What to expect from TMVA - The Toolkit for Multivariate Analysis in ROOT

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(for TMVA A.Hoecker, E.v.Toerne, H.Voss, J.Teerhag, J.Stelzer, P.Speckmayer)

ROOT Users Workshop , Saas Fee, 11-14 March 2013

Outline

- **Introduction to TMVA**
  - Classification and Regression
  - Highlight of what is “new”-ish
- **Using TMVA**
  - example walk through
  - general remarks on MVA’s
    - do’s and don’ts
    - what about systematic errors

  } too bad but: → backup slides only
  - real application examples
- **Plans**
- **Summary**

Event Classification

- **Discriminate *Signal* from *Background***
  - select events of type *S* ?
  - we have discriminating variables x_1, x_2, …

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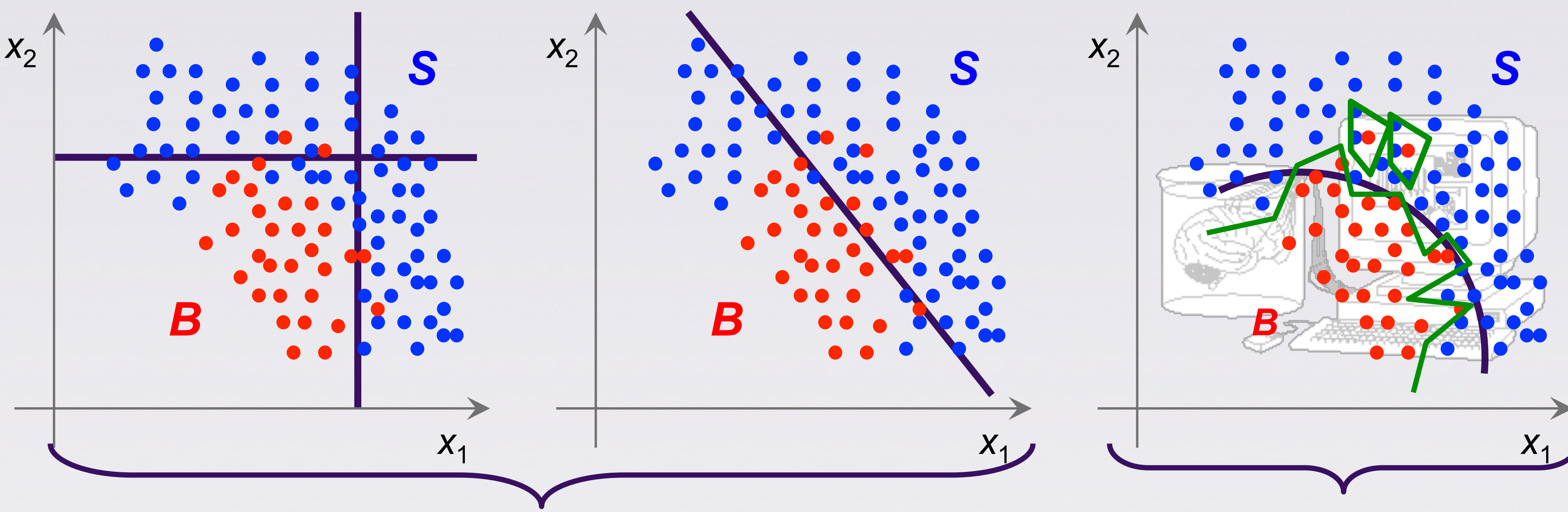
Rectangular cuts? | A linear boundary? | A nonlinear one?



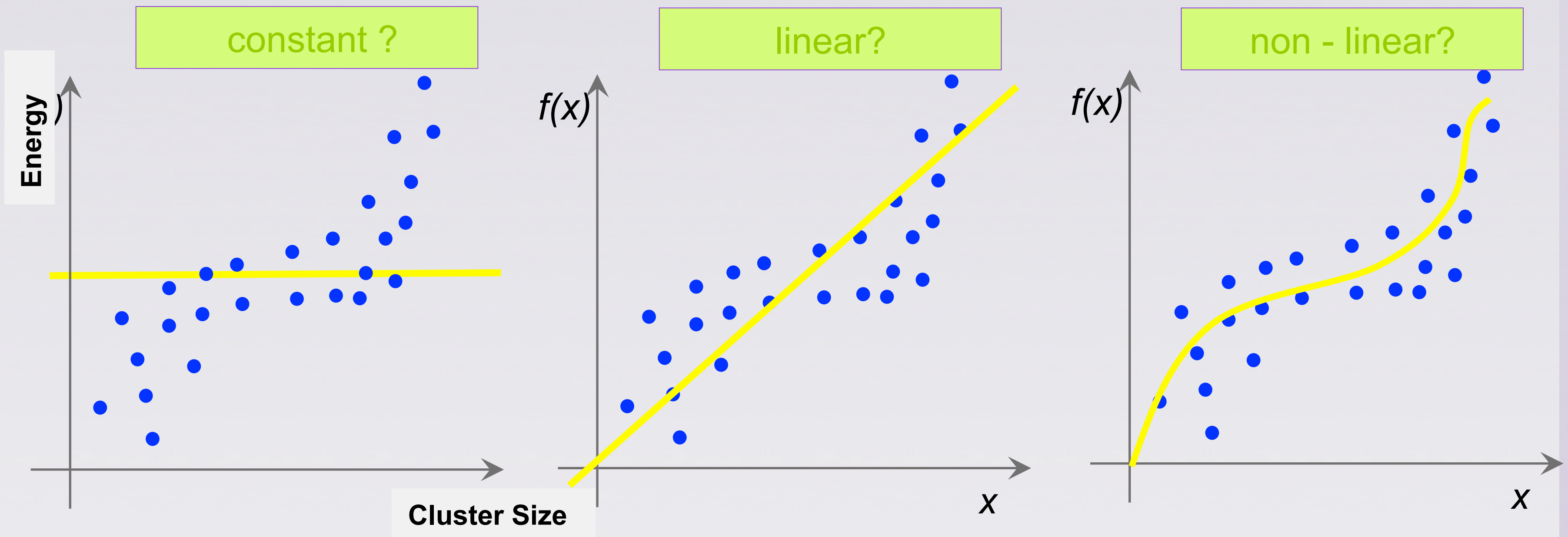
Low variance (stable), high bias methods

High variance, small bias methods

- Which model/class ? Pro and cons ?
- ***T*MVA** helps to decide on the model and finds the "optimal" boundary!

Regression

- estimate "functional behaviour" from a set of 'known measurements" ?
- e.g. : photon energy as function "D"-variables ECAL shower parameters + …



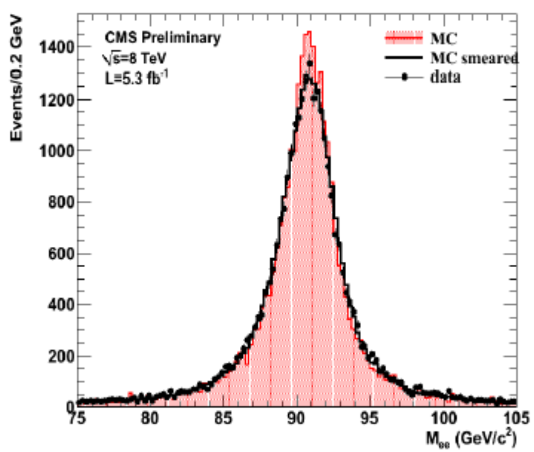
- known analytic model (i.e. n^{th} -order polynomial) → Maximum Likelihood Fit)
- no model ?
  - → "draw any kind of curve" and parameterize it?
- seems trivial ? → human brain has very good pattern recognition capabilities!
- what if you have **many** input variables? → Use ***T*MVA**

CMS Higgs Discovery
(such a nice example for MVA usage)

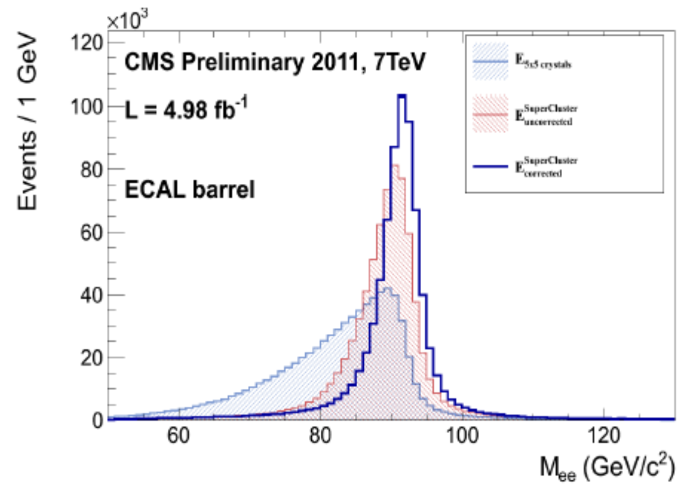
- MVA regression for energy calibration

Photon Energy Corrections, Scale and Resolution

- ECAL cluster energies corrected using a MC trained multivariate regression
  - Improves resolution and restores flat response of energy scale versus pileup
  - Inputs: Raw cluster energies and positions, lateral and longitudinal shower shape variables, local shower positions w.r.t. crystal geometry, pileup estimators
- Regression also used to provide a per photon energy resolution estimate
- **Energy Scale and resolution:** use $Z \to e^+e^-$



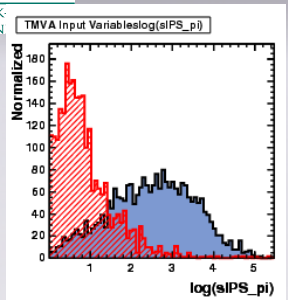
Non converted photons in the barrel |η|<1

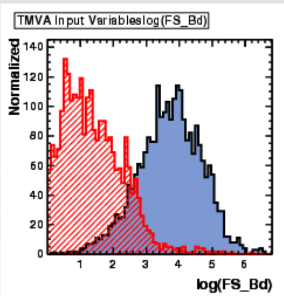


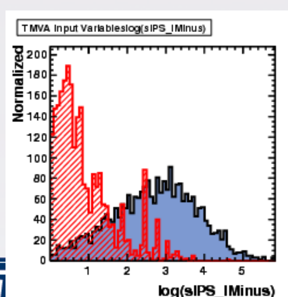
Effect of the regression on the $Z \to e^+e^-$ peak

MVA Classification

- "D" variables (sensitivity to Signal and Background)
- D-dim. variable space → one combined variable

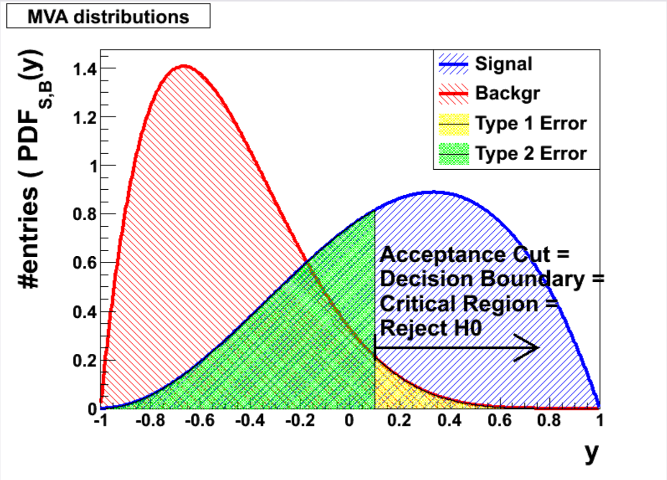






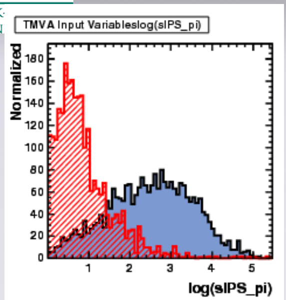
D variable (feature) space

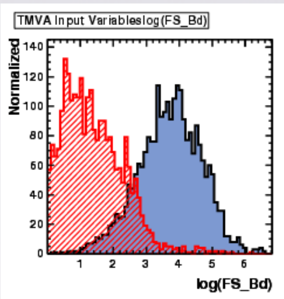
y(x): $R^D \rightarrow R$:

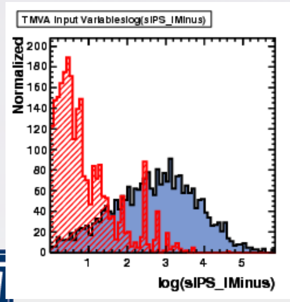


- simple cut on y → complex decision boundary in feature space
- how to find such magical y(x)?

MVA Classification



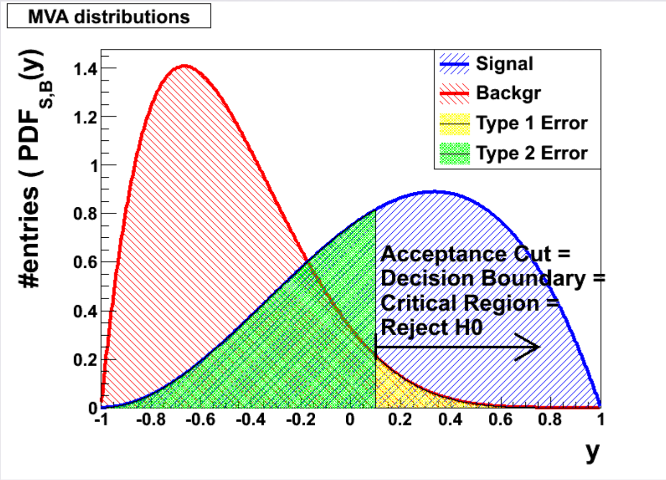




D variable (feature) space

- simple cut on y → complex decision boundary in feature space
- how to find such magical y(x)?

$y(x): R^D \rightarrow R$:

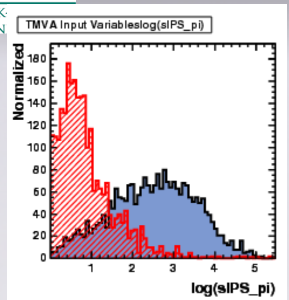


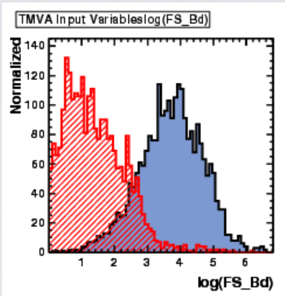
- take model for y(x)
  - linear, nonlinear, piecewiese, flexible, less flexible …
  - fit free parameters to do best (minimize a loss function – i.e. how many misclassified events)

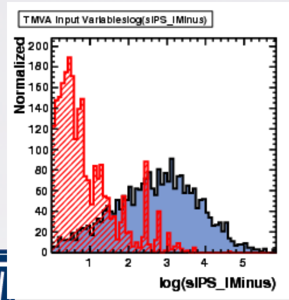
MVA Clas…tion

Regression

Forget about all "blue" and only look at "red" histograms

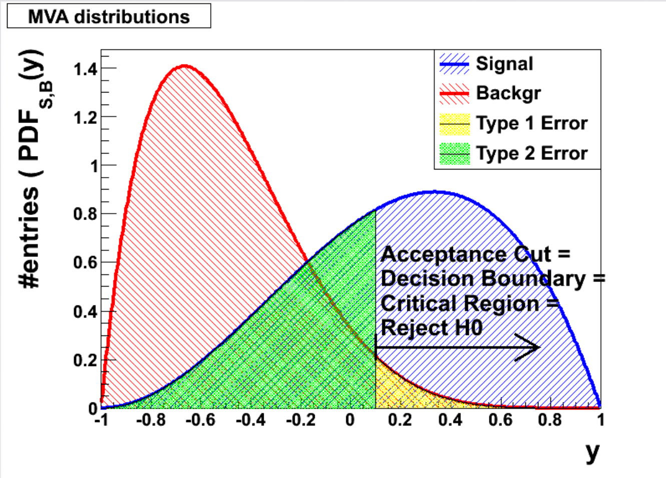






D variable (feature) space

y(x): $R^D \rightarrow R$:



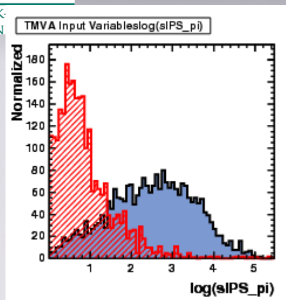
- take model for y(x)
  - linear, nonlinear, piecewiese, flexible, less flexible …
  - fit free parameters to do best (minimize a loss function – i.e. how m… …ents)

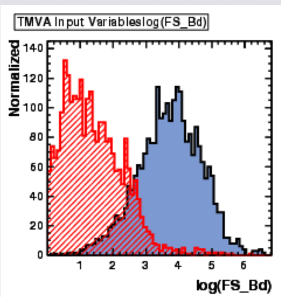
residual $(f(x)$

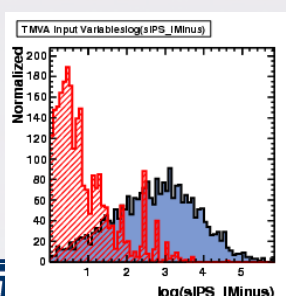
MVA Classification

Regression

Forget about all "blue" and only look at "red" histograms

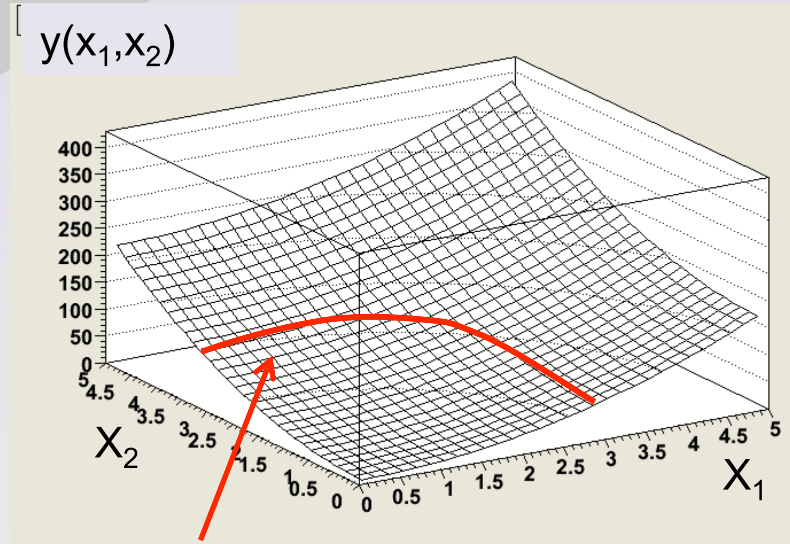






D variable (feature) space

y(x): $R^D \rightarrow R$:



Regression: y=const → contour line

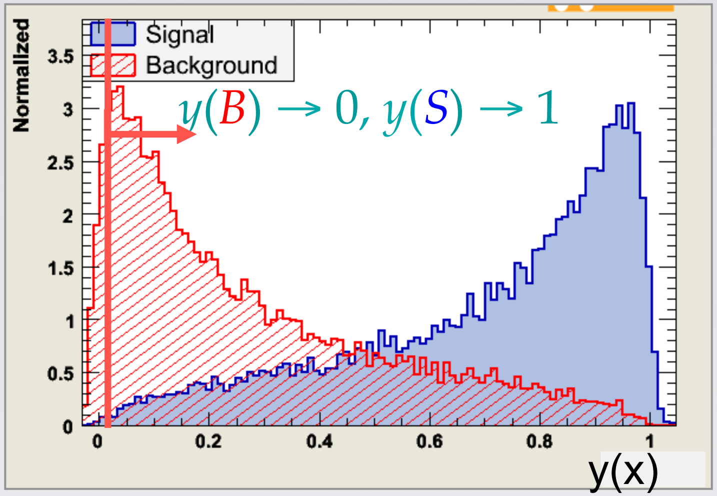
Classification: → decision Boundary

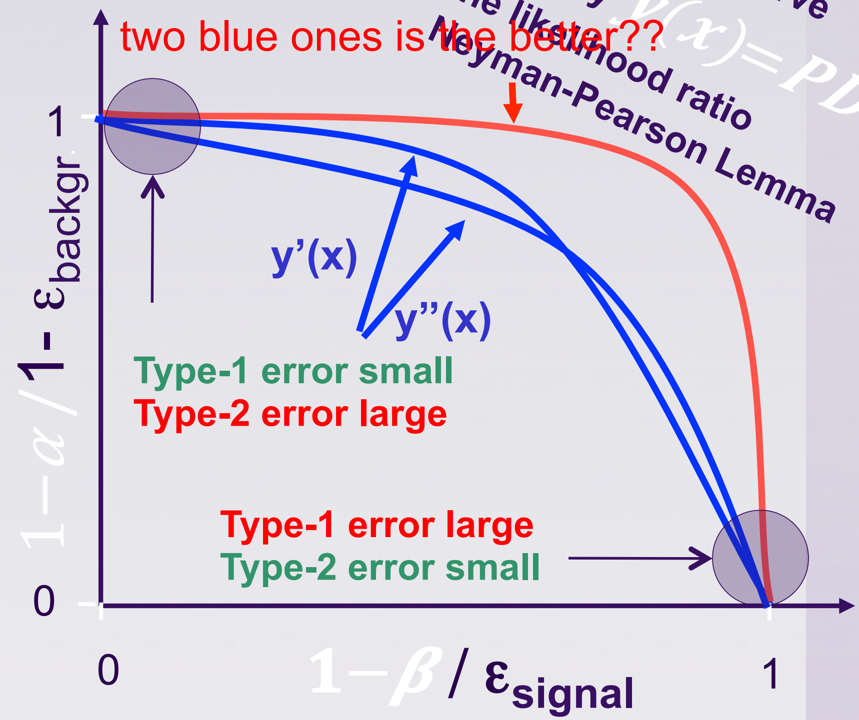
- take model for y(x)
  - linear, nonlinear, piecewiese, flexible, less flexible …
  - fit free parameters to do best (minimize a loss function – i.e. h… …ents)

residual $(f(x)$

Receiver Operation Characteristic (ROC) curve

Signal(H_1) /Background(H_0) discrimination:





Signal(H_1) /Background(H_0) :

- **Type 1 error: reject H_0 although true → background contamination**
  - Significance α: background sel. efficiency **1− α: background rejection**
- **Type 2 error: accept H_0 although false → loss of efficiency**
  - Power: **1− β signal selection efficiency**

What is TMVA doing for you?

- Finds $y(x) : R^n \rightarrow R$
  - given a certain type of model class y(x)
  - "fits" (learns) from events with known type parameters in y(x)
    such that y:
    - CLASSIFICATION: separates well Signal from Background in training data
    - REGRESSION: fits well the target function for training events
  - use for yet unknown events → predictions

→ supervised machine learning

TMVA Content

- **implemented classifiers and regression methods**
  - Rectangular cut optimisation (classification only)
  - Projective and multidimensional likelihood estimator
  - k-Nearest Neighbour algorithm (kNN)
  - LD, Fisher and H-Matrix discriminants (classification only)
  - Function discriminant (classification only)
  - Artificial neural network (MLP) → Bayesian Network features, BFGS
  - Boosted/bagged decision trees (BDT) → RealAdaBoost, Gradient-Boost
  - Rule Fitting (classification only)
  - Support Vector Machine (SVM)
- **implemented data preprocessing stages:**
  - De-correlation, Principal Value Decomposition, Normalisation, "Gaussianisation", Flattening (uniform)
- **combination methods:**
  - Boosting, Categorisation, MVA Committees

Using TMVA

2 main steps:

1. Training phase:

train(build), test and evaluate classifiers using data samples with known signal and background events

2. Application phase:

use to classify unknown data samples

ROOT script for Training

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

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

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

  factory->AddSignalTree         ( (TTree*)input->Get("TreeS") );
  factory->AddBackgroundTree ( (TTree*)input->Get("TreeB") );

  factory->AddVariable("var1+var2", 'F');
  factory->AddVariable("var1-var2", 'F');
  factory->AddVariable("var3", 'F');
  factory->AddVariable("var4", 'F');

  factory->PrepareTrainingAndTestTree("", “nTrain_Signal=3000:nTrain_Background=3000:SplitMode=Random:!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->TestAllMethods();
  factory->EvaluateAllMethods();

  outputFile->Close();
  delete factory;
}
```

← create *Factory*

← give training/test trees

← register input variables

← select MVA methods and options

← train, test and evaluate

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ROOT script for Application

TMVA

```
void TMVClassificationApplication( )
{
  TMVA::Reader *reader = new TMVA::Reader();

  Float_t var1, var2, var3, var4;
  reader->AddVariable( "var1+var2", &var1 );
  reader->AddVariable( "var1-var2",  &var2 );
  reader->AddVariable( "var3", &var3 );
  reader->AddVariable( "var4", &var4 );

  reader->BookMVA( "MLP classifier", "weights/MyMVAnalysis_MLP.weights.txt");

  TFile *input = TFile::Open("yourDataFile.root");
  TTree* theTree = (TTree*)input->Get("TreeS");

  // … set branch addresses for user TTree
  for (Long64_t  iev=3000;  iev<theTree->GetEntries(); iev++) {
    theTree->GetEntry(iev);

    var1 = userVar1 + userVar2;
    var2 = userVar1 - userVar2;
    var3 = userVar3;
    var4 = userVar4;

    Double_t   mvaValue =  reader->EvaluateMVA(  "MLP classifier"  );

    // do something with it …
  }
  delete reader;
}
```

- create *Reader*
- register the variables
- read trained classifier(s)
- event loop
- compute input variables
- classifier output

TMVA

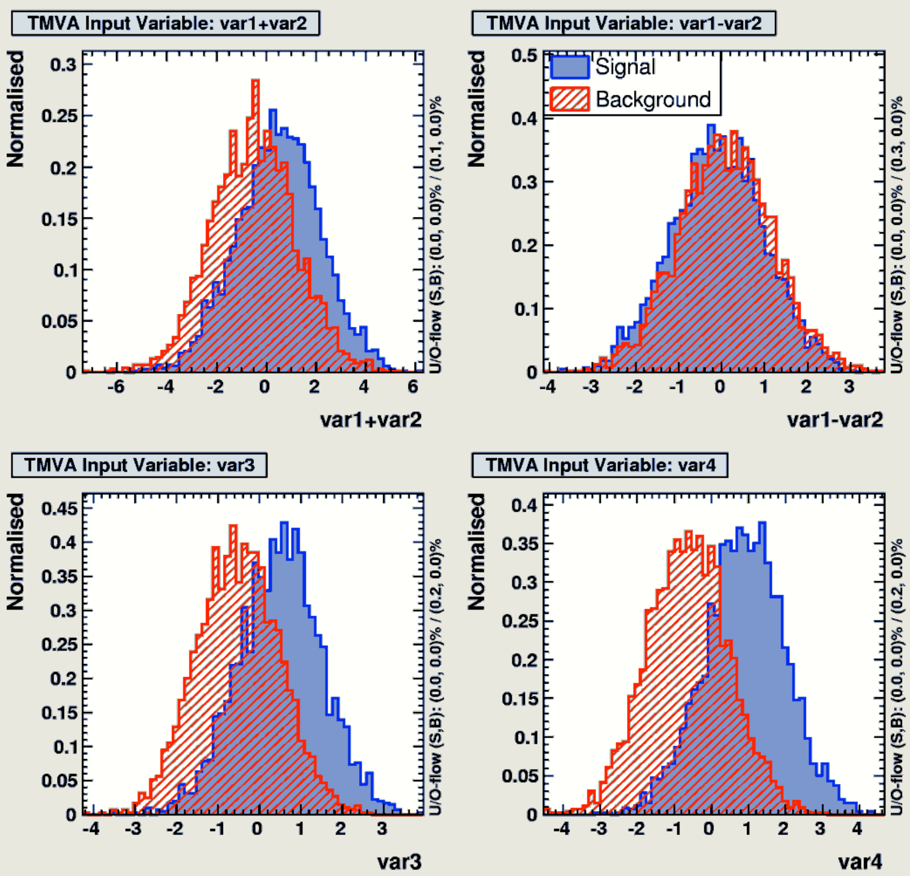
Running TMVA

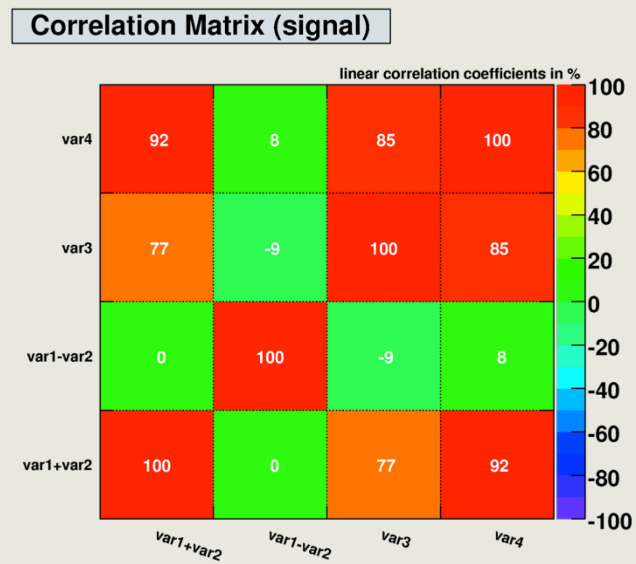
- provide data: ROOT TTree , ASCII-file or event-by-event
- choose variables (or functions ROOT Expressions thereof)
- pre-selection cuts (independent for signal and bkg)
- define global event weights for signal or background input files
- define individual event weight (any variable present in training data)
- choose splitting into training and test samples:
  - Block wise, Randomly, Periodically (i.e. periodically 3 test ev., 2 train ev., etc..)
  - User defined training and test trees
- choose pre-processing of input variables (e.g., de-correlation)
- choose classifiers(s) and it's configuration options
- train/test/evealuate

  → look at the results and diagnostics
- if happy, use trained classifier in the analysis

Toy Example Training:

- Data set with 4 linearly correlated Gaussian distributed variables:



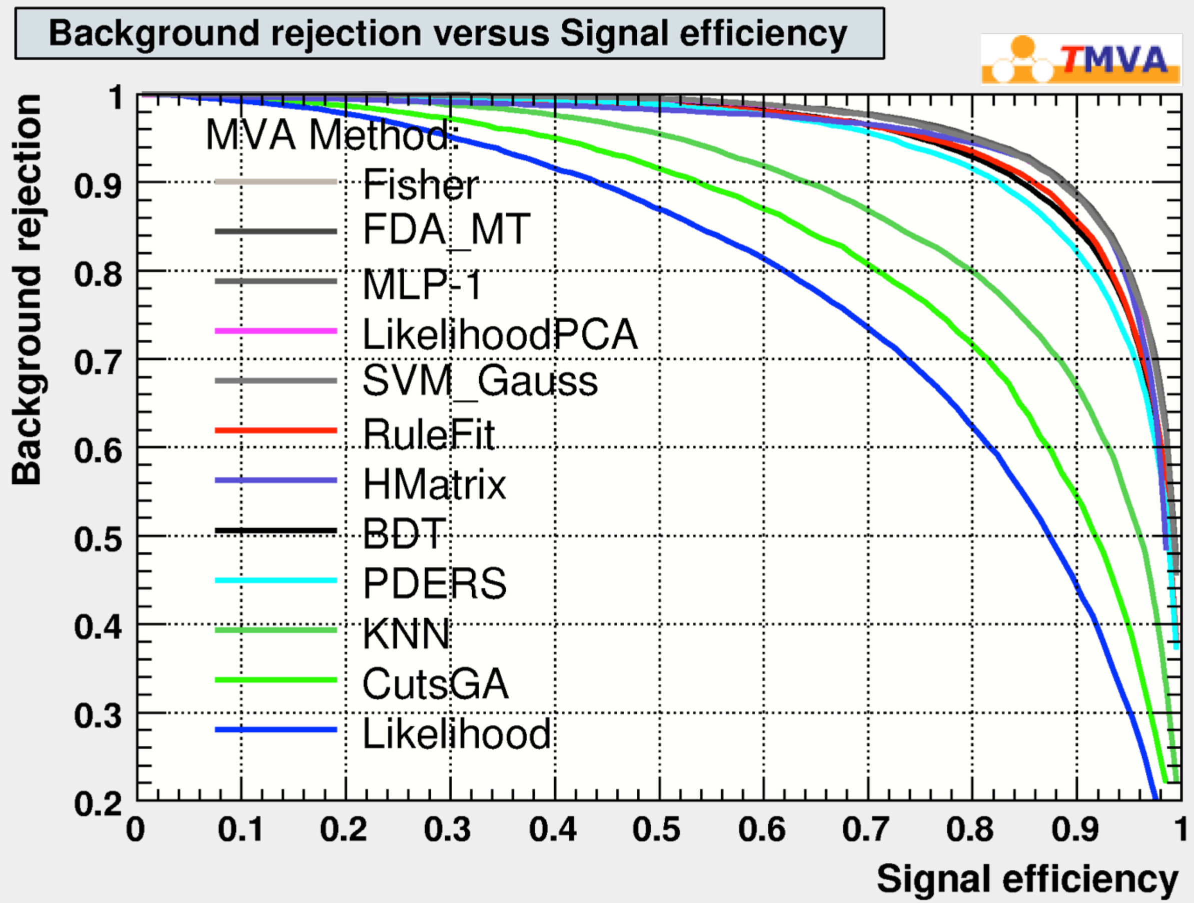



```
--------------------------------------
Rank : Variable   : Separation
--------------------------------------
   1 : var4       : 0.606
   2 : var1+var2  : 0.182
   3 : var3       : 0.173
   4 : var1-var2  : 0.014
--------------------------------------
```

Receiver Operation Characteristics (ROC) Curve

- Smooth background rejection versus signal efficiency curve:
  (from cut on classifier output)

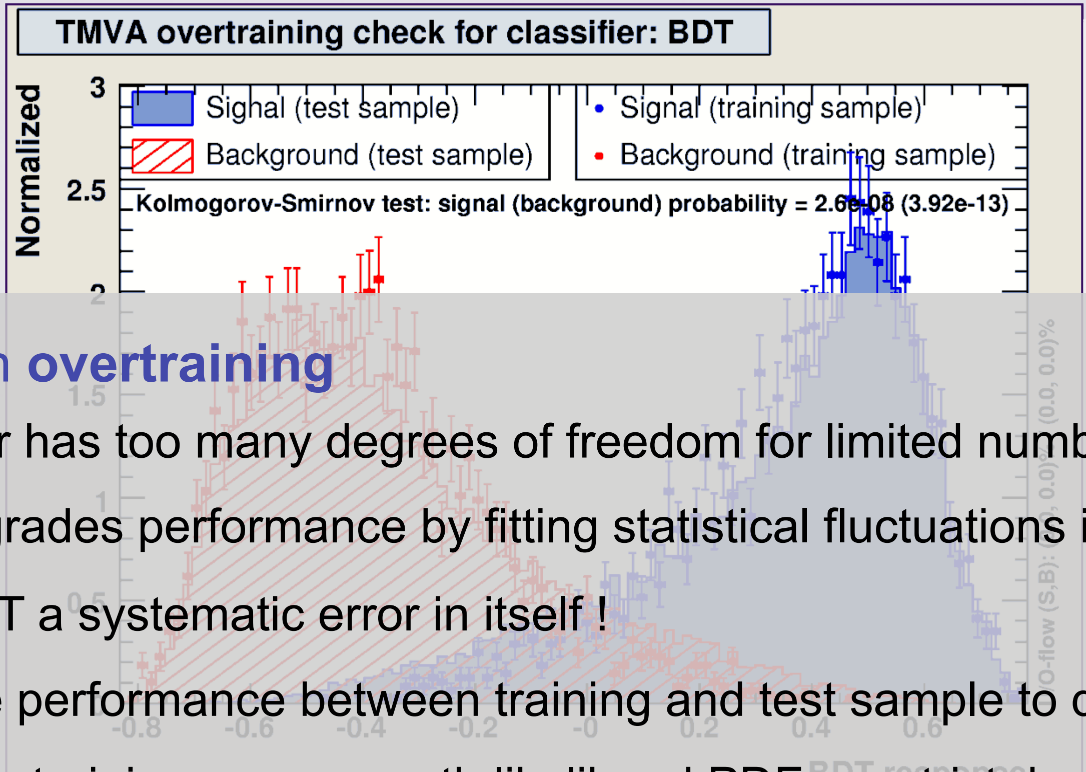
“Specificity” (probability to predict B if true B)



“Sensitivity” (probability to predict S if true S)

Evaluating the Classifier Training

- inspect classifier output distribution
- compare for test *and* training samples …

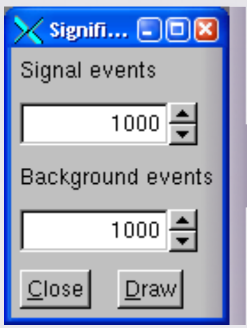


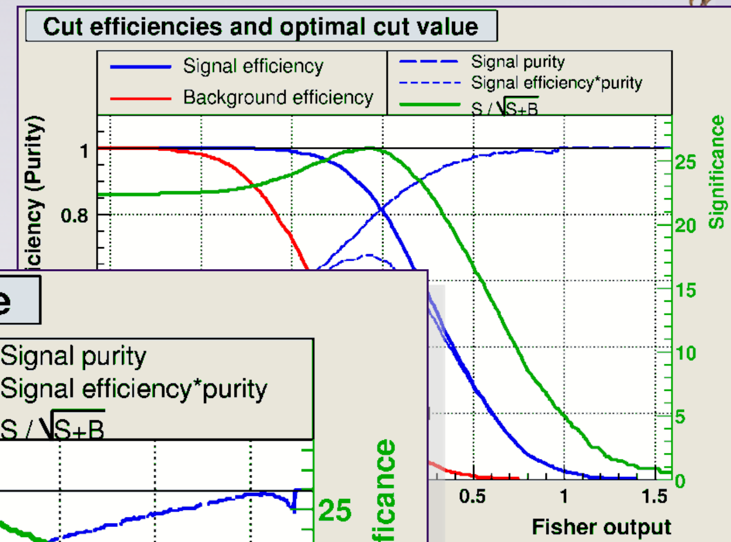
- Remark on **overtraining**
  - classifier has too many degrees of freedom for limited number of training events
    - degrades performance by fitting statistical fluctuations in training sample
    - NOT a systematic error in itself !
  - Compare performance between training and test sample to detect overtraining
  - Avoid overtraining: *e.g.*, smooth likelihood PDFs, restrict decision tree depth, increase kernel parameter size, …

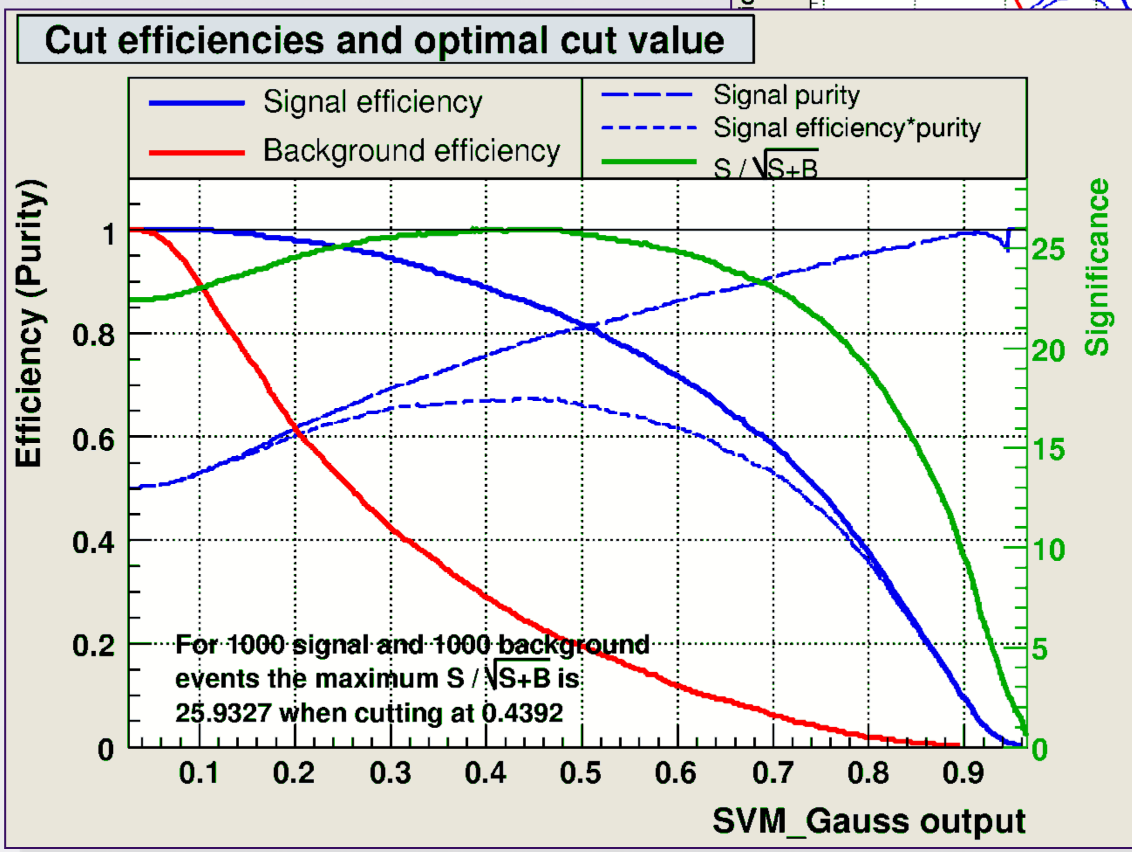
Evaluating the Classifier Training

- Optimal cut for each classifiers …

  Determine the optimal cut (working point) on a classifier output

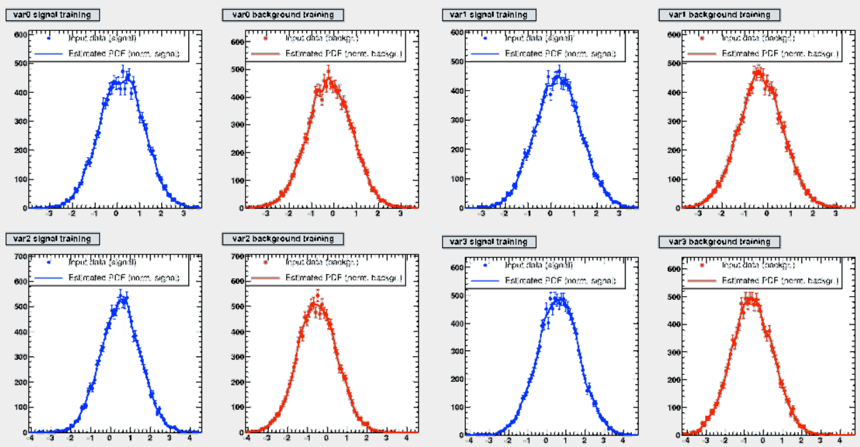


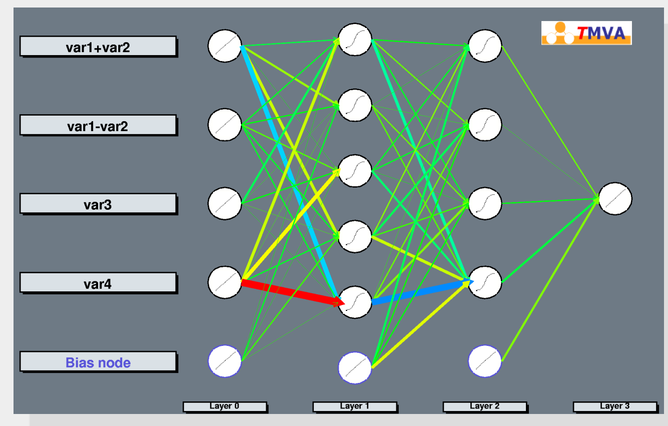


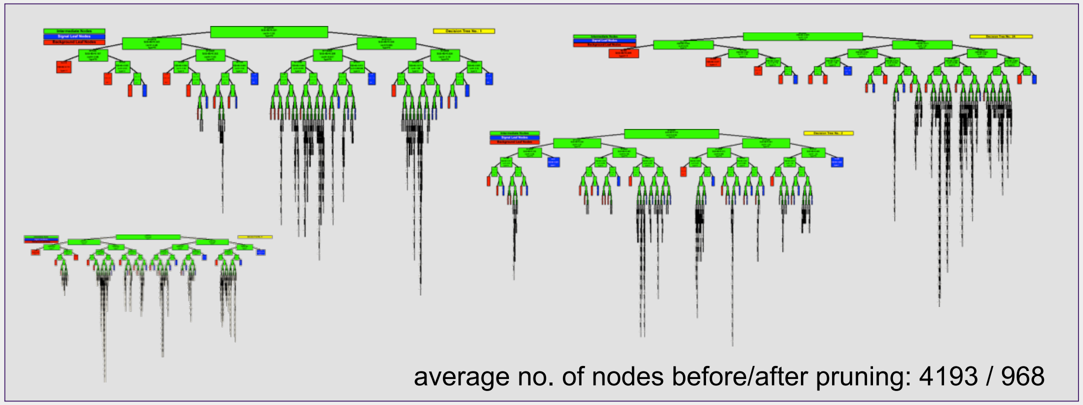


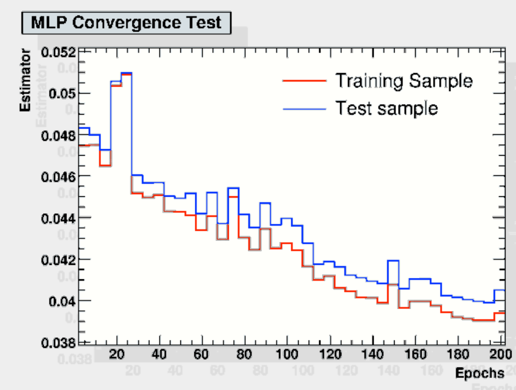
Evaluating the Classifier Training

- Projective likelihood PDFs, MLP training, BDTs, …



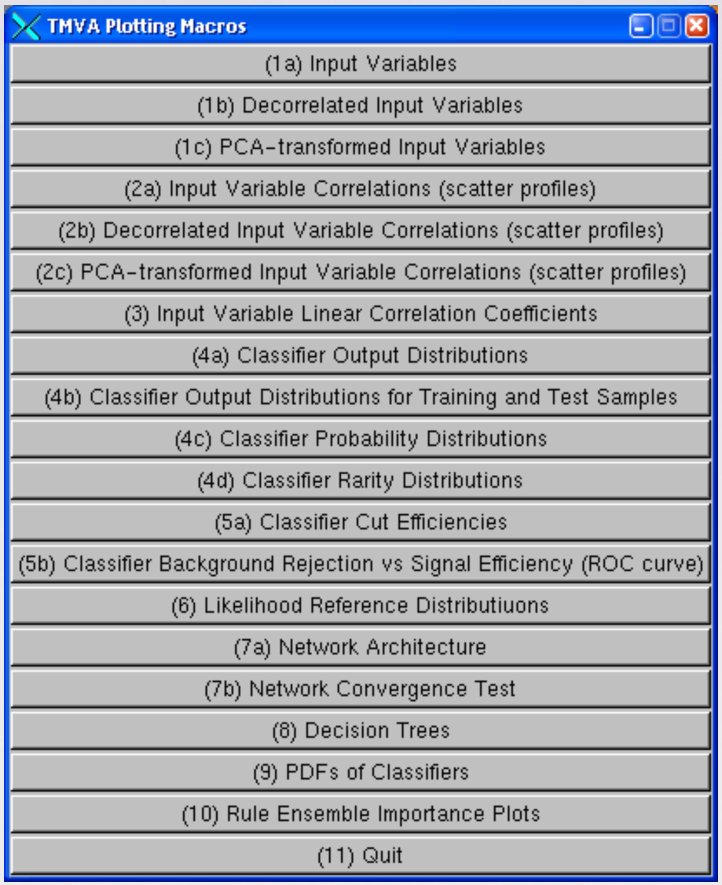






TMVA Evaluation „Framework“

- TMVA helps to understand/optimise your training results !
  - ROOT evaluation/diagnostic scripts (through GUI)



Plot all signal (S) and background (B) input variables with and without pre-processing

Correlation scatters and linear coefficients for S & B

Classifier outputs (S & B) for test and training samples (spot overtraining)

Classifier *Rarity* distribution

Classifier significance with optimal cuts

B rejection versus S efficiency – ROC curve

Classifier-specific plots:
- Likelihood reference distributions
- Classifier PDFs (for probability output and Rarity)
- Network architecture, weights and convergence
- Rule Fitting analysis plots
- Visualise decision trees+ control plots

Evaluating the Classifiers Training (taken from TMVA output…)

Input Variable Ranking

Better variable

```
--- Fisher        : Ranking result (top variable is best ranked)
--- Fisher        : ---------------------------------------------
--- Fisher        : Rank : Variable  : Discr. power
--- Fisher        : ---------------------------------------------
--- Fisher        :    1 : var4      : 2.175e-01
--- Fisher        :    2 : var3      : 1.718e-01
--- Fisher        :    3 : var1      : 9.549e-02
--- Fisher        :    4 : var2      : 2.841e-02
--- Fisher        : ---------------------------------------------
```

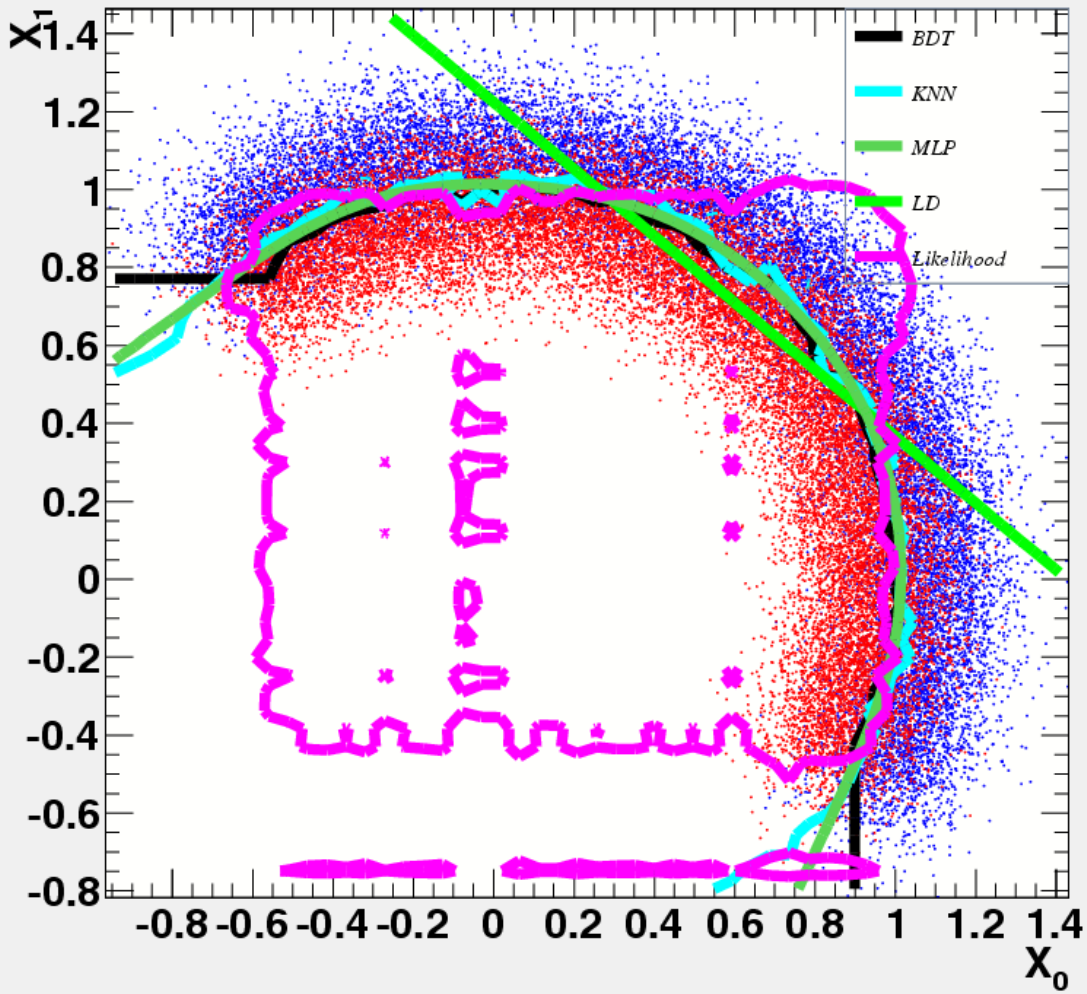
- How discriminating is a variable ? (treat with care, check also the variable separations themselves)

Correlation and Overlap Between Different Classifiers

```
--- Factory       : Inter-MVA overlap matrix (signal):
--- Factory       : ------------------------------
--- Factory       :              Likelihood  Fisher
--- Factory       : Likelihood:      +1.000  +0.667
--- Factory       :     Fisher:      +0.667  +1.000
--- Factory       : ------------------------------
```

- Do classifiers select the same events as signal and background ? If not, there is something to gain !

Decision Boundaries



BDT

kNN

MLP

LD

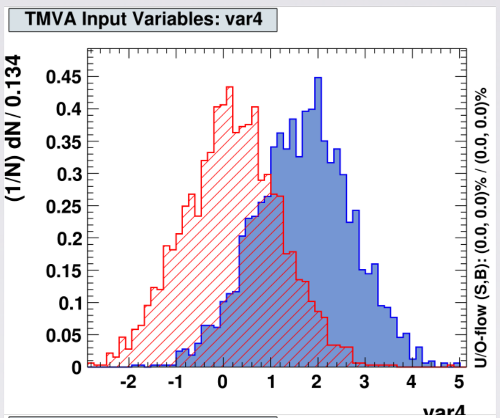
Likelihood

*T*MVA Categories

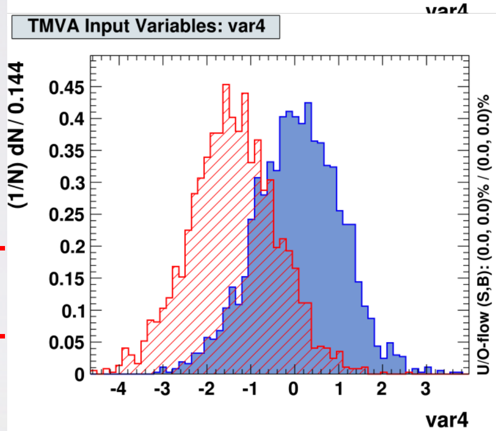
- **TMVA Categories: one classifier per 'region'**
- 'regions' in the detector (data) with different features treated <u>independent</u>
  - improves performance
  - avoids additional correlations where otherwise the variables would be uncorrelated!

Example: var4 depends on some variable "eta"

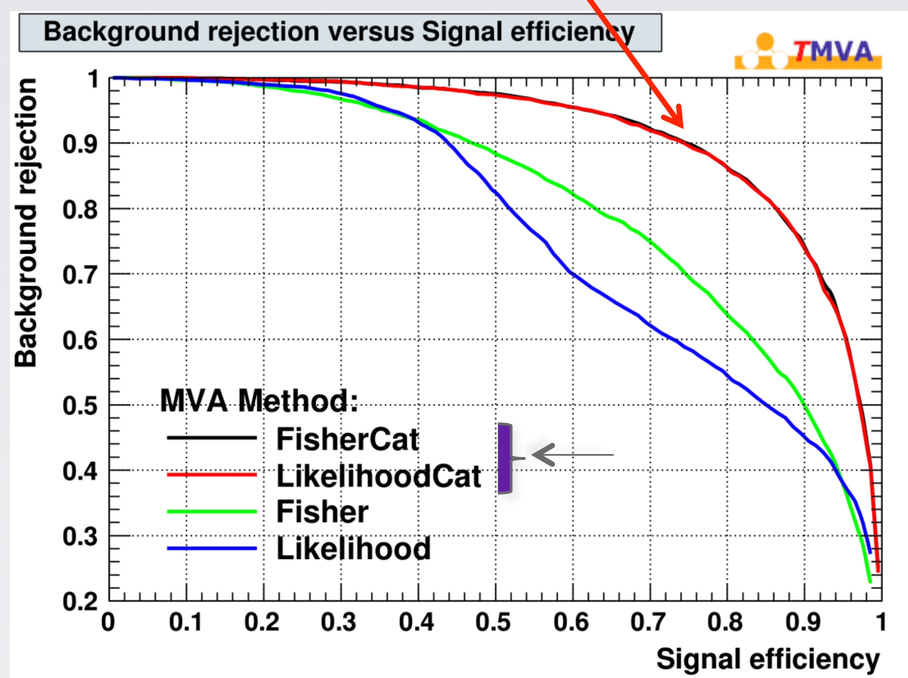
|eta| > 1.3



|eta| < 1.3



Recover optimal performance after splitting into categories



(T)MVA and Systematic Uncertainties

- minimize "systematic" uncertainties (robustness)

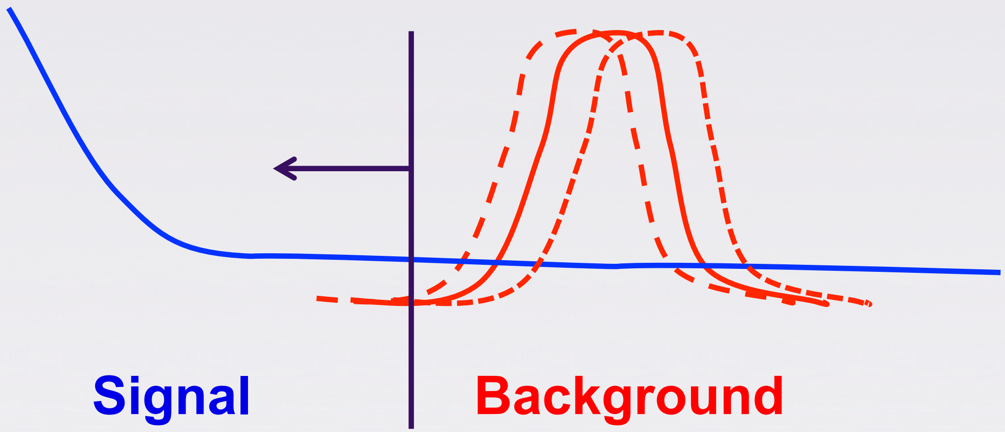
→ "classical cuts" : do not cut near steep edges, or in regions of large sys. uncertainty

→ hard to translate to MVAs:

  → artificially degrade discriminative power (shifting/smearing) of systematically "uncertain" observables IN THE TRAINING

    → remove/smooth the 'edges' → MVA does not try to exploit them

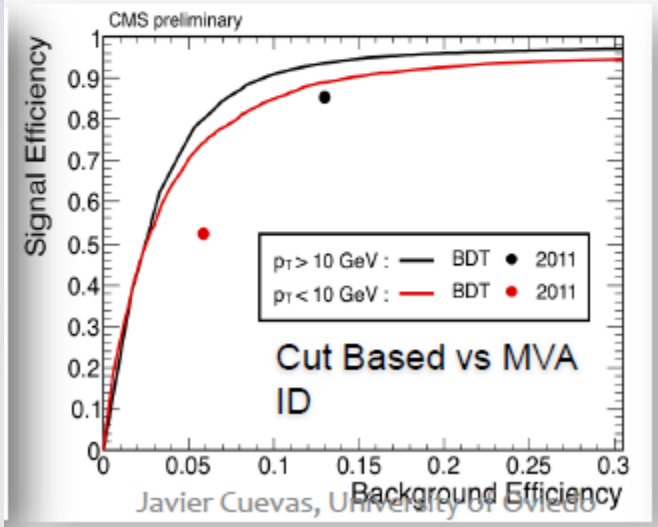
  → First attempts to automatize this are on the way



CMS Higgs Discovery

(such a nice example for MVA usage)

- Multivariate electron identification in 2012
  - ECAL, tracker, ECAL-tracker-HCAL matching and impact parameter (IP) observables



$H \rightarrow \gamma\gamma$

- Analysis selection (MultiVariate Analysis MVA)
  - Vertex ID
    - Input variables: $\Sigma p_T^{2\,(tracks)}$, p_T balance wrt $\gamma\gamma$, conversions information
  - ID photons $p_{T1} > m_{\gamma\gamma} / 3$ $p_{T2} > m_{\gamma\gamma} / 4$
- MVA Diphoton discriminant categories
  - High score
    - signal-like events
    - good $m_{\gamma\gamma}$ resolution
  - Designed to be $m_{\gamma\gamma}$ independent
  - Trained on signal and background MC
  - Input variables:
    - Kinematic variables: $p_{T\gamma} / m_{\gamma\gamma}$, η_γ, $\cos(\varphi_1 - \varphi_2)$
    - Photon ID MVA output for each photon
    - Per-event mass resolutions for the correct and incorrect choice of vertex

PPC 2012 - KIAS - Nov 5th Javier Cuevas, University of Oviedo

LHCb $B_s \rightarrow \mu\mu$ "evidence"

EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH (CERN)

LHCb-PAPER-2012-043
CERN-PH-EP-2012-zzz
October 31, 2012

First evidence of the $B_s^0 \rightarrow \mu^+\mu^-$ decay

LHCb collaboration

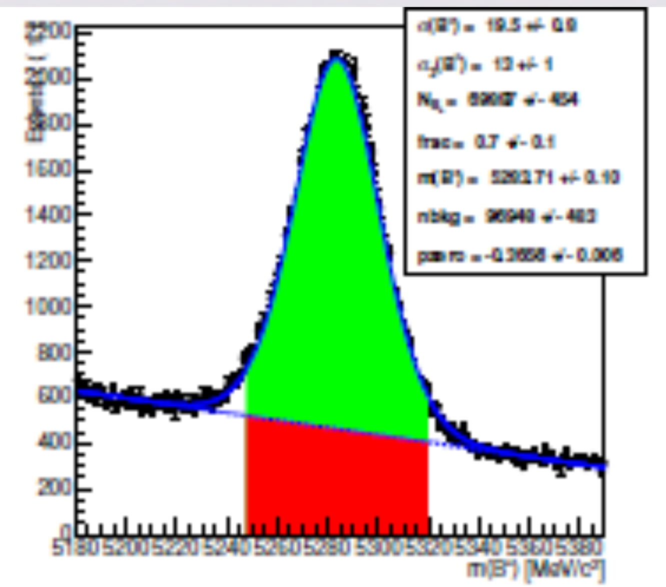
A two-stage multivariate selection, based on boosted decision trees [13], is applied. The first multivariate discriminant, the MVS, removes 80 % of the background while retaining 92 % of signal. The output of the second multivariate discriminant, called BDT in the following, and the dimuon invariant mass are used to classify the selected candidates in a binned two-dimensional space.

You don't even need Monte Carlo to train!

- "sWeights" allow to generate signal and data distributions of any variable that is uncorrelated to one variable where one can fit already a signal +background PDF to.

First observation of the $B^*_{s2}(5840)^0 \to B^{*+}K^-$ decay and properties of the orbitally excited B^0_s mesons

The LHCb collaboration†



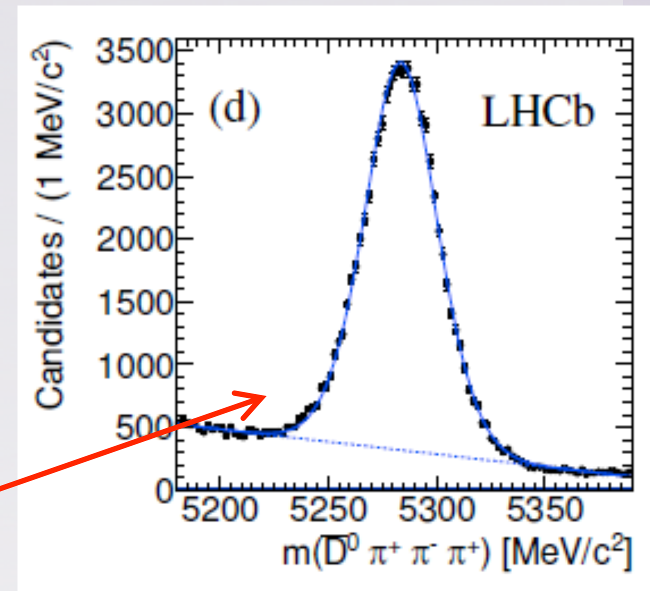
mass distribution

→ fit sig/bkg pdfs

→ sWeights

→ BDT training variables from data

mass distribution after BDT selection



- Negative event weights work FINE in TMVA
  - also BDTs (as proven above) where boosting negative weights is tricky! → we also experiment with alternative "global event pairing"

TMVA Outlook

- **Currently working on:**
  - alternative negative event weight treatment for BDT (and general)
  - user help to increase robustness w.r.t. systematic uncertainties
  - (automatic option parameter tuning)
  - update of Users Guide (ready but valied for ‘next release’ only)
- **Thoughts for the future**
  - constant improvement of the classifiers
    - improve SVM implementation (automatic setting of tuning parameters, training time estimate, ..) and promote its usage
    - speed up ?
  - start thinking about “parallelisation” : starting points
    - serialize processing of different methods → should be easy to parallelise for different CPU cores
    - BDT training (each node split →loops serially over each variable)
    - Genetic fitting algorithm
    - GPU usage ? → one user already tried, need to follow up
    - PROOF-lite ? (well, I’m one of those that …)

Summary

- **Multivariate Classifiers (Regressors)**

  → (fit) decision boundary (target function)
- **TMVA provides:**
  - May different machine learing algorithms, all easily accessible witht the same e.g.
    - PDF based: multi-dimensional (and projective) Likelihood
    - Linear: Linear Classifier (e.g. Fisher Discriminant)
    - Non-Linear: ANN, BDT, SVM
- **TMVA helps to understand/judge/improve your training**
  - carefully study the control plots
  - compare different MVAs !
  - find working point on ROC curve
- **MVAs are not magic:**
  - systematic uncertainties don't lie in the training !!
  - estimate them similar as you'd do in classical cuts

Generalities for (T)MVA Analyses

- There is no magic in MVA-Methods:
  - “black boxes” ? → they are not sooo hard to understand
  - you typically still need to make careful tuning and do some “hard work”
  - no “artificial intelligence” … just “fitting decision boundaries” in a given model

- The most important thing at the start is finding good observables
  - good separation power between S and B
  - little correlations amongst each other
  - watch correlation between selection variables and the parameters you try to measure!

- Think also about possible combination of variables
  - this may allow you to eliminate correlations
    - rem.: you are MUCH more intelligent than what the algorithm will do

Generalities for (*T*)MVA Analyses

- Apply pure preselection cuts and let the MVA only do the difficult part.

- "Sharp features should be avoided" → numerical problems, loss of information when binning is applied
  - simple variable transformations (i.e. log(variable)) can often smooth out these areas and allow signal and background differences to appear in a clearer way

Systematic Uncertainties

- Multivariate Classifiers THEMSELVES don't have systematic uncertainties
  → even if trained on a "phantasy Monte Carlo sample"
  - there are only "bad" and "good" performing classifiers !
    - OVERTRAINING is NOT a systematic uncertainty !!
    - difference between two classifiers resulting from two different training runs DO NOT CAUSE SYSTEMATIC ERRORS
  - same as with "well" and "badly" tuned classical cuts
  - MVA classifiers: → only select a region(s) in observable space
- Efficiency estimate (Monte Carlo) → statistical/systematic uncertainty
  - involves "estimating" (uncertainties in) distribution of $PDF_{y_{S(B)}}$

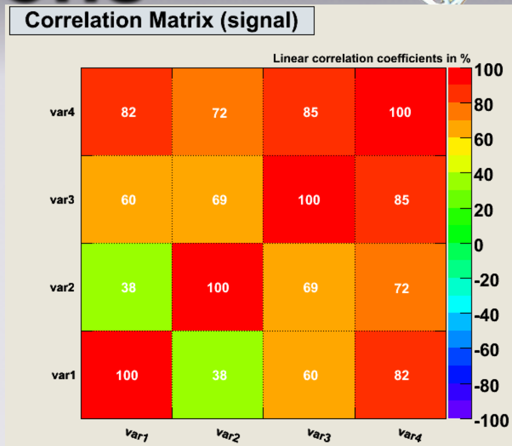
  → estimate systematic error/uncertainty on efficiencies
    - statistical "fluctuations" → re-sampling (Bootstrap)
    - "smear/shift/change" input distributions and determine $PDF_{y_{S(B)}}$
    - simple "cut variation" has never been the best test ☺
- Only involves "test" samples…
  - systematic uncertainties have nothing to do with the training !!

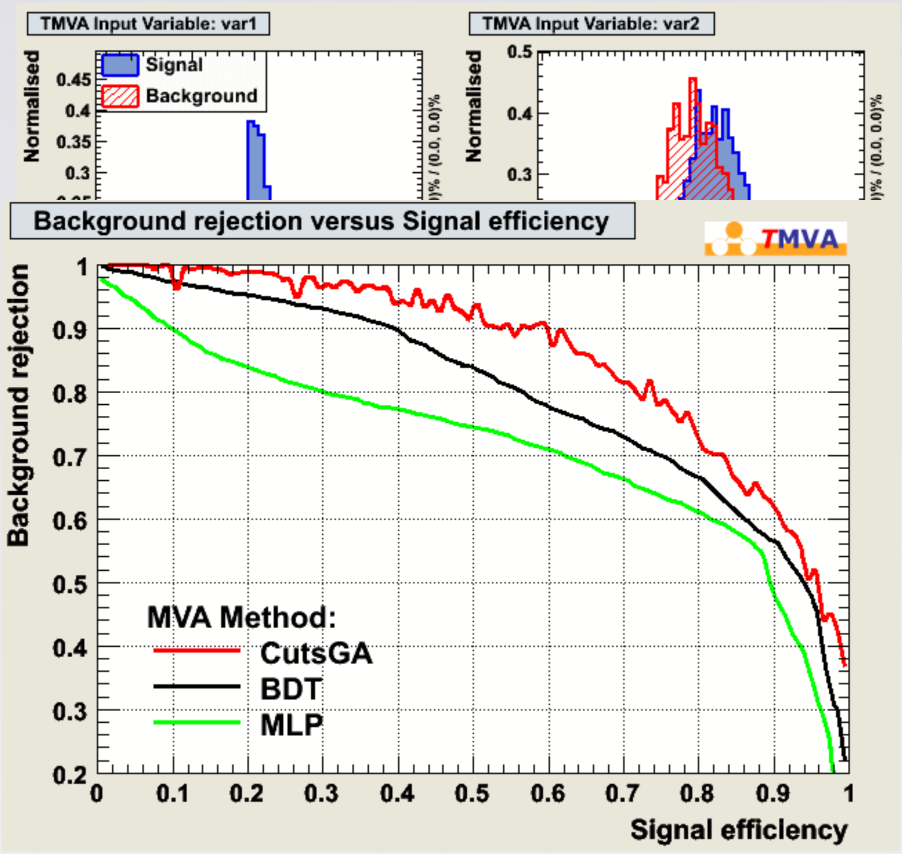
(T)MVA and Systematic Uncertainties

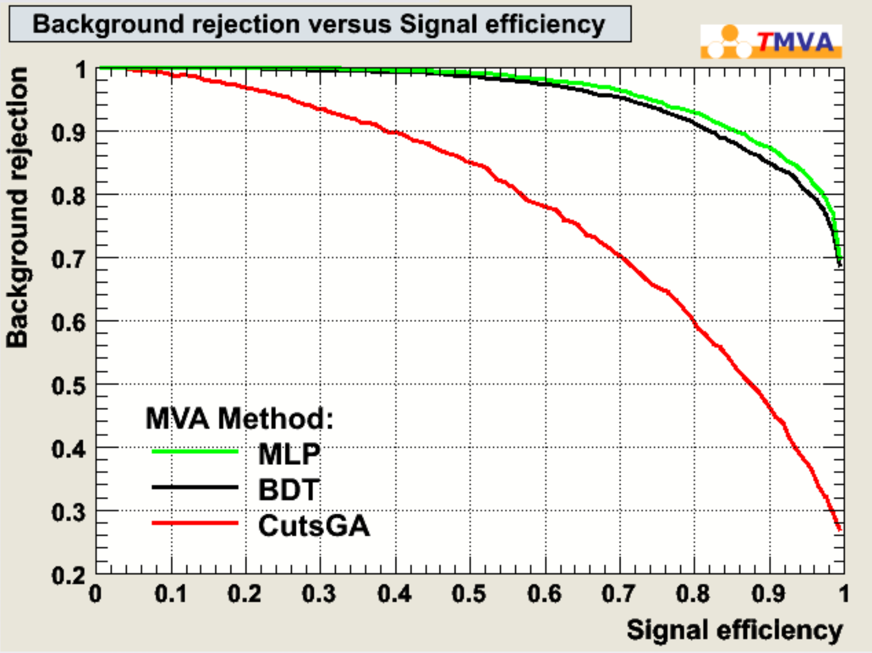
- → Don't be afraid of correlations!
  - → typically "kinematically generated" → easily modeled correctly
  - → "classical cuts" are also affected by "wrongly modeled correlations"
  - → MVA method let's you spot mis-modeled correlations!
    - → "projections" of input variables
    - → + the combined MVA test statistic "y(x)" !

Systematic "Error" in Correlations

- Use as training sample events that have correlatetions
  - optimize CUTs
  - train an propper MVA (e.g. Likelihood, BDT)



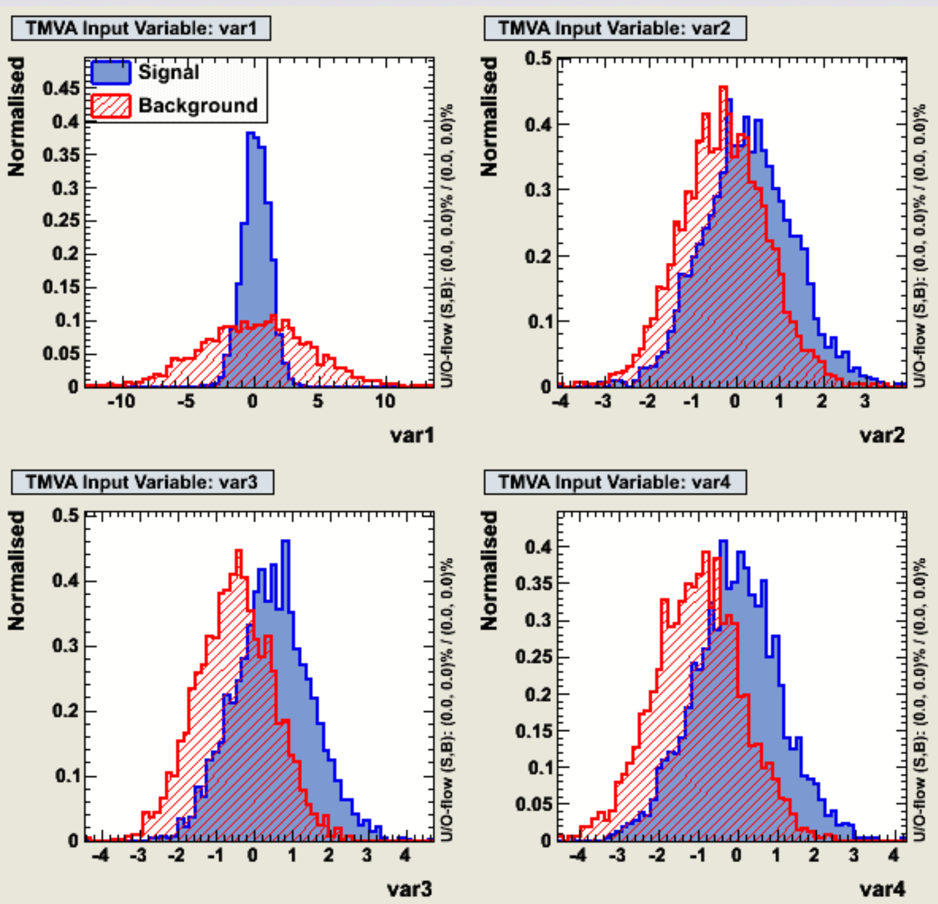


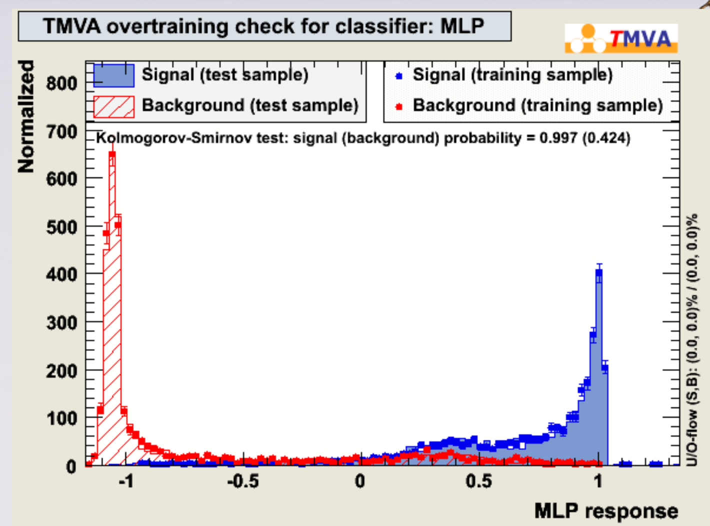


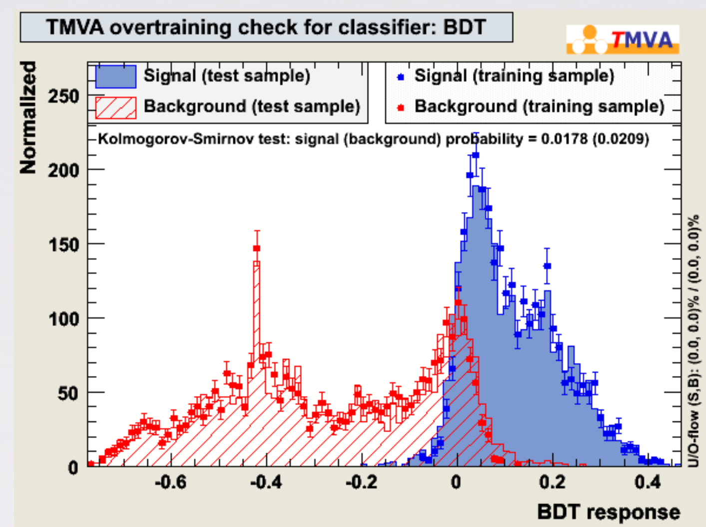
- Assume in "real data" there are NO correlations → SEE what happens!!

Systematic “Error” in Correlations

- Compare “Data” (TestSample) and Monte-Carlo
- both taken from the same underlying distributions

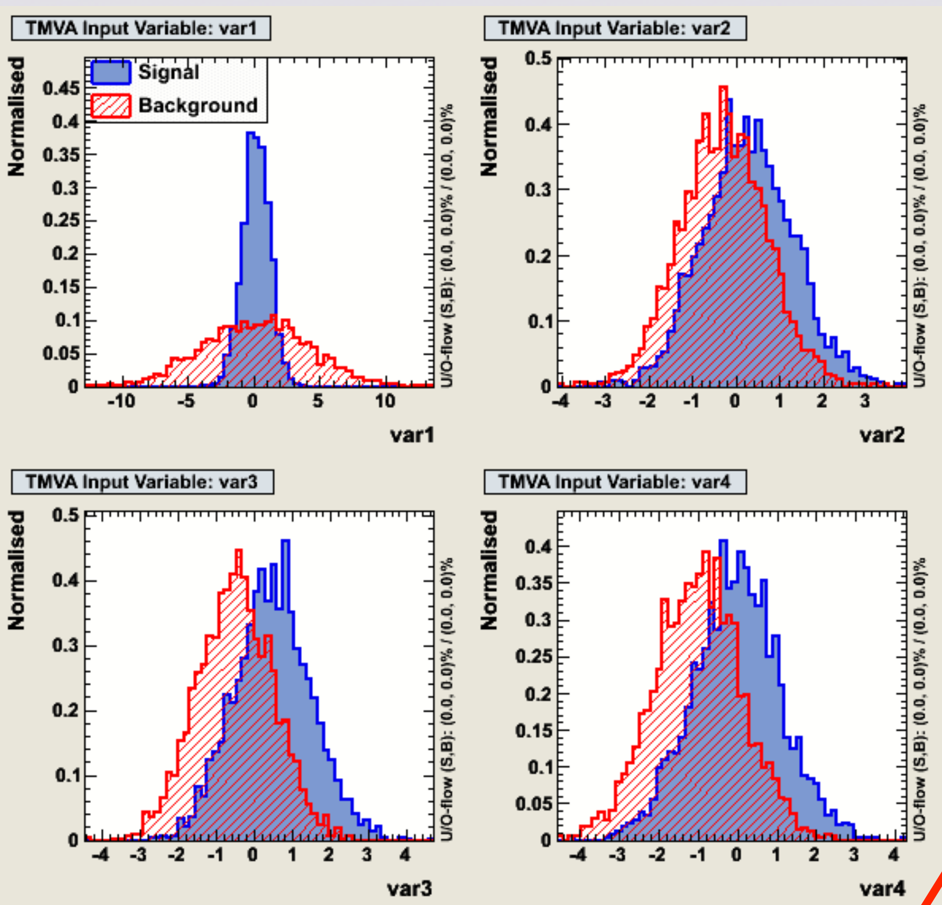


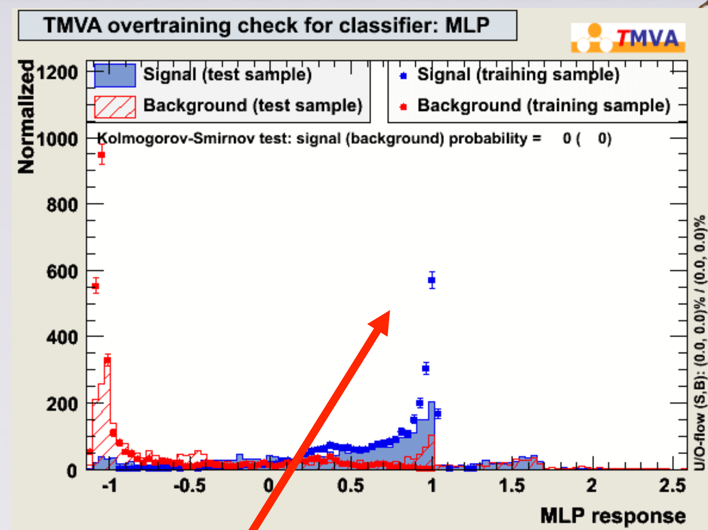


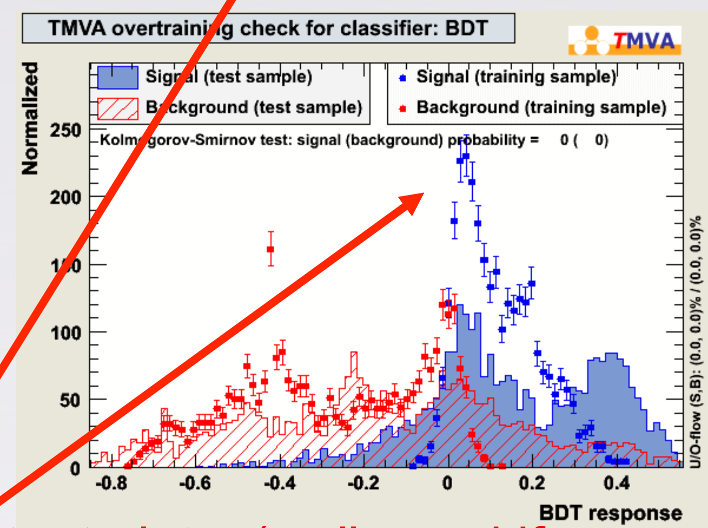


Systematic "Error" in Correlations

- Compare "Data" (TestSample) and Monte-Carlo
- both taken from the same underlying distributions that differ by the correlation!!!







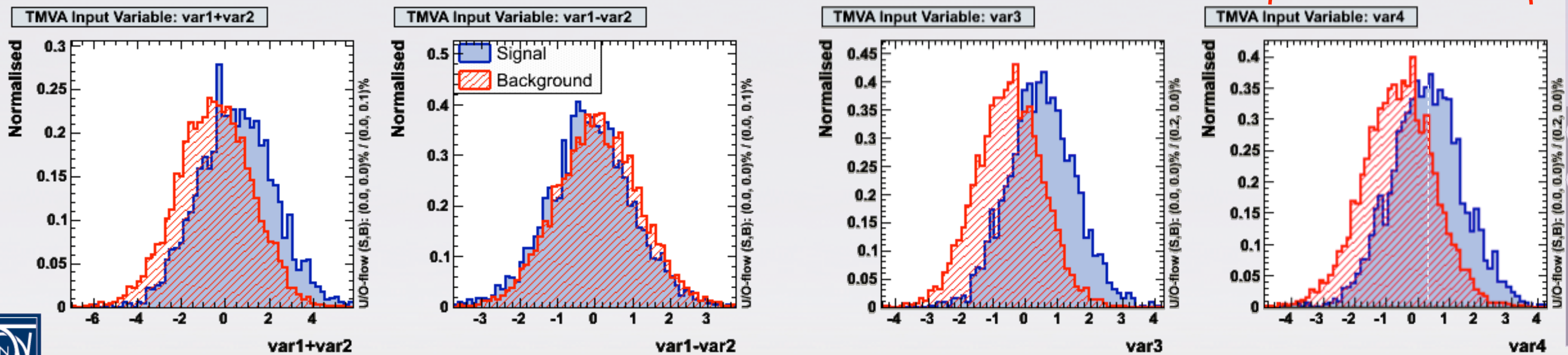
Differences are ONLY visible in the MVA-output plots (well…and if you were to study the 'cut sequences')

Robustness Against Systematics

- Is there a strategy however to become 'less sensitive' to possible systematic uncertainties
  - i.e. classically: variable that is prone to uncertainties → do not cut in the region of steepest gradient
  - classically one would not choose the most important cut on an uncertain variable
- Try to make classifier less sensitive to "uncertain variables"
  - i.e. re-weight events in training to decrease separation
  - in variables with large systematic uncertainty

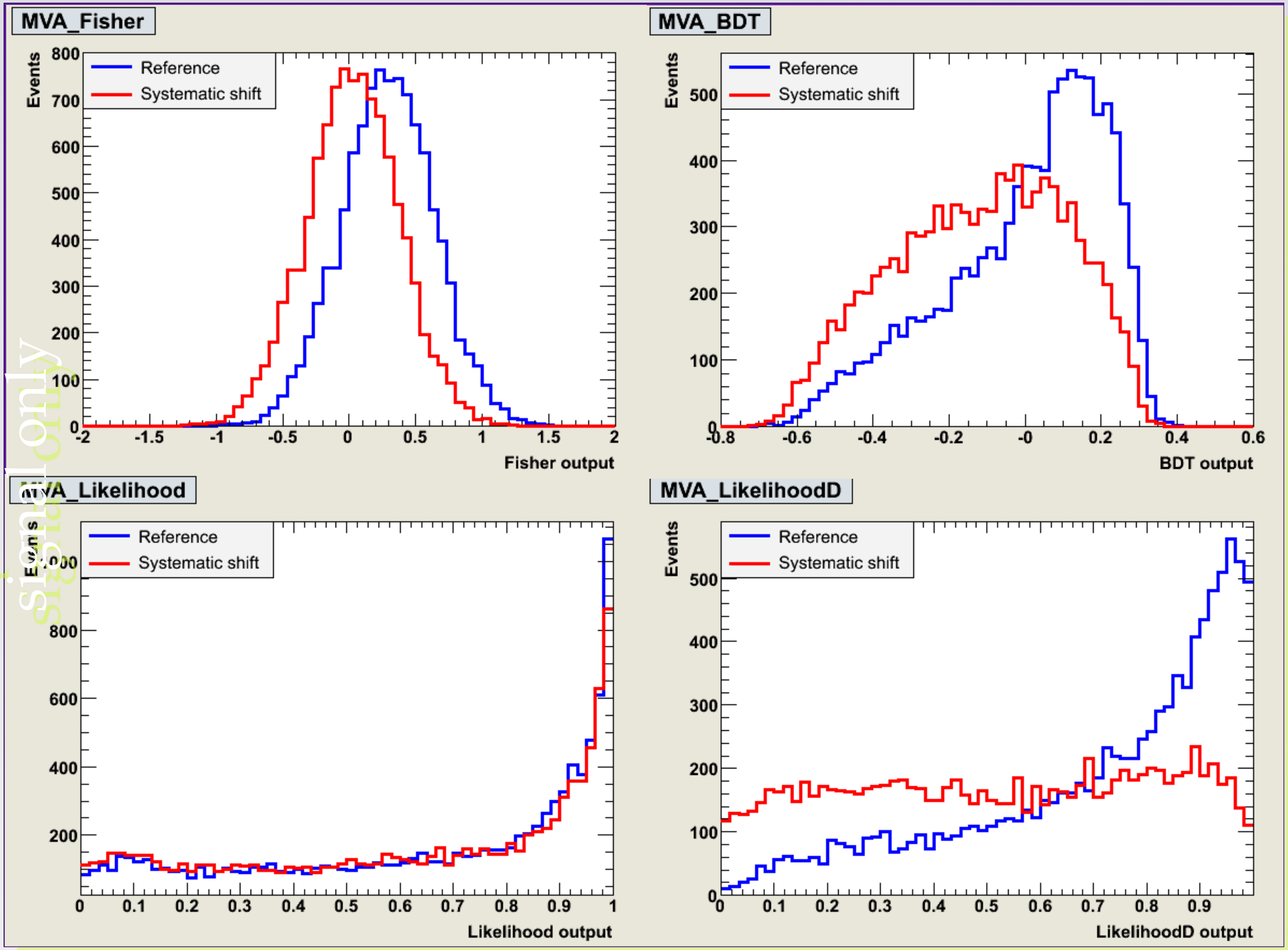
(certainly not yet a recipe that can strictly be followed, more an idea of what could perhaps be done)

"Calibration uncertainty"
→ possible shift
→ worsen (or increase) the discrimination power of "var4"



Robustness Against Systematics

Classifier output distributions for signal only



Robustness Against Systematics

Classifier output distributions for signal only