*T*MVA — Status and Developments

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And the contributors: See acknowledgments on page 28

On the web: http://tmva.sf.net/ (home), https://twiki.cern.ch/twiki/bin/view/TMVA/WebHome (tutorial)

Motivation / Outline

- ROOT: is the analysis framework used by most (HEP)-physicists
- Idea: rather than just implementing new MVA techniques and making them available in ROOT (*i.e*. like TMulitLayerPercetron does):
  - Have one common platform / interface for all MVA classifiers
  - Have data pre-processing capabilities
  - Train / test all classifiers on same data sample and evaluate consistently
  - Provide common analysis (ROOT scripts) and application framework
  - Provide access with and without ROOT, through macros, C++ executables or python

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- Outline of this talk
  - The TMVA project
  - Quick survey of available classifiers
  - Recent developments and outlook

New development highlighted

Planned developments highlighted

TMVA Development and Distribution

- TMVA is a sourceforge (SF) package for world-wide access
  - Home page ……………….http://tmva.sf.net/
  - SF project page …………. http://sf.net/projects/tmva
  - View CVS …………………http://tmva.cvs.sf.net/tmva/TMVA/
  - Mailing list ………………..http://sf.net/mail/?group_id=152074
  - Tutorial TWiki ……………. https://twiki.cern.ch/twiki/bin/view/TMVA/WebHome

- Active project → fast response time on feature requests
  - Currently 4 core developers, and 27 registered contributors at SF
  - >2200 downloads since March 2006 (not accounting CVS checkouts and ROOT users)

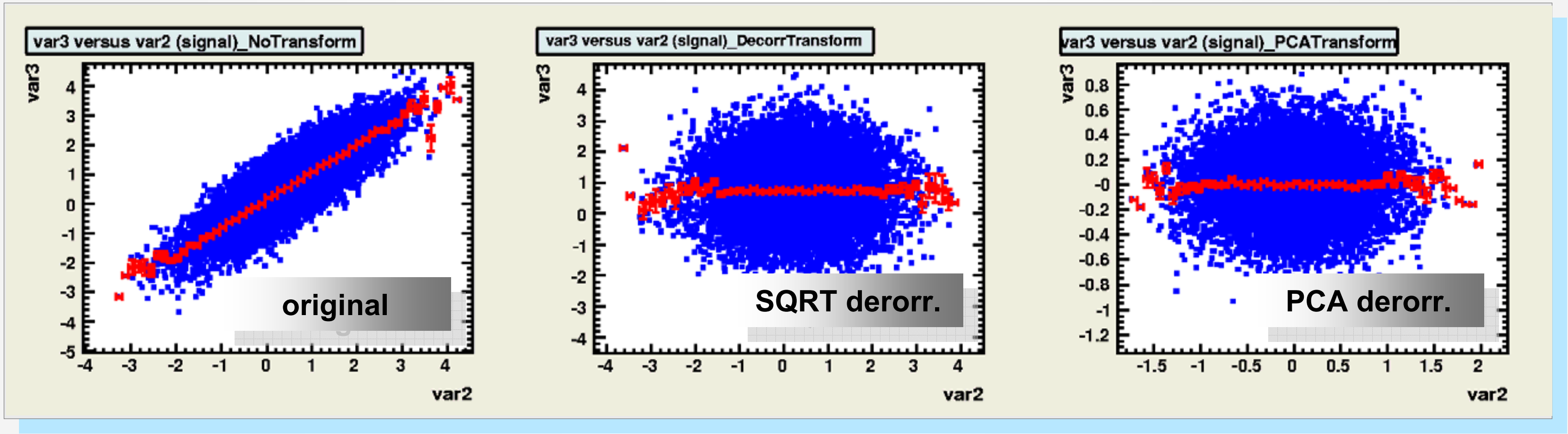
- Integrated and distributed with ROOT since ROOT v5.11/03
  (newest version 3.8.14 in ROOT production release 5.18)

The *T*MVA Classifiers

- Currently implemented classifiers :
  - Rectangular cut optimisation
  - Projective and multidimensional likelihood estimator
  - k-Nearest Neighbor algorithm
  - Fisher and H-Matrix Discriminants
  - Function Discriminant
  - Artificial neural networks (3 *multilayer perceptron* implementations)
  - Boosted/bagged decision trees with node pruning
  - Rule Ensemble Fitting
  - Support Vector Machine
- Currently implemented data preprocessing :
  - Linear decorrelation
  - Principal component analysis

Example for Data Preprocessing: Decorrelation

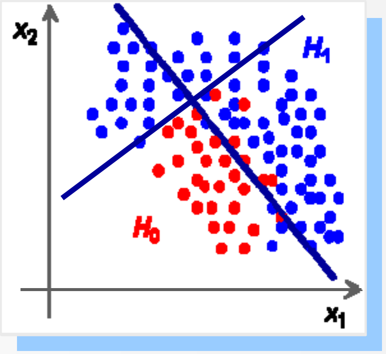
- Commonly realised for all classifiers in *T*MVA (centrally in `DataSet` class)
- Removal of linear correlations by rotating input variables
  - using the "square-root" of the correlation matrix
  - using the Principal Component Analysis
- Note that decorrelation is only complete, if
  - Correlations are linear
  - Input variables are Gaussian distributed



Rectangular Cut Optimisation

- Simplest method: cut in rectangular variable volume

$$x_{\text{cut}}(i_{\text{event}}) \in \{0,1\} = \bigcap_{v \in \{\text{variables}\}} \left(x_v(i_{\text{event}}) \subset [x_{v,\min}, x_{v,\max}] \right)$$

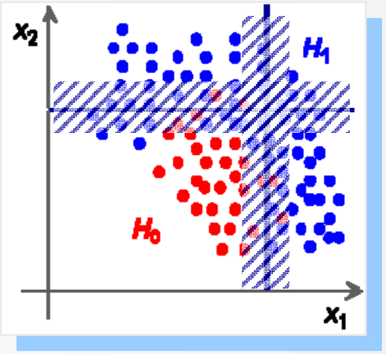


- Cuts usually benefit from prior decorrelation of cut variables
- Technical challenge: how to find optimal cuts ?
  - MINUIT fails due to non-unique solution space
  - *T*MVA uses: **Monte Carlo sampling**, **Genetic Algorithm**, **Simulated Annealing**
  - Huge speed improvement of volume search by sorting events in binary tree

New development (ongoing):
Implementation of new Simulated Annealing algorithm
(collaboration with team of Polish mathematics students)

Projective Likelihood Estimator (PDE Approach)

- Probability density estimators for each input variable combined in likelihood estimator (ignoring correlations)
  - Optimal approach if zero correlations (or linear → decorrelation)
  - Otherwise: significant performance loss



- Technical challenge: how to estimate the PDF shapes

➡ **3 ways:** **parametric fitting (function)** | **event counting** | **nonparametric fitting**

parametric fitting (function): Difficult to automate for arbitrary PDFs

event counting: Automatic, unbiased, but suboptimal

nonparametric fitting: Easy to automate, can create artefacts/suppress information

- **TMVA uses binned shape interpolation using spline functions**
- **Or: unbinned adaptive Gaussian kernel density estimation**

➡ *T*MVA performs automatic validation of goodness-of-fit

New development:
Adaptive smoothing

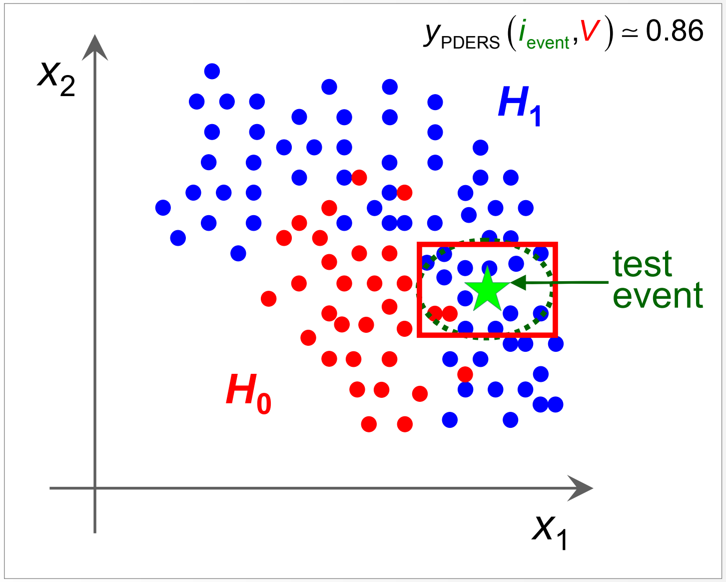
Planned:
Extend PDF class to RooFit multi-D models

Multidimensional PDE Approach

- Use a single PDF per event class (sig, bkg), which spans N_{var} dimensions
  - PDE Range-Search: count number of signal and background events in "vicinity" of test event → preset or **adaptive** volume defines "vicinity"

Carli-Koblitz, NIM A501, 576 (2003)

  - Improve simple event counting by use of kernel functions to penalise large distance from test event
  - Increase counting speed with binary search tree



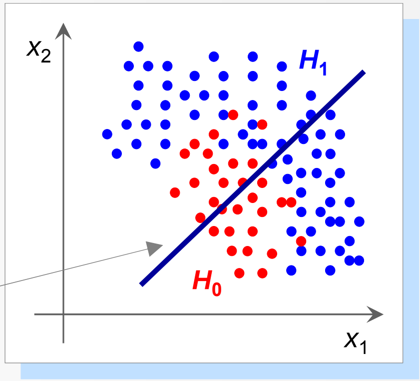
New developments:
- Improve binary search tree by tuning sort algorithm to achieve equal-length branches
- Use ROOT's TFoam cellular algorithm

New developments:
- **Genuine k-NN algorithm** (author R. Ospanov)
- Intrinsically adaptive approach
- Very fast search with kd-tree event sorting
- Recently added: event weight support
- Planned: support of kernel functions

Fisher's Linear Discriminant Analysis (LDA)

- Well known, simple and elegant classifier
  - LDA determines axis in the input variable hyperspace such that a projection of events onto this axis pushes signal and background as far away from each other as possible

projection axis



- Classifier response couldn't be simpler:

"Fisher coefficients"

$$y_{\mathrm{Fi}}\left(i_{\mathrm{event}}\right) = F_0 + \sum_{k\in\{\mathrm{variables}\}} x_k\left(i_{\mathrm{event}}\right)\cdot F_k$$

New developments:

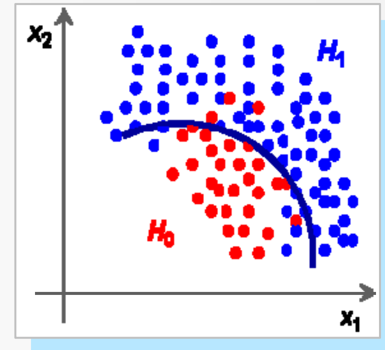
Function discriminant analysis (FDA)

Fit any user-defined function of input variables requiring that signal events return →1 and background →0

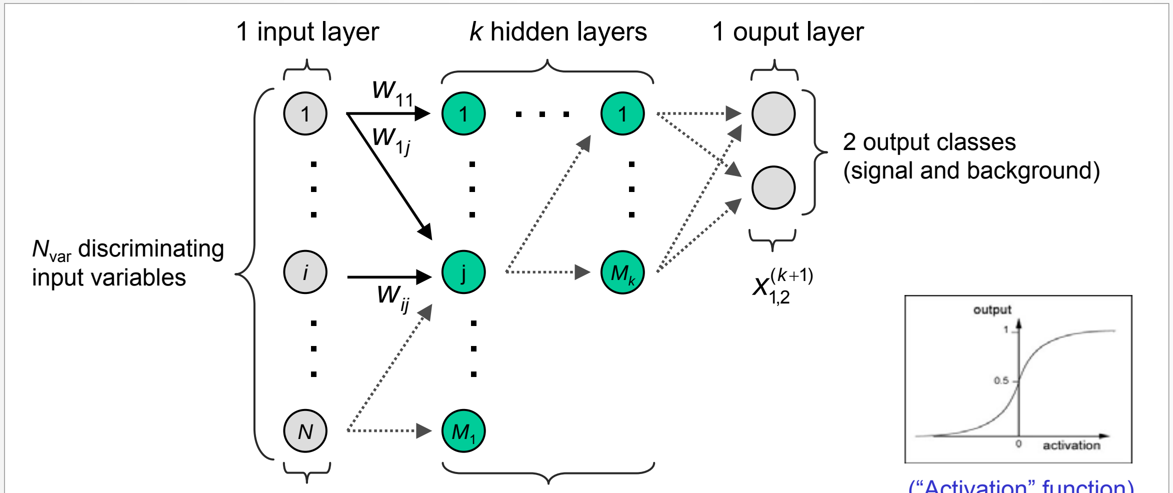
- Parameter fitting: Genetics Alg., MINUIT, MC and combinations
- Easy reproduction of Fisher result, but can add nonlinearities
- Very transparent discriminator

Nonlinear Analysis: Artificial Neural Networks

- Achieve nonlinear classifier response by "activating" output nodes using nonlinear weights



Feed-forward Multilayer Perceptron



$$x_j^{(k)} = A\left(w_{0j}^{(k)} + \sum_{i=1}^{M_{k-1}} w_{ij}^{(k)} \cdot x_i^{(k-1)}\right) \quad \text{with:} \quad A(x) = \left(1+e^{-x}\right)^{-1}$$

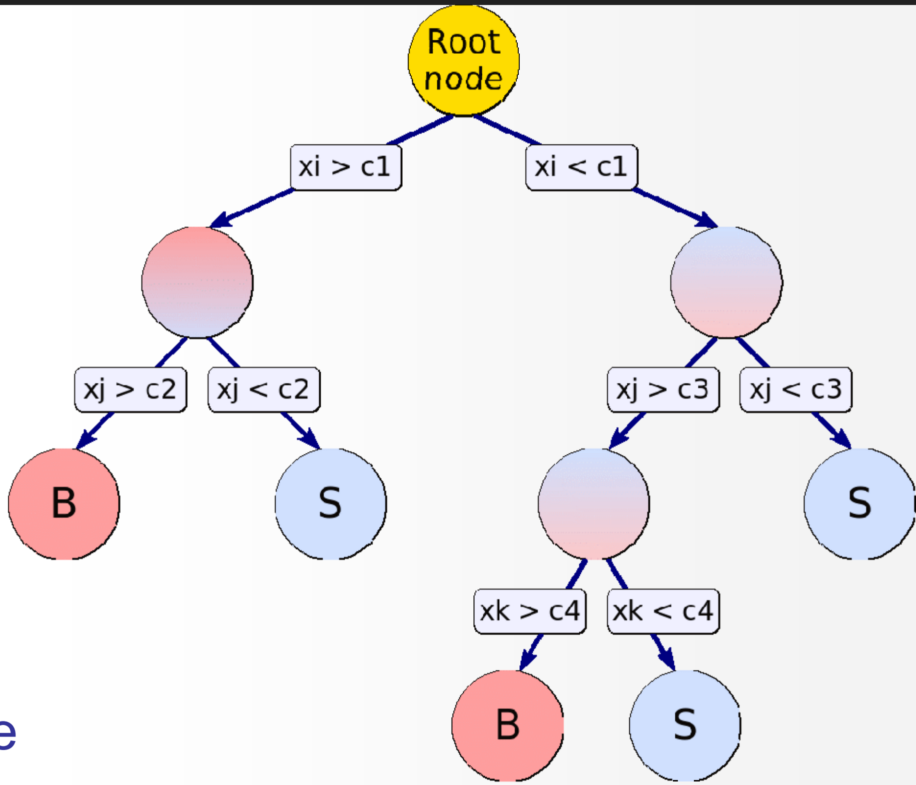
- Three different implementations in TMVA (all are Multilayer Perceptrons)
  - **TMlpANN:** Interface to ROOT's MLP implementation
  - **MLP:** TMVA's own MLP implementation for increased speed and flexibility
  - **CFMlpANN:** ALEPH's Higgs search ANN, translated from FORTRAN

Boosted Decision Trees (BDT)

- DT: Sequential application of cuts splits the data into nodes, where the final nodes (leafs) classify an event as signal or background

- BDT: combine forest of DTs, with differently weighted events in each tree (trees can also be weighted)
  - *e.g.*, "AdaBoost": incorrectly classified events receive larger weight in next DT
  - "Bagging": random event weights $\approx$ resampling with replacement
  - Boosting or bagging create set of "basis functions": final classifier is linear combination of these → improves stability

- Bottom-up "pruning" of a decision tree
  - Remove statistically insignificant nodes to reduce tree overtraining



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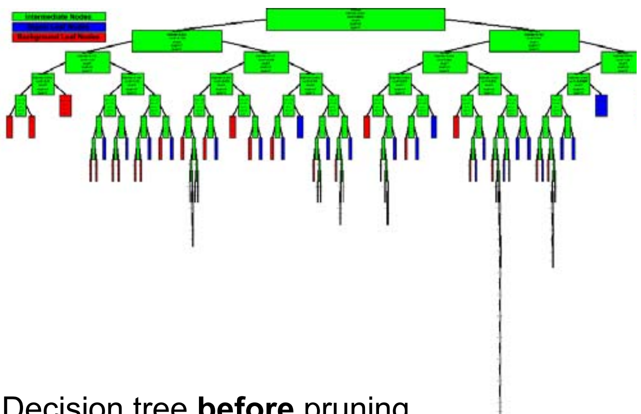
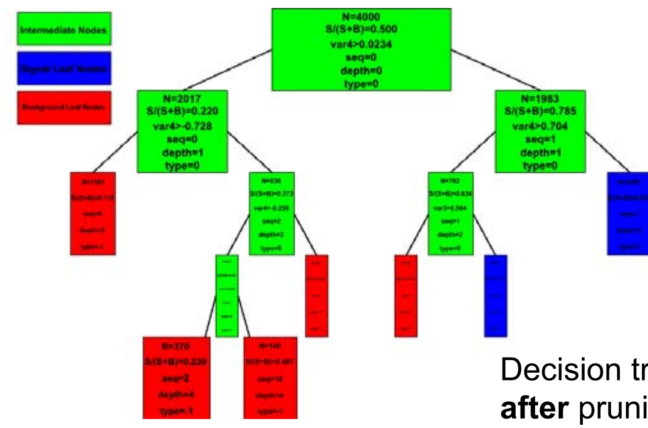


Decision tree **before** pruning



Decision tree **after** pruning

- Bottom-up "pruning" of a decision tree
  - Remove statistically insignificant nodes to reduce tree overtraining

"New developments:"

- Reduced memory consumption by pruning each DT right after its construction.
- More flexible "tree displaying" GUI

Predictive Learning via Rule Ensembles (Rule Fitting)

- Following RuleFit approach by Friedman-Popescu

Friedman-Popescu, Tech Rep, Stat. Dpt, Stanford U., 2003

- Model is linear combination of *rules*, where a rule is a sequence of cuts

RuleFit classifier

rules (cut sequence → r_m=1 if all cuts satisfied, =0 otherwise)

normalised discriminating event variables

$$y_{\mathrm{RF}}\left(\vec{x}\right) = a_0 + \underbrace{\sum_{m=1}^{M_R} a_m r_m\left(\hat{\vec{x}}\right)}_{\text{Sum of rules}} + \underbrace{\sum_{k=1}^{n_R} b_k \hat{x}_k}_{\text{Linear Fisher term}}$$

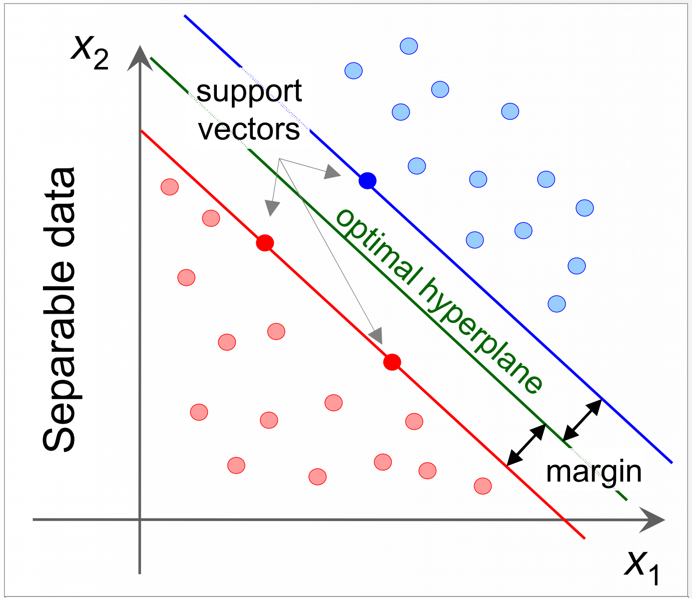
- The problem to solve is
  - Create rule ensemble: use forest of decision trees
  - Fit coefficients a_m, b_k: gradient direct regularization minimising *Risk* (Friedman et al.)

- Pruning removes topologically equal rules" (same variables in cut sequence)

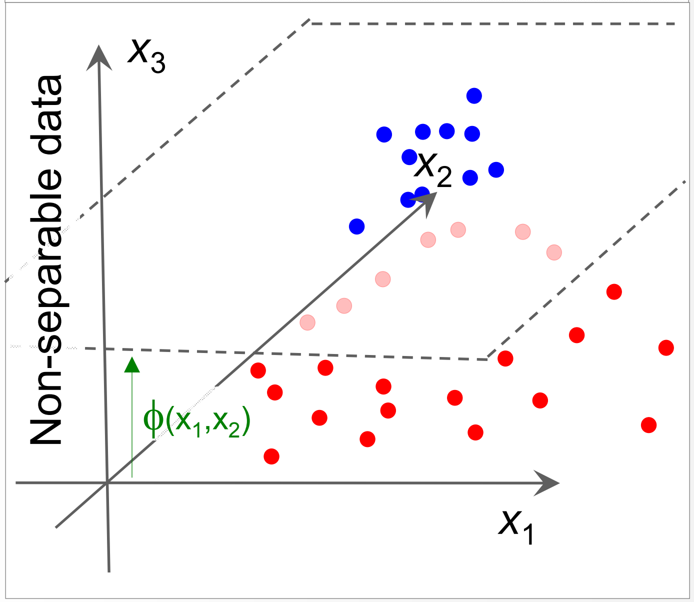
One of the elementary cellular automaton rules (Wolfram 1983, 2002). It specifies the next color in a cell, depending on its color and its immediate neighbors. Its rule outcomes are encoded in the binary representation $30=00011110_2$.

Support Vector Machine (SVM)

- Linear case: find hyperplane that best separates signal from background
  - Best separation: maximum distance (margin) between closest events (*support*) to hyperplane
  - Linear decision boundary
  - If data non-separable add *misclassification cost* parameter to minimisation function



- Non-linear cases:
  - Transform variables into higher dim. space where a linear boundary can fully separate the data
  - Explicit transformation not required: use kernel functions to approximate scalar products between transformed vectors in the higher dim. space
  - Choose Kernel and fit the hyperplane using the techniques developed for linear case



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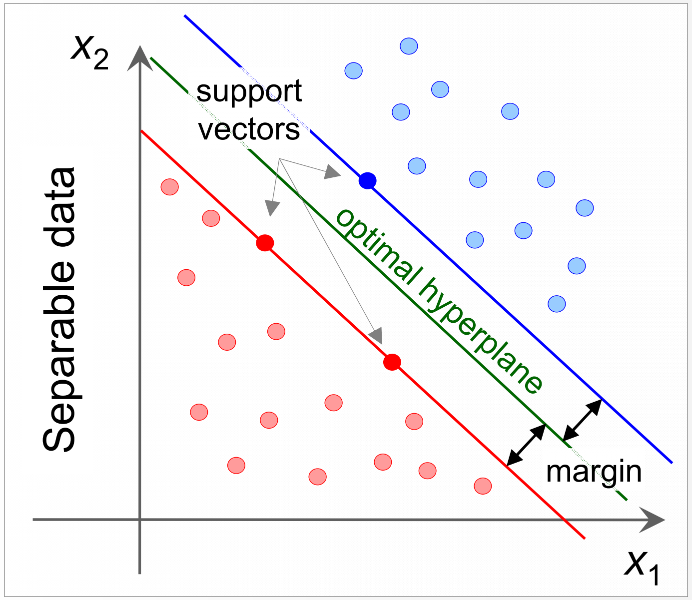

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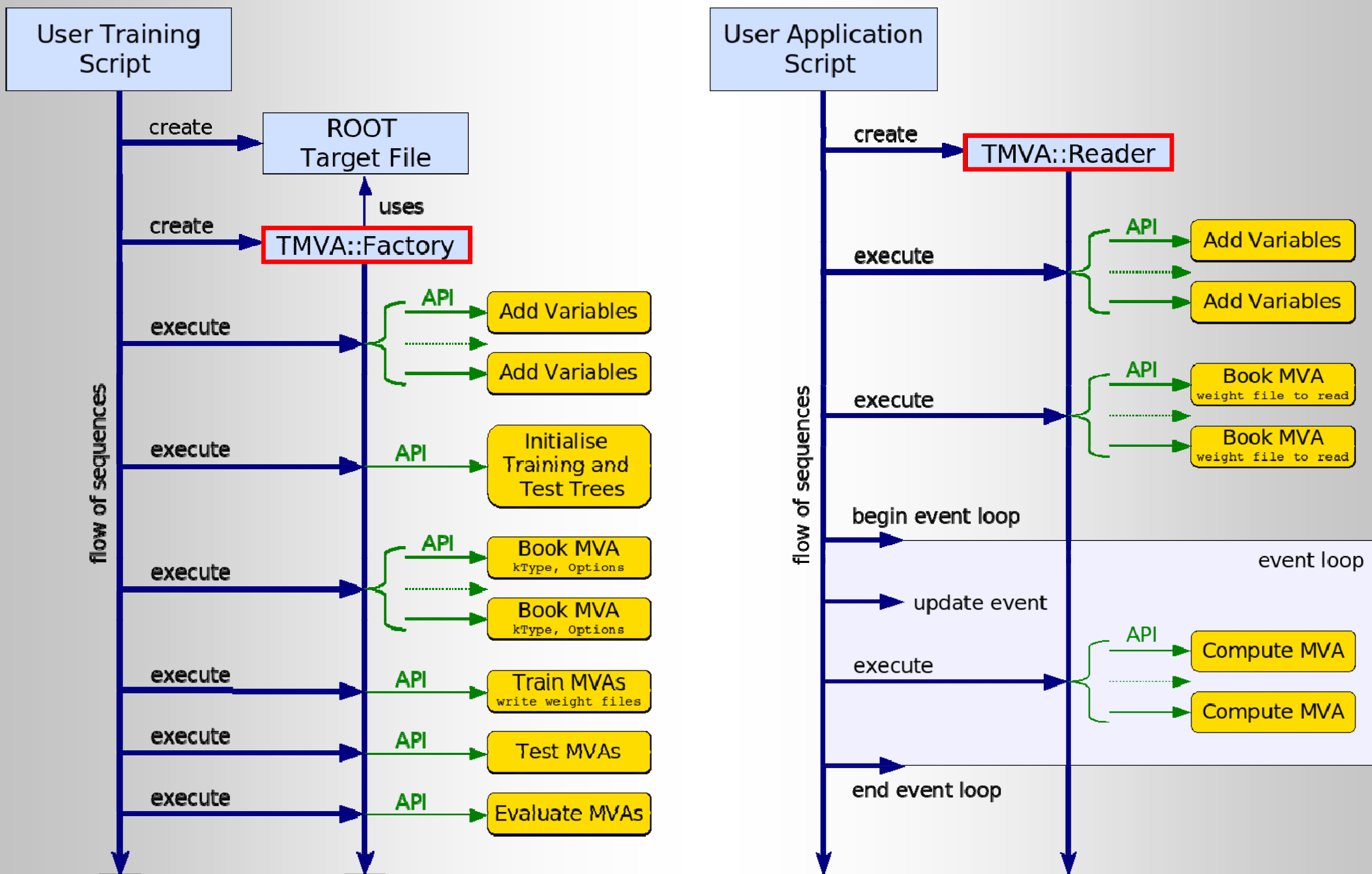
New developments (ongoing):
- SVM requires substantial tuning for optimal performance

➡ Implementation of automatic parameter tuning

Data Preparation

- Data input format: ROOT TTree or ASCII
- Supports selection of any subset or combination or function of available variables
- Supports application of pre-selection cuts (possibly independent for signal and bkg)
- Supports global event weights for signal or background input files
- Supports use of any input variable as individual event weight
- Supports various methods for splitting into training and test samples:
  - Block wise
  - Randomly
  - Periodically (*i.e*. periodically 3 testing ev., 2 training ev., 3 testing ev, 2 training ev. ….)
  - User defined training and test trees (in upcomming release)
- Preprocessing of input variables (*e.g.*, decorrelation)

Code Flow for *Training* and *Application* Phases

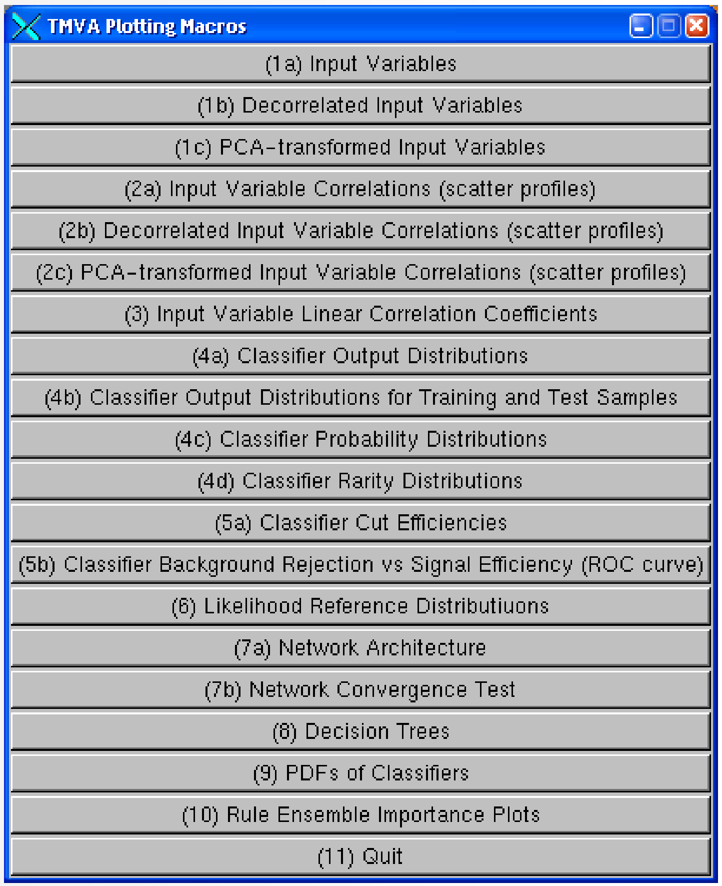


Scripts can be ROOT scripts, C++ executables or python scripts (via PyROOT)

→ *T*MVA tutorial

MVA Evaluation Framework

- TMVA is not only a collection of classifiers, but an MVA framework
- After training, TMVA provides ROOT evaluation 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

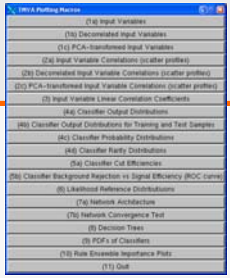
Classifier significance with optimal cuts

B rejection versus S efficiency

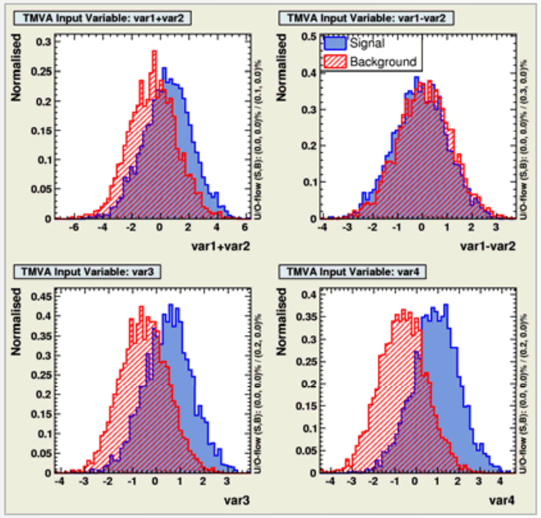
Classifier-specific plots:
- Likelihood reference distributions
- Classifier PDFs (for probability output and Rarity)
- Network architecture, weights and convergence
- Rule Fitting analysis plots

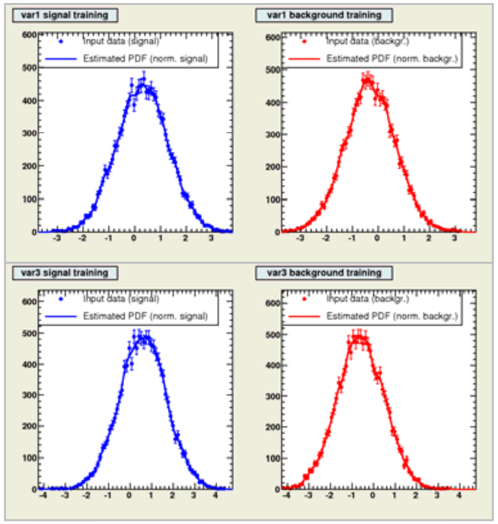
- Visualise decision trees

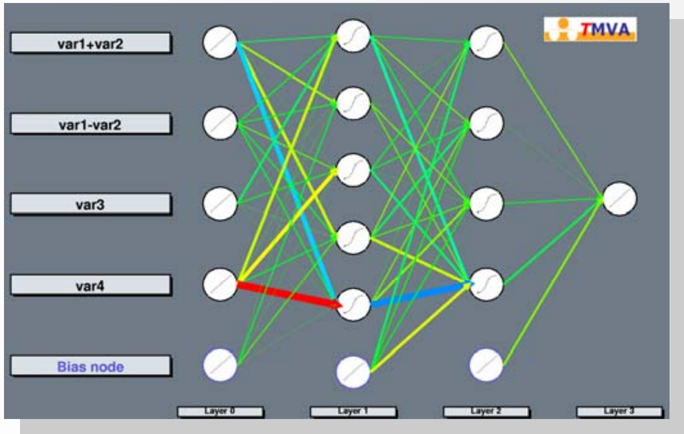
Evaluating the Classifier Training

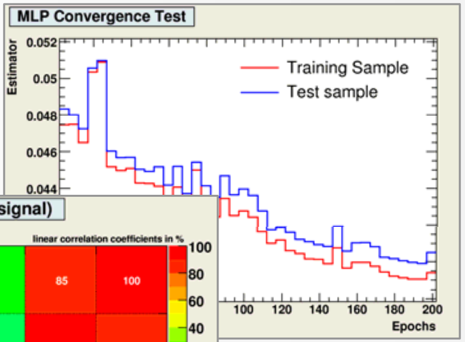


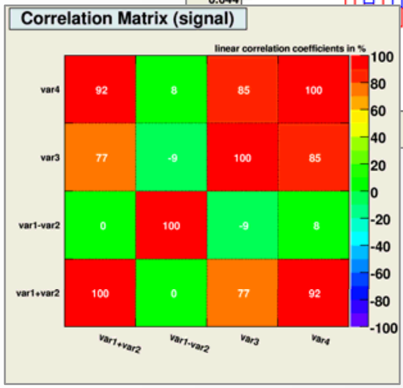
- Projective likelihood PDFs, MLP training, BDTs, …

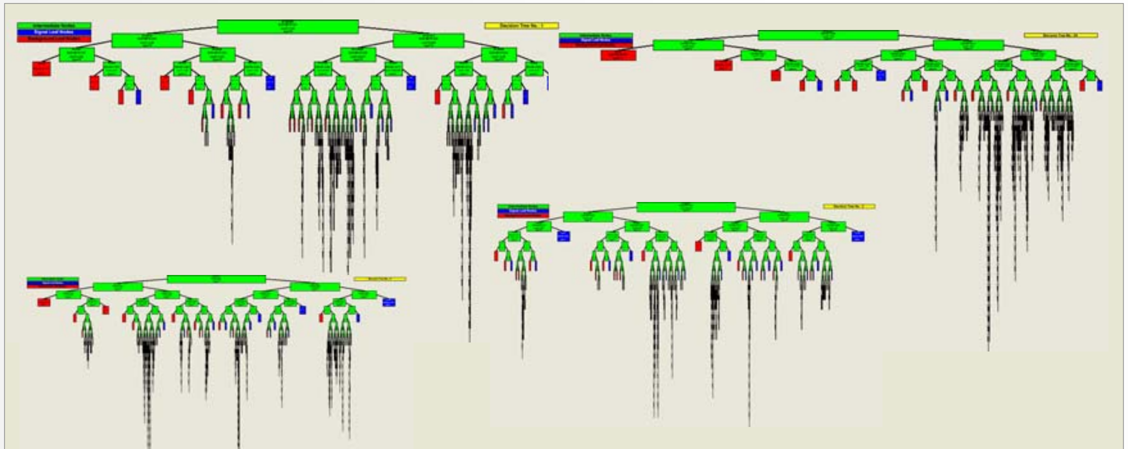






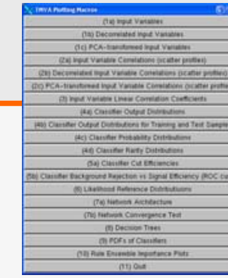




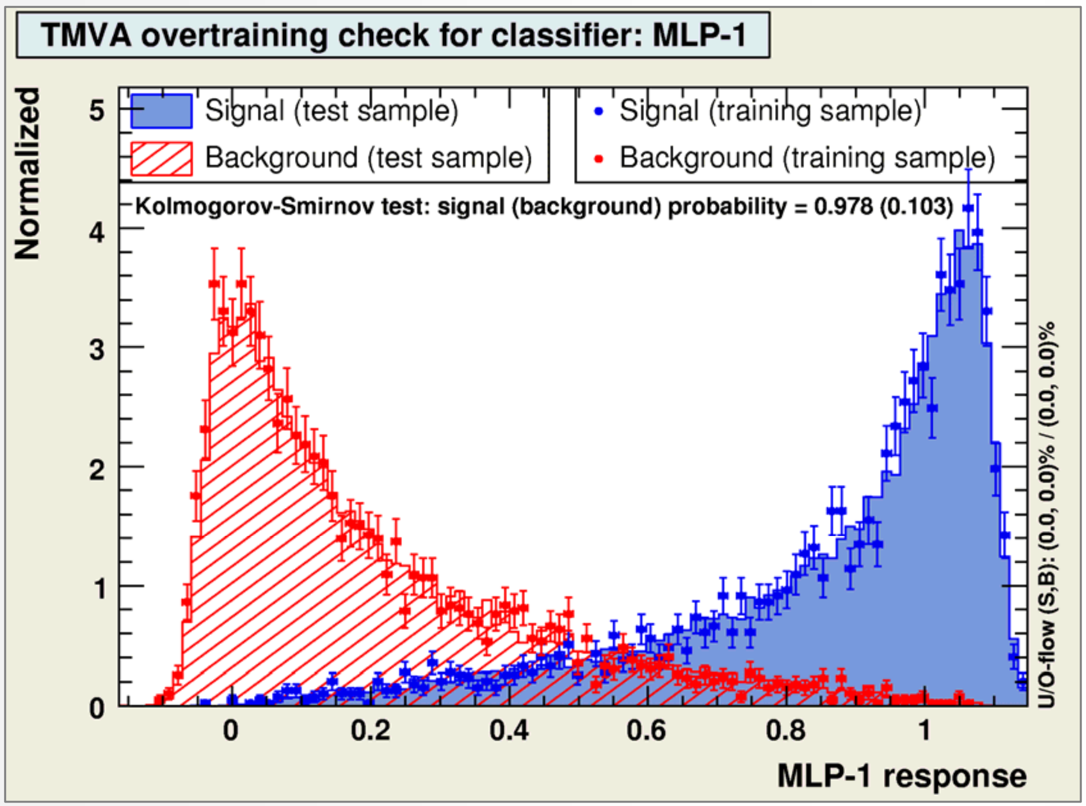


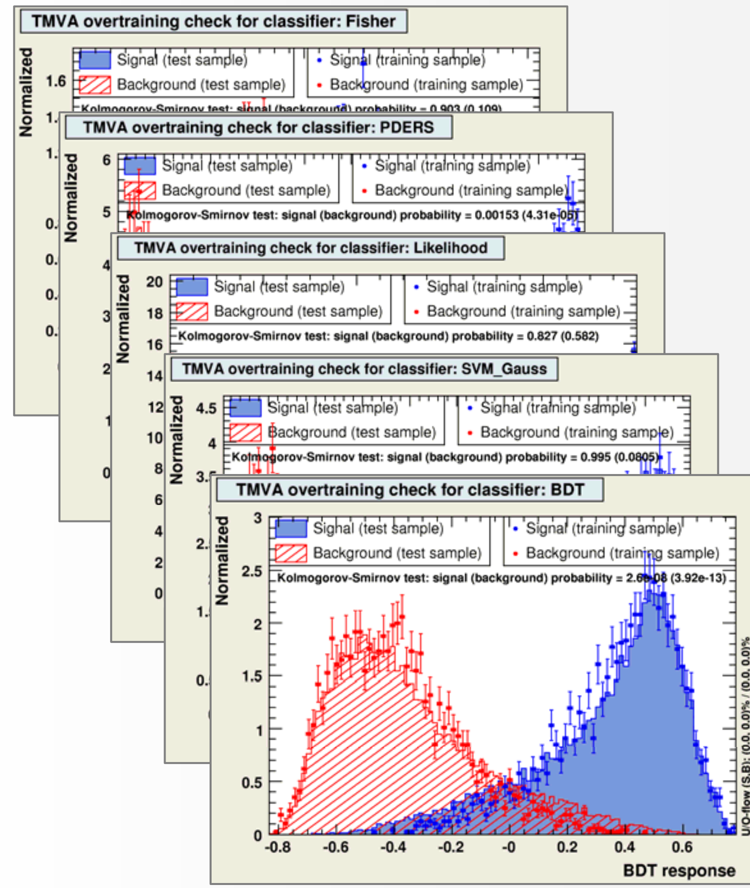
average no. of nodes before/after pruning: 4193 / 968

Evaluating the Classifier Training

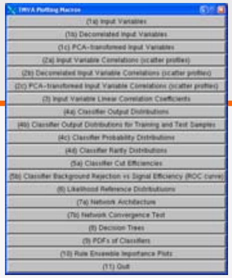


- Classifier output distributions for test *and* training samples …



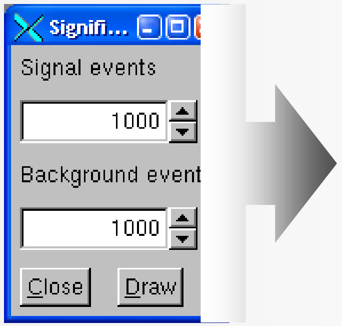


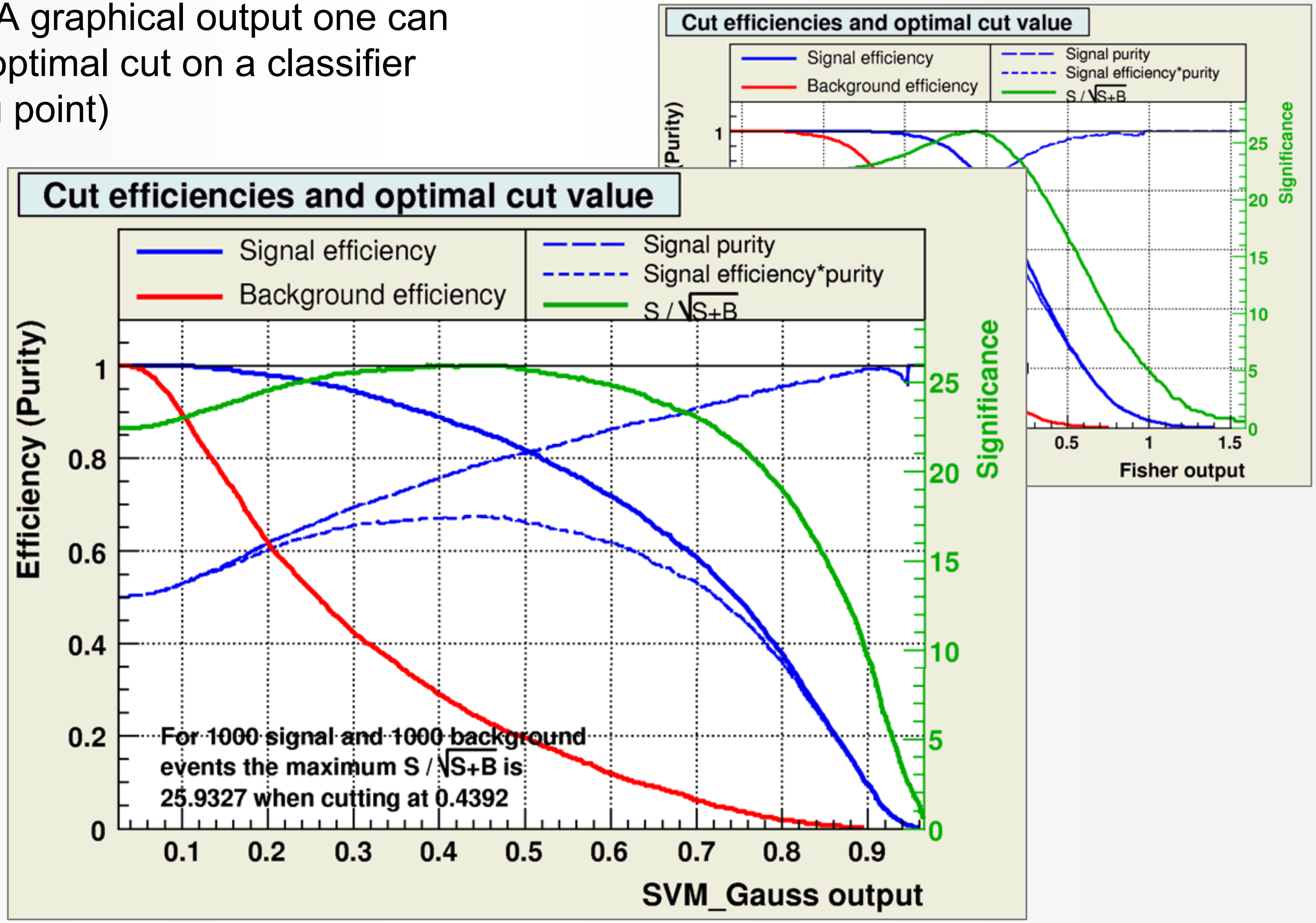
Evaluating the Classifier Training



- Optimal cut for each classifiers …

Using the TMVA graphical output one can determine the optimal cut on a classifier output (working point)

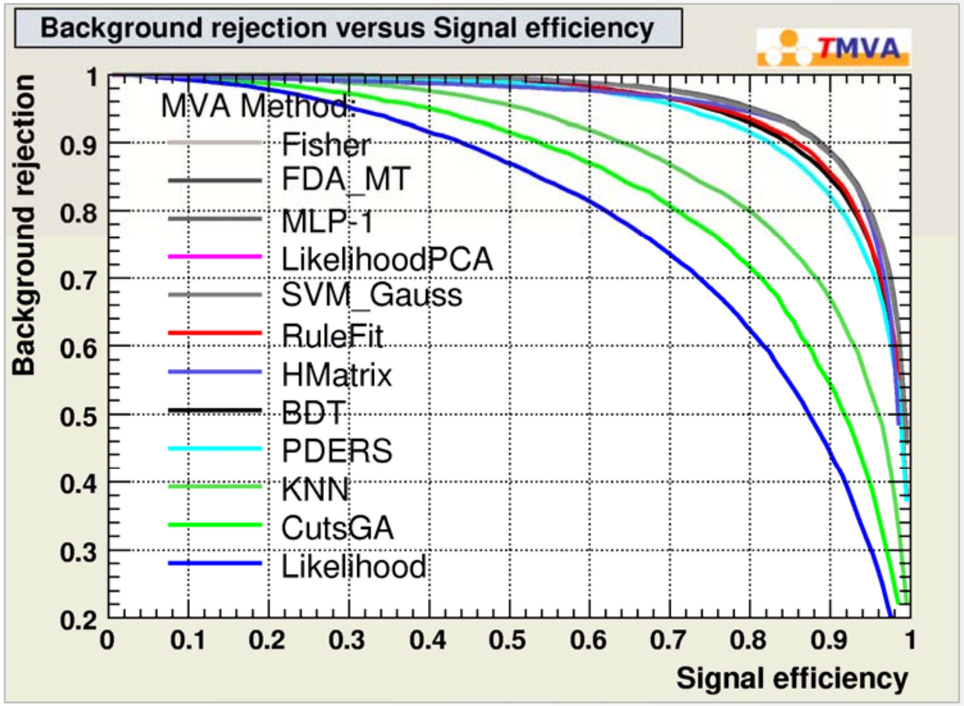


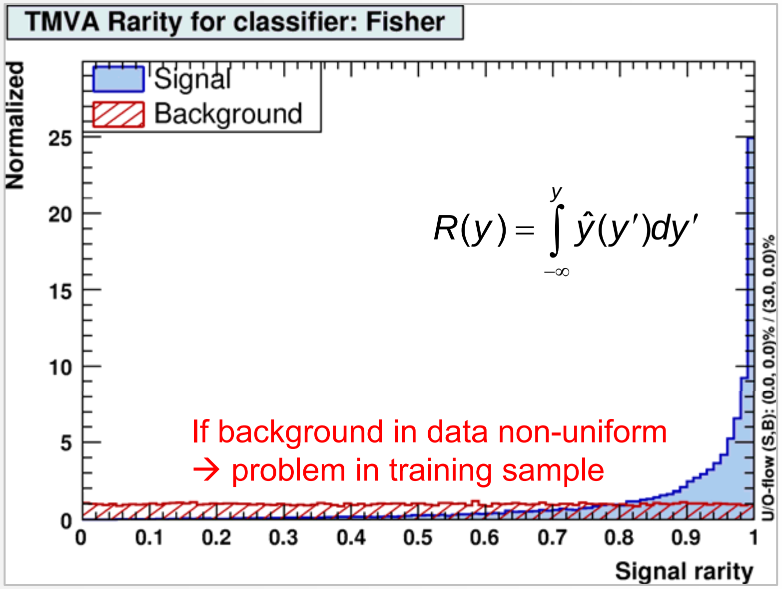


Evaluating the Classifier Training

- Background rejection versus signal efficiencies …

Best plot to compare classifier performance

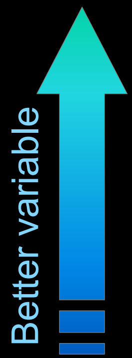




An elegant variable is the *Rarity*: transforms to uniform background. Height of signal peak direct measure of classifier performance

Evaluating the Classifiers (taken from TMVA output…)

Input Variable Ranking




```
--- 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 ?

Classifier correlation and overlap

```
--- 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 !

Evaluating the Classifiers (taken from TMVA output…)

Evaluation results ranked by best signal efficiency and purity (area)

MVA Methods:	Signal efficiency at bkg eff. (error): @B=0.01	@B=0.10	@B=0.30	Area	Separation:	Significance:
Fisher	0.268(03)	0.653(03)	0.873(02)	0.882	0.444	1.189
MLP	0.266(03)	0.656(03)	0.873(02)	0.882	0.444	1.260
LikelihoodD	0.259(03)	0.649(03)	0.871(02)	0.880	0.441	1.251
PDERS	0.223(03)	0.628(03)	0.861(02)	0.870	0.417	1.192
RuleFit	0.196(03)	0.607(03)	0.845(02)	0.859	0.390	1.092
HMatrix	0.058(01)	0.622(03)	0.868(02)	0.855	0.410	1.093
BDT	0.154(02)	0.594(04)	0.838(03)	0.852	0.380	1.099
CutsGA	0.109(02)	1.000(00)	0.717(03)	0.784	0.000	0.000
Likelihood	0.086(02)	0.387(03)	0.677(03)	0.757	0.199	0.682

Better classifier

Testing efficiency compared to training efficiency (overtraining check)

MVA Methods:	Signal efficiency: from test sample (from traing sample) @B=0.01	@B=0.10	@B=0.30
Fisher	0.268 (0.275)	0.653 (0.658)	0.873 (0.873)
MLP	0.266 (0.278)	0.656 (0.658)	0.873 (0.873)
LikelihoodD	0.259 (0.273)	0.649 (0.657)	0.871 (0.872)
PDERS	0.223 (0.389)	0.628 (0.691)	0.861 (0.881)
RuleFit	0.196 (0.198)	0.607 (0.616)	0.845 (0.848)
HMatrix	0.058 (0.060)	0.622 (0.623)	0.868 (0.868)
BDT	0.154 (0.268)	0.594 (0.736)	0.838 (0.911)
CutsGA	0.109 (0.123)	1.000 (0.424)	0.717 (0.715)
Likelihood	0.086 (0.092)	0.387 (0.379)	0.677 (0.677)

Check for over-training

Subjective Summary of TMVA Classifier Properties

Criteria		Cuts	Likeli-hood	PDERS / k-NN	H-Matrix	Fisher	MLP	BDT	Rule fitting	SVM
Perfor-mance	no / linear correlations	😐	☺	☺	😐	☺	☺	😐	☺	☺
	nonlinear correlations	😐	☹	☺	☹	☹	☺	☺	😐	☺
Speed	Training	☹	☺	☺	☺	☺	😐	☹	😐	☹
	Response	☺	☺	☹/😐	☺	☺	☺	😐	😐	😐
Robust-ness	Overtraining	☺	😐	😐	☺	☺	☹	☹	😐	😐
	Weak input variables	☺	☺	☹	☺	☺	😐	😐	😐	😐
Curse of dimensionality		☹	☺	☹	☺	☺	😐	☺	😐	😐
Transparency		☺	☺	😐	☺	☺	☹	☹	☹	☹

The properties of the Function discriminant (FDA) depend on the chosen function

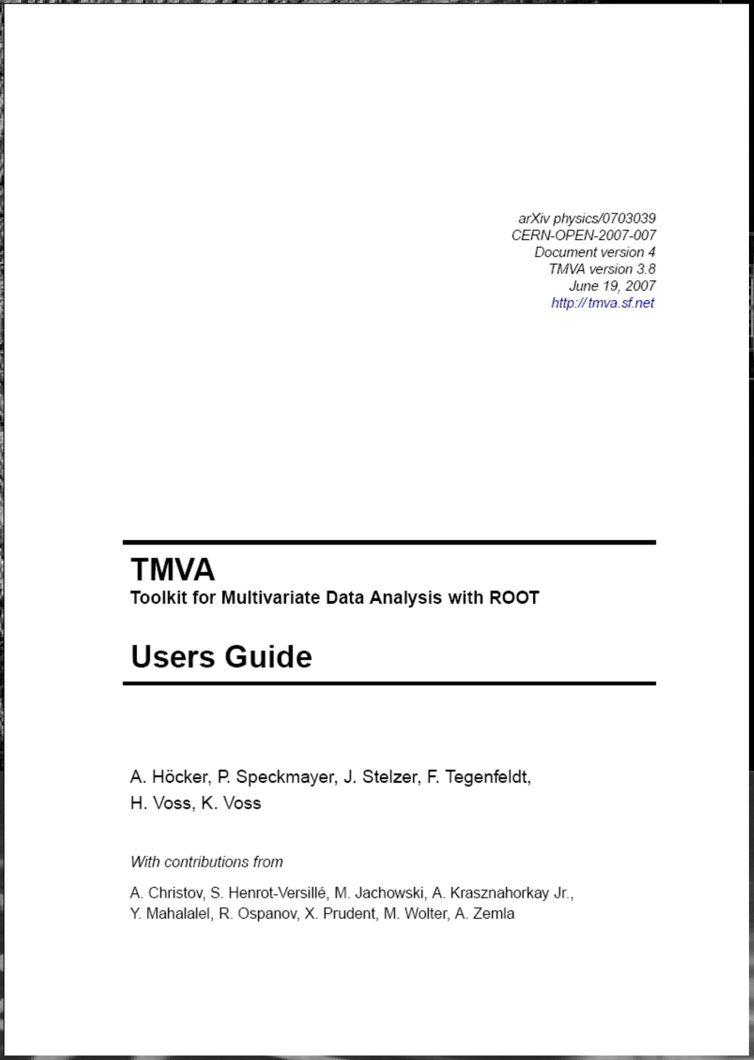
Framework Developments

New and planned framework developments:

- Use ROOT's plugin mechanism to insert user-written classifiers into TMVA (example application: NeuroBayes)
- Primary development from last Summer: Generalised classifiers
  Redesign of classifier creation and data handling to prepare:
  - Combine *any* classifier with *any other* classifier
  - Boost or bag any classifier
  - *Categorisation*: use *any* combination of input variables and classifiers in *any* phase space region
  - Redesign is ready – now in testing mode. Dispatched really soon ;-)

TMVA Users Guide !

Available on http://tmva.sf.net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TMVA
Toolkit for Multivariate Data Analysis with ROOT

Users Guide

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TMVA Users Guide
97pp, incl. code examples
arXiv physics/0703039

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Backup slides on:
(i) some illustrative toy examples
(ii) treatment of systematic uncertainties
(iii) sensitivity to weak input variables

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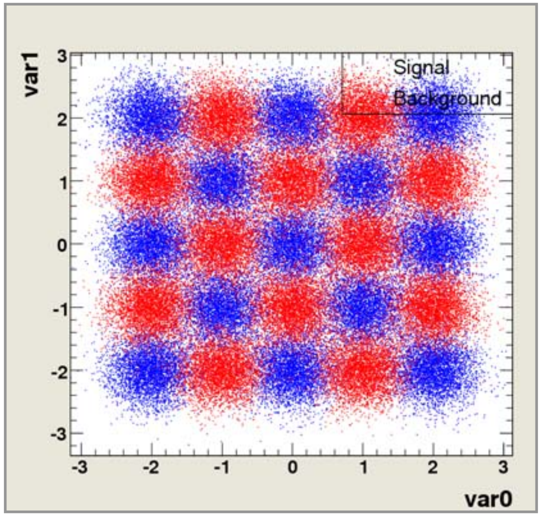
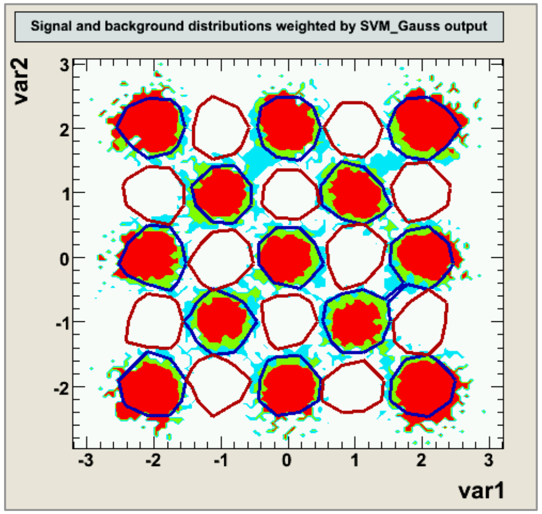
More Toy Examples

The “Schachbrett” Toy (chess board)

Event distribution

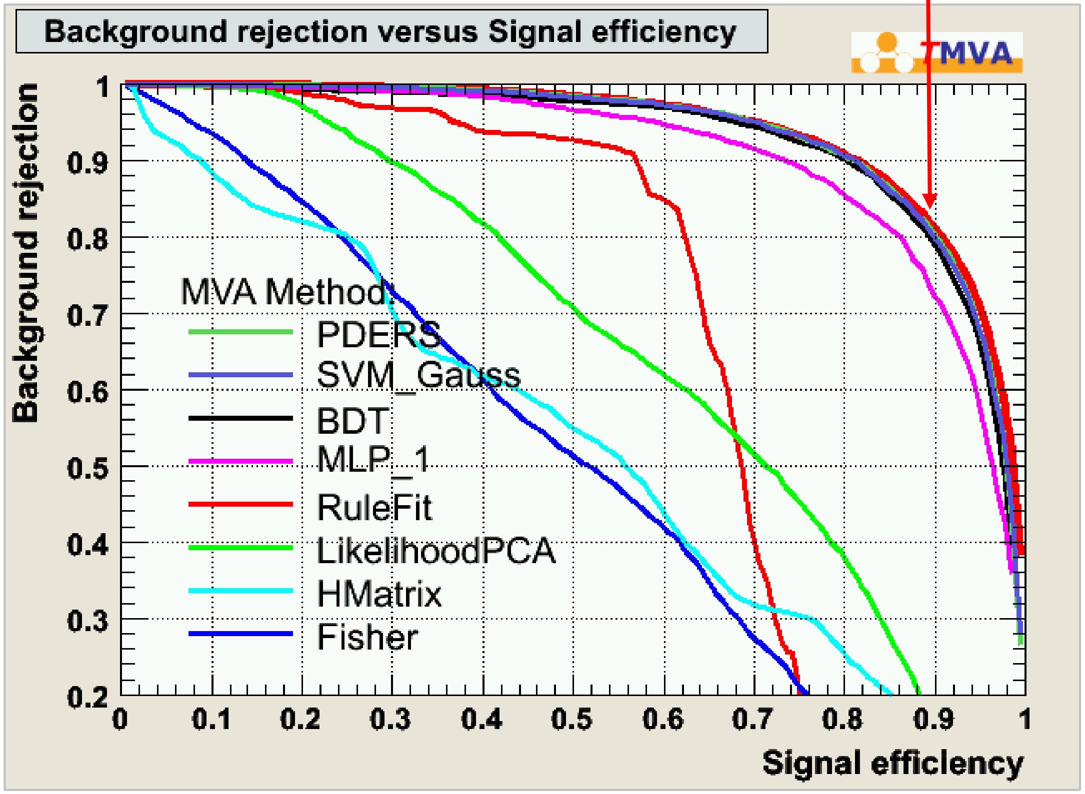


Events weighted by SVM response



- **Performance achieved without parameter tuning: PDERS and BDT best “out of the box” classifiers**
- **After some parameter tuning, also SVM und ANN(MLP) perform equally well**

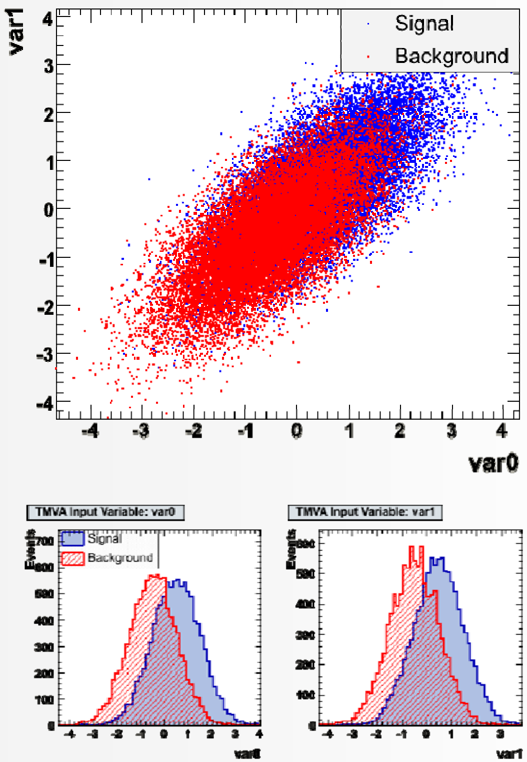
Theoretical maximum



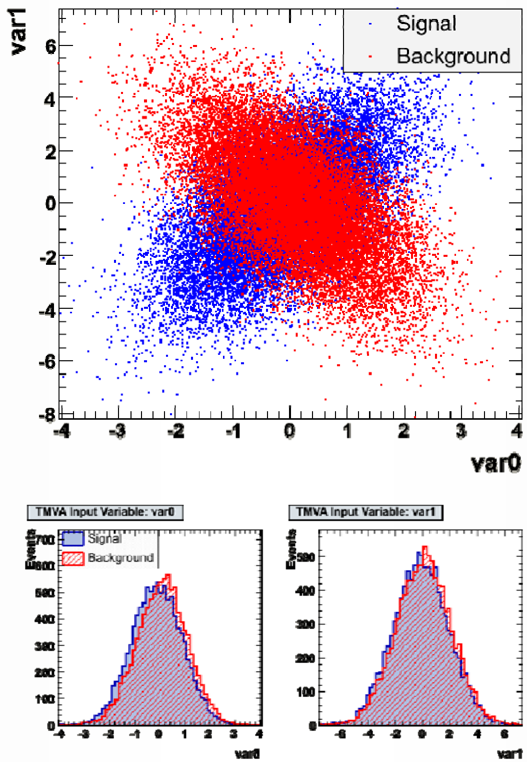
More Toys: Linear-, Cross-, Circular Correlations

- Illustrate the behaviour of linear and nonlinear classifiers

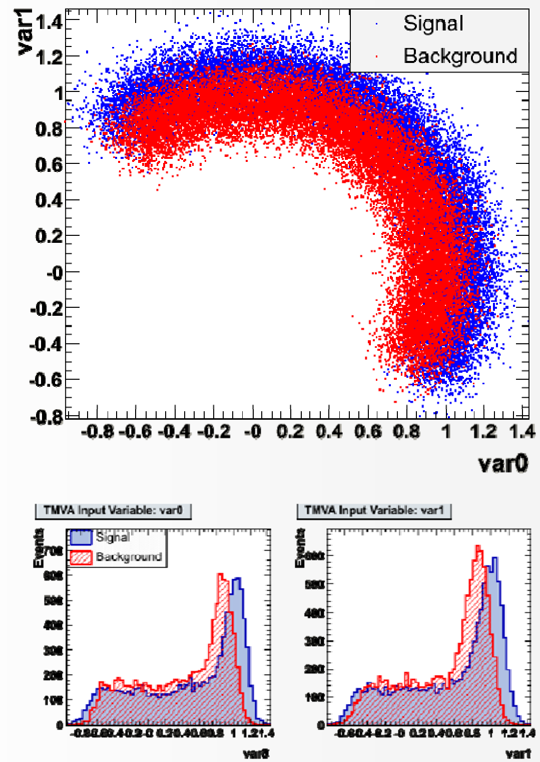
Linear correlations
(same for signal and background)



Linear correlations
(opposite for signal and background)



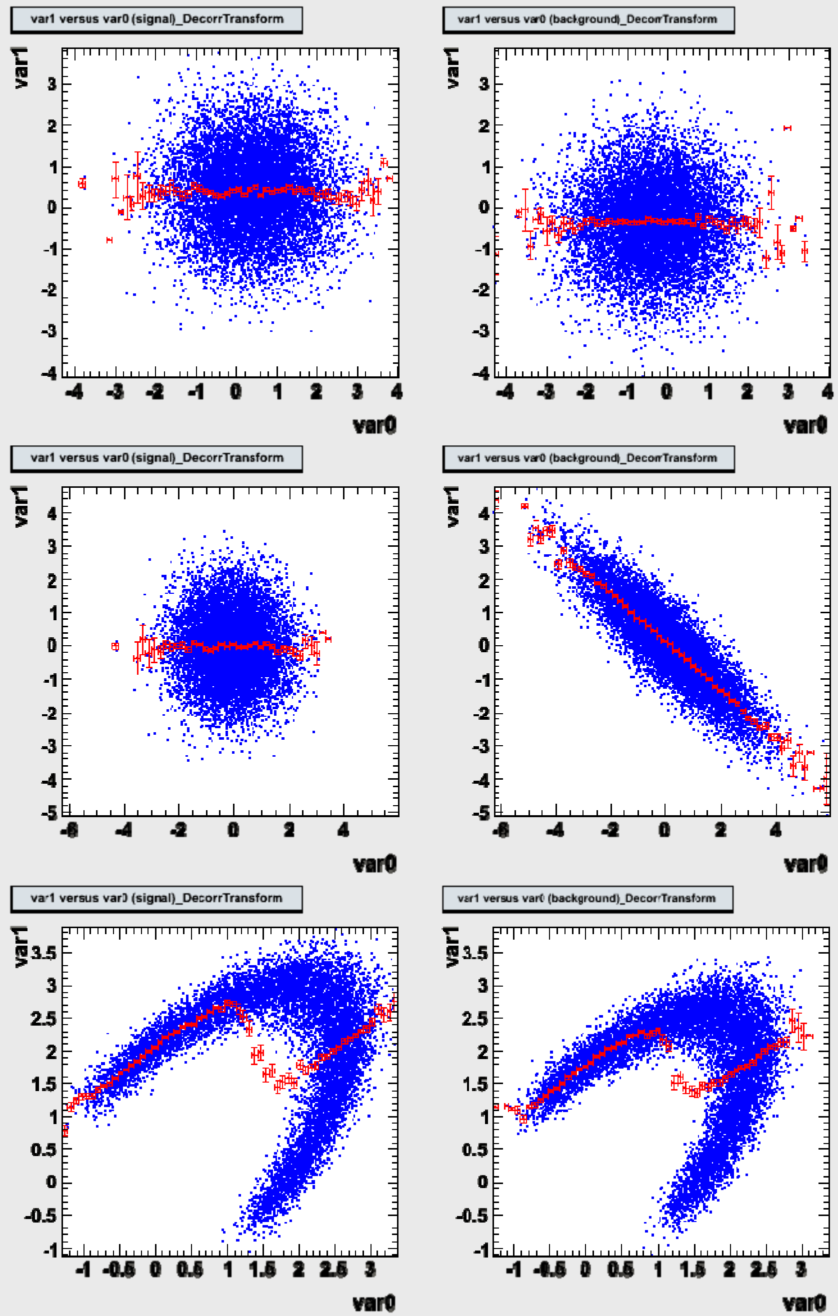
Circular correlations
(same for signal and background)



- How does linear decorrelation affect strongly nonlinear cases ?

Original correlations

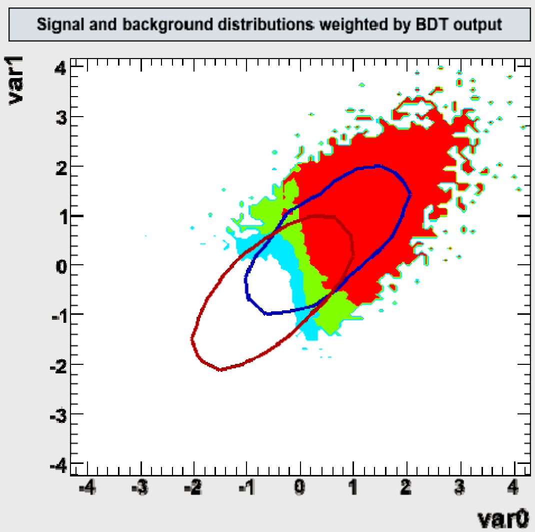
SQRT decorrelation



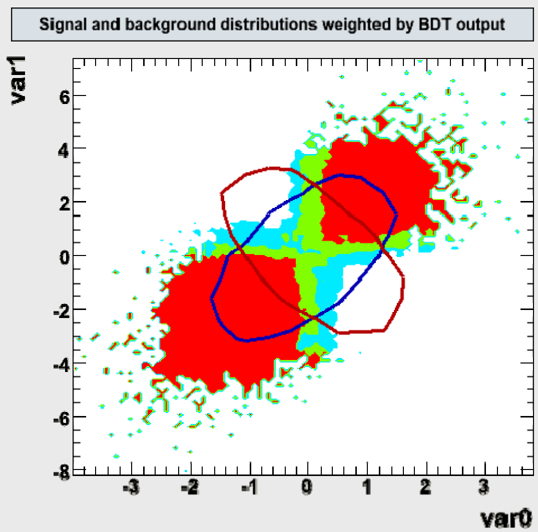
Weight Variables by Classifier Output

- How well do the classifier resolve the various correlation patterns ?

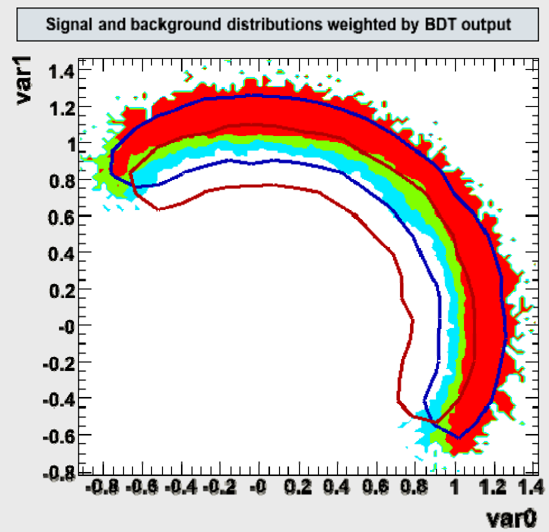
Linear correlations
(same for signal and background)



Cross-linear correlations
(opposite for signal and background)



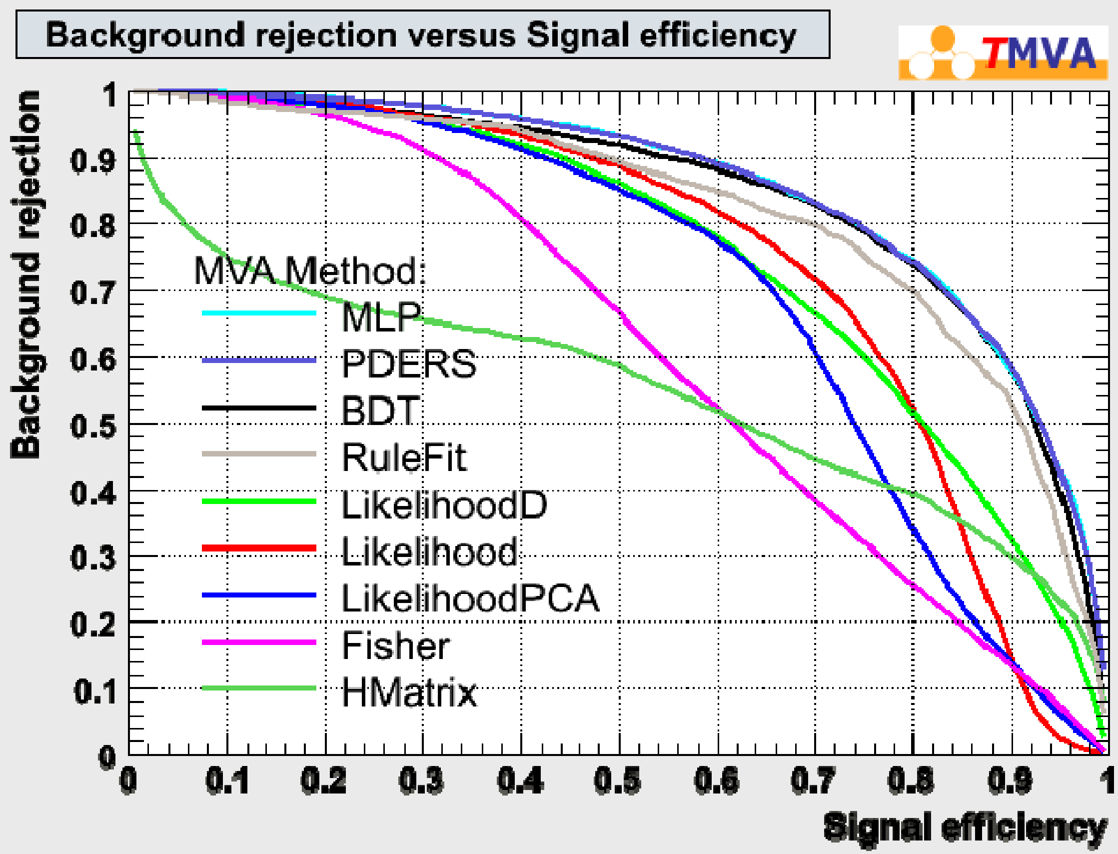
Circular correlations
(same for signal and background)



BDT

Final Classifier Performance

- Background rejection versus signal efficiency curve:

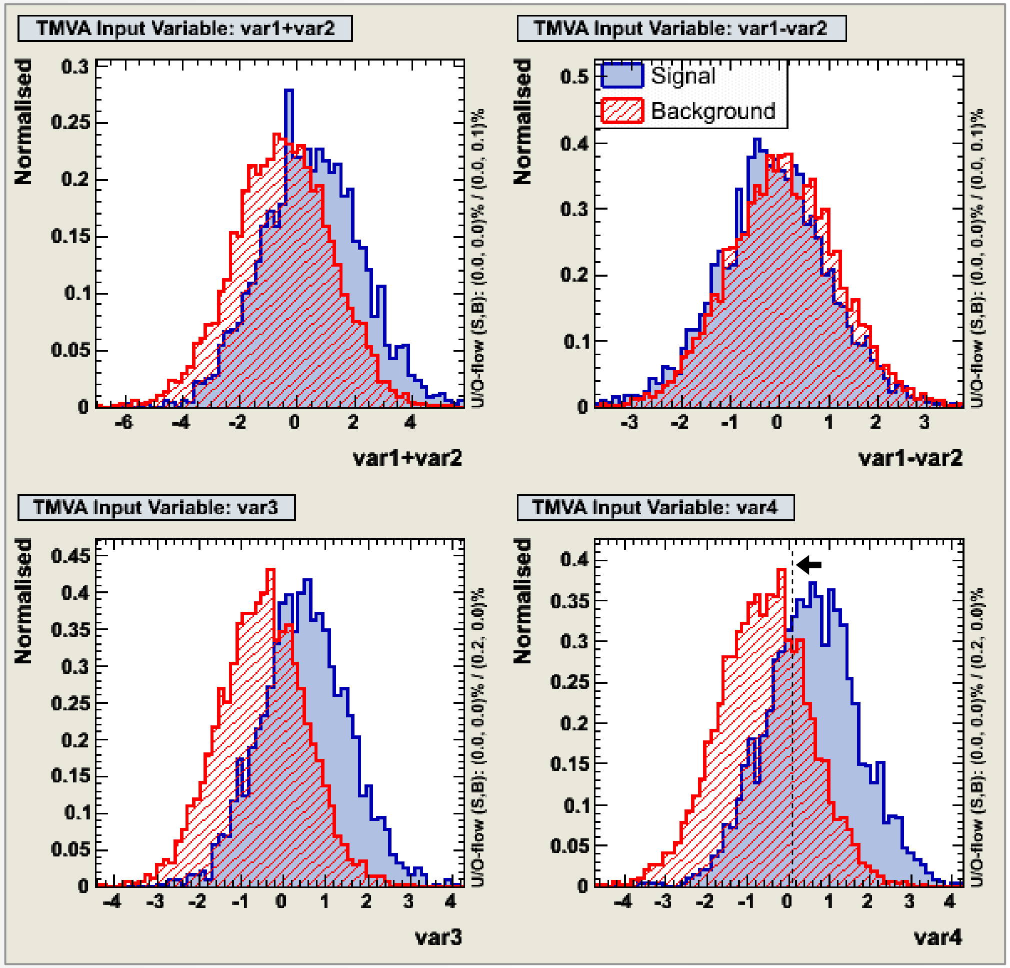


Circular Example

Some words on systematics

Treatment of Systematic Uncertainties

- Assume strongest variable “var4” suffers from systematic uncertainty



“Calibration uncertainty” may shift the central value and hence worsen the discrimination power of “var4”

Treatment of Systematic Uncertainties

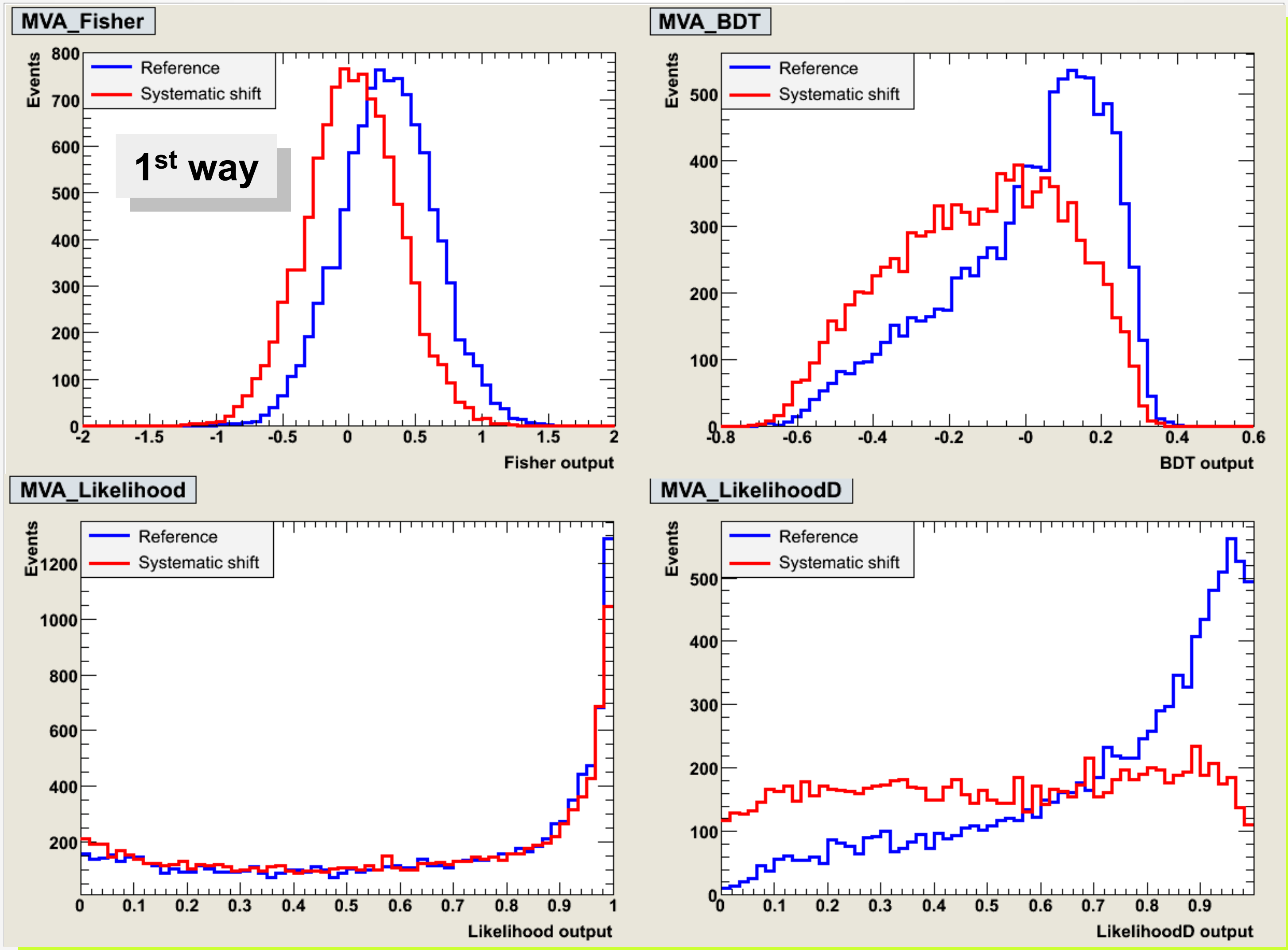
- Assume strongest variable “var4” suffers from systematic uncertainty
- (at least) Two ways to deal with it:

1. Ignore the systematic in the training, and evaluate systematic error on classifier output
   - Drawbacks:
     - “var4” appears stronger in training than it might be → suboptimal performance
     - Classifier response will strongly depend on “var4”
2. Train with shifted (= weakened) “var4”, and evaluate systematic error on classifier output
   - Cures previous drawbacks

- If classifier output distributions can be validated with data control samples, the second drawback is mitigated, but not the first one (the performance loss) !

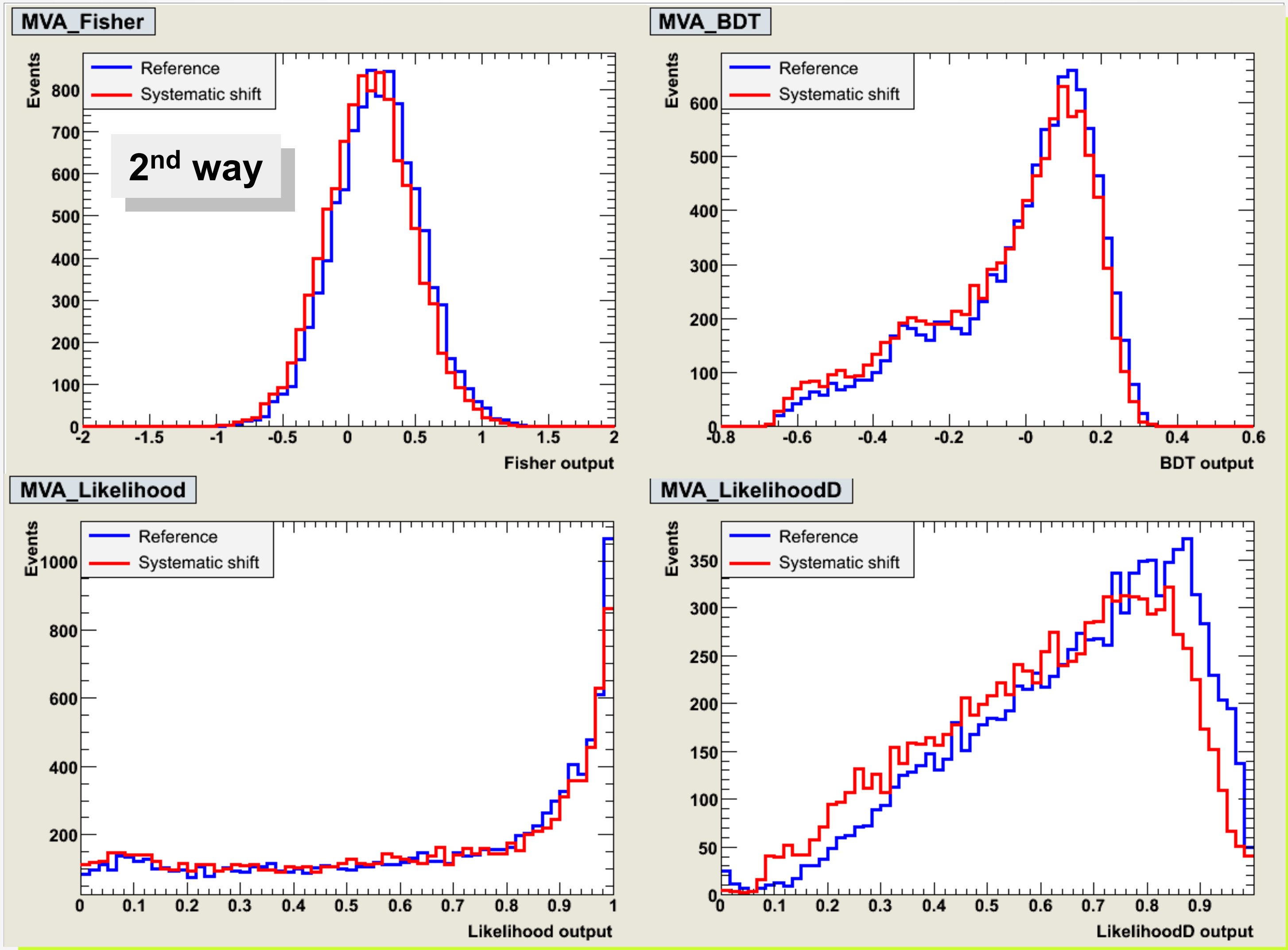
Treatment of Systematic Uncertainties

Classifier output distributions for signal only



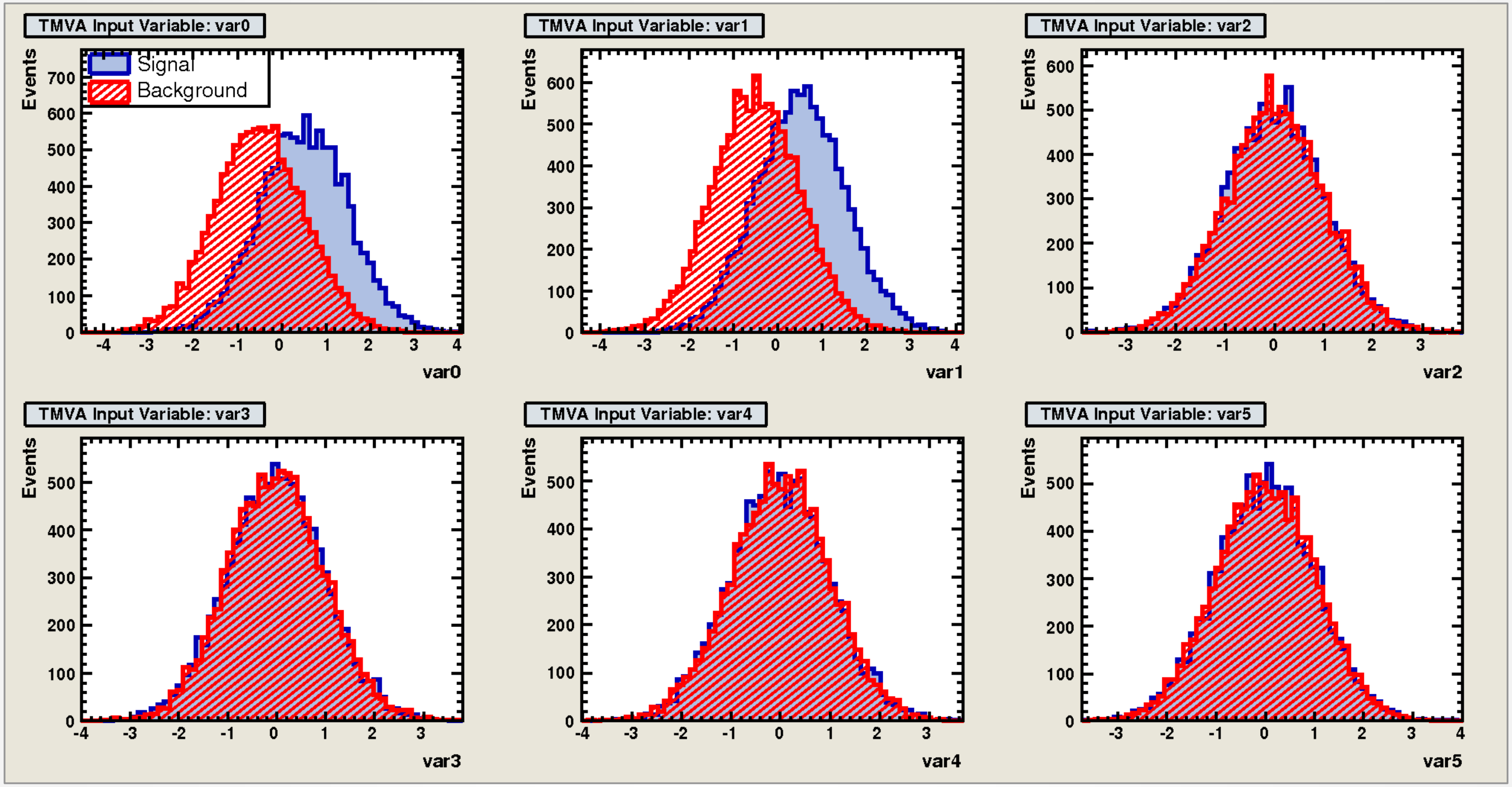
Treatment of Systematic Uncertainties

Classifier output distributions for signal only



Stability with Respect to Irrelevant Variables

- Toy example with 2 discriminating and 4 non-discriminating variables ?



Stability with Respect to Irrelevant Variables

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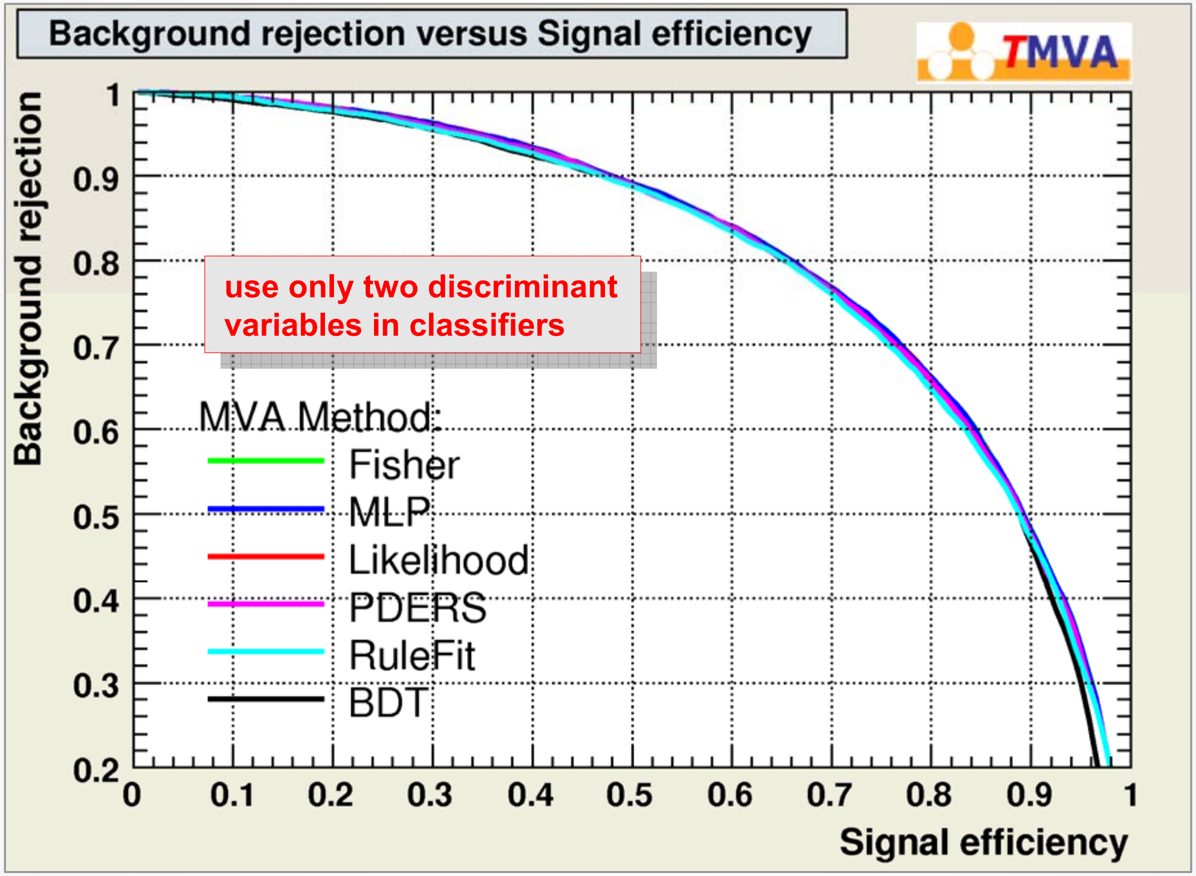

Stability with Respect to Irrelevant Variables

- Toy example with 2 discriminating and 4 non-discriminating variables ?