TMVA Tutorial

L. Moneta

IML

2nd IML Machine Learning Workshop / 9-12 April 2018

TMVA

- ROOT Machine Learning tools are provided in the package TMVA (Toolkit for MultiVariate Analysis)
- Provides a set of algorithms for standard HEP usage
- Used in LHC experiment production and in several analysis (e.g. Higgs studies)
- Main ML Tool until few years ago (e.g. 2013)
- Easy interface for beginners, powerful for experts
- Several active contributors and several features added recently (e.g. deep learning)

TMVA

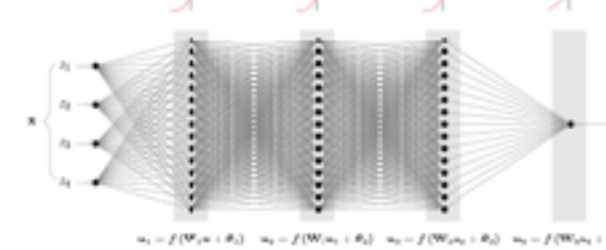
- TMVA is not only a collection of multi-variate methods. It is a
  - common interface to different methods
    - common interface for classification and regression
  - easy training and testing of different methods on the same dataset
    - consistent evaluation and comparison
    - same data pre-processing
  - several tools provided for pre-processing
  - embedded in ROOT

TMVA Methods

The available methods are (up-to 2015 version):

- Rectangular cut optimisation
- Projective likelihood estimation (PDE approach)
- Multidimensional probability density estimation (PDE - range-search approach)
- Multidimensional k-nearest neighbour classifier
- Linear discriminant analysis (H-Matrix and Fisher discriminants)
- Function discriminant analysis (FDA)
- Artificial neural networks (various implementations)
- Boosted/Bagged decision trees
- Predictive learning via rule ensembles (RuleFit)
- Support Vector Machine (SVM)

New Features



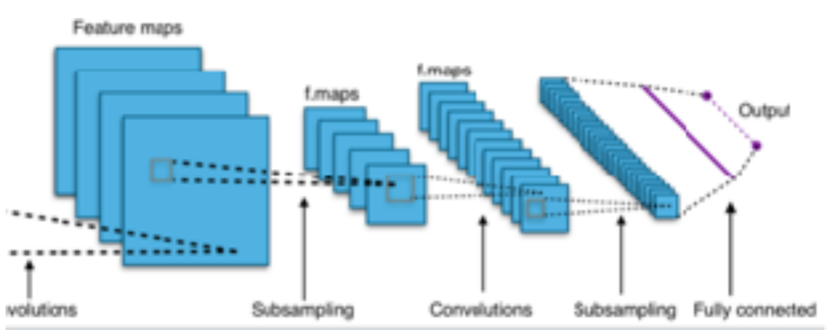
New major features added since 2016 and available in the ROOT version 6.12:

- Deep Learning
  - support for parallel training on CPU and GPU (with CUDA and OpenCL)
- Cross Validation and Hyper-parameter optimisation
- Improved loss functions for regression
- Interactive training and visualization for Jupyter notebooks
- new pre-processing features (variance threshold)

Most Recent Features

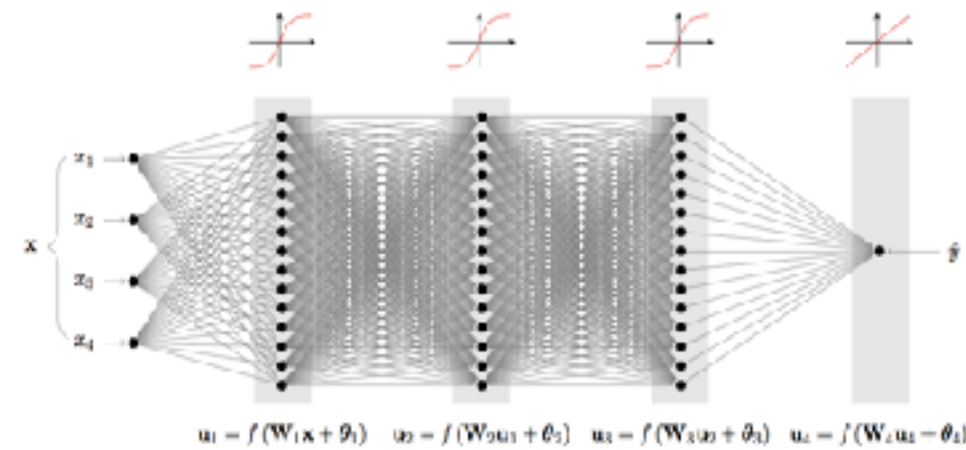
Features available in ROOT master and/or being released for the ROOT version 6.14:

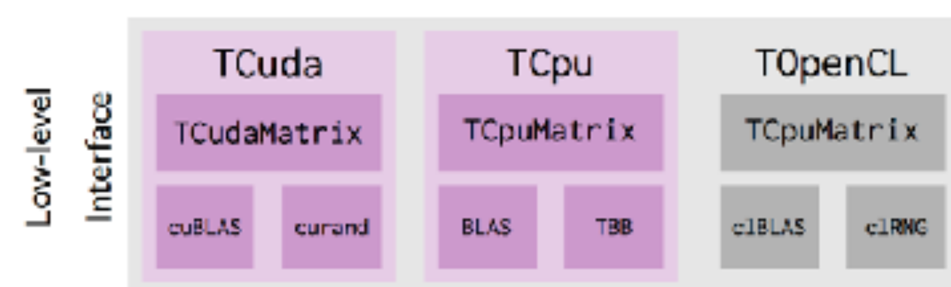
- Deep Learning Module with
  - Convolutional Layer
  - Recurrent Layer
- Improved Cross Validation
- Improved BDT performance using multi-thread parallelisation



Deep Learning in TMVA

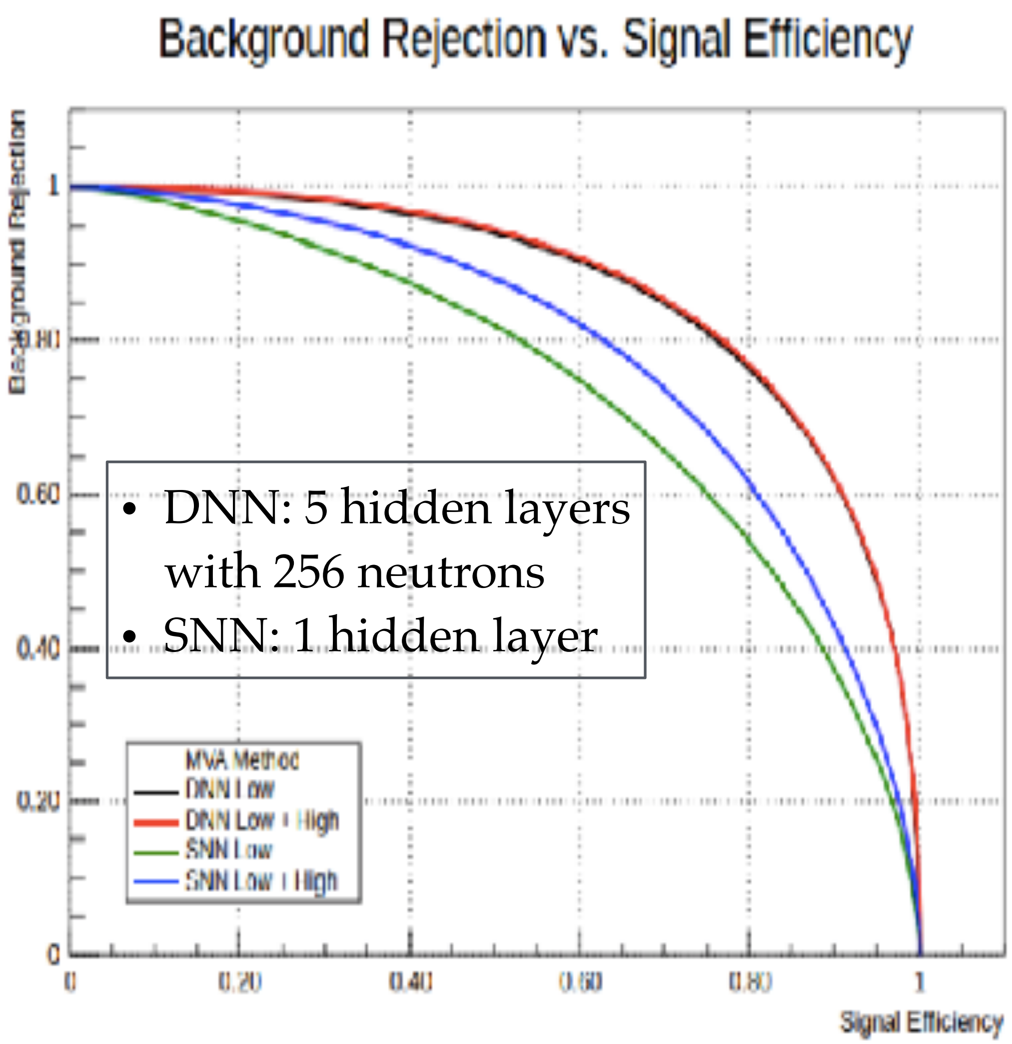
- Deep Learning library in ROOT/TMVA
  - parallel evaluation on CPU
    - implementation using OpenBLAS and TBB
  - GPU support
    - CUDA
    - OpenCL
  - Excellent performance and high numerical throughput
- For more information see
  - https://indico.cern.ch/event/565647/contributions/2308666/attachments/1345668/2028738/tmva_dnn_gpu.pdf



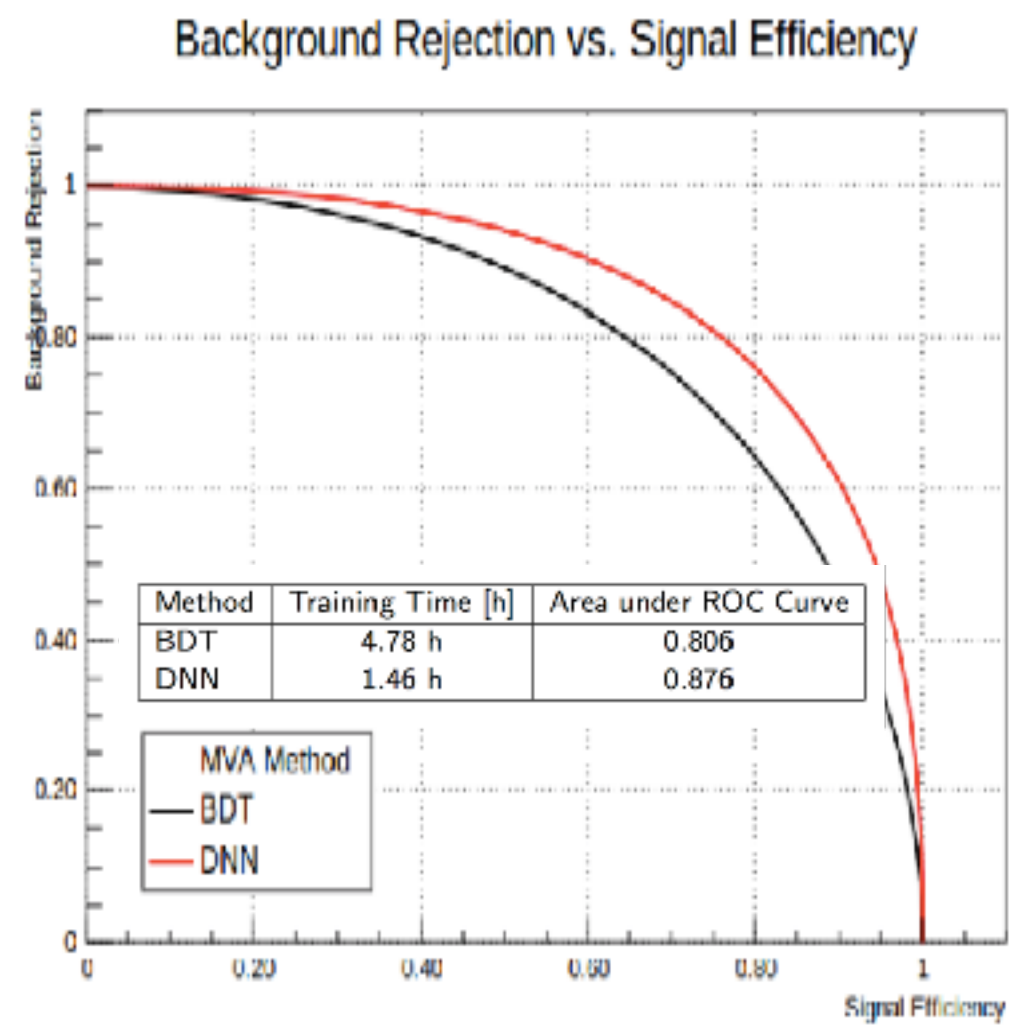


Deep Learning Performance

DNN vs Standard ANN



DNN vs BDT

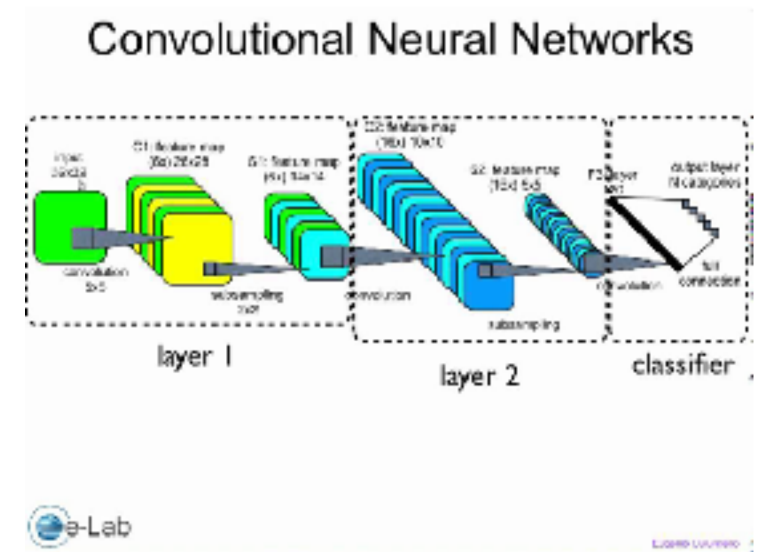


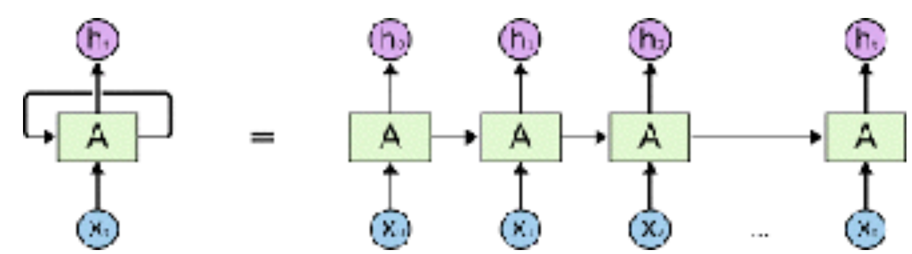
Method	Training Time [h]	Area under ROC Curve
BDT	4.78 h	0.806
DNN	1.46 h	0.876

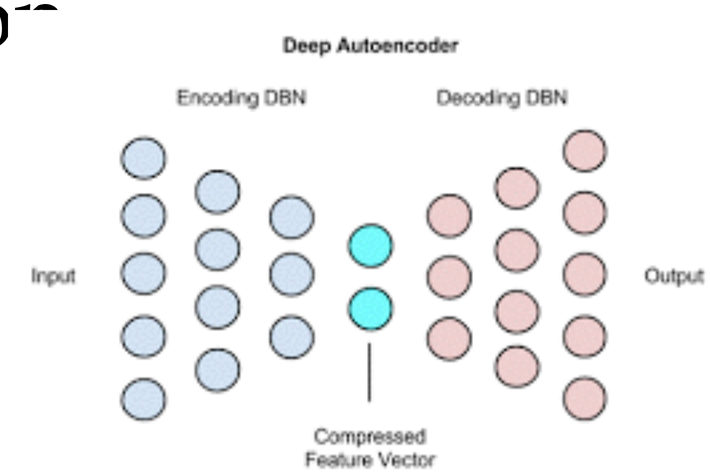
- Using Higgs public dataset with 11M events
- Significant improvements compared to shallow networks and BDT

Deep Learning Developments in TMVA

- Extend existing Deep Neural Network classes by adding:
  - Convolutional Neural Network
    - very powerful for image data sets
  - Recurrent Neural Network
    - useful for time-dependent data
  - Deep Auto Encoder
    - useful for dimensionality reductio
      (pre-processing tool)
    - can be used as unsupervised tool
      (e.g. for anomaly detection)

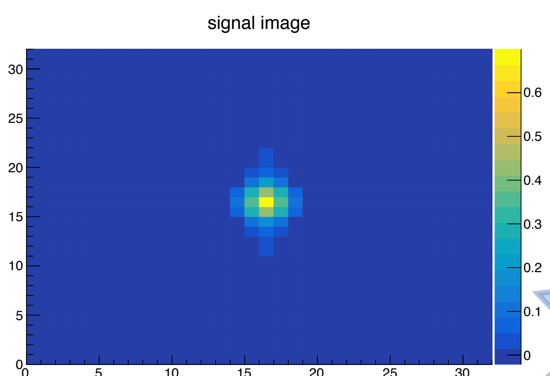


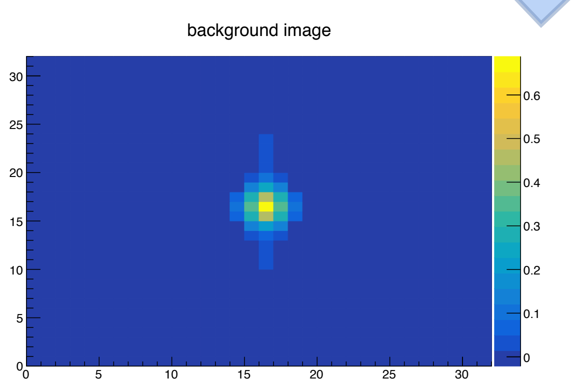




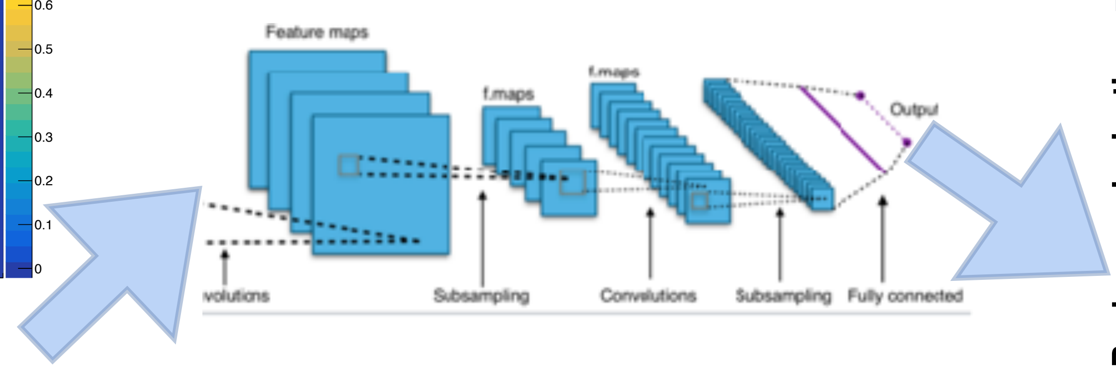
Convolutional Neural Network

- Integrated in ROOT master, for next ROOT release (6.14)
- Supporting now CPU parallelization, GPU support will come in the summer
  - parallelisation and code optimisation is essential

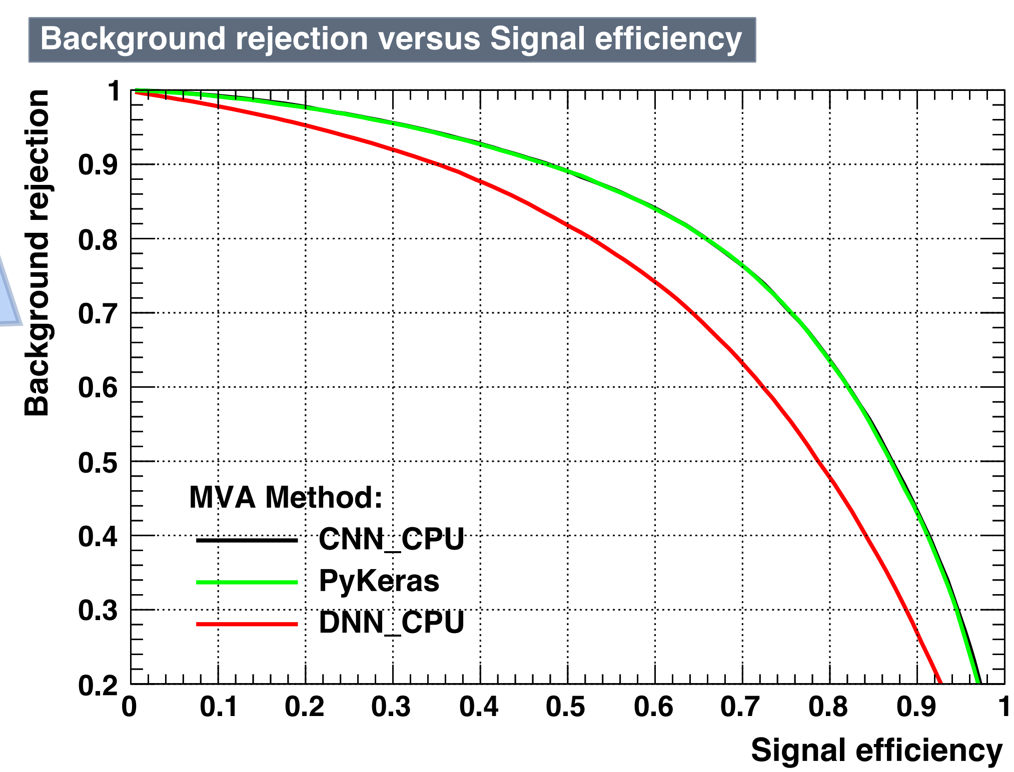




input 32x32 images

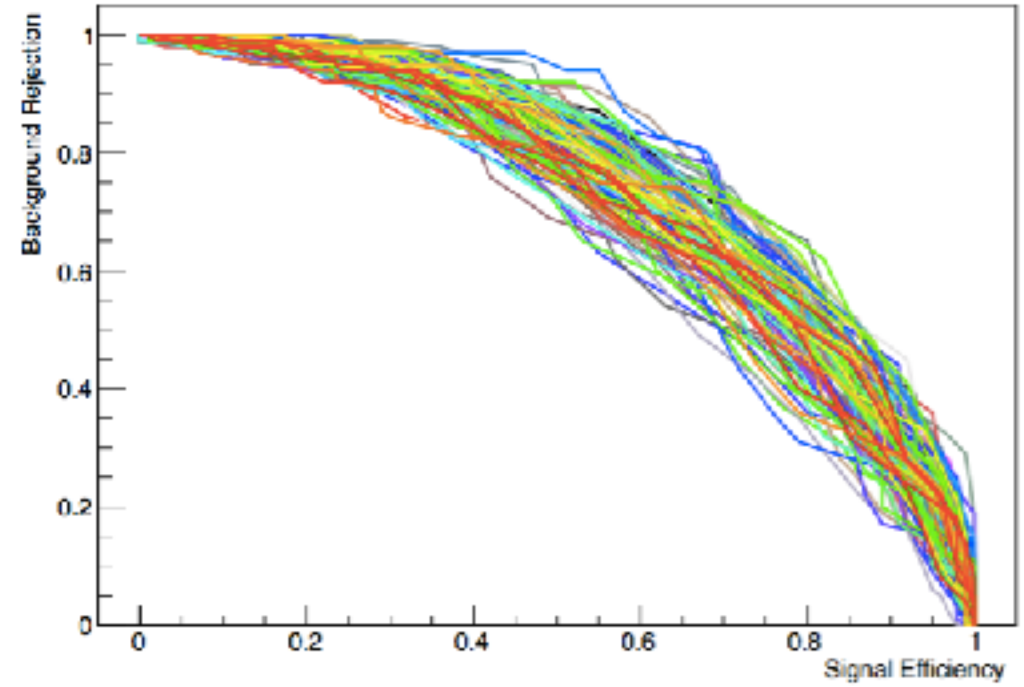


Convolutional + Pooling + Dense layers



Cross Validation in TMVA

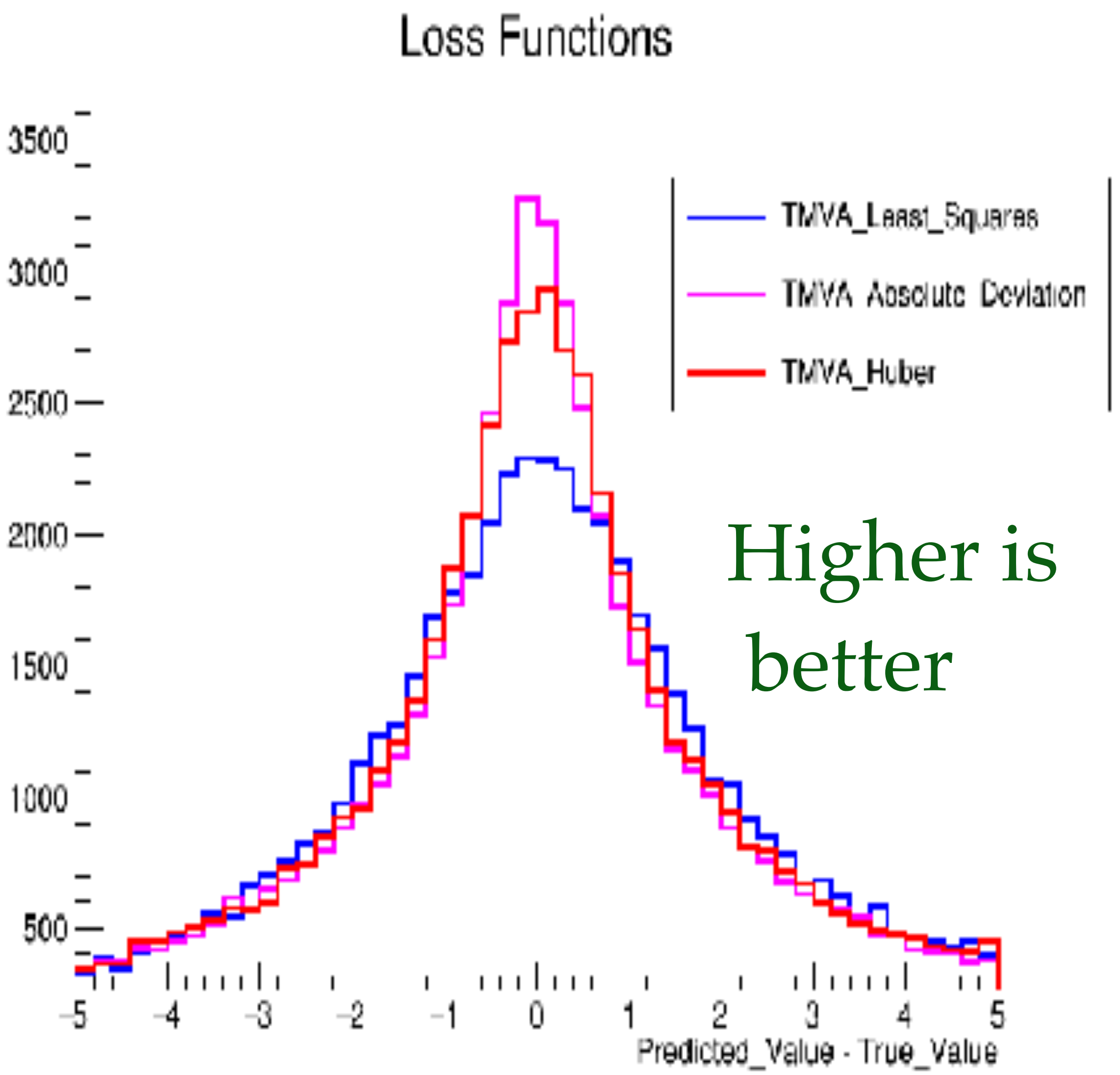
- TMVA supports k-fold cross-validation



- Hyper-parameter tuning
  - find optimised parameters (BDT-SVM)
- Foreseen providing support for parallel execution
  - multi-process/multi-threads and on a cluster using Spark or MPI

Regression in TMVA

- New Regression Features:
  - Loss function
    - Huber (default)
    - Least Squares
    - Absolute Deviation
    - Custom Function



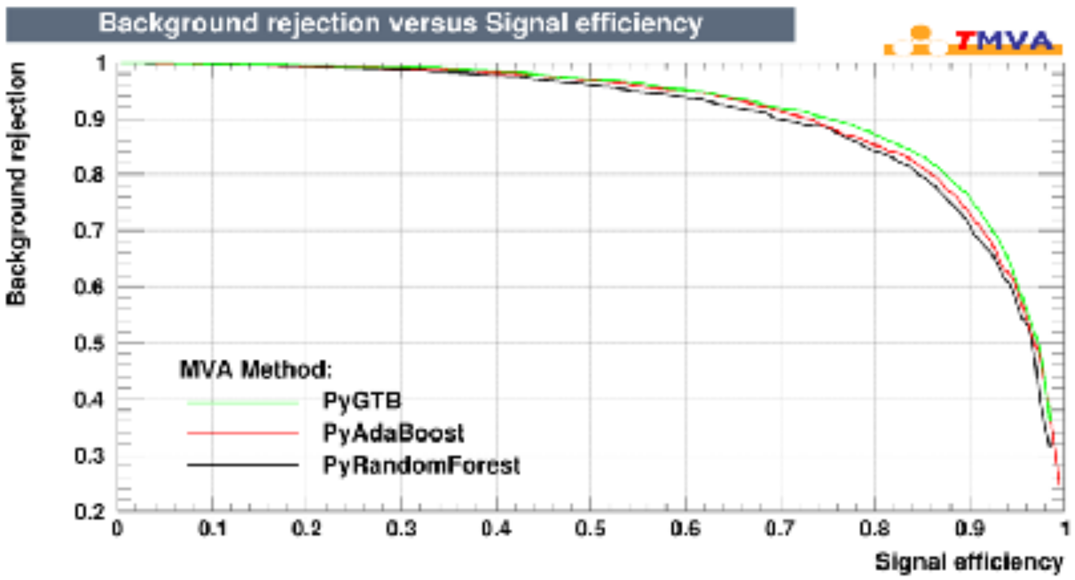
Higher is better

Important for regression performance

TMVA Interfaces

External tools are available as additional methods in TMVA and they can be trained and evaluated as any other internal ones.

- RMVA: Interface to Machine Learning methods in R
  - c50, xgboost, RSNNS, e1071
    - see http://oproject.org/RMVA
- PYMVA: Python Interface
  - **skikit-learn** with RandomForest, Gradiend Tree Boost, Ada Boost)
    - see http://oproject.org/PYMVA
  - **Keras** (Theano + Tensorflow)
    - support model definition in Python
    - see https://indico.cern.ch/event/565647/contributions/2308668/attachments/1345527/2028480/29Sep2016_IML_keras.pdf
  - Input data are copied internally from TMVA to Numpy array



Example PyMVA with Keras

Define the Keras model in Python

Define model for Keras

In [5]:
```
# Define model
model = Sequential()
model.add(Dense(32, init='glorot_normal', activation='relu',
        input_dim=numVariables))
model.add(Dropout(0.5))
model.add(Dense(32, init='glorot_normal', activation='relu'))
model.add(Dropout(0.5))
model.add(Dense(2, init='glorot_uniform', activation='softmax'))

# Set loss and optimizer
model.compile(loss='categorical_crossentropy', optimizer=Adam(),
        metrics=['categorical_accuracy',])

# Store model to file
model.save('model.h5')

# Print summary of model
model.summary()
```

Book the method as any others of TMVA

Book methods

Just run the cells that contain the classifiers you want to try.

In [6]:
```
# Keras interface with previously defined model
factory.BookMethod(dataloader, ROOT.TMVA.Types.kPyKeras, 'PyKeras',
        'H:!V:VarTransform=G:FilenameModel=model.h5:'+\
        'NumEpochs=10:BatchSize=32:'+\
        'TriesEarlyStopping=3')
```

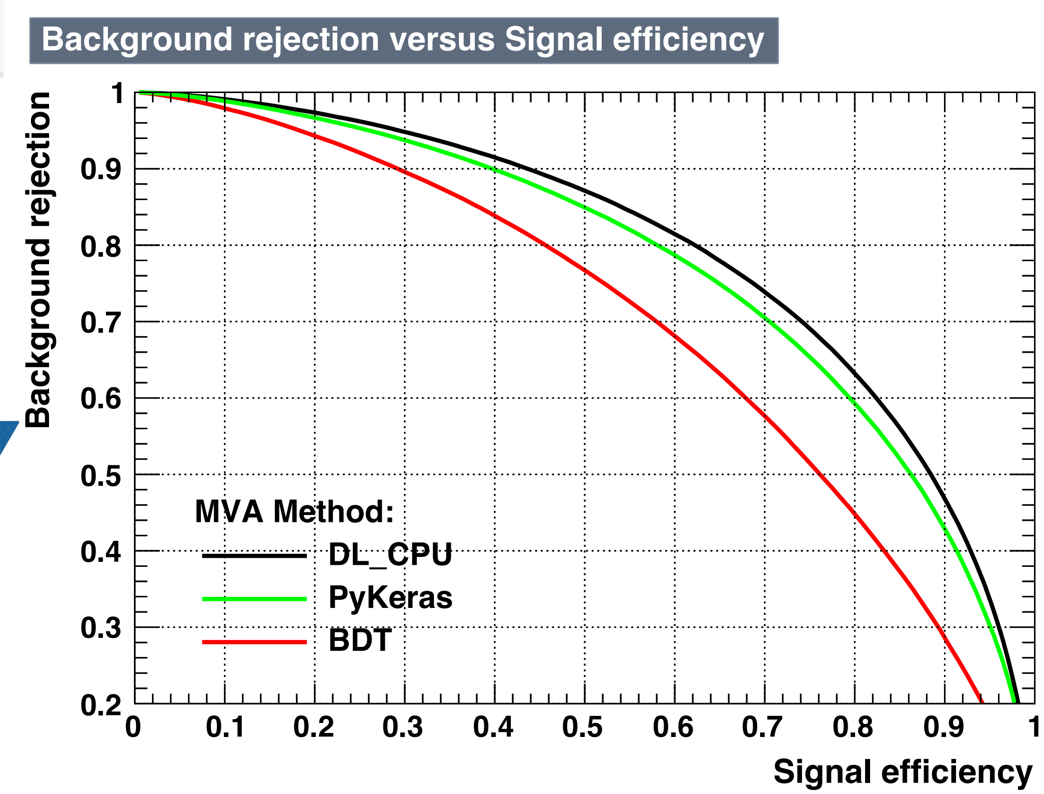
Out[6]:
```
<ROOT.TMVA::MethodPyKeras object ("PyKeras") at 0x77e48b0>
```

PyMVA with Keras

Train,Test and Evaluate inside TMVA (using TMVA::Factory)

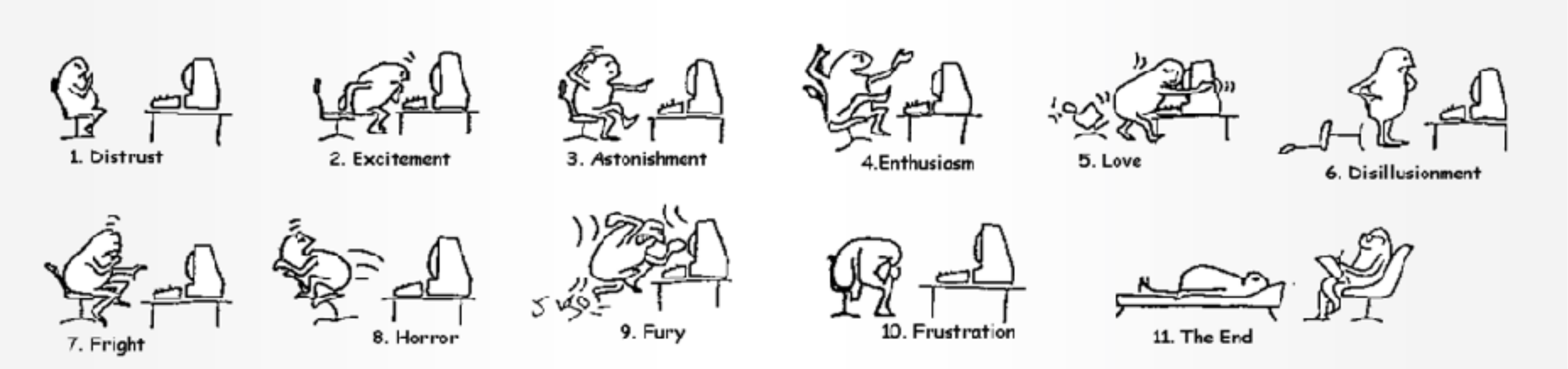
Run training, testing and evaluation

```
In [8]: factory.TrainAllMethods()

Factory                  : Train all methods

In [9]: factory.TestAllMethods()

Factory                  : Test all methods
Factory                  : Test method: PyKeras
                         .

In [10]: factory.EvaluateAllMethods()

Factory                  : Evaluate all methods
Factory                  : Evaluate classifier: PyKeras
                         :
```



Examine result with TMVA GUI

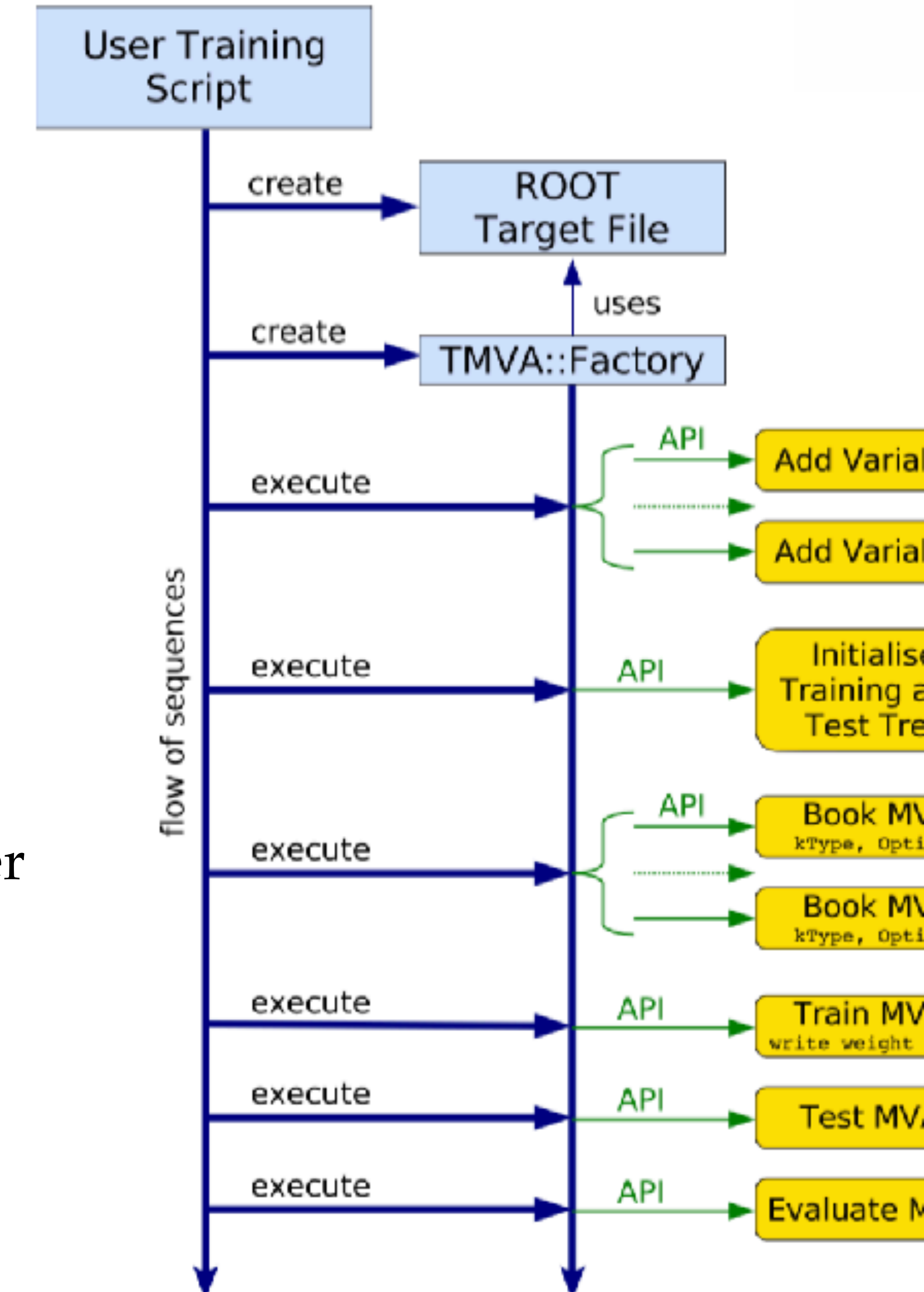
Using TMVA



1. Distrust
2. Excitement
3. Astonishment
4.Enthusiasm
5. Love
6. Disillusionment
7. Fright
8. Horror
9. Fury
10. Frustration
11. The End

Workflow in TMVA

- Reading input data
- Select input features and preprocessing
- **Training**
  - find optimal classification or regression parameters using data with known labels (e.g. signal and background MC events)
- **Testing**
  - evaluate performance of the classifier in an independent test sample
  - compare different methods
- **Application**
  - apply classifier/regressor to real data where labels are not known



TMVA Custumizations and Features

TMVA supports:

- ROOT Tree input data (or ASCII, e.g. csv)
- pre-selection cuts on input data
- event weights (negative weights for some methods)
- various method for splitting training/test samples
- k-fold cross-validation
- support variable importance
- hyper-parameter optimisations

TMVA Session

```
void TMVAnalysis( )
{
 TFile* outputFile = TFile::Open( "TMVA.root", "RECREATE" );

 TMVA::Factory *factory = new TMVA::Factory( "MVAnalysis", outputFile,"!V");

 TFile *input = TFile::Open("tmva_example.root");

 factory->AddVariable("var1+var2", 'F');
 factory->AddVariable("var1-var2", 'F');   //factory->AddTarget("tarval", 'F');

 factory->AddSignalTree ( (TTree*)input->Get("TreeS"), 1.0 );
 factory->AddBackgroundTree ( (TTree*)input->Get("TreeB"), 1.0 );
 //factory->AddRegressionTree ( (TTree*)input->Get("regTree"), 1.0 );
 factory->PrepareTrainingAndTestTree( "", "",
 "nTrain_Signal=200:nTrain_Background=200:nTest_Signal=200:nTest_Background=200:!V" );

 factory->BookMethod( TMVA::Types::kLikelihood, "Likelihood",
 "!V:!TransformOutput:Spline=2:NSmooth=5:NAvEvtPerBin=50" );
 factory->BookMethod( TMVA::Types::kMLP, "MLP",
 "!V:NCycles=200:HiddenLayers=N+1,N:TestRate=5" );

 factory->TrainAllMethods();  // factory->TrainAllMethodsForRegression();
 factory->TestAllMethods();
 factory->EvaluateAllMethods();
 outputFile->Close();
 delete factory;
}
```

Create Factory

Add variables/ targets

Initialize Trees

Book MVA methods

Train, test and evaluate

[E. v. Toerne]

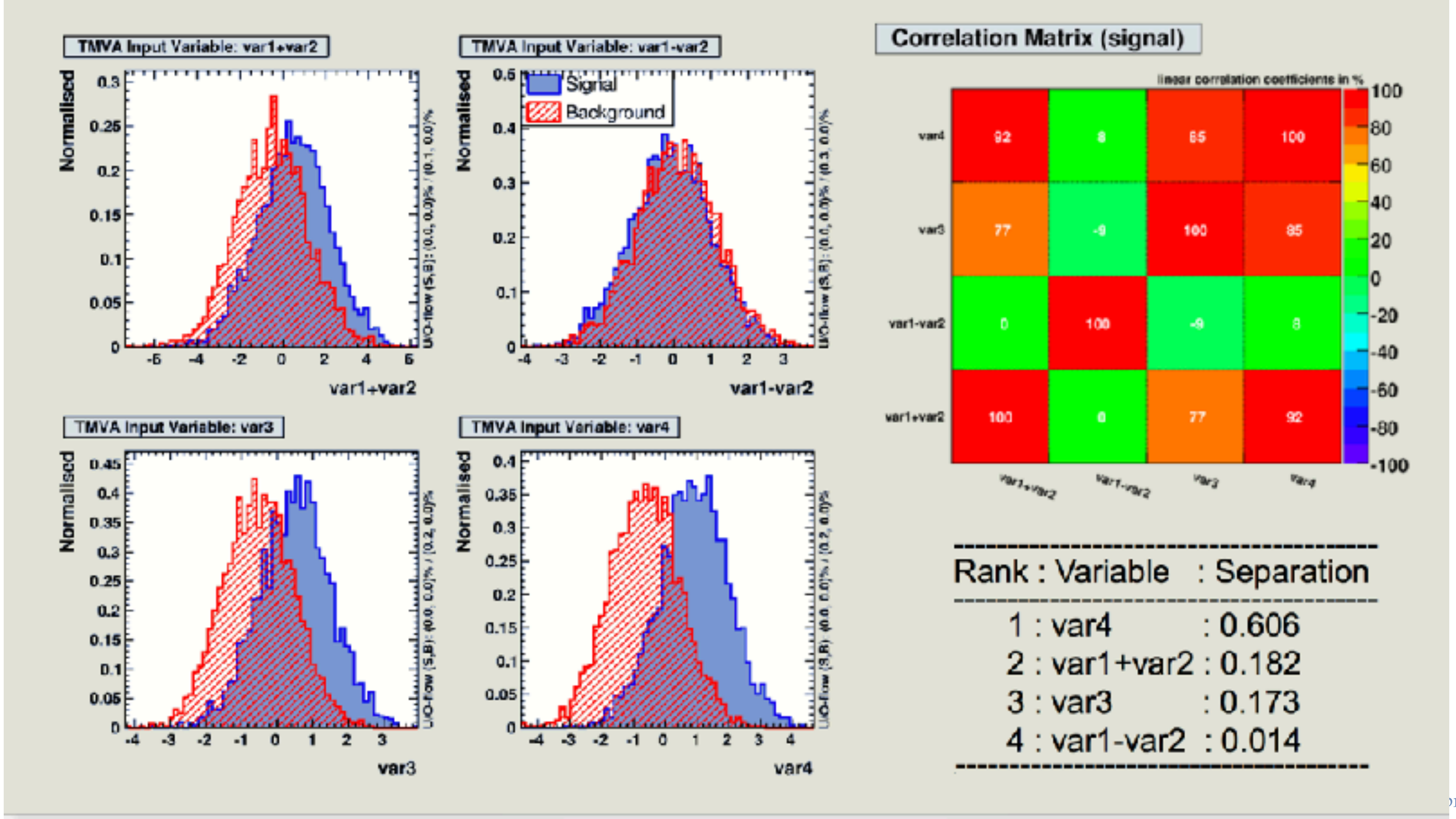
We will see better with a real example
(e.g. TMVAClassification.C tutorial)

TMVA Toy Example

4 Gaussian variable with linear correlations

$$\{x_1 = v_1 + v_2,\ x_2 = v_1 - v_2,\ x_3 = v_3,\ x_4 = v_4\}$$

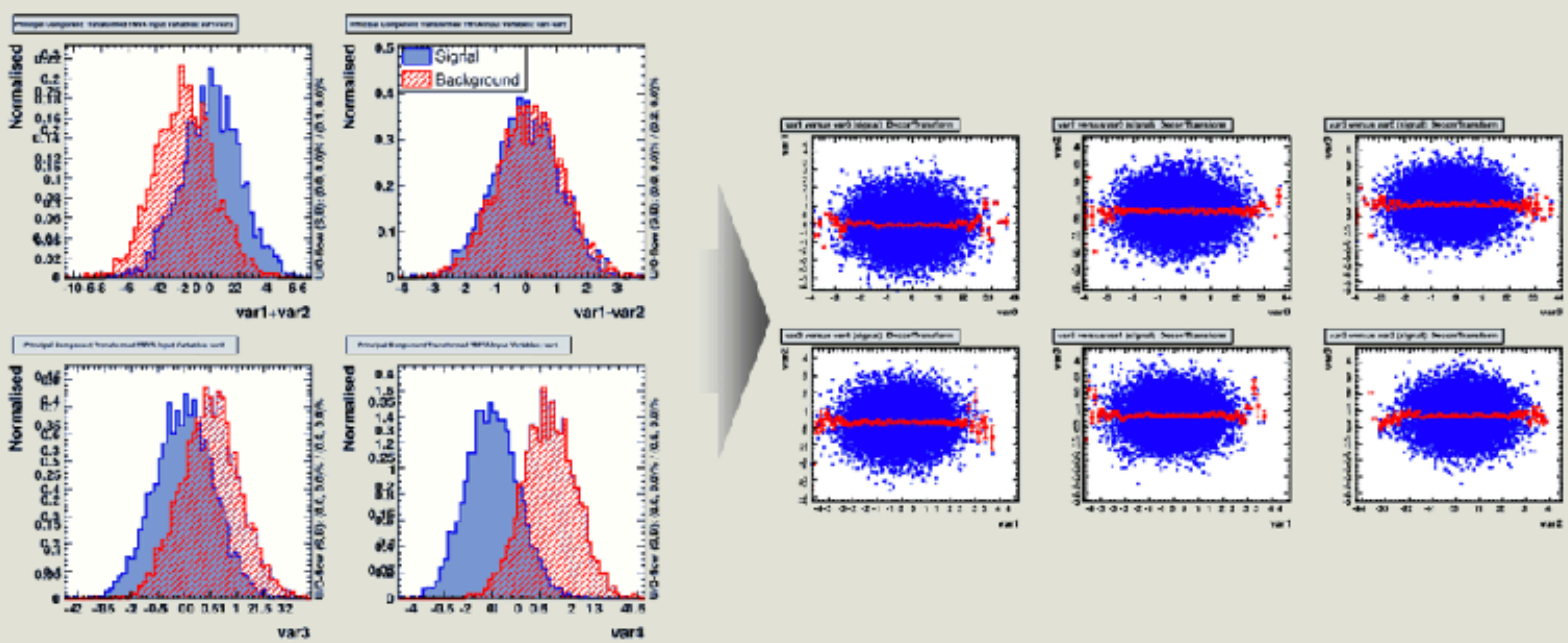
where $\{v_1, ..v_4\}$ are normal variables



Rank	Variable	Separation
1	var4	0.606
2	var1+var2	0.182
3	var3	0.173
4	var1-var2	0.014

Pre-processing of the Input Variables

- Example: decorrelation of variable before training can be useful



- Note that in cases with non-Gaussian distributions and/or nonlinear correlations decorrelation may do more harm than any good

Several others pre-processing available (see Users Guide)

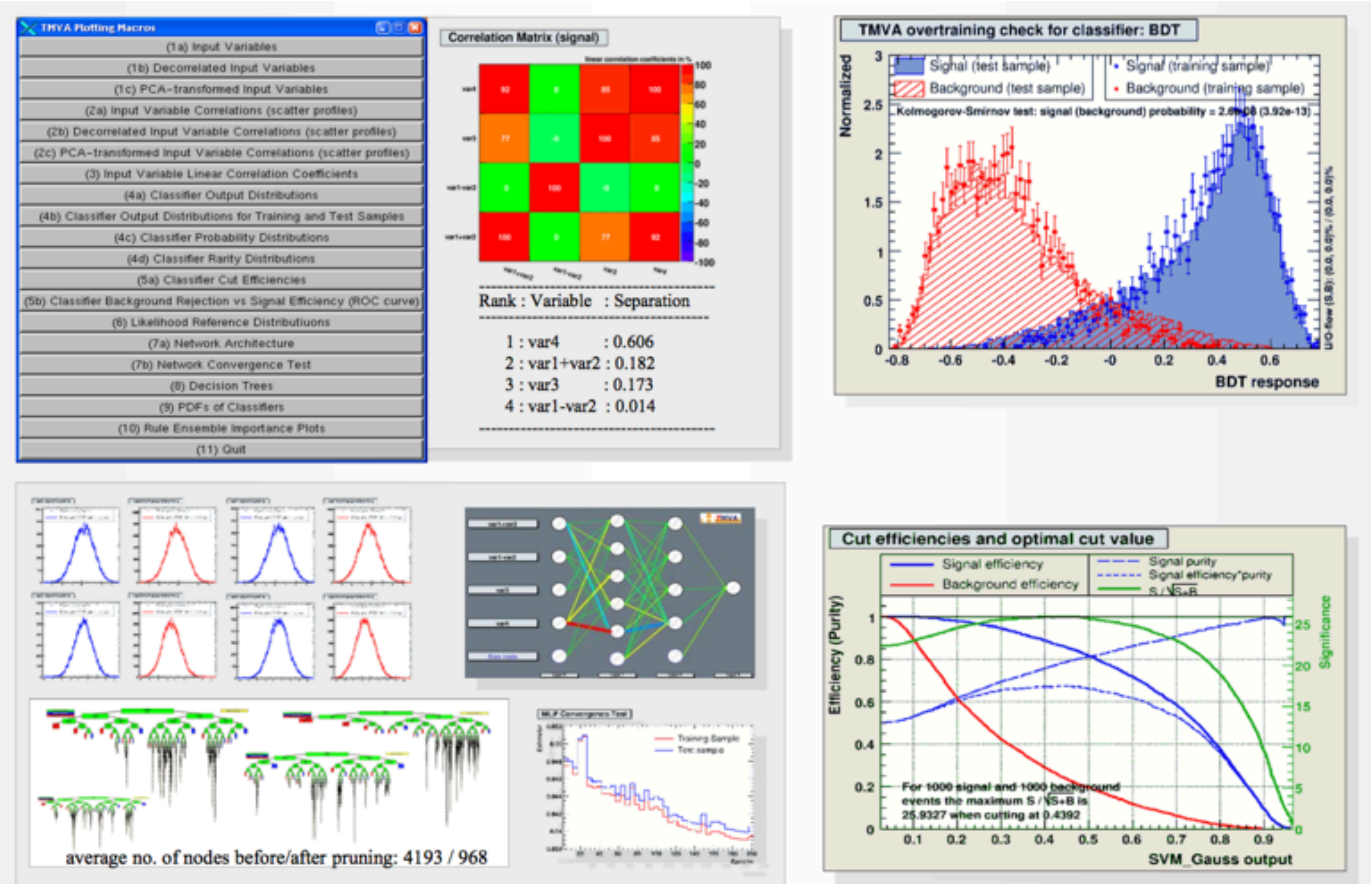
Available Preprocessing

- List of available pre-processing in TMVA
  - Normalization
  - Decorrelation (using Cholesky decomposition)
  - Principal Component Analysis
  - Uniformization
  - Gaussianization

- Can be selected individually for each single method (when booking)

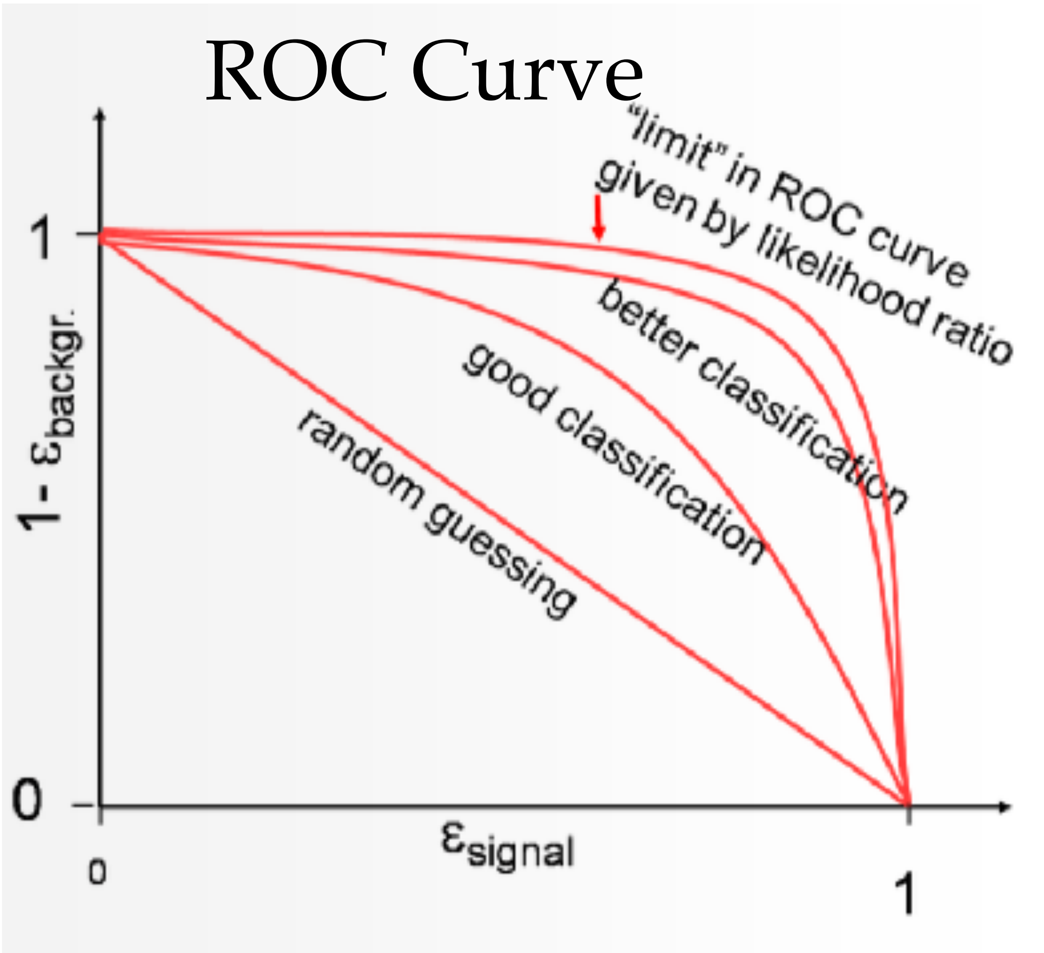
TMVA GUI

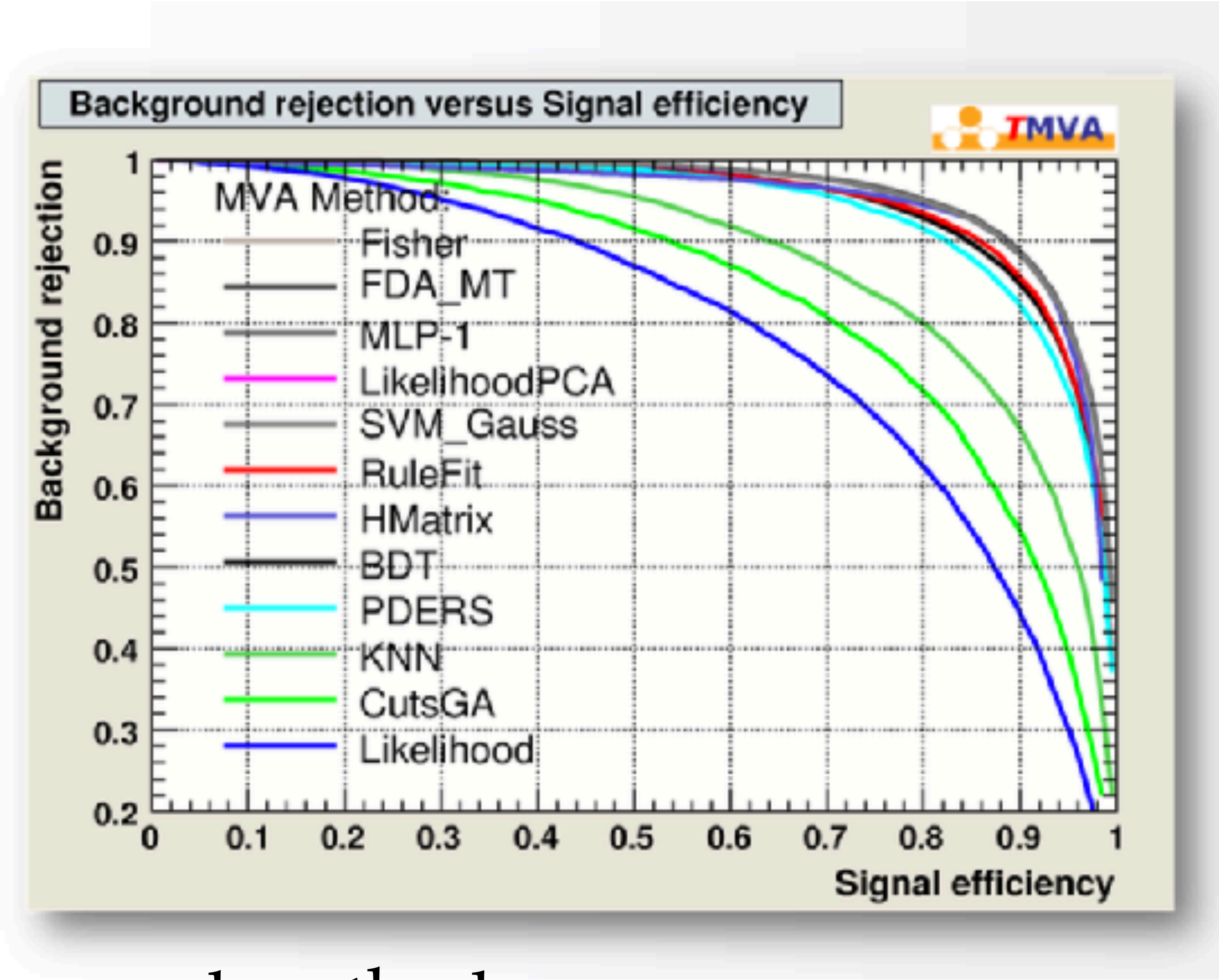
At the end of training + test phase, TMVA produces an output file that can be examined with a special GUI (**TMVAGui**)



ROC Curve in TMVA

For example from GUI one can obtain a ROC curve for each method trained and tested on an independent data set

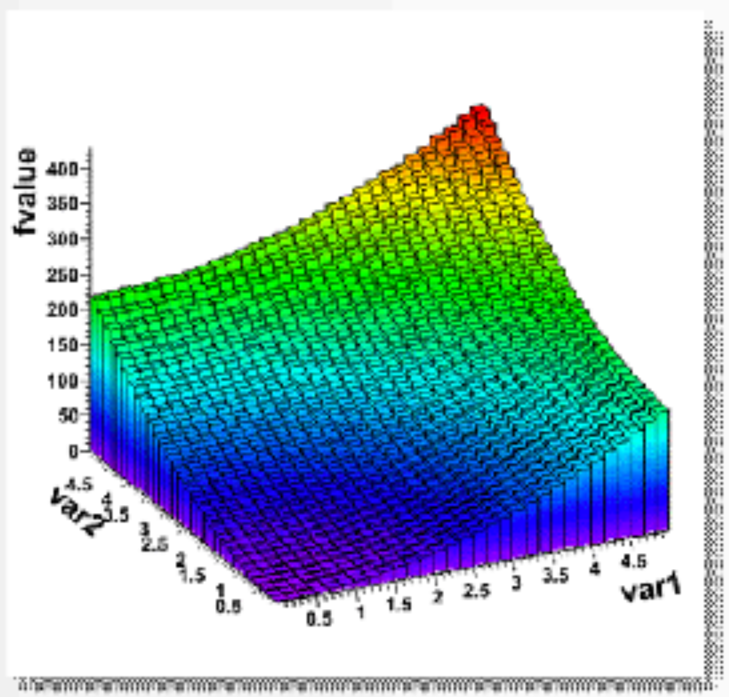


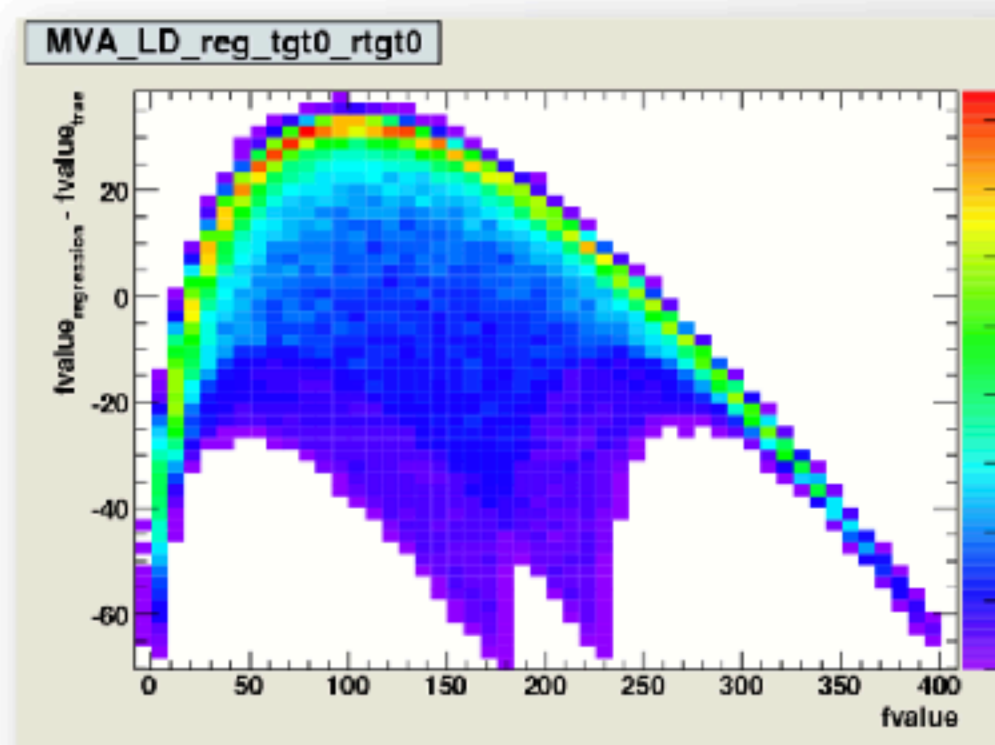


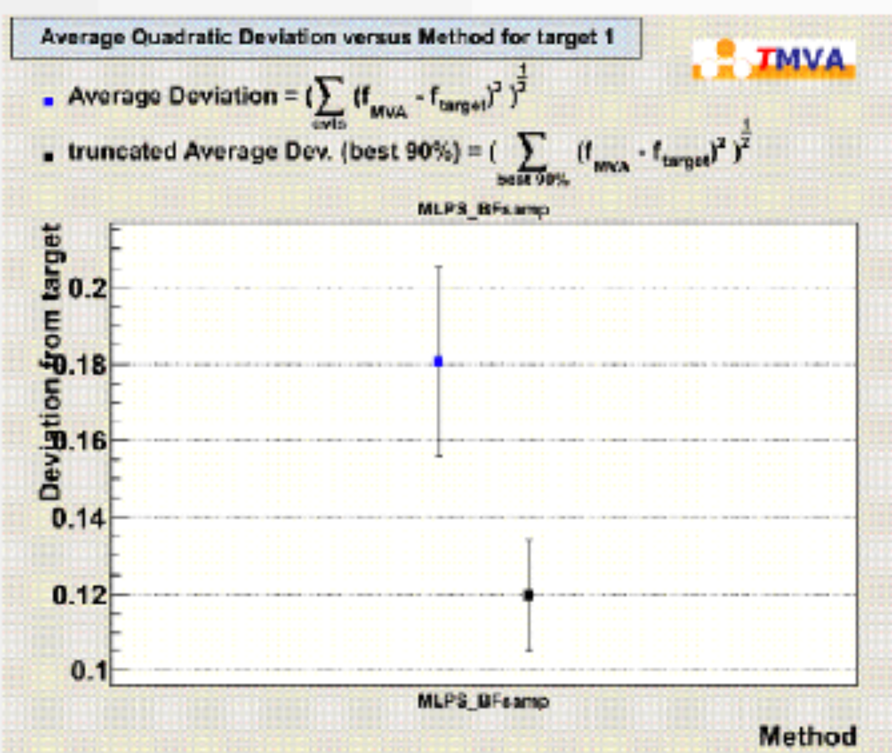
➜ Comparison of several methods

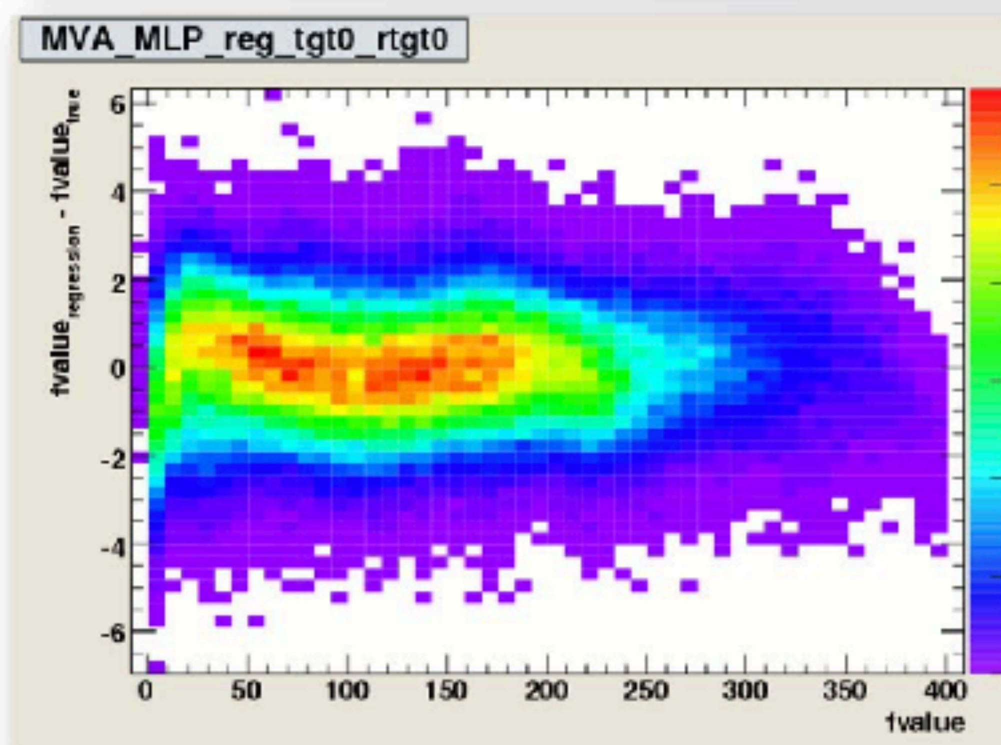
TMVA Regression GUI

A dedicated GUI exists for regression (**TMVARegGui**)





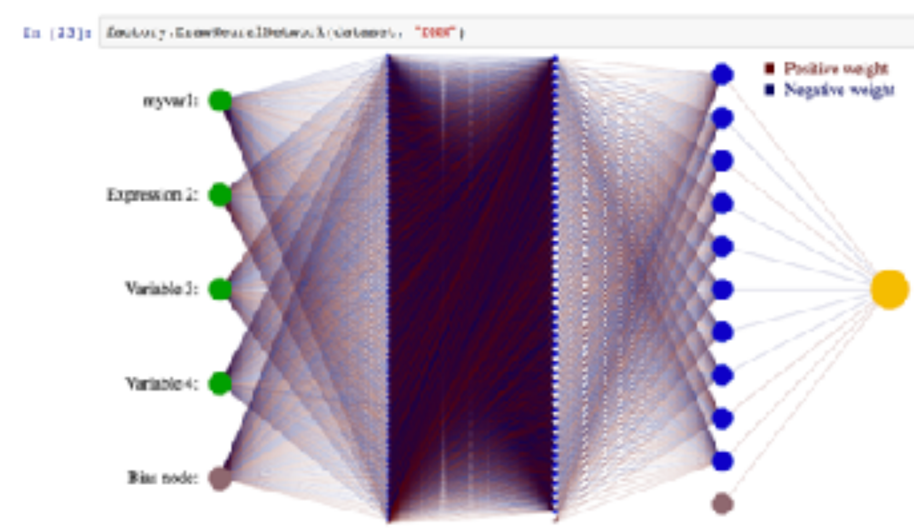


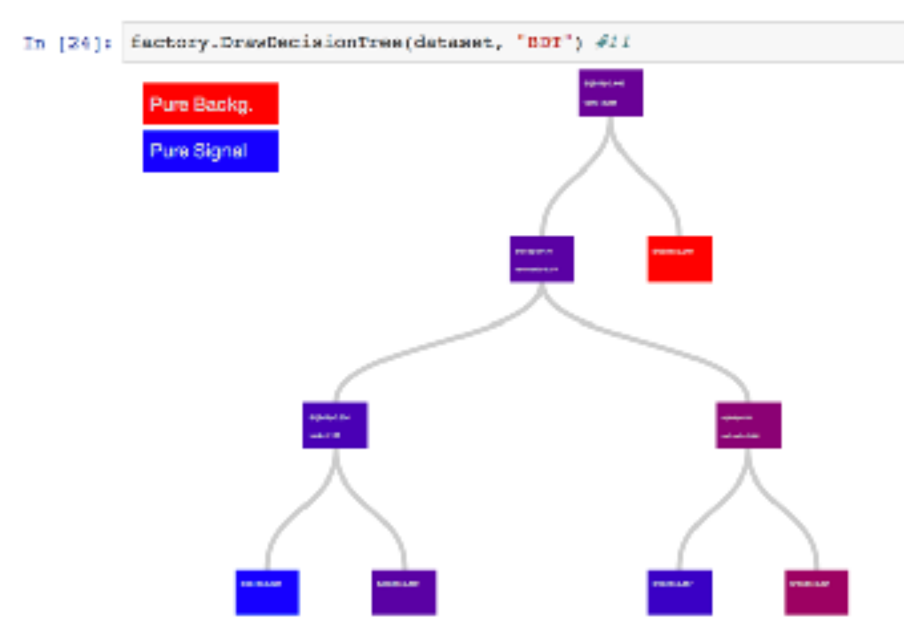


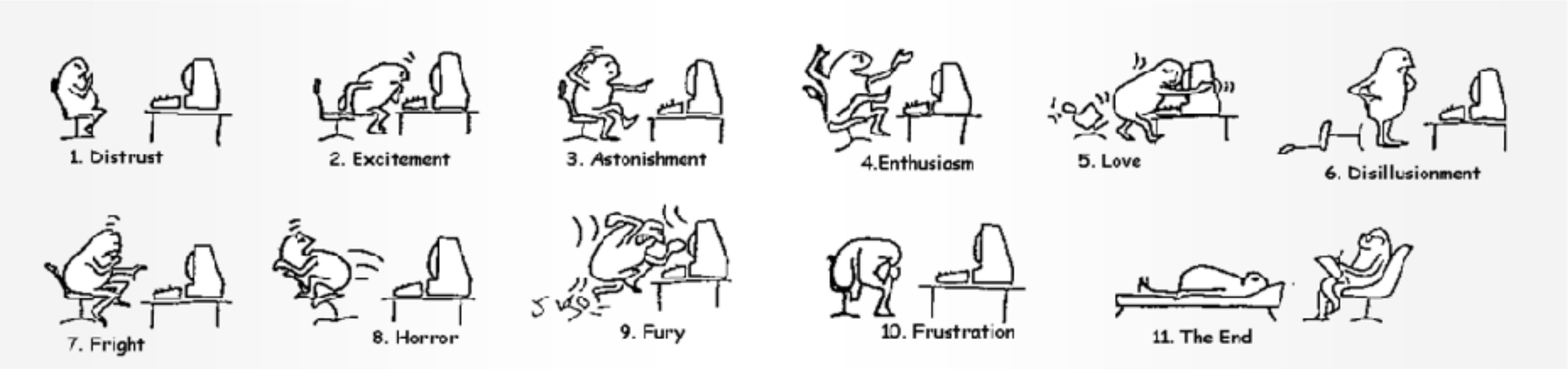
Jupyter Integration

New Python package for using TMVA in Jupyter notebook (jsmva)

- Improved Python API for TMVA functions
- Visualisation of BDT and DNN
- Enhanced output and plots (e.g. ROC plots)
- Improved interactivity (e.g. pause/resume/stop of training)
- see example in SWAN gallery
  https://swan.web.cern.ch/content/machine-learning







Let’s start using TMVA

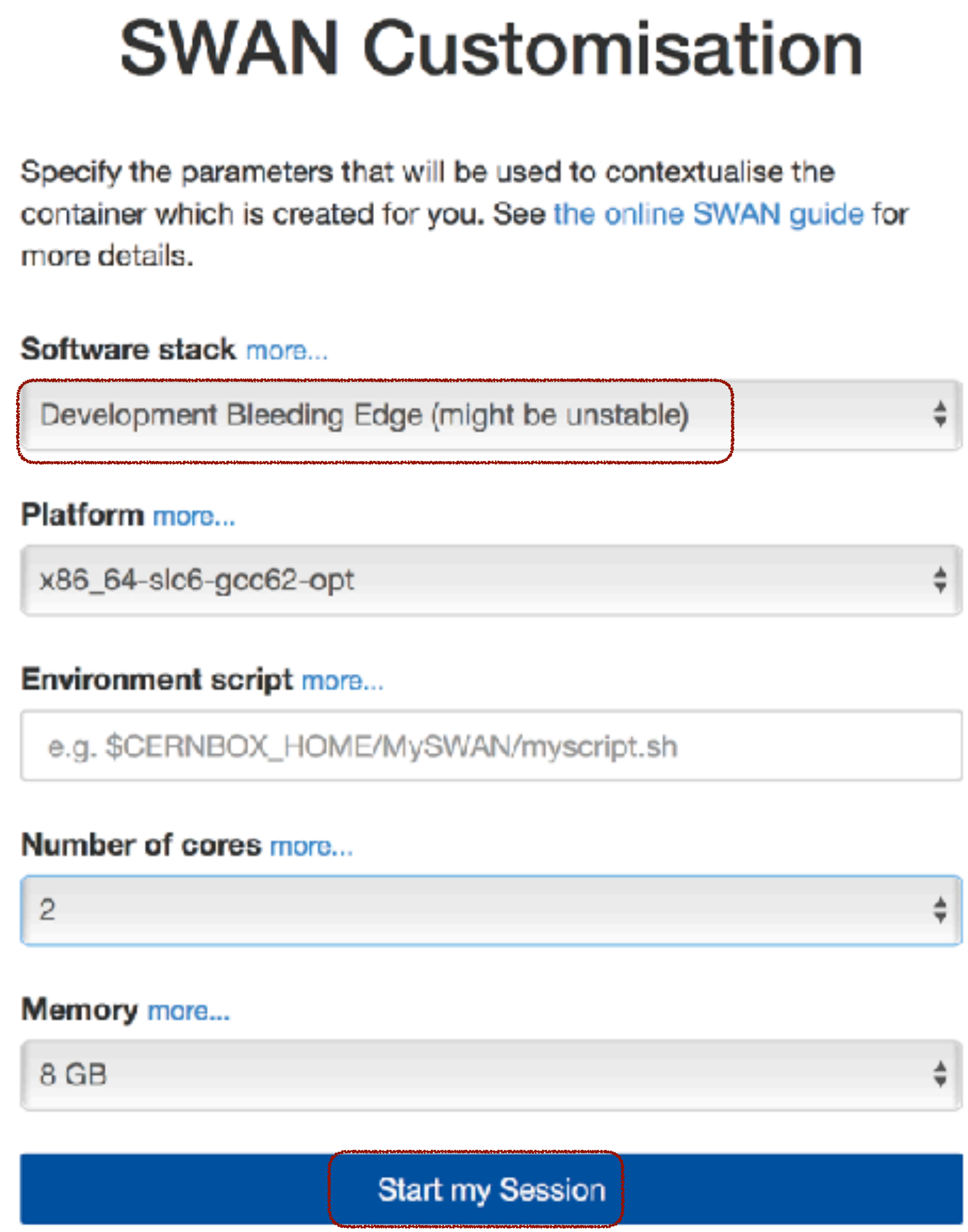
TMVA Tutorial

- **Run tutorial on notebook**
  - use **SWAN**
    - go to swan.cern.ch

  - **or running local notebooks**
    - root —notebook

If you don't have CERN account for using SWAN please contact me
Some temporary account can be made available
But before please feel the online form available **here**

Starting SWAN

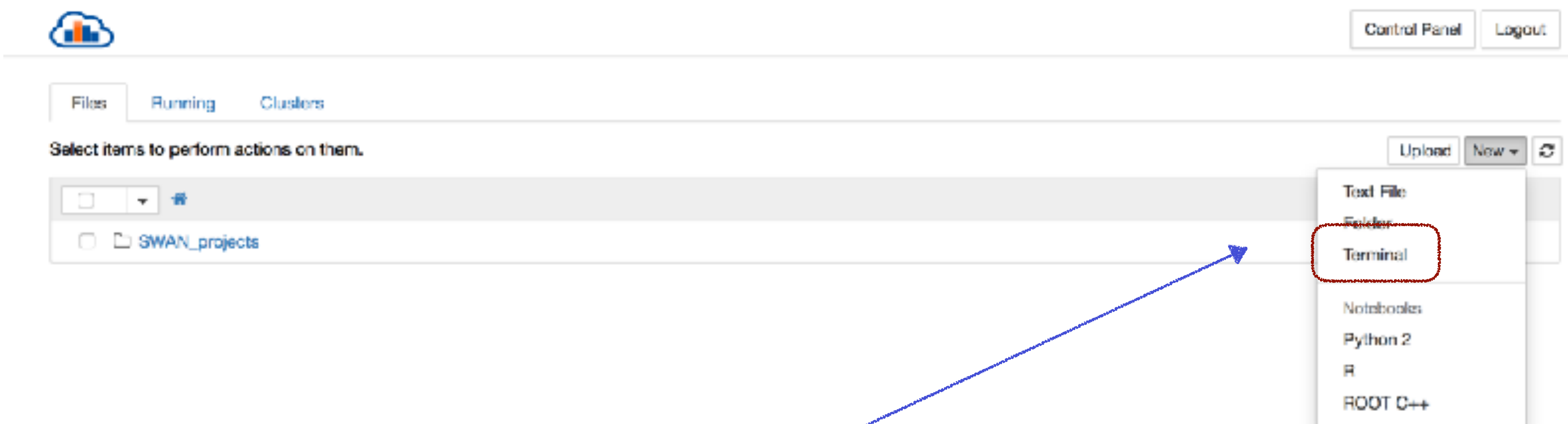


Select to use new Deep Learning

click here to start

Starting a Terminal in SWAN

After login cernbox home directory will be visible



Start a terminal window

Getting the Notebooks

- **Clone the git repository of the tutorials**

  https://github.com/lmoneta/tmva-tutorial.git

  - get directly the **IML-tutorial-2018** branch
  - git clone —branch IML-tutorial-2018 https://github.com/lmoneta/tmva-tutorial.git

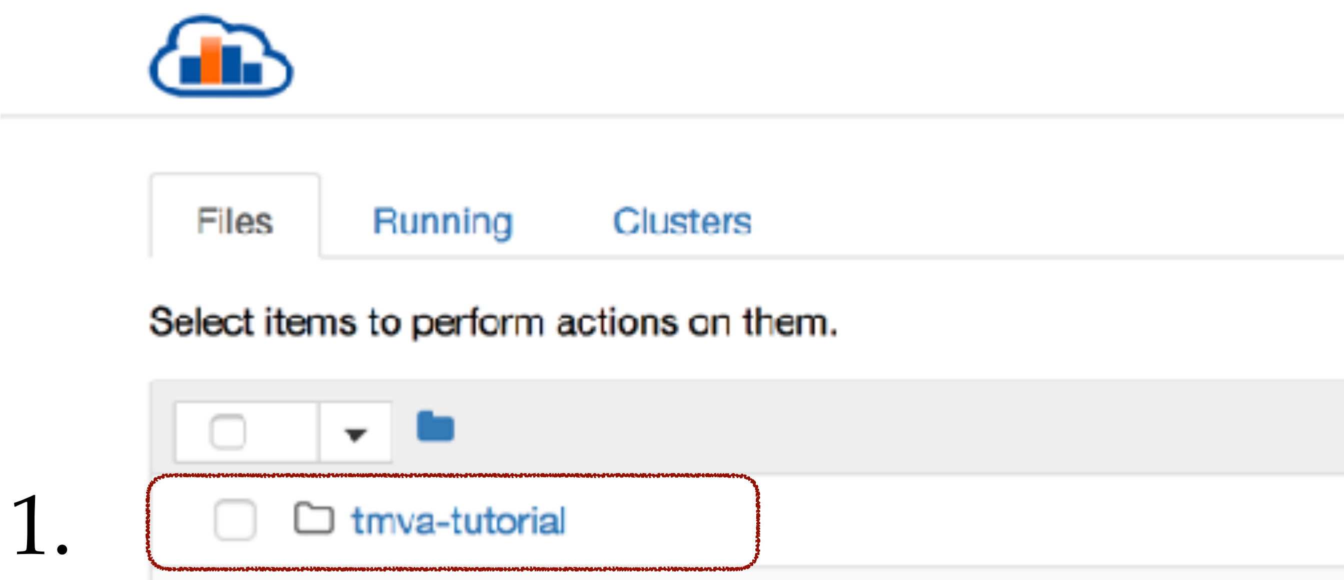
If directory already exists delete it before or update its git repository doing:
git fetch; git checkout -b IML-tutorial-2018 origin/IML-tutorial-2018

```
bash-4.1$ git clone --branch IML-tutorial-2018 https://github.com/lmoneta/tmva-tutorial.git
Initialized empty Git repository in /eos/user/m/moneta/tmva-tutorial/.git/
remote: Counting objects: 72, done.
remote: Compressing objects: 100% (25/25), done.
remote: Total 72 (delta 11), reused 24 (delta 5), pack-reused 42
Unpacking objects: 100% (72/72), done.
bash-4.1$ ls tmva-tutorial
README.md  tutorial_IML2017  tutorial_IML2018  tutorial_Lisbon
bash-4.1$
```

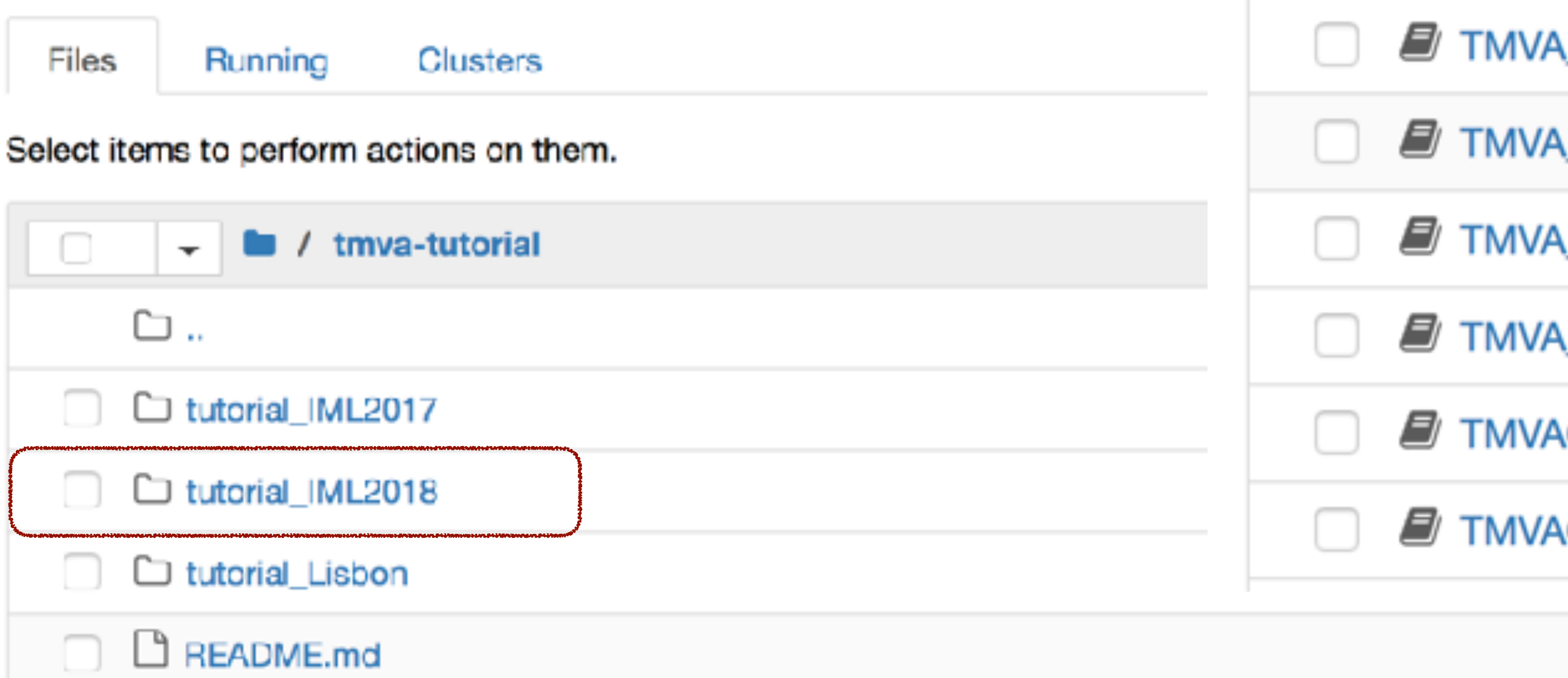
- Go back to SWAN Home page and select the directory **tmva-tutorial/tutorial_IML2018**
  - Start using the notebooks

Notebooks

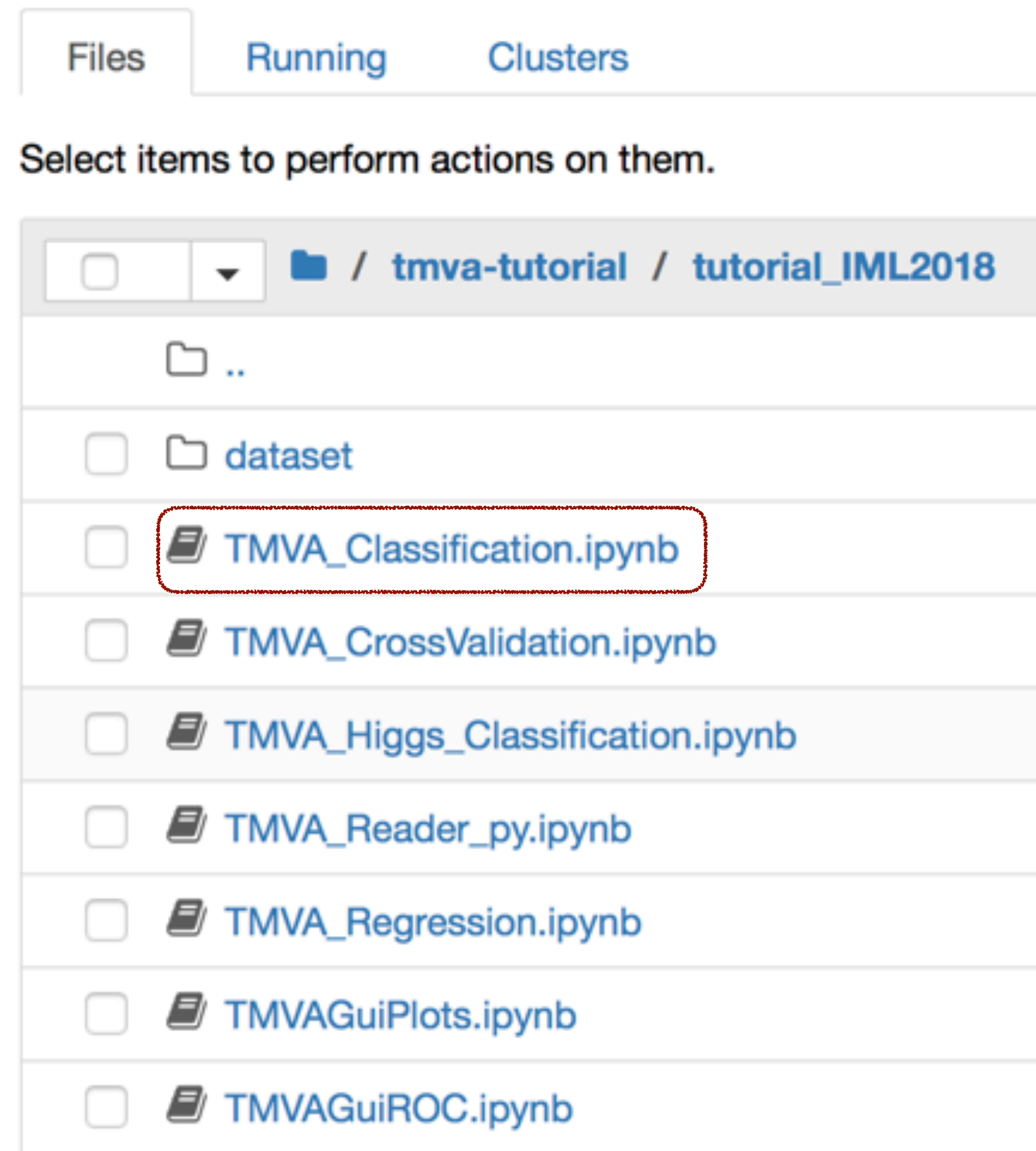
1.



2.



3.



TMVA Classification

TMVA_Classification (autosaved)

Control Panel Logout

File Edit View Insert Cell Kernel Help

Not Trusted ROOT C++

Markdown

TMVA Classification Example

Declare Factory

Create the Factory class. Later you can choose the methods whose performance you'd like to investigate.

The factory is the major TMVA object you have to interact with. Here is the list of parameters you need to pass

- The first argument is the base of the name of all the output weightfiles in the directory weight/ that will be created with the method parameters
- The second argument is the output file for the training results
- The third argument is a string option defining some general configuration for the TMVA session. For example all TMVA output can be suppressed by removing the "!" (not) in front of the "Silent" argument in the option string

In [1]:

```
TMVA::Tools::Instance();
```

Outlook for TMVA

- Very active development happening in TMVA
  (thanks to contribution from doctoral students, summer students and Google Summer of Code students)
  - e.g. New Deep Learning tools
- Important to have a rich set of modern ML tools in ROOT and at the same time provide interfaces to popular external libraries
- New planned developments (GSOC projects for 2018)
  - Complete Deep Learning module (add GPU support)
  - GAN for fast simulation
  - Direct interface to Tensorflow
- Improve big data (I/O) handling for ML
  - avoid un-needed extra data copies and optimise memory usage
  - better interface to external tools

Conclusions

- Very active development in TMVA
  - expect several new features in next release
- Feedback from users is essential
  - we are defining ROOT plan of work for next year, requests and feedback from experiments will be taken into account
- Users contributions are extremely important
  - best way to contribute is opening a Pull Request in GitHub (https://github.com/root-project/root)
- For support use ROOT Forum : https://root.cern.ch/phpBB3/
  - with categories dedicated on TMVA
- For reporting ROOT bugs: https://sft.its.cern.ch/jira
- or just contact us directly

TMVA Contributors

Lorenzo Moneta	Algorithm development, Integration and support
Sergei Gleyzer	Analyzer Tools, Algorithm Development
Omar Zapata Mesa	PyMVA, RMVA, Modularity, Parallelization and Integration
Kim Albertsson	Multi-class for BDT, cross validation/evaluation and support
Stefan Wunsch	KERAS Interface
Peter Speckmeyer	Deep Learning CPU
Simon Pfreundschuh	Deep Learning CPU and GPU
Vladimir Ilievski	New Deep Learning module, CNN layers
Saurav Shekkar	New Deep Learning module and Recurrent layer
Akshay Vashistha	Deep Auto Encoder development
Mark Huwiler	Deep Auto Encoder and Deep Learning integration tests
Mammad Hagili	Parallelisation of Cross-Validation
Adrian Bevan, Tom Stevenson	SVMs, Cross-Validation, Hyperparameter Tuning
Attila Bagoly	Jupyter Integration, Visualization, Output
Paul Seyfert	Performance optimization
Andrew Carnes	Regression, Loss Functions, BDT Parallelization

- Continued invaluable contributions from Andreas Hoecker, Helge Voss, Eckhard v.Thorne, Jörg Stelzer, and key support from CERN EP-SFT Group