

Multivariate Data Analysis with **TMVA**

Andreas Hoecker^(*) (CERN)

Statistical Tools Workshop, DESY, Germany, June 19, 2008

(*) On behalf of the present core team: A. Hoecker, P. Speckmayer, J. Stelzer, H. Voss And the contributors: A. Christov, Or Cohen, Kamil Kraszewski, Krzysztof Danielowski, S. Henrot-Versillé, M. Jachowski, A. Krasznahorkay Jr., Maciej Kruk, Y. Mahalalel, R. Ospanov, X. Prudent, A. Robert, F. Tegenfeldt, K. Voss, M. Wolter, A. Zemla

See acknowledgments on page 43

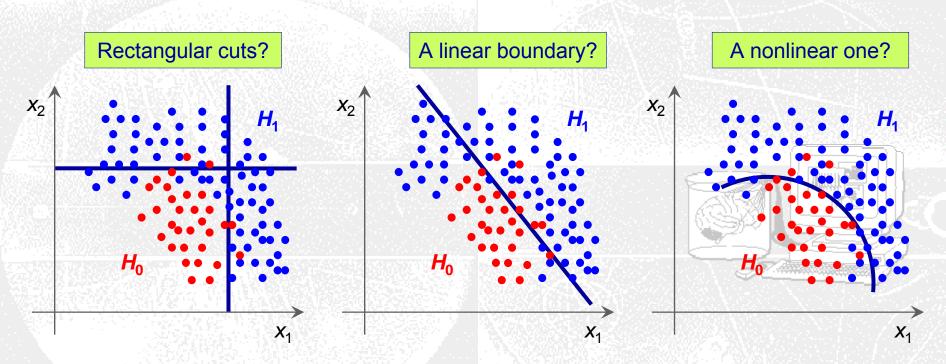
On the web: http://tmva.sf.net/ (home), https://w/kccern.ch/(wiki/bin/view/TMVA/WebHome (tutorial)

DESY, June 19, 2008

Event Classification

Suppose data sample with two types of events: H_0 , H_1

- We have found discriminating input variables $x_1, x_2, ...$
- What decision boundary should we use to select events of type H_1 ?

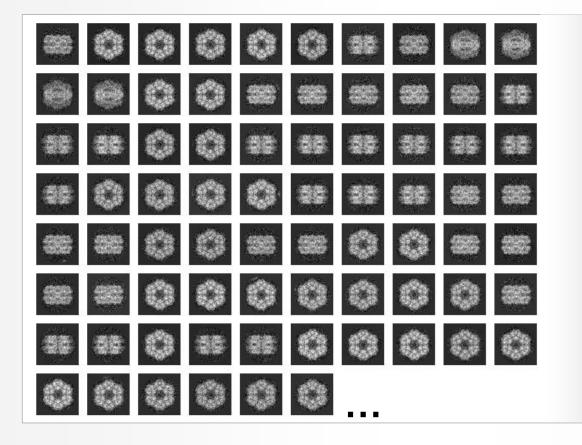


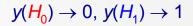
How can we decide this in an optimal way ? \rightarrow Let the machine learn it !

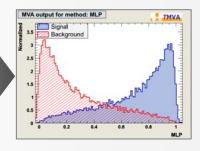


Multivariate Event Classification

- All multivariate classifiers have in common to condense (correlated) multi-variable input information in a single scalar output variable
 - It is a $R^n \rightarrow R$ regression problem; classification is in fact a *discretised regression*







MV regression is also interesting ! In work for TMVA !



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A. Hoecker — Multivariate Data Analysis with **T**MVA

What is **T**MVA

- 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 common data pre-processing capabilities
 - Train and 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

Эu	tline of this talk
	The T MVA project
-	Quick survey of available classifiers and processing steps
	Evaluation tools

TMVA

7MVA Development and Distribution

TMVA is a sourceforge (SF) package for world-wide access

- Home page<u>http://tmva.sf.net/</u>
- SF project page<u>http://sf.net/projects/tmva</u>
- View CVS<u>http://tmva.cvs.sf.net/tmva/TMVA/</u>
- Mailing list<u>http://sf.net/mail/?group_id=152074</u>
- Tutorial TWiki<u>https://twiki.cern.ch/twiki/bin/view/TMVA/WebHome</u>

Active project \rightarrow fast response time on feature requests

- Currently 4 core developers, and 16 active contributors
- >2400 downloads since March 2006 (not accounting cvs checkouts and ROOT users)
- Written in C++, relying on core ROOT functionality

Integrated and distributed with ROOT since ROOT v5.11/03

MVA

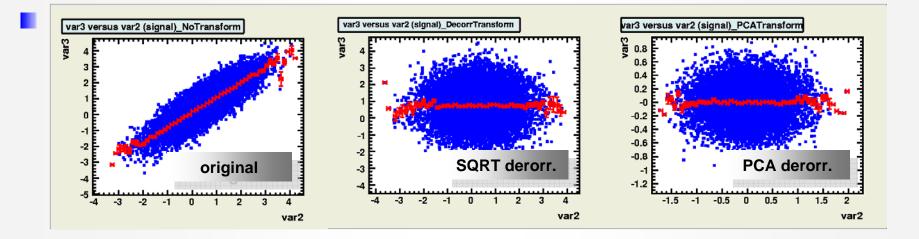
The TMVA Classifiers

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 automatic node pruning
- RuleFit
- Support Vector Machine
- Currently implemented data preprocessing stages:
 - Decorrelation
 - Principal Value Decomposition
 - Transformation to uniform and Gaussian distributions (coming soon)

Data Preprocessing: Decorrelation

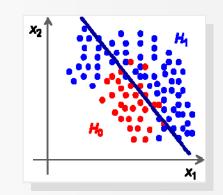
- Commonly realised for all methods in TMVA (centrally in DataSet class)
- Removal of linear correlations by rotating input variables
 - using the "square-root" of the correlation matrix
 - using the Principal Component Analysis



Rectangular Cut Optimisation

Simplest method: cut in rectangular variable volume

$$\boldsymbol{X}_{\text{cut}}\left(\boldsymbol{i}_{\text{event}}\right) \in \left\{\boldsymbol{0},\boldsymbol{1}\right\} = \bigcap_{\boldsymbol{v} \in \{\text{variables}\}} \left(\boldsymbol{X}_{\boldsymbol{v}}\left(\boldsymbol{i}_{\text{event}}\right) \subset \left[\boldsymbol{X}_{\boldsymbol{v},\min}, \boldsymbol{X}_{\boldsymbol{v},\max}\right]\right)$$



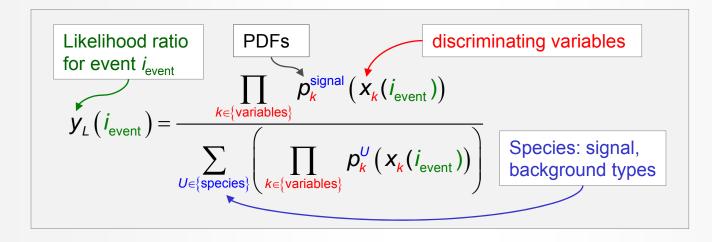
Technical challenge: how to find optimal cuts ?

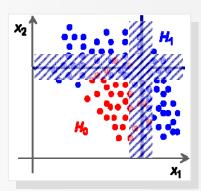
- MINUIT fails due to non-unique solution space
- TMVA uses: Monte Carlo sampling, Genetic Algorithm, Simulated Annealing
- Huge speed improvement of volume search by sorting events in binary tree

Cuts usually benefit from prior decorrelation of cut variables

Projective Likelihood Estimator (PDE Approach)

Much liked in HEP: probability density estimators for each input variable combined in likelihood estimator





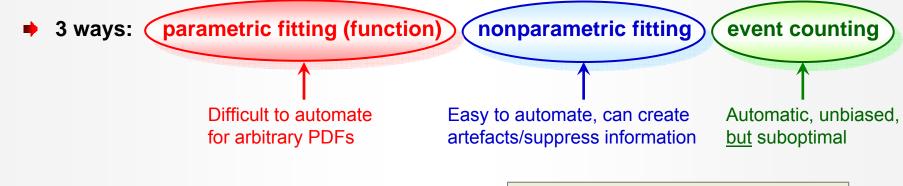
PDE introduces fuzzy logic

I Ignores correlations between input variables

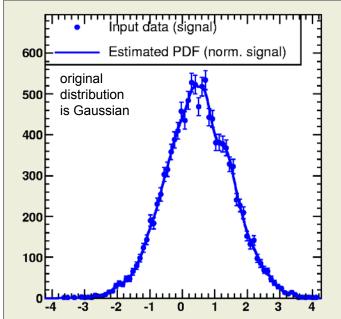
- Optimal approach if correlations are zero (or linear \rightarrow decorrelation)
- Otherwise: significant performance loss

PDE Approach: Estimating PDF Kernels

Technical challenge: how to estimate the PDF shapes



- We have chosen to implement <u>nonparametric fitting</u> in **T**MVA
 - Binned shape interpolation using spline functions and adaptive smoothing
 - Unbinned adaptive kernel density estimation (KDE) with Gaussian smearing
 - TMVA performs automatic validation of goodness-of-fit

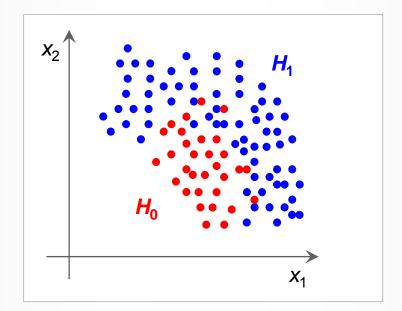


Multidimensional PDE Approach

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)

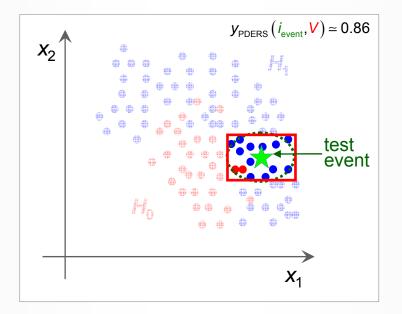


Multidimensional PDE Approach

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Carli-Koblitz, NIM A501, 576 (2003)



Improve y_{PDERS} estimate within V by using various N_{var} -D kernel estimators

Enhance speed of event counting in volume by binary tree search

k-Nearest Neighbor

Better than searching within a volume (fixed or floating), count adjacent reference events till statistically significant number reached

- Method intrinsically adaptive
- Very fast search with kd-tree event sorting

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 Classifier response couldn't be simpler: \$\mathcal{Y}_{Fi}(i_{event}) = F_0 + \sum_{k \text{variables}} x_k(i_{event}) \cdot F_k\$ (Figure 1)

- Compute Fisher coefficients from signal and background covariance matrices
- Fisher requires distinct sample means between signal and background
- Optimal classifier for linearly correlated Gaussian-distributed variables

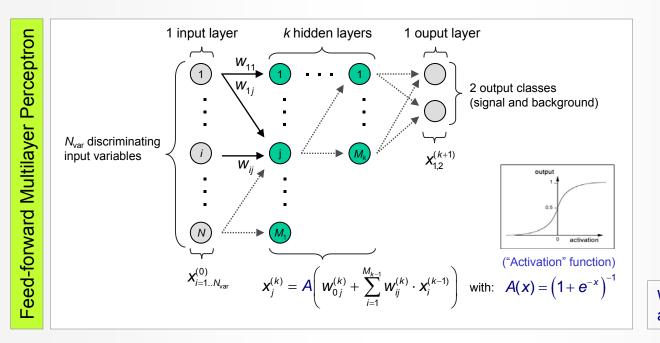
Function discriminant analysis (FDA)

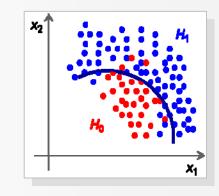
Fit any user-defined function of input variables requiring that signal events return $\rightarrow 1$ and background $\rightarrow 0$

- 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





Weight adjustment using analytical back-propagation

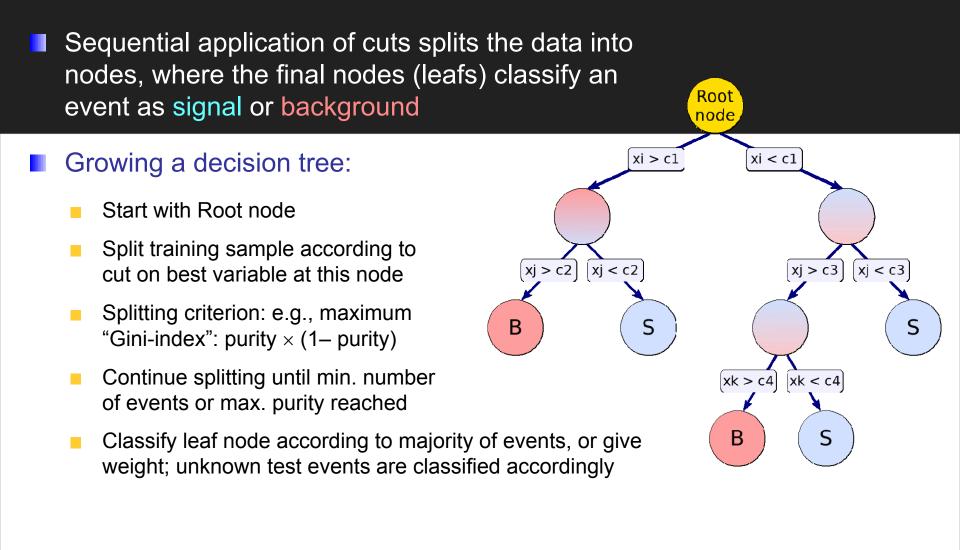
Three different implementations in TMVA (all are Multilayer Perceptrons)

- **TMIPANN:** Interface to ROOT's MLP implementation
- MLP: TMVA's own MLP implementation for increased speed and flexibility
- CFMIpANN: ALEPH's Higgs search ANN, translated from FORTRAN

Decision Trees

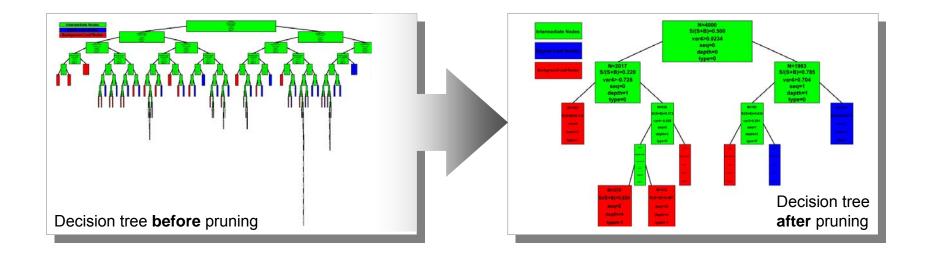
Sequential application of cuts splits the data into nodes, where the final nodes (leafs) classify an event as signal or background X_2

Decision Trees



Decision Trees

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



Bottom-up "pruning" of a decision tree

Remove statistically insignificant nodes to reduce tree overtraining

Boosted Decision Trees (BDT)

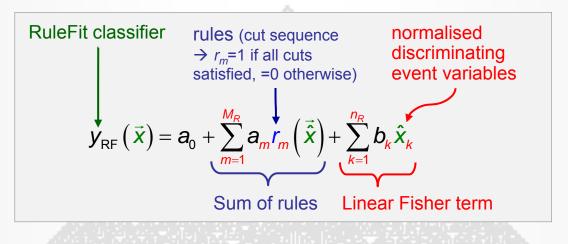
- Data mining with decision trees is popular in science (so far mostly outside of HEP)
 - Advantages:
 - Independent of monotonous variable transformations, immune against outliers
 - Weak variables are ignored (and don't (much) deteriorate performance)
 - Shortcomings:
 - Instability: small changes in training sample can dramatically alter the tree structure
 - Sensitivity to overtraining (\rightarrow requires pruning)
- Boosted decision trees: combine forest of decision trees, with differently weighted events in each tree (trees can also be weighted), by majority vote
 - e.g., "AdaBoost": incorrectly classified events receive larger weight in next decision tree
 - Bagging" (instead of boosting): random event weights, resampling with replacement
 - Boosting or bagging are means to create set of "basis functions": the final classifier is linear combination (*expansion*) of these functions → improves stability !

Predictive Learning via Rule Ensembles (RuleFit)

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



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.)

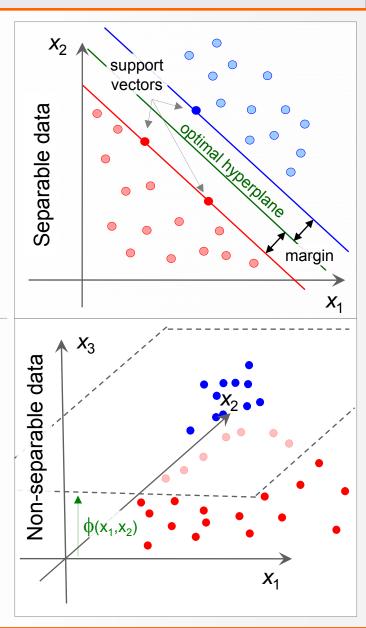
Pruning removes topologically equal rules" (same variables in cut sequence)

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=00011110₂.

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

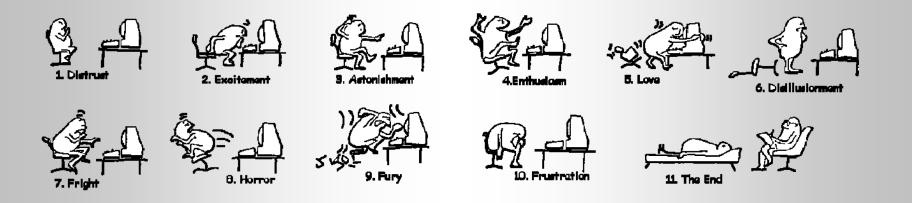
- Non-linear cases:
 - Transform variables into higher dim. space where a linear boundary can fully separate the data
 - Explicit transformation not required: use kernel functions to approximate scalar products between transformed vectors in the higher dim. space
 - Choose Kernel and fit the hyperplane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



Using TMVA

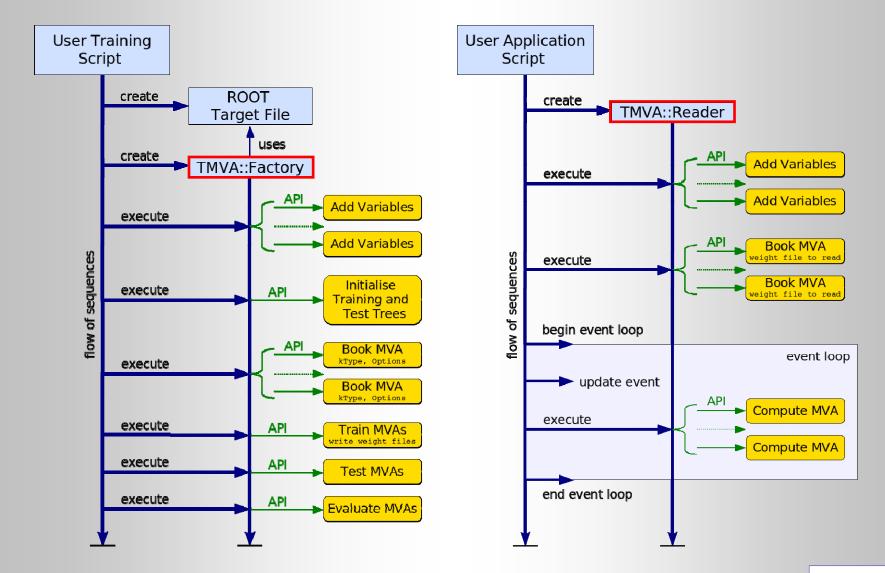
A typical *T*MVA analysis consists of two main steps:

- 1. Training phase: training, testing and evaluation of classifiers using data samples with known signal and background composition
- 2. Application phase: using selected trained classifiers to classify unknown data samples
- Illustration of these steps with toy data samples



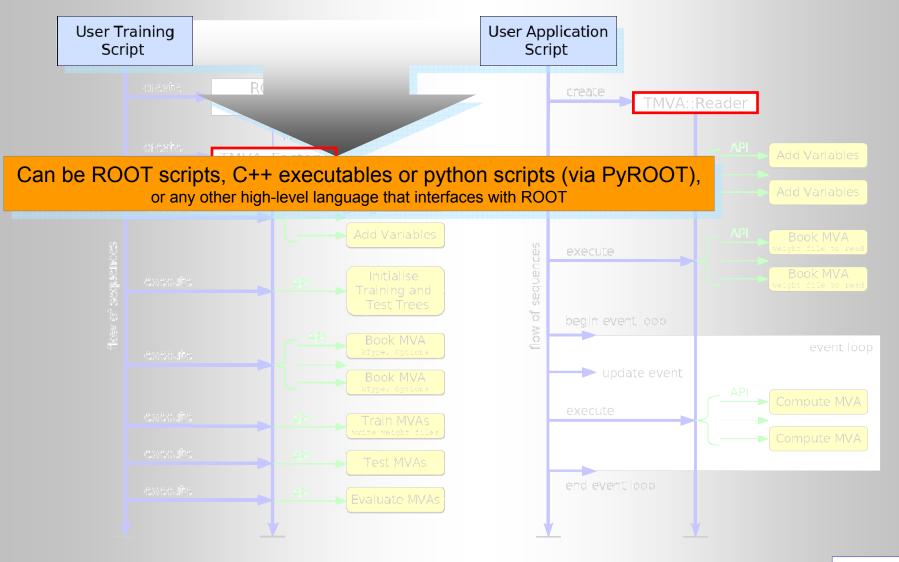
→ TMVA tutorial

Code Flow for Training and Application Phases



→ TMVA tutorial

Code Flow for Training and Application Phases



→ TMVA tutorial

A Simple Example for *Training*

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");

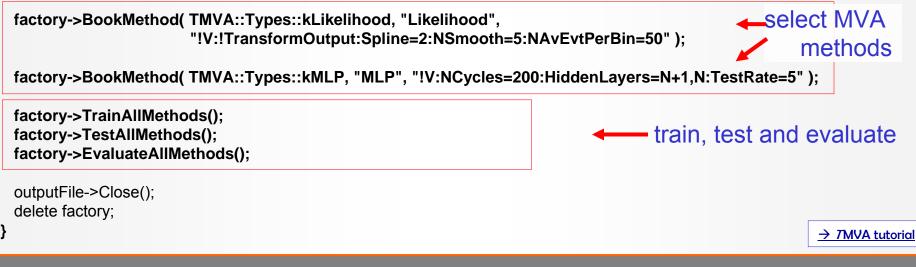
```
factory->AddSignalTree ((TTree*)input->Get("TreeS"), 1.0);
factory->AddBackgroundTree ((TTree*)input->Get("TreeB"), 1.0);
```

factory->AddVariable("var1+var2", 'F'); factory->AddVariable("var1-var2", 'F'); factory->AddVariable("var3", 'F'); factory->AddVariable("var4", 'F'); give training/test trees

- create *Factory*

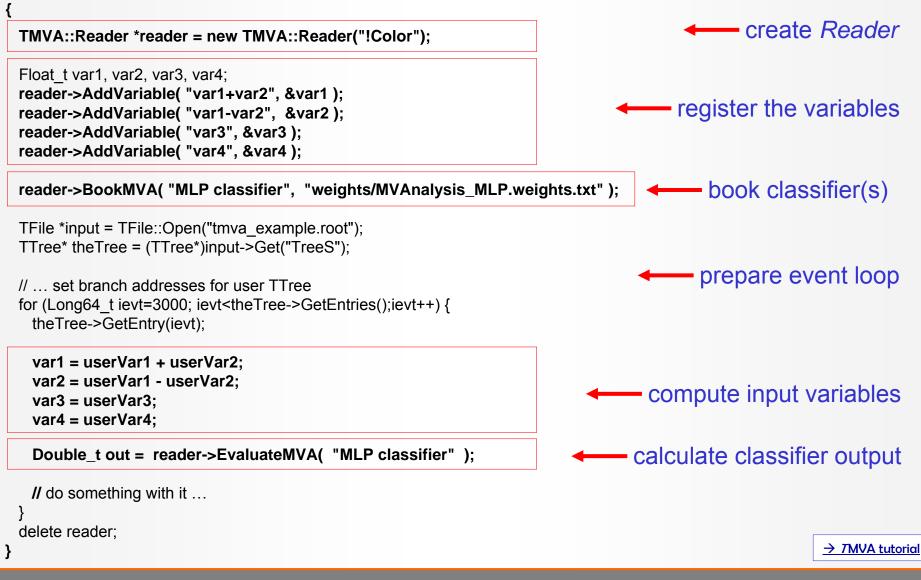
register input variables

factory->PrepareTrainingAndTestTree("", "NSigTrain=3000:NBkgTrain=3000:SplitMode=Random:!V");



A Simple Example for an Application

void TMVApplication()



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

Preprocessing of input variables (e.g., decorrelation)

MVA Evaluation Framework

TMVA is not only a collection of classifiers, but an MVA framework

After training, TMVA provides ROOT evaluation scripts (through GUI)

🔀 TMVA Plotting Macros
(1a) Input Variables
(1b) Decorrelated Input Variables
(1c) PCA-transformed Input Variables
(2a) Input Variable Correlations (scatter profiles)
(2b) Decorrelated Input Variable Correlations (scatter profiles)
(2c) PCA-transformed Input Variable Correlations (scatter profiles)
(3) Input Variable Linear Correlation Coefficients
(4a) Classifier Output Distributions
(4b) Classifier Output Distributions for Training and Test Samples
(4c) Classifier Probability Distributions
(4d) Classifier Rarity Distributions
(5a) Classifier Cut Efficiencies
(5b) Classifier Background Rejection vs Signal Efficiency (ROC curve)
(6) Likelihood Reference Distributiuons
(7a) Network Architecture
(7b) Network Convergence Test
(8) Decision Trees
(9) PDFs of Classifiers
(10) Rule Ensemble Importance Plots
(11) Quit

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

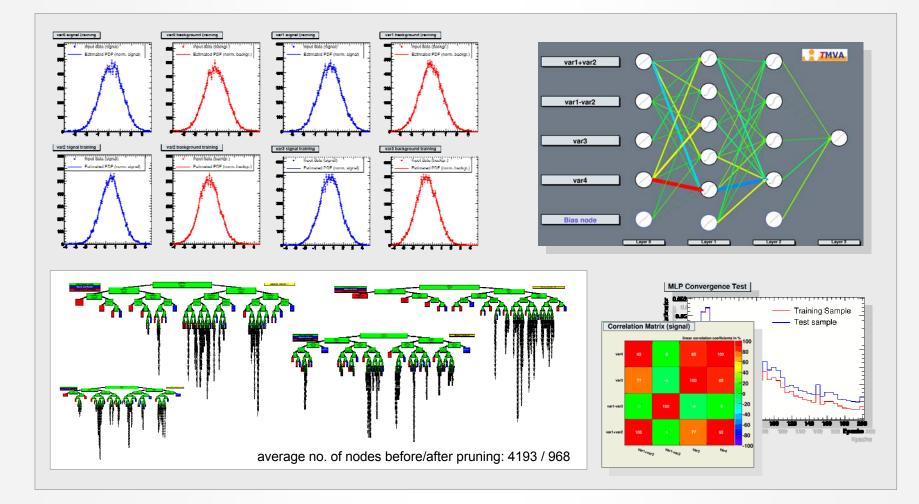
B rejection versus S efficiency

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

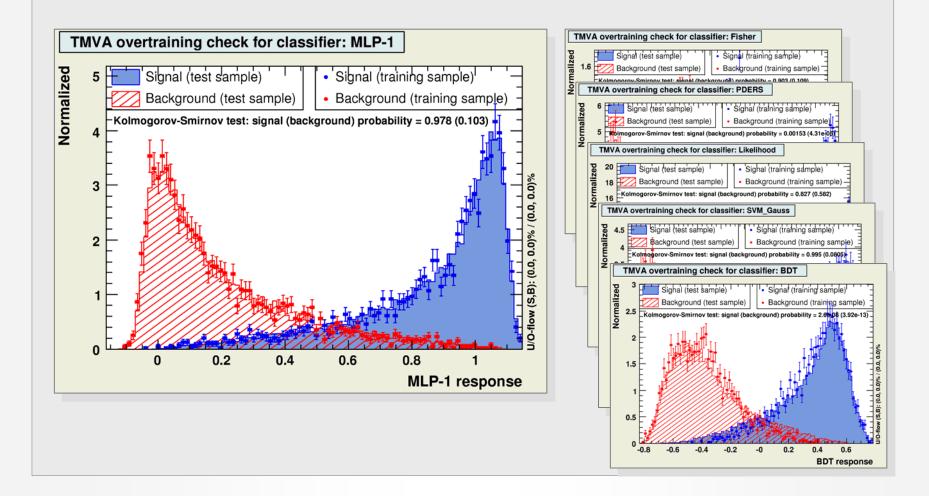
Evaluating the Classifier Training (I)

Projective likelihood PDFs, MLP training, BDTs, ...

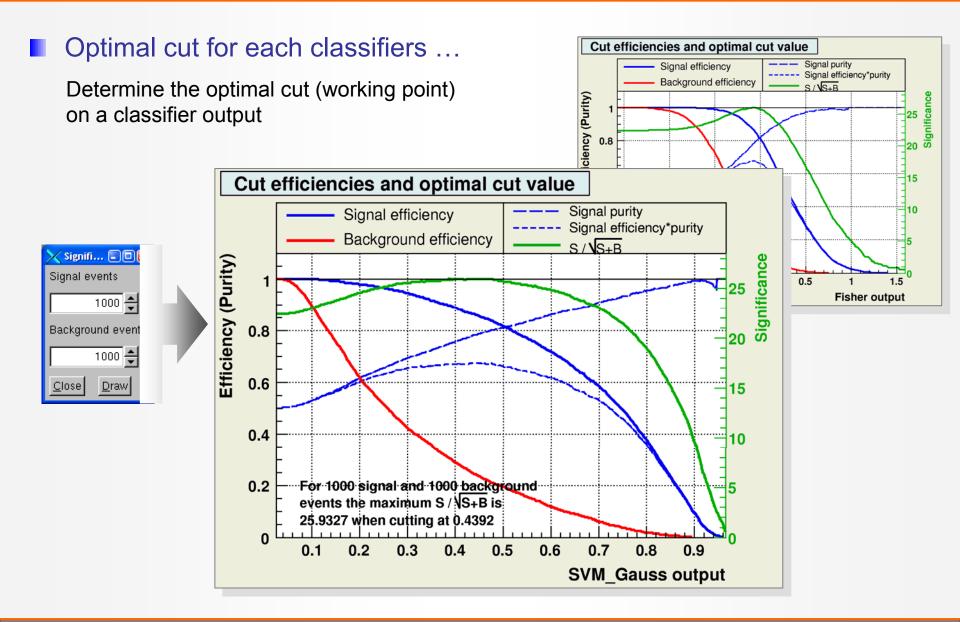


Evaluating the Classifier Training (II)

Classifier output distributions for test and training samples ...

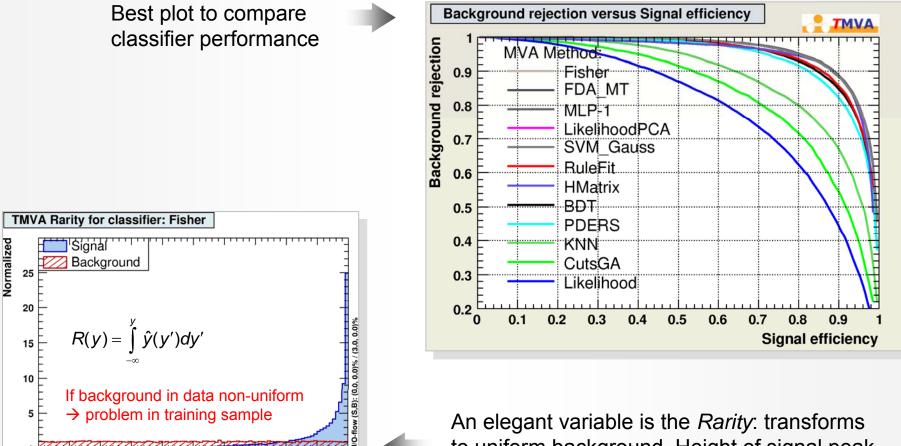


Evaluating the Classifier Training (III)



Evaluating the Classifier Training (IV)

Background rejection versus signal efficiencies ...



02

0.4

0.5

0.6

0.7

0.8

0.9

Signal rarity

Evaluating the Classifiers (taken from 7MVA 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 (a

MVA Methods:	Signal eff @B=0.01	iciency at @B=0.10	bkg eff. (e @B=0.30	rror): Area	Sepa- ration:	Signifi- cance:
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



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Better classifier

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Evaluating the Classifiers (taken from 7MVA output...)

MVA	Signal eff	iciency at	bkg eff. (e	rror):	Sepa-	Signifi-
Methods:	@B=0.01	@B=0.10	@B=0.30	Area	ration:	cance:
Fisher MLP LikelihoodD PDERS RuleFit HMatrix BDT	: 0.268(03) : 0.266(03) : 0.259(03) : 0.223(03) : 0.196(03) : 0.058(01) : 0.154(02)	0.653(03) 0.656(03) 0.649(03) 0.628(03) 0.607(03) 0.622(03) 0.594(04)	0.873(02) 0.873(02) 0.871(02) 0.861(02) 0.845(02) 0.868(02) 0.838(03)	0.882 0.882 0.880 0.870 0.870 0.859 0.855 0.852	0.444 0.444 0.441 0.417 0.390 0.410 0.380	1.189 1.260 1.251 1.192 1.092 1.093 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

Testing efficiency compared to training efficiency (overtraining check)

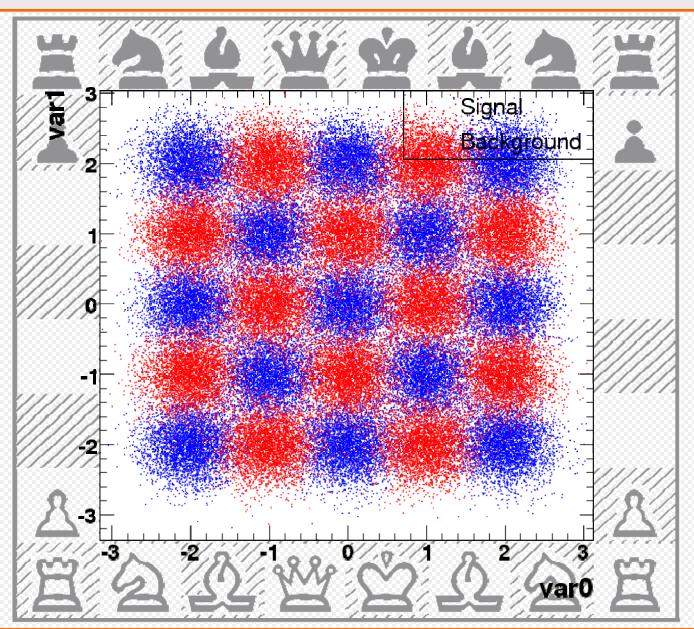
_	MVA	Signal efficiency:	from test sample	(from traing sample)		
	Methods:	@B=0.01	@B=0.10	@B=0.30		
Check or over- –	Fisher MLP LikelihoodD PDERS RuleFit HMatrix BDT CutsGA Likelihood	<pre>: 0.268 (0.275) : 0.266 (0.278) : 0.259 (0.273) : 0.223 (0.389) : 0.196 (0.198) : 0.058 (0.060) : 0.154 (0.268)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

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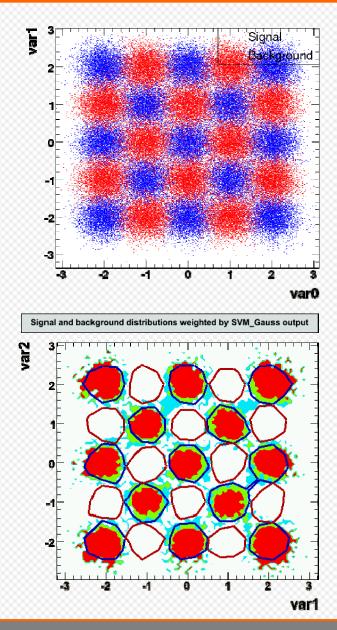
Better classifier

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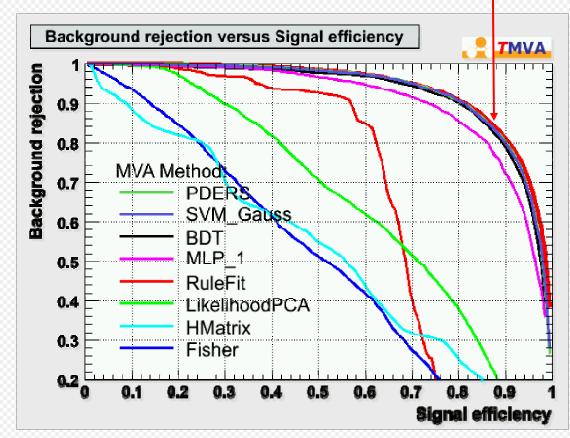
The "Schachbrett" Toy



The "Schachbrett" Toy



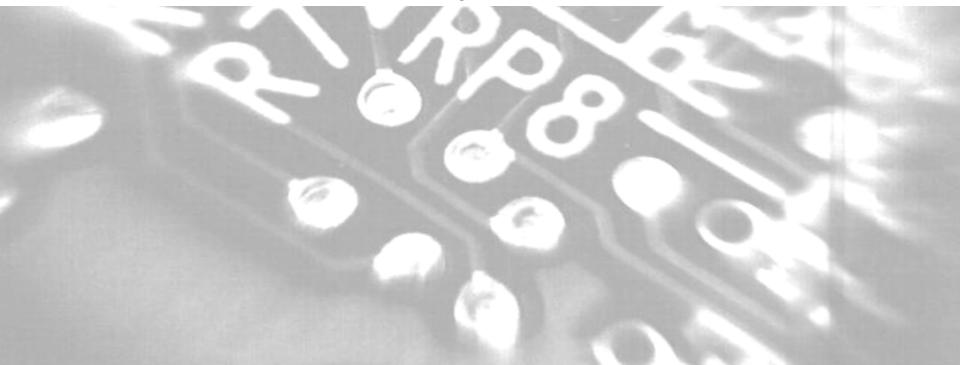
- Performance achieved without parameter tuning: PDERS and BDT best "out of the box" classifiers
- After specific tuning, also SVM und MLP perform well



Theoretical maximum

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Summary & Plans



TMVA

Summary of the Classifiers and their Properties

Criteria		Classifiers								
		Cuts	Likeli- hood	PDERS / k-NN	H-Matrix	Fisher	MLP	BDT	RuleFit	SVM
Perfor- mance	no / linear correlations	:		\odot		\odot	\odot		\odot	
	nonlinear correlations		\bigotimes	\odot	$\overline{\mathbf{S}}$	$\overline{\mathbf{S}}$	\odot	\odot		\odot
Speed	Training	8			\odot	\odot		8	æ	8
	Response	\odot		8/9		\odot	\odot		÷	
Robust -ness	Overtraining	\odot			\odot	\odot	8	8		
	Weak input variables	\odot	\odot	$\overline{\mathbf{S}}$	\odot	\odot			e	(
Curse of dimensionality			\odot	$\overline{\mathbf{S}}$	\odot	\odot		\odot	()	(
Transparency		\odot	\odot	(\odot	\odot	\bigotimes	\bigotimes	end on the chos	\bigotimes

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

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Outlook

Primary development from last Summer: Generalised classifiers

- Combine any classifier with any other classifier using any combination of input variables in any phase space region
- Be able to boost or bag any classifier
- Categorisation: use any combination of input variables and classifiers in any phase space region
- Code is ready now in testing mode. Dispatched soon hopefully...

This summer: Extend TMVA to multivariate

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

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regression

<u>advert isement</u>

We have a Users Guide

Available on http://tmva.sf.net

arXiv physics/0703039 CERN-OPEN-2007-007 Document version 4 TMVA version 3.8 June 19, 2007 http://tmva.sf.net

TMVA Toolkit for Multivariate Data Analysis with ROOT

Users Guide

A. Höcker, P. Speckmayer, J. Stelzer, F. Tegenfeldt, H. Voss, K. Voss

With contributions from

A. Christov, S. Henrot-Versillé, M. Jachowski, A. Krasznahorkay Jr., Y. Mahalalel, R. Ospanov, X. Prudent, M. Wolter, A. Zemla

7MVA Users Guide 97pp, incl. code examples arXiv <u>physics</u>/0703039

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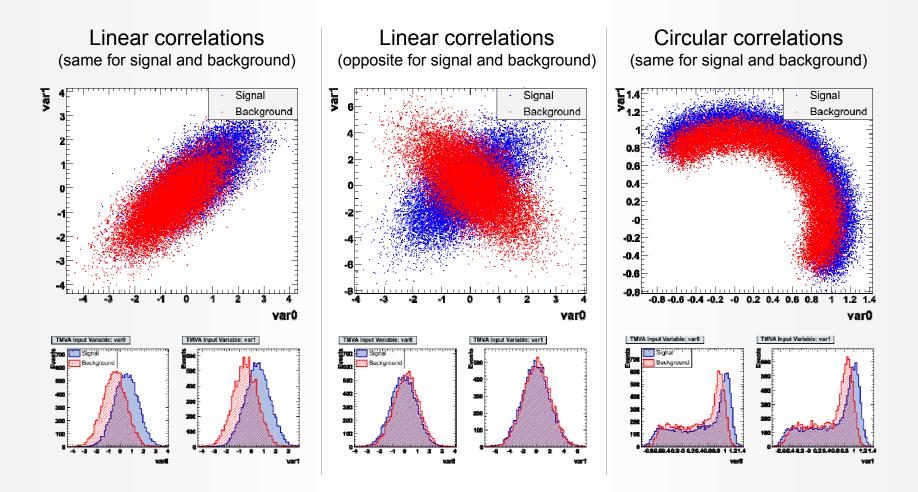
- **T**MVA is open source software
- Use & redistribution of source permitted according to terms in <u>BSD license</u>
- Several similar data mining efforts with rising importance in most fields of science and industry
- Important for HEP:
 - Parallelised MVA training and evaluation pioneered by Cornelius package (BABAR)
 - Also frequently used: *StatPatternRecognition* package by I. Narsky
 - Many implementations of individual classifiers exist

Acknowledgments: The fast development of TMVA would not have been possible without the contribution and feedback from many developers and users to whom we are indebted. We thank in particular the CERN Summer students Matt Jachowski (Stanford) for the implementation of TMVA's new MLP neural network, Yair Mahalalel (Tel Aviv) and three genius Krakow mathematics students for significant improvements of PDERS, the Krakow student Andrzej Zemla and his supervisor Marcin Wolter for programming a powerful Support Vector Machine, as well as Rustem Ospanov for the development of a fast k-NN algorithm. We are grateful to Doug Applegate, Kregg Arms, René Brun and the ROOT team, Tancredi Carli, Zhiyi Liu, Elzbieta Richter-Was, Vincent Tisserand and Alexei Volk for helpful conversations.

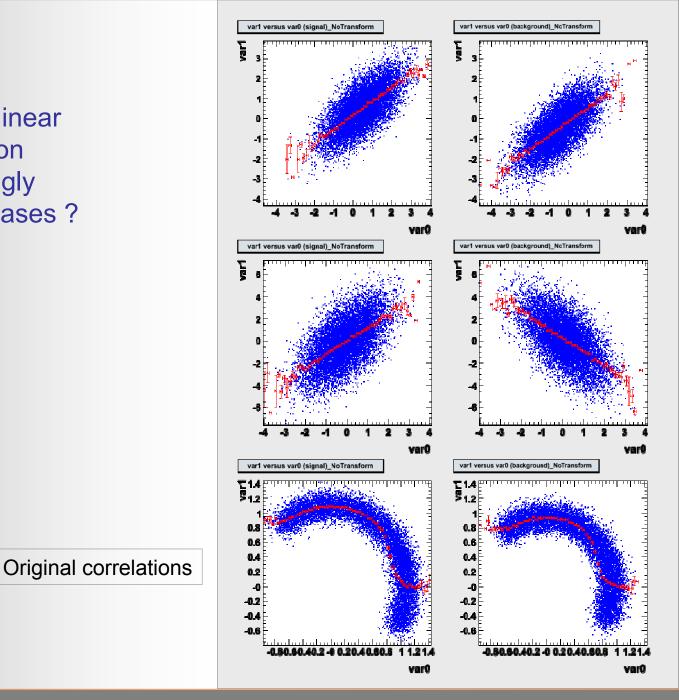
More Toy Examples

More Toys: Linear-, Cross-, Circular Correlations

Illustrate the behaviour of linear and nonlinear classifiers



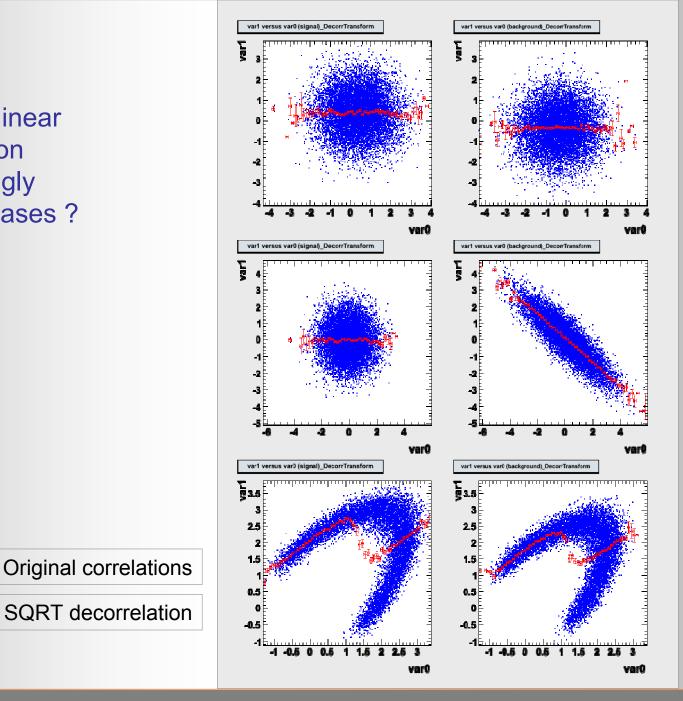
How does linear decorrelation affect strongly nonlinear cases ?



DESY, June 19, 2008

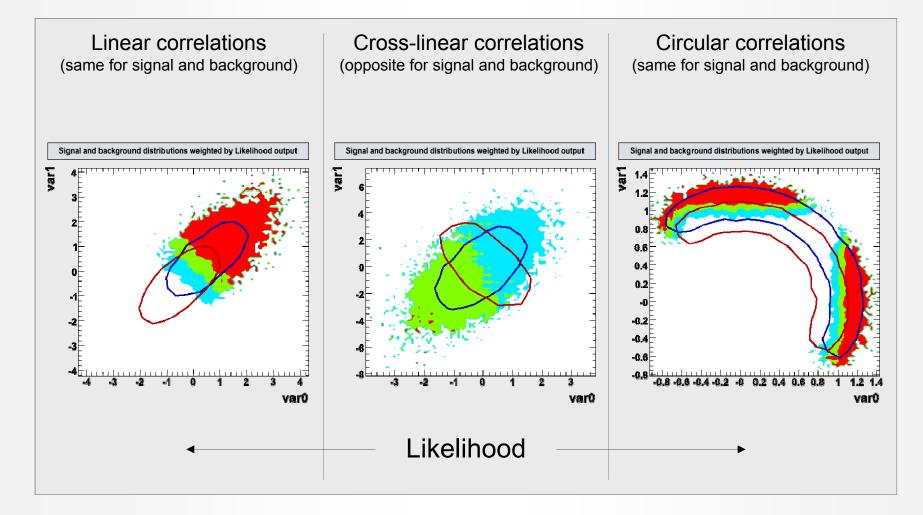
A. Hoecker — Multivariate Data Analysis with TMVA

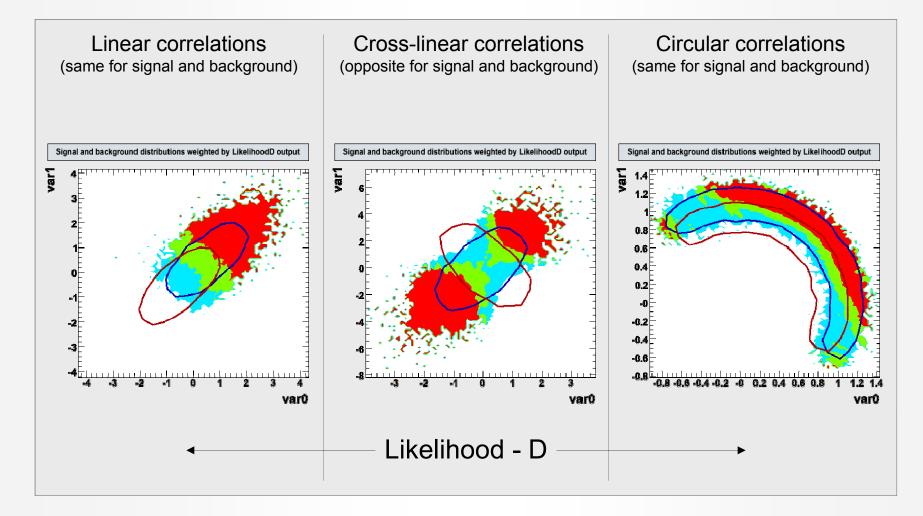
How does linear decorrelation affect strongly nonlinear cases ?

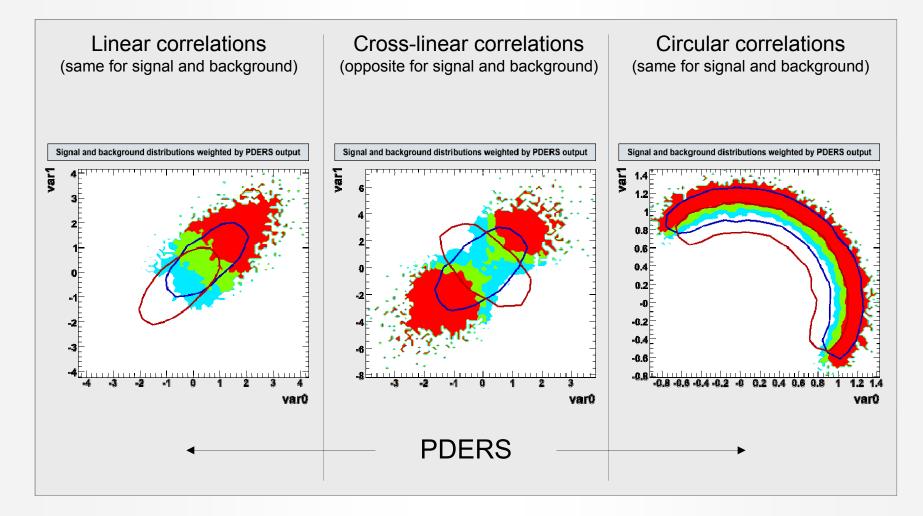


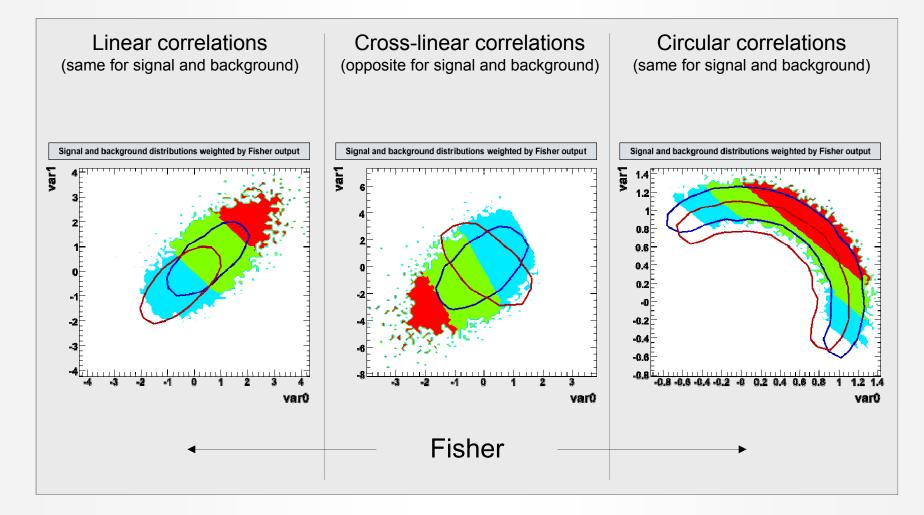
DESY, June 19, 2008

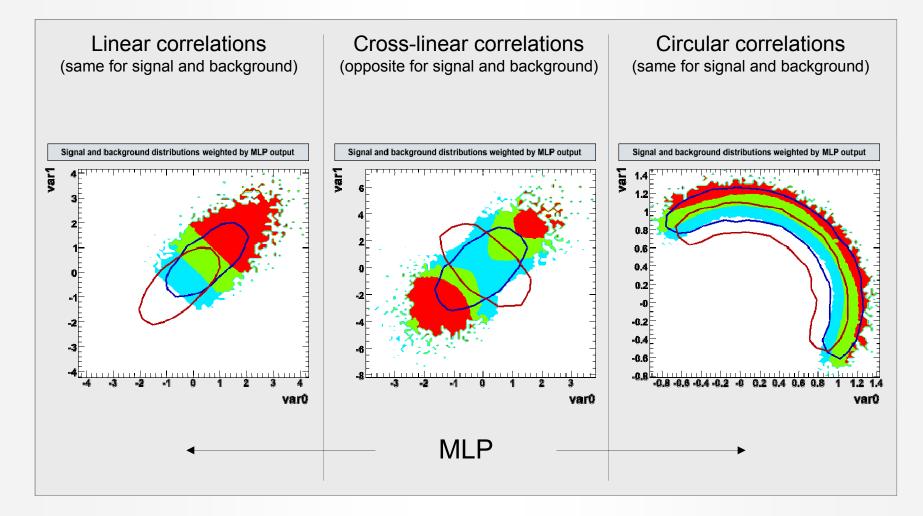
A. Hoecker — Multivariate Data Analysis with TMVA

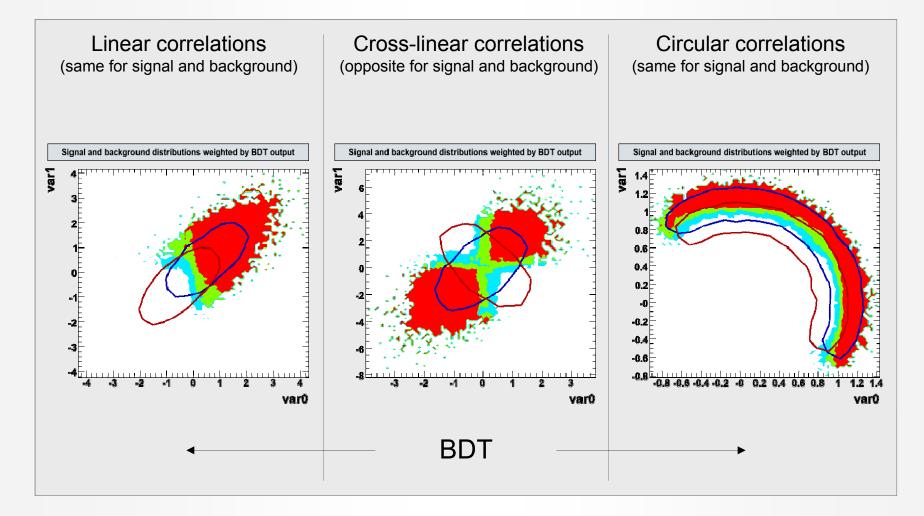






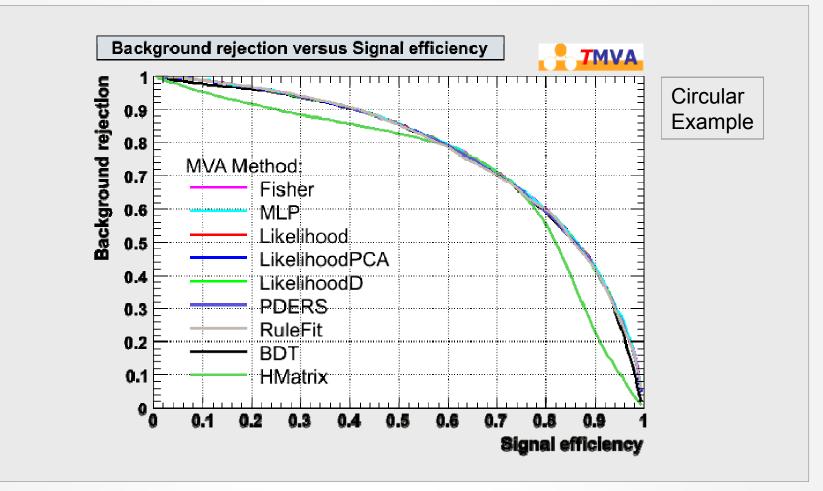






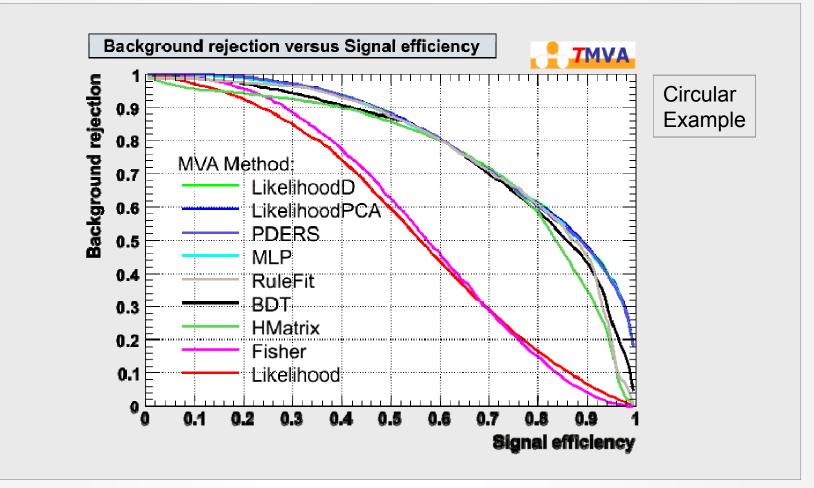
Final Classifier Performance

Background rejection versus signal efficiency curve:



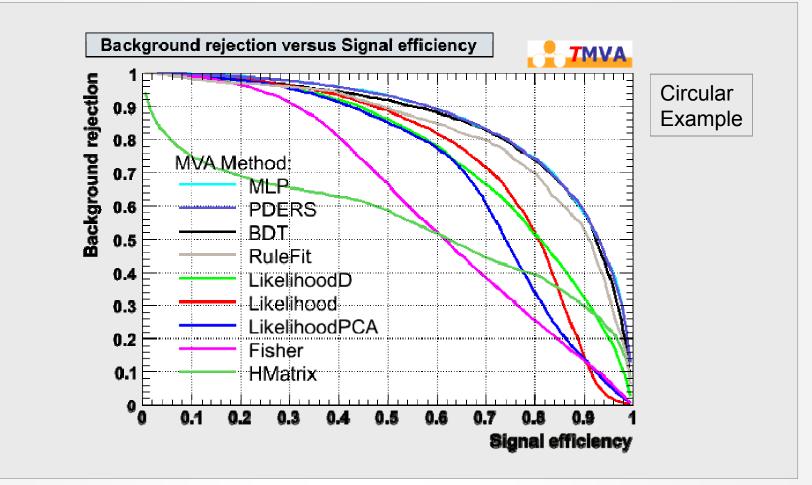
Final Classifier Performance

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Final Classifier Performance

Background rejection versus signal efficiency curve:

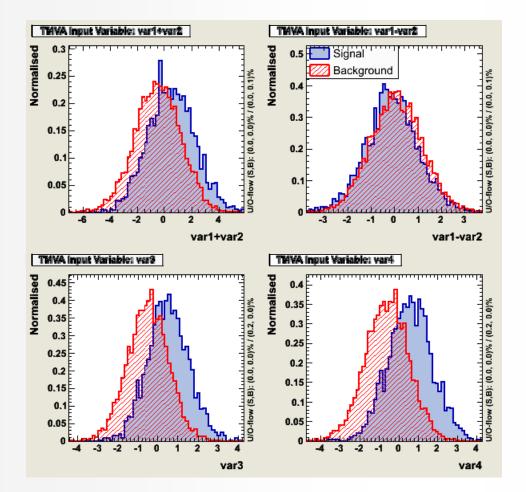


Some words on systematics

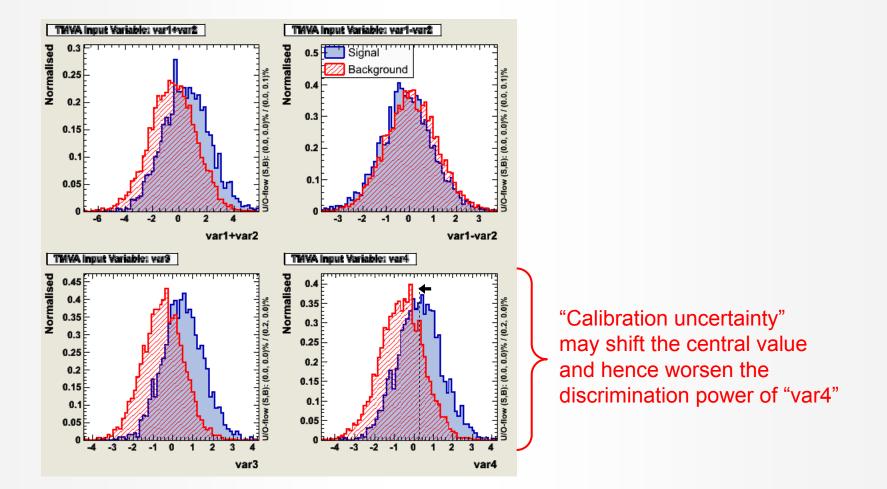
DESY, June 19, 2008

A. Hoecker — Multivariate Data Analysis with TMVA

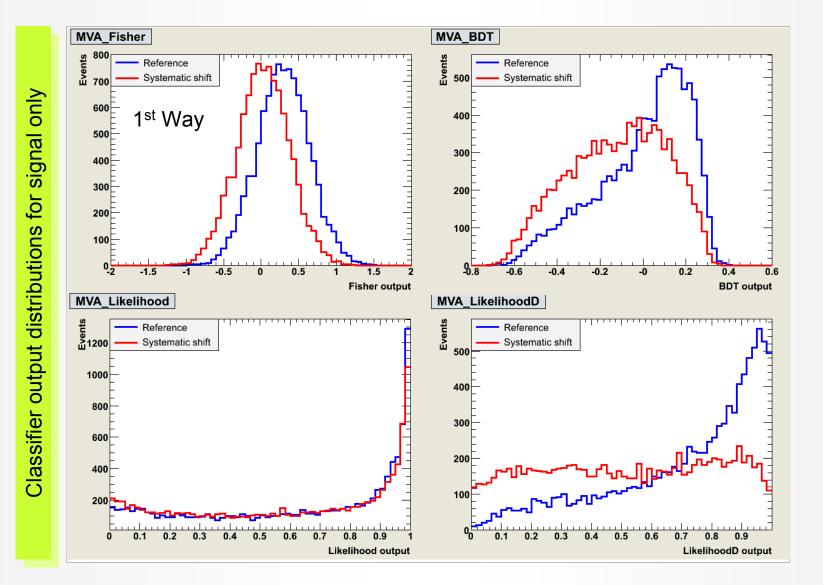
Assume strongest variable "var4" suffers from systematic uncertainty

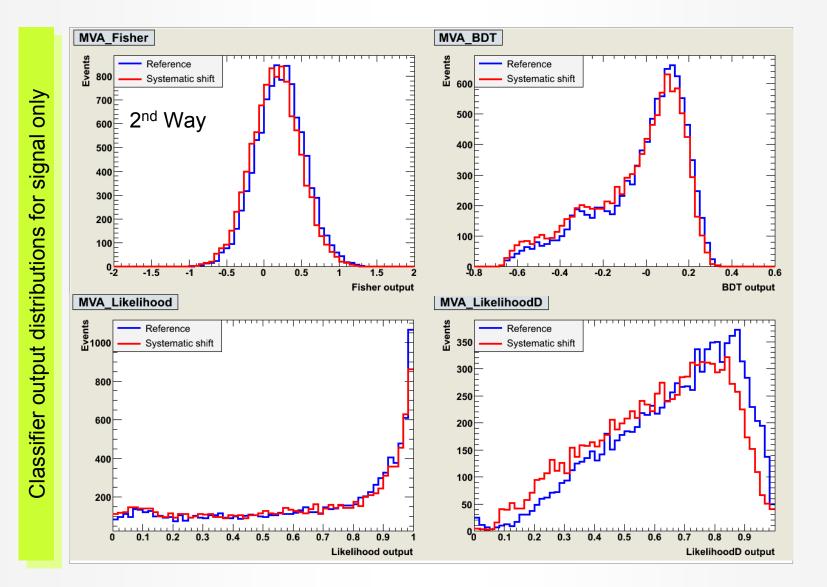


Assume strongest variable "var4" suffers from systematic uncertainty



- 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 \rightarrow 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) !

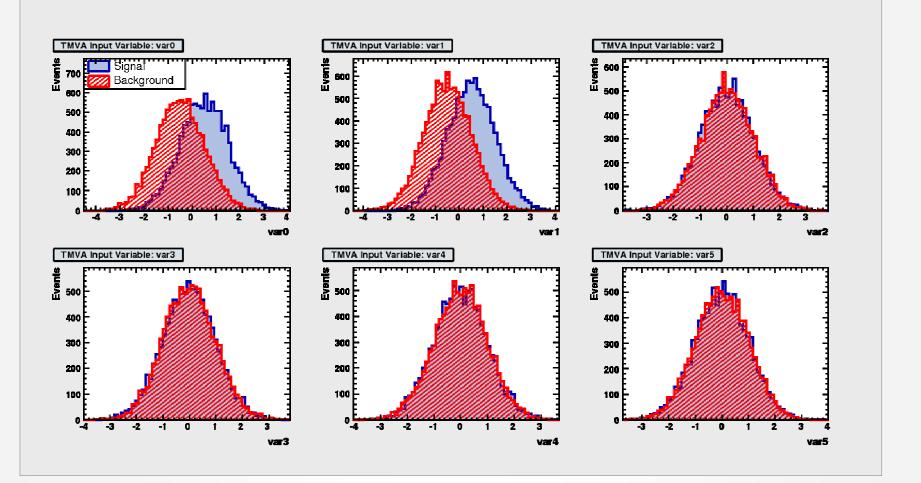




DESY, June 19, 2008

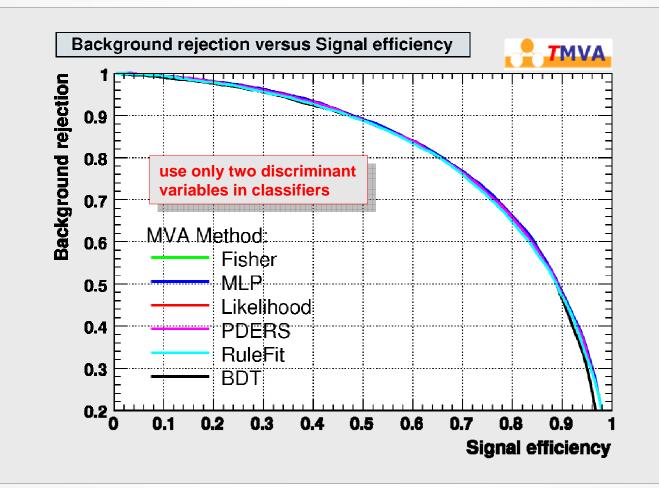
Stability with Respect to Irrelevant Variables

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



Stability with Respect to Irrelevant Variables

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



Stability with Respect to Irrelevant Variables

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

