ML framework and QC tools in ALICE.

Measure the uncertainty

Robust regression and model compression

MVA wrapper+AliNDFunctionInterface

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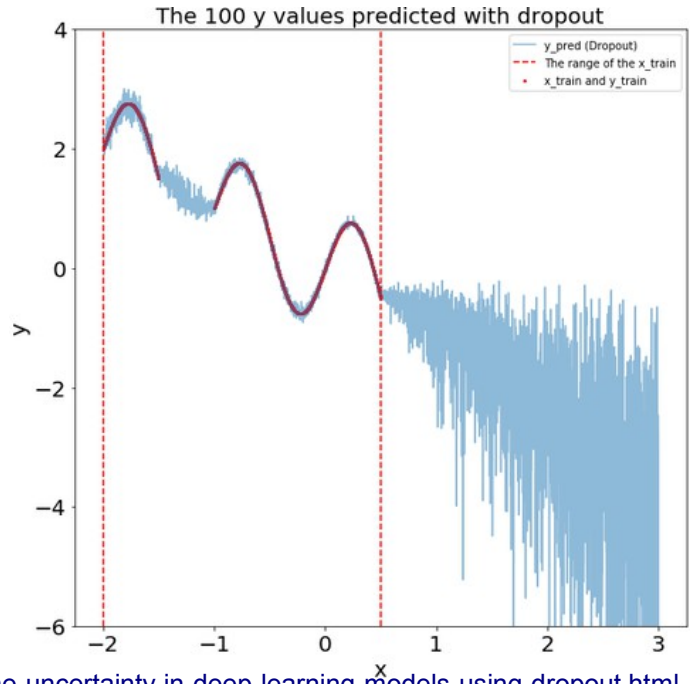


https://fairyonice.github.io/Measure-the-uncertainty-in-deep-learning-models-using-dropout.html

Outlook

N dimensional analysis pipeline in ALICE

(T)MVA interface wrapper (Python/C++)

- quantiles
- prediction/confidence intervals
- model compression

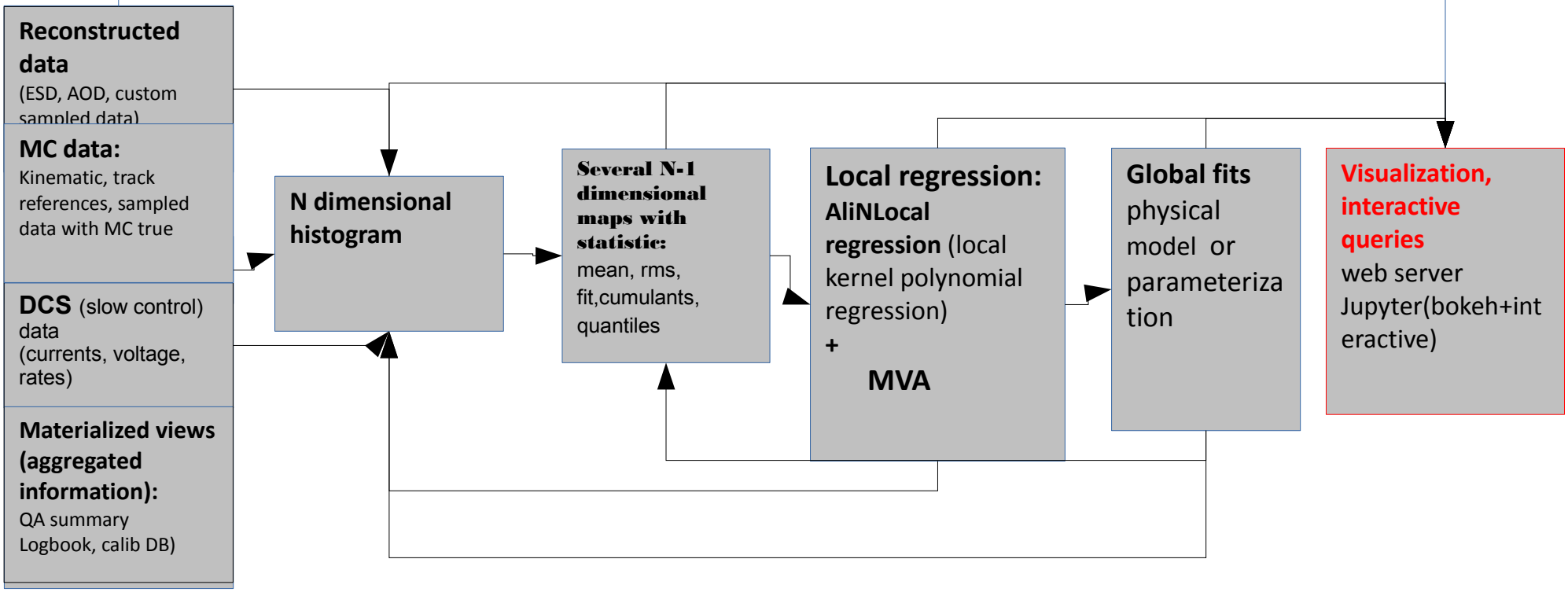
TMVA wrapper

- first example of user interface for MVA wrapper

Jupyter notebook tutorial:

- Example usage of the MVA interface in time series analysis
- Space point distortion time series, regression (sklearn.RandomForest, KNN, Keras) with error predictions
- https://indico.cern.ch/event/766450/contributions/3225232/attachments/1764699/286

Alice - Standard ND pipeline



$$f(p_0, p_1, p_2, \ldots) \neq f_0(p_0) \oplus f_1(p_1) \oplus f_2(p_2) \oplus \ldots.$$

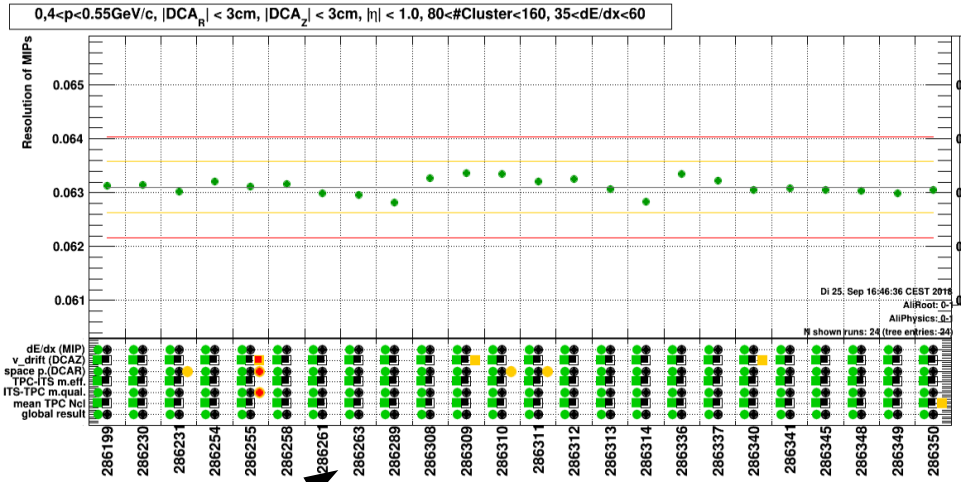
Standard calibration/performance maps and QA done and interpreted in multidimensional space

dimensionality depends on the problem to study (and on available resources)

Data →Histogram → set of ND maps → set of NDlocal regression/MVA → Global fits

Some steps can be skipped, e.g local regression (TMVA/AliNDLocal) can be done using unbinned input data

Alice - automatic alarms



Status bar

Status bar decomposition

Aggregated summary data used as an input for automatic alarms

User defined alarm. Usually combination

outliers - **n sigma bands around "predicted value"** (median,mean)

"physically accepatable" performance

logical &&, || of the state for sub-component

MVA algortihm/regression to be used to predict expected value and error of prediction

MVA AliNDFunctionInterface to machine learning

AliNDFunctionInterface : TMVA wrapper in ALICE analysis framework AliRoot (C++ implementation usable aslo in Python)

- Simple and compact user interface
  - similar to TTree::Draw and Histogram::Fit queries
- Store all the data as ROOT objects in ROOT files (instead of weight files, no xml files)
  - possibility to store data in Alice calibration DB
- Easy usage providing TFormula/TTreeformula interface
  - possibility to combine/normalize/operate with other formulas (other TMVA, global fits, NDimensional local tables (e.g AliNDLocalRegression object)

New wrapper (written in Python - to be interfaced also to C++)

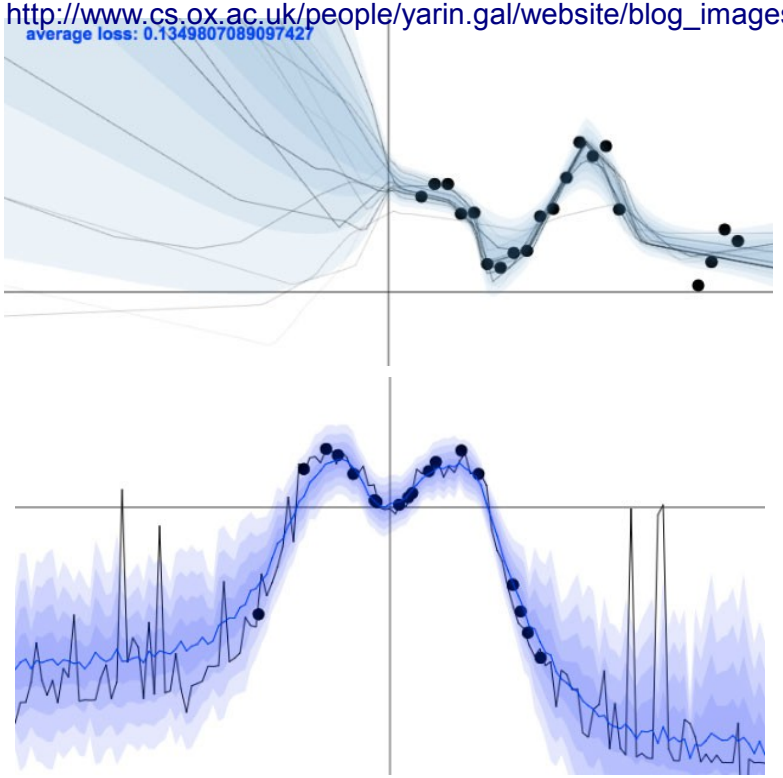
- **Local error estimates** (reducible and irreducible errors) and local robust estimators
- Combined/weighted evaluation, caching and model compression **(WORK IN progress)**

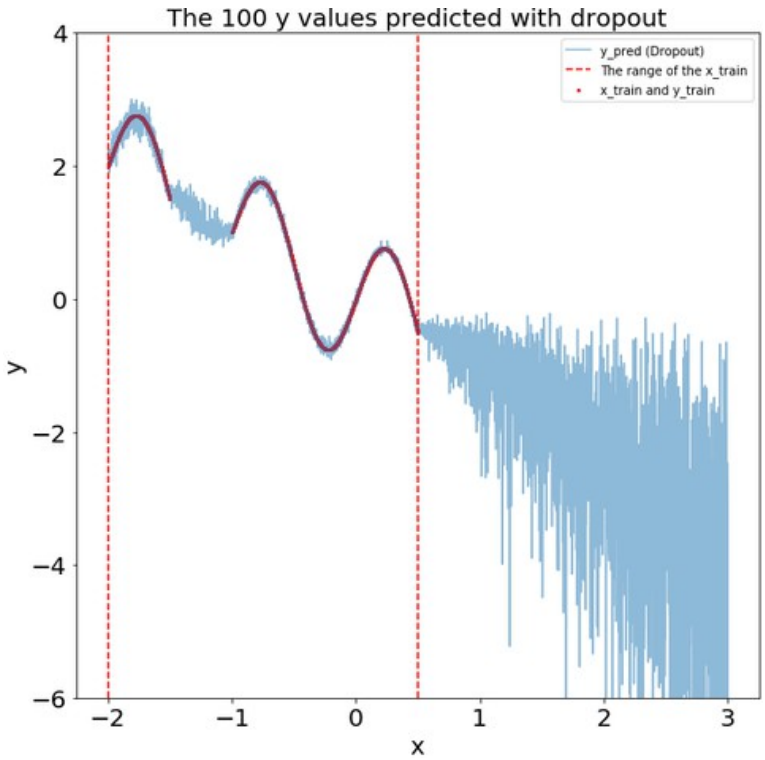
Goal - make the usage of the MVA almost as easy as standard fits in root

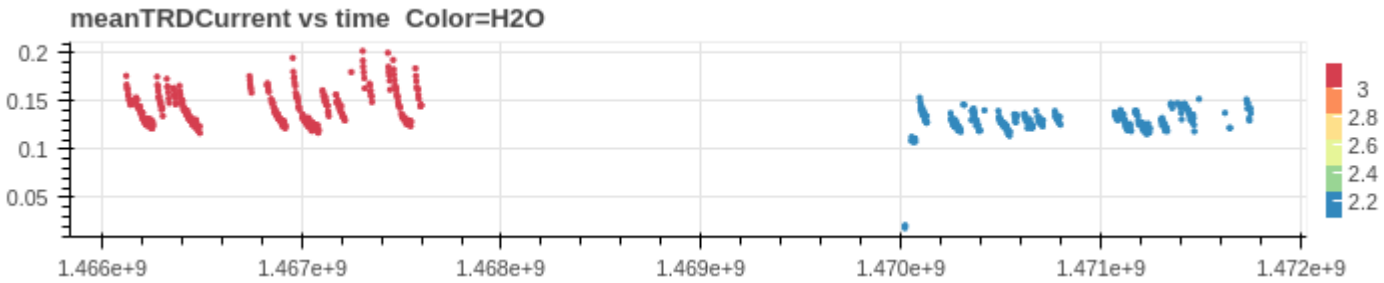
Why Should we Care About Uncertainty?

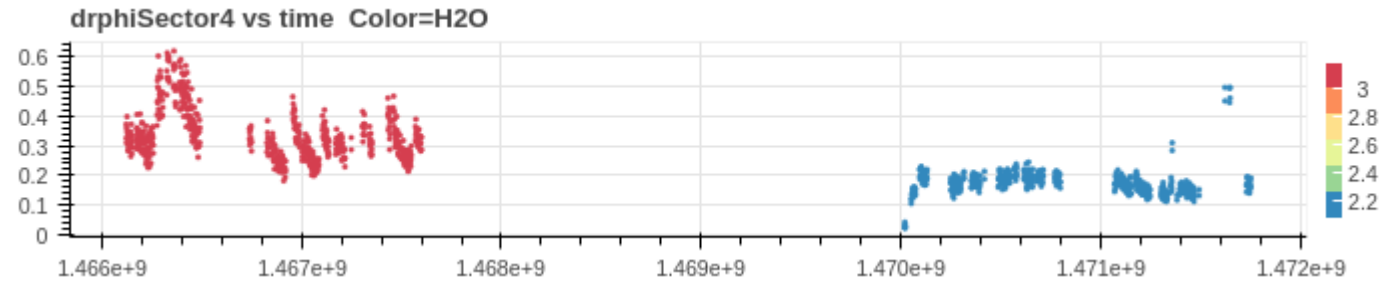
http://www.cs.ox.ac.uk/people/yarin.gal/website/blog_images/reg_demo_small.jpg

https://fairyonice.github.io/Measure-the-uncertainty-in-deep-learning-models-using-dropout.html









Example:
Alice example time series flux, gas composition and distortion

What is the prediction error for non seen data ?

Confidence/prediction intervals

Currently not standard libraries to estimate reducibble and irreducible error of the ML models.

Confidence Intervals for Scikit Learn Random Forests

http://contrib.scikit-learn.org/forest-confidence-interval/

https://github.com/scikit-learn-contrib/forest-confidence-interval

forestci package

This package adds to scikit-learn the ability to calculate confidence intervals of the predictions generated from scikit-learn

Neural network prediction:

1: Delta method

2: Bayesian method

3: Mean variance estimation

4: Bootstrap

Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning (https://arxiv.org/abs/1506.02142 - 2015)

test-time dropout can be seen as Bayesian approximation to a Gaussian process related to the original network

Quantile regression and prediction intervals

Currently not standard libraries to estimate reducibble and irreducible error of the ML models.

Most estimators during prediction return E(Y|X), which can be interpreted as the answer to the question, what is the expected value of your output given the input?

Quantile methods, return y at q for which F(Y=y|X)=q where q is the percentile and y is the quantile.

Quantile regression forest:

https://scikit-garden.github.io/examples/QuantileRegressionForests/

Deep Quantile Regression

Quantile Regression Loss function (March 2018)

https://towardsdatascience.com/deep-quantile-regression-c85481548b5a

Ensemble method (work in progress)

Combination of the different methods based on the local error properties

Problem to solve - significant extrapolation error in some local regions

e.g KNN conservative extrapolation less sensitive than BDT and Random forest

local error estimate using methods from previous slides

combine methods using weighted average

Speed up MVA evaluation using caching:

In case of small number of dimensions tabulated kernel local regression (AliNDLocalRegression)

In case of multidimensional problem cache “results” and feed it into fast methods (Neural network?)

Model compression - KERAS

https://www.cs.cornell.edu/~caruana/compression.kdd06.pdf

An ensemble is a collection of models whose predictions are combined by weighted (local) averaging or voting.

Well known ensemble methods include bagging[2], boosting [14], random forests[3], Bayesian averaging [9] and stacking [17].

Ensembles - disadvantage: many ensembles are large and slow

Goal: compress the function that is learned by a complex model into a much smaller, faster model that has comparable performance (within prediction intervals)

To be used in reconstruction

The main idea behind model compression is to use a fast and compact model to approximate the function learned by a slower, larger, but better performing model.

Unlike the true function that is unknown, the function learned by a high performing model is available and can be used to label large amounts of pseudo data.

Current assumption: KERAS to be used as an compression model.

Problem - current ROOT interface too slow. Need to speed up evaluation.

AliNDFunctionInterface

AliNDFunctionInterface TMVA usage

Step 1: Register methods

Step 2: Register factory

Step 3: Fit Method(s)

Step x: Compress model

Step 4: Load /Register reader

Step 5: Eval MVA as an formula

Step 1: Register (regression/classification) methods

AliNDFunctionInterface::registerMethod() with parameters:

std::string method: assign name

std::string content: method registration string used in TMVA

TMVA::Types::EMVA: type within TMVA

Example:

```
AliNDFunctionInterface::registerMethod("MLPBNN", "H:!
   V:NeuronType=tanh:VarTransform=N:NCycles=20:HiddenLayers=N+5:Te
   stRate=5:TrainingMethod=BFGS:UseRegulator",TMVA::Types::kMLP);
```

Experts provide default methods (for particular categories of problems)

In example experts provided function MLPBNN as equivalent of other function (e.g gauss or exp functions)

Step 2: Register factory

AliNDFunctionInterface::registerFactory() with parameters:

std::string factory: assign name

std::string content: string used in PrepareTrainingAndTestTree() to define sample size etc.

If empty or unavailable: use default settings

Example:

```
AliNDFunctionInterface::registerFactory("testFactory",
   "nTrain_Regression=50%:nTest_Regression=50%:SplitMode=Random:No
   rmMode=NumEvents:!V");
```

Experts provide default methods

Step 3: Fit Method - Regression

Training and testing for Regression provided by:
AliNDFunctionInterface::FitMVARegression()

Parameters:

const char * output: output root file and directory separated by “#”

TTree *tree: input tree

const char *varFit: variable to fit in regression separated by “:”

TCut cut

const char * variables: variables used for training

const char *methods: previously registered method names

const char * factoryString: previously registered strings to define sample for training and testing

```
Int_t  AliNDFunctionInterface::FitMVARegression(const char *
output, TTree *tree, const char *varFit, TCut cut, const char *
variables, const char *methods,const char * factoryString);
```

```
AliNDFunctionInterface::FitMVARegression("TMVA_RegressionOutput.ro
   ot#test",regTree,"fvalue","var1>3","var1:var2","MLPBNN:BDT","te
   st_factory");
```

Step 3: Fit Method Regression

Interface:

```
Int_t  AliNDFunctionInterface::FitMVARegression(const char *
   output, TTree *tree, const char *varFit, TCut cut, const char *
   variables, const char *methods,const char * factoryString);
```

Example:

```
AliNDFunctionInterface::FitMVARegression("TMVA_RegressionOutput.ro
   ot#test",regTree,"fvalue","var1>3","var1:var2","MLPBNN:BDT","te
   st_factory");
```

Step 4: Load /Register reader

Load TMVA Reader via AliNDFunctionInterface::LoadMVAReader()

Weights from xml file and variables are stored to root file before and are loaded via LoadMVAReader to apply the methods to independent data

Parameters:

Int_t id: to identify booked reader

const char * inputFile: root file where parameters are stored

const char *method: method to be booked

const char *dir: directory of stored method

Example:

```
AliNDFunctionInterface::LoadMVAReader(0,"TMVA_Output.root","PyRandomForest","cleanK0");
```

Step 5: Eval MVA as an formula

Evaluate MVA (variadic function)

TMVA mathod to be loaded (regisetered using id) before

`EvalMVA(int id, T v, Args... args);` (Regression)

`EvalMVAClasification(int id, T v, Args... args);` (Classification)

Parameters: Reader ID (usually registered using hash value) and variables

Example usage:

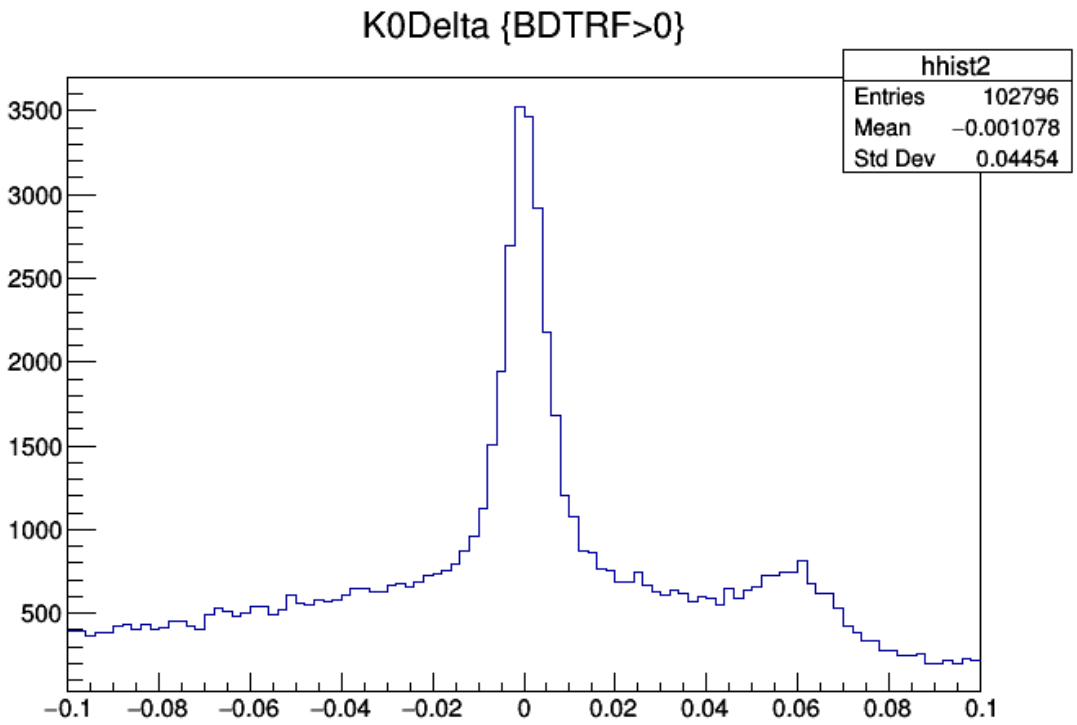
register TMVA as an function in tree and use it in queries

```
treeMVA
   ->SetAlias("BDTRF","AliNDFunctionInterface::EvalMVAClassificati
   on(2,errChi2,v0ErrM,pointAngleN,mpt,armV0S,fRr+0)");


treeMVA->Draw("K0Delta>>hist(100,-0.1,0.1)","BDTRF>0")
```

Step 5: Eval MVA as an formula

Example:

```
treeMVA
   ->SetAlias("BDTRF","AliNDFunctionInterface::EvalMVAClassificati
   on(2,errChi2,v0ErrM,pointAngleN,mpt,armV0S,fRr+0)");


treeMVA->Draw("K0Delta>>hist(100,-0.1,0.1)","BDTRF>0")
```



Conclusion

N dimensional analysis pipeline in ALICE

(T)MVA interface wrapper

- quantiles
- prediction/confidence intervals
- model compression

TMVA wrapper

- MVA regression almost as simple as gaussian fit

New MVA wrapper

- Work in progress
- See Jupyter notebook demo - ML based anaysis of the time series 0distortion data

Backup

Step 3: Fit Method - Classification

Training and testing for classification provided by:
AliNDFunctionInterface::FitMVAClassification()

Parameters:

const char * output: output root file and directory separated by “#”

const char *input_trees: root file and tree separated by “#” - the trees define the classes

const char *cuts: cuts for each tree separated by “:”. If only one tree available, the cuts define the classes

const char * variables: variables used for training

const char *methods: previously registered method names

const char * factoryString: previously registered strings to define sample for training and testing

Example:

```
Int_t  AliNDFunctionInterface::FitMVAClassification(const char *
   output, const char *inputTrees, const char *cuts, const char *
   variables, const char *methods, const char * factoryString)
```

```
AliNDFunctionInterface::FitMVAClassification("TMVA_Output.root#cle
   anK0","TMVAInput.root#MVAInput","cleanK0:isBackground","errChi2
   :v0ErrM:pointAngleN:mpt:armV0S:fRr","BDTRF:PyRandomForest:KNN",
   "");
```

Interface:

```
Int_t  AliNDFunctionInterface::FitMVAClassification(const char *
   output, const char *inputTrees, const char *cuts, const char *
   variables, const char *methods, const char * factoryString)
```

Example one tree:

```
AliNDFunctionInterface::FitMVAClassification("TMVA_Output.root#cle
   anK0","TMVAInput.root#MVAInput","cleanK0:isBackground","errChi2
   :v0ErrM:pointAngleN:mpt:armV0S:fRr","BDTRF:PyRandomForest:KNN",
   "");
```

Example multiple trees:

```
AliNDFunctionInterface::FitMVAClassification("TMVA_Output.root#cle
   anK0","TMVAInput.root#MVAInput1:TMVAInput.root#MVAInput2","","e
   rrChi2:v0ErrM:pointAngleN:mpt:armV0S:fRr","BDTRF:PyRandomForest
   :KNN","");
```