, False Negative
- Punzi measure

$\frac{S}{\sqrt{S+B}}, \frac{S}{\sqrt{B}}, \dots$

Efficiency flatness?



Complexity indicators

- ‘I can’t remember which version of the code I used to generate figure 13’
- ‘The new student wants to reuse that model I published three years ago but he can’t reproduce the figures’
- ‘I thought I used the same parameters but I’m getting different results!?’
- ‘It worked yesterday!’
- ‘Why did I do that?’
- ‘Where are events selected with previous version of reconstruction software?’

Complexity sources

- Domain (Physics)
- Datasources & formats
- Analysis strategy
- Analysis steps
- Team (distributed) communication

Research reproducibility degree

- By yourself
- By your team members
- By member of another team in the same domain (HEP, Cosmology, ...)
- By someone else

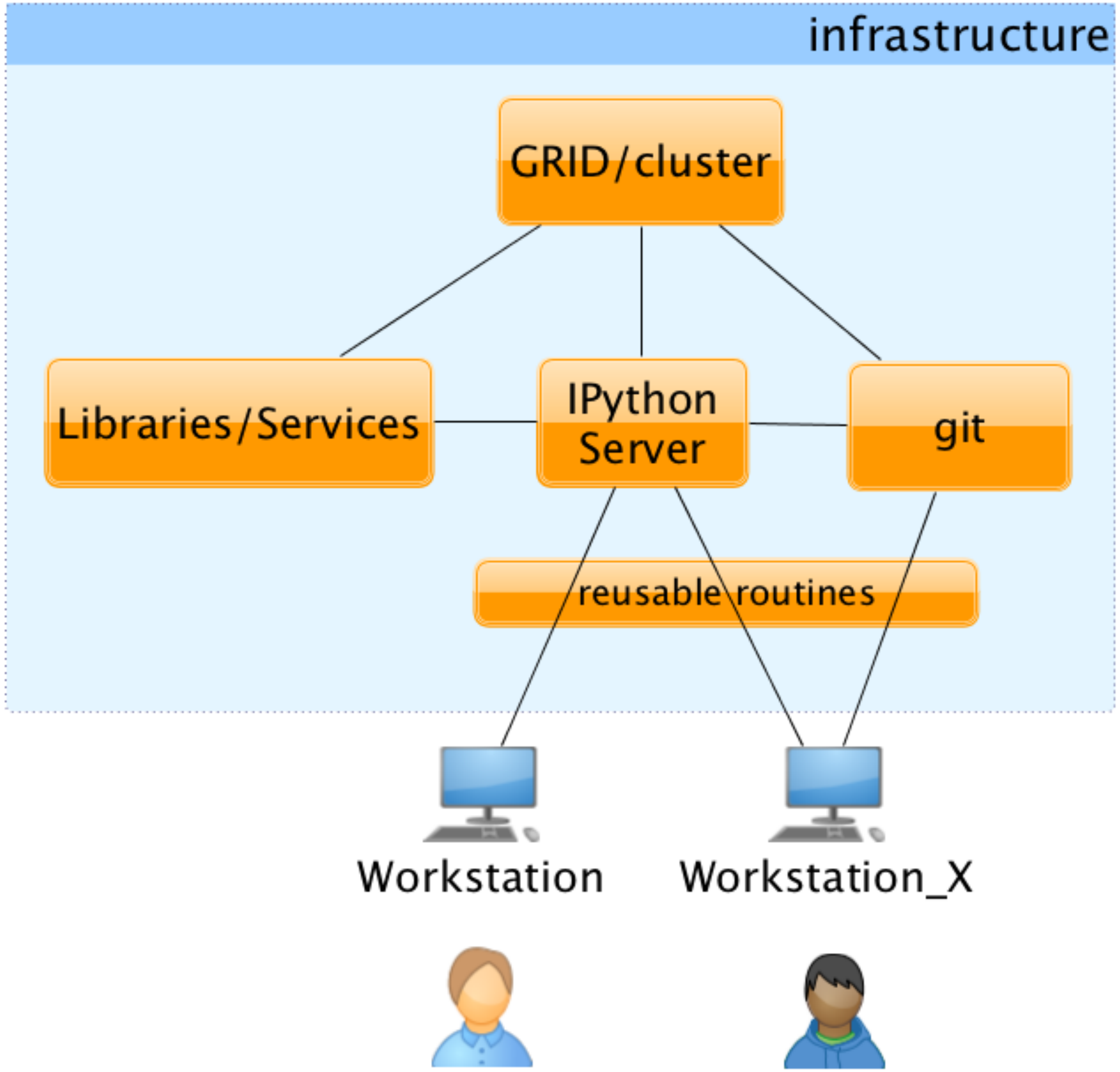
Requires dedicated framework!

Reproducible Experiment Platform (REP)

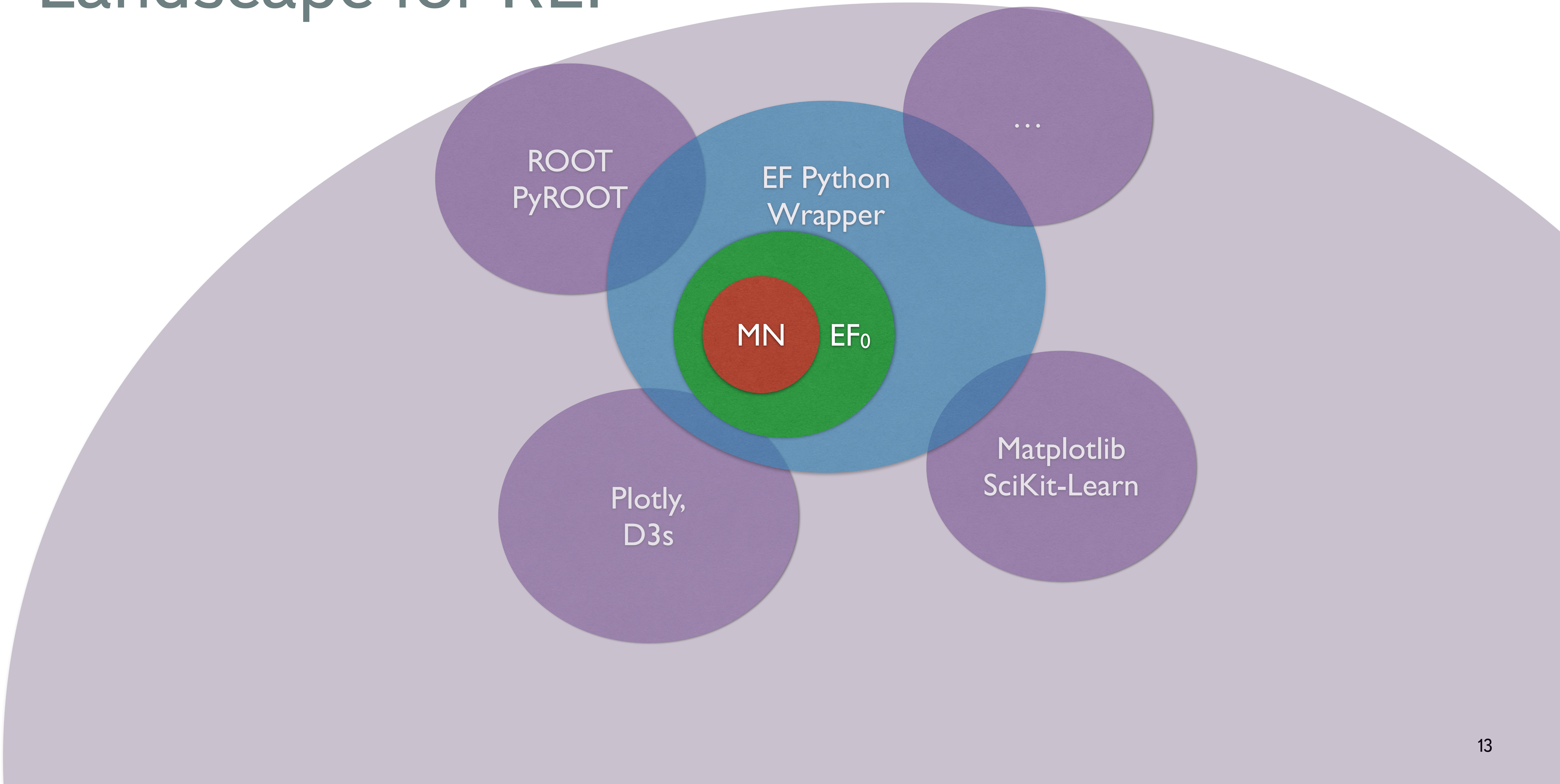
software infrastructure to support a collaborative ecosystem for computational science. It is a solution for team of researchers that allows

- running computational experiments on big shared datasets,
- obtaining reproducible and repeatable results,
- comparing measurable result consistently.

Main Components



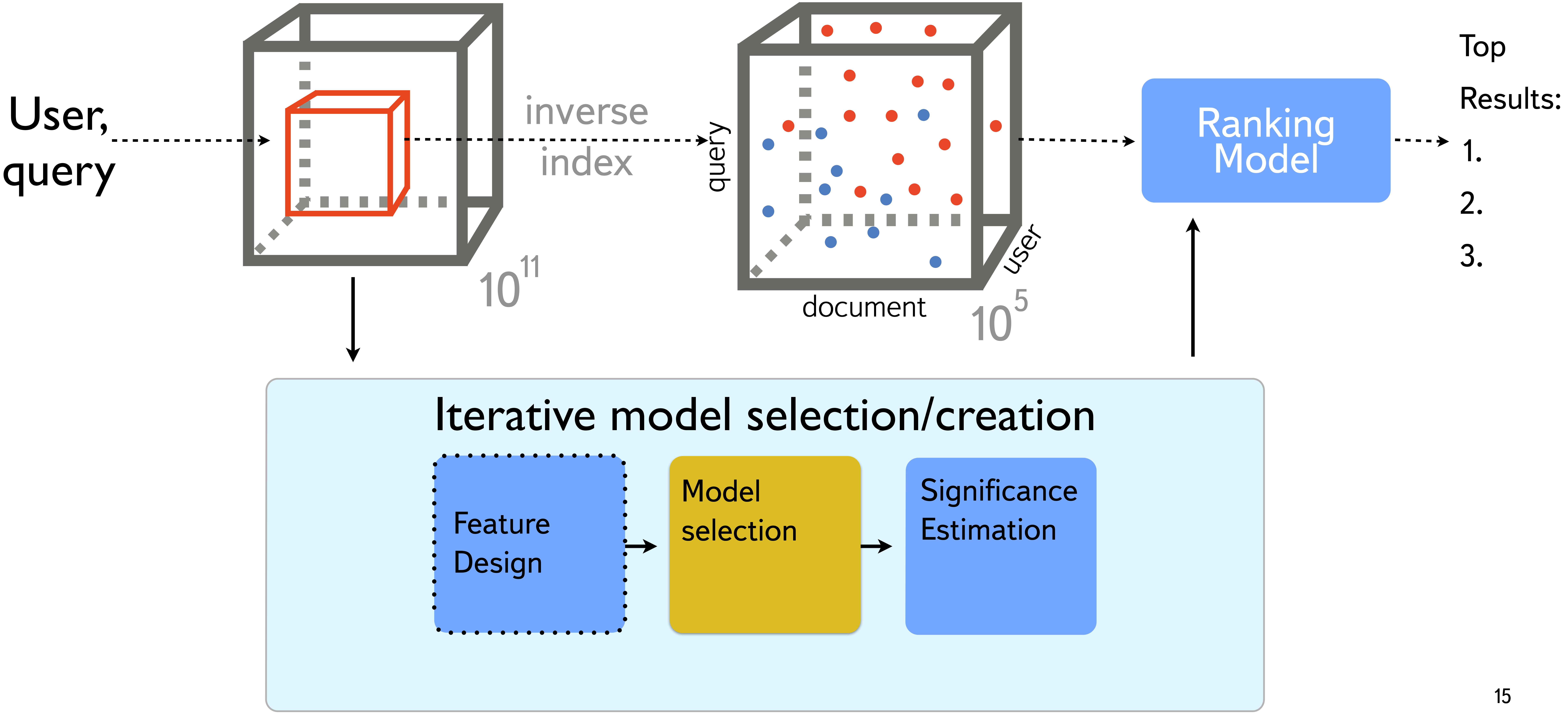
Landscape for REP



REP features / requirements

1. research automation, i.e. defining modules that can be reused later on,
2. consistent automatic cross-check,
3. online visually enhanced shared interactive environment,
4. result reproducibility (code / data provenance),
5. support for existing standard modules,
6. scalability (performance increase as additional [hardware] resources are available),
7. [flat learning curve]

Web Search Workflow



User, query

inverse index

Ranking Model

Top Results:

1.

2.

3.

Iterative model selection/creation

Feature Design

Model selection

Significance Estimation

Collaborative work redux

CVS
Programming language
Fixed platform

Continuous Integration
Deployment
Beta-testing

1 person

- Total «freedom»

10 people

- Formal agreements
- Experiments repository
  - share of experience, source code reuse
  - data specification, parameters, version

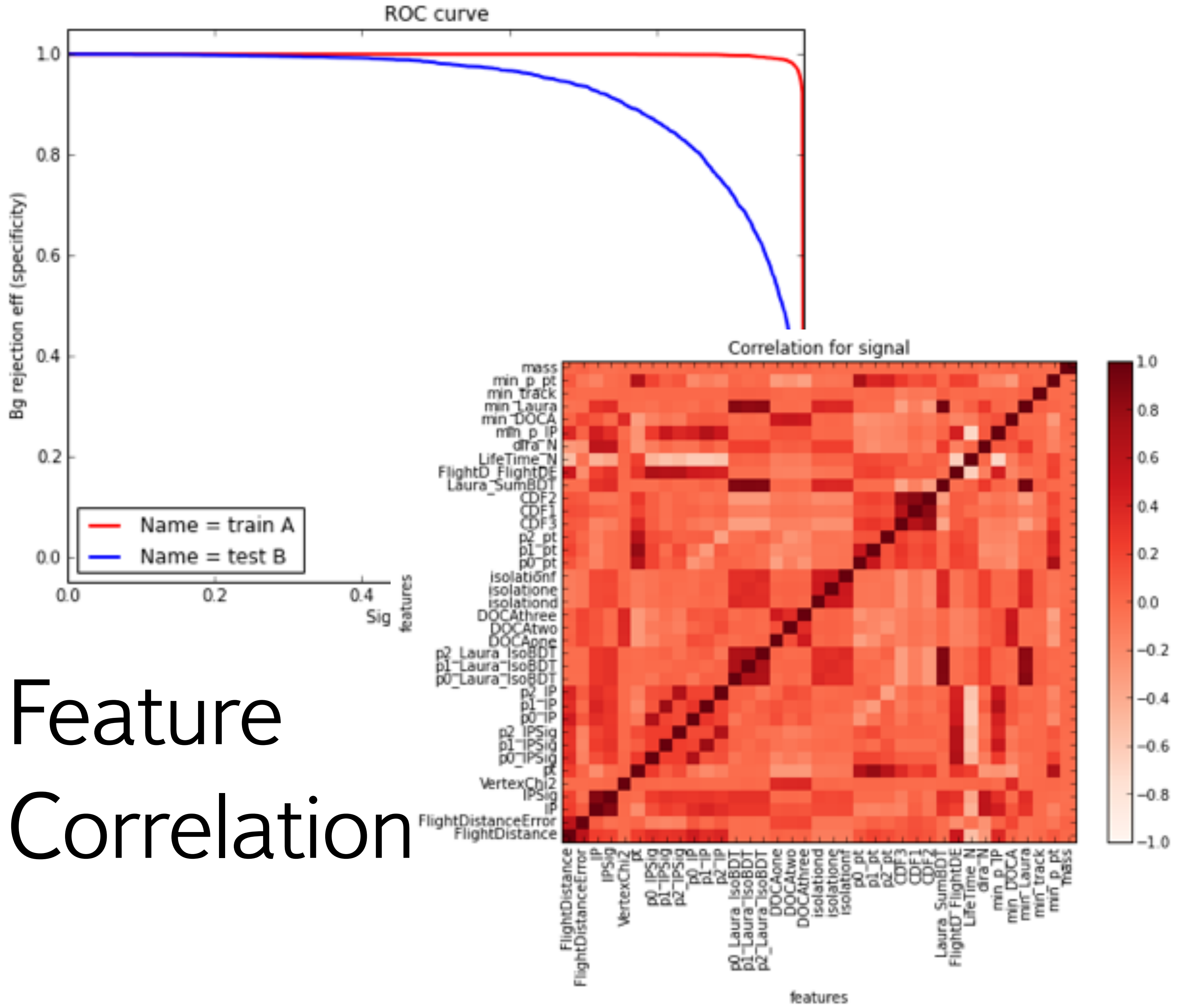
100 people

- Regulative infrastructure
- Automated hypotheses testing
  - **10s per week ⟹ 1000s per week**

REP for Particle Physics

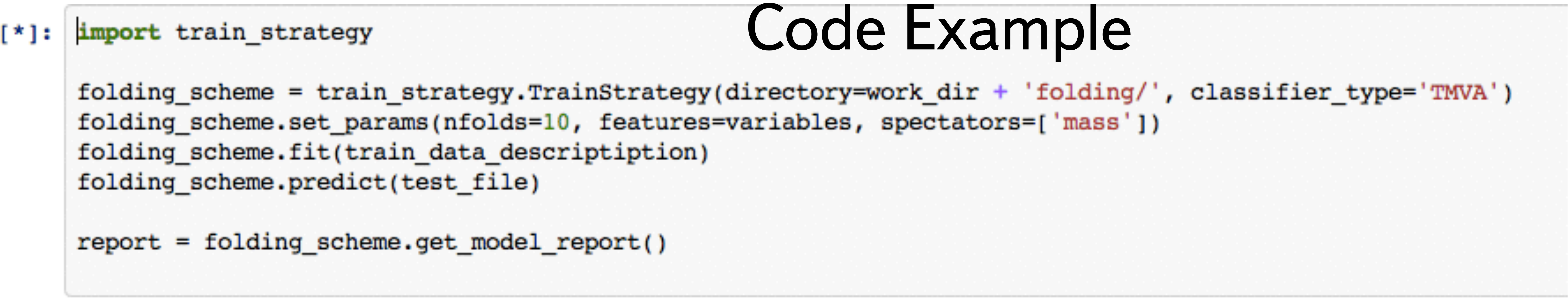
- Online & Interactive
- Support for ROOT & Python & TMVA
- Support for 3rd party classifier (e.g Matrixnet and SKLearn)
- Run heavy jobs on cluster

ROC



Feature Correlation

Code Example

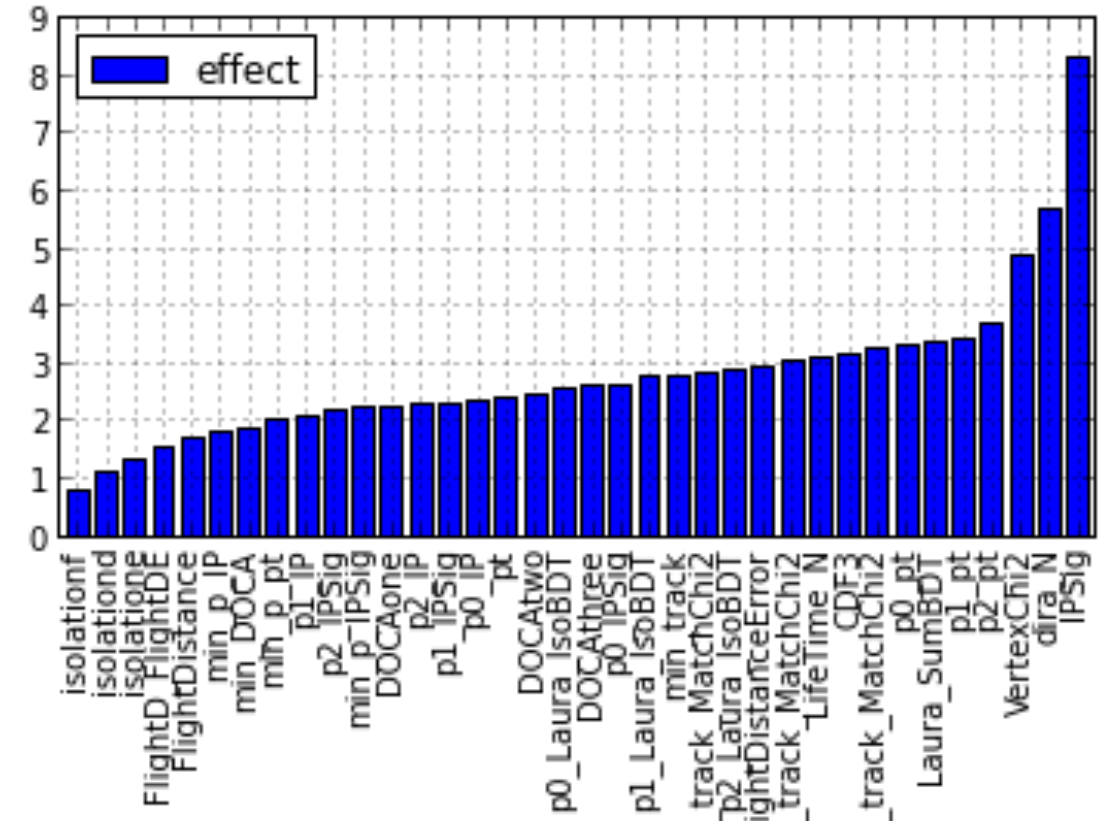


```
[*]: import train_strategy

     folding_scheme = train_strategy.TrainStrategy(directory=work_dir + 'folding/', classifier_type='TMVA')
     folding_scheme.set_params(nfolds=10, features=variables, spectators=['mass'])
     folding_scheme.fit(train_data_description)
     folding_scheme.predict(test_file)

     report = folding_scheme.get_model_report()
```

Feature Strength



More details: http://bit.ly/1fCjEqg (tomorrow)

Cases

- Teaching Data Science / Machine Learning
- Information Retrieval Research
- Physics Research
- Interdisciplinary Research

$$B_s \to \mu^+\mu^-$$
$$B_s \to 4\mu$$
$$\tau \to 3\mu$$
$$B \to K^*\mu^+\mu^-$$
$$\ldots$$

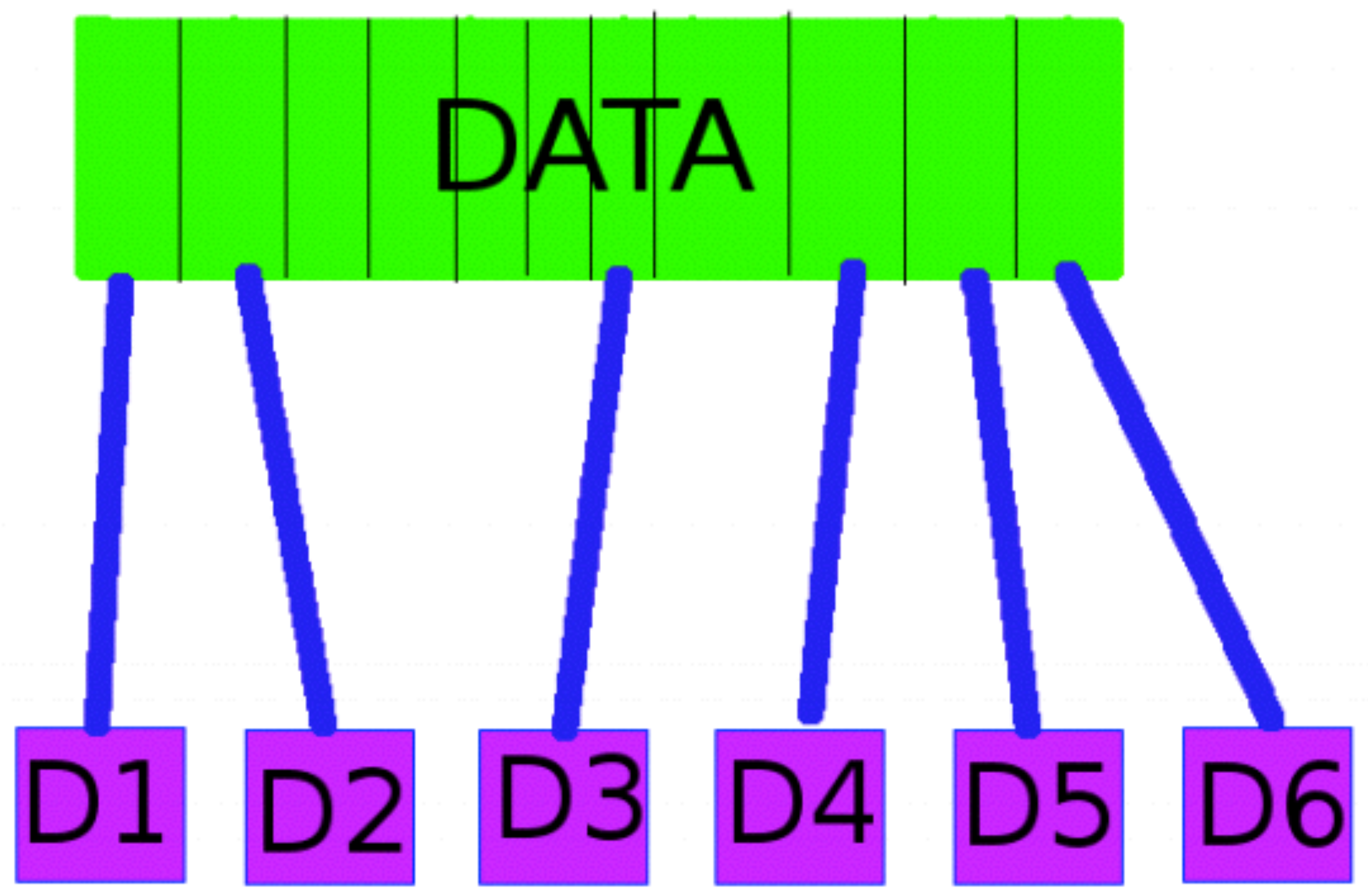
Instead of Conclusion

- New source of tools & metrics: **data science**
  - …as well as source of complexity
- Research reproducibility = defeat of complexity
  - Environment (http://bit.ly/1fCjEqg)
  - Status: **looking for new cases, adopters**
- Would like to try?
  - andrey.ustyuzhanin@cern.ch

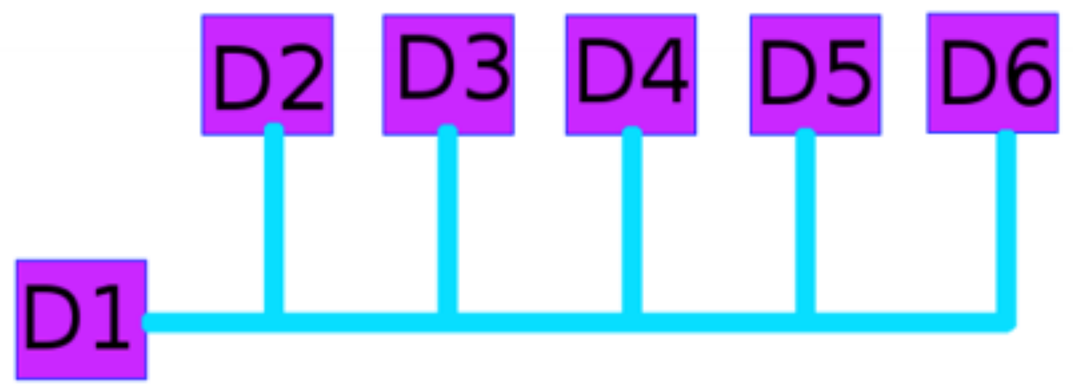
Backup

N-folding, training scheme example

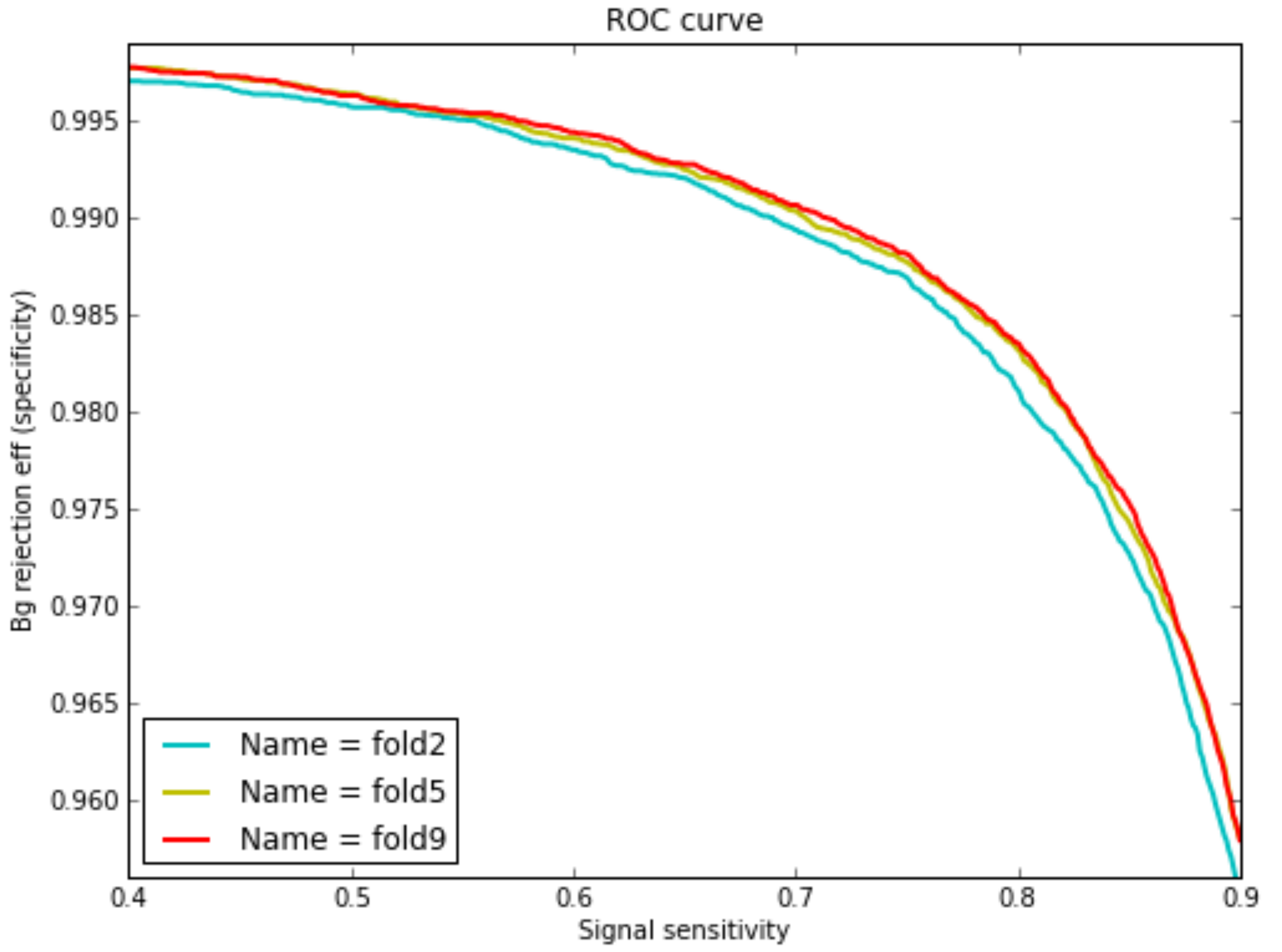
(works well for limited statistics)



Split data in N folds randomly



Take i-th fold,
train formula on remaining folds,
apply to selected one



See the difference