Machine Learning Techniques for HEP Data Analysis with TMVA

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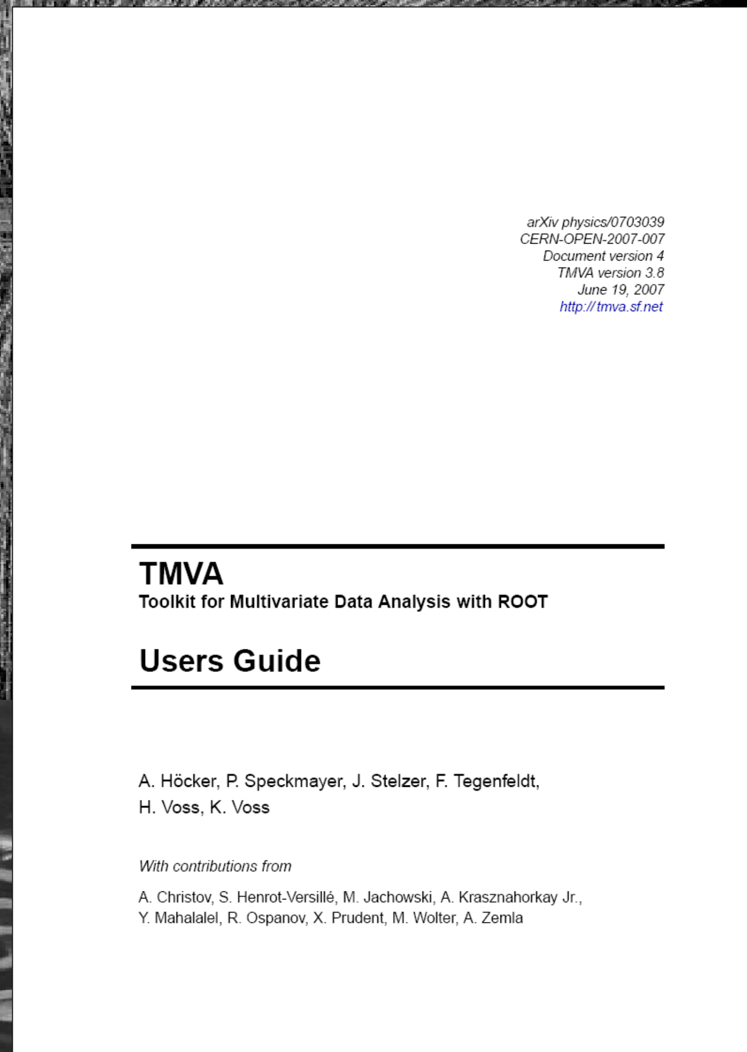
See acknowledgments on page 43

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

advertisement

We (finally) have a 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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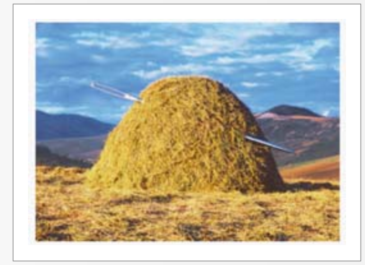
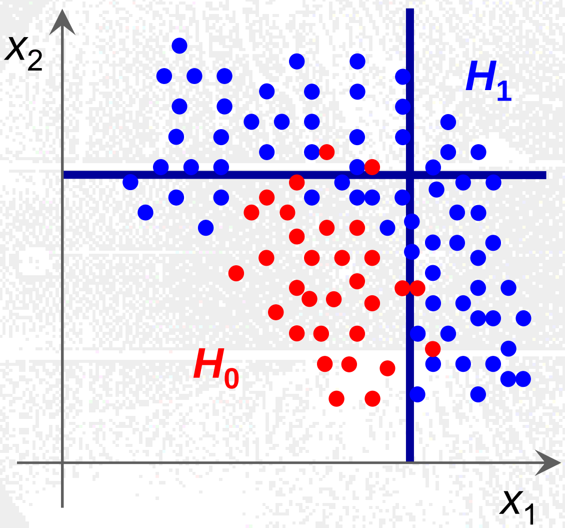
TMVA Users Guide
97pp, incl. code examples
arXiv physics/0703039

Event Classification

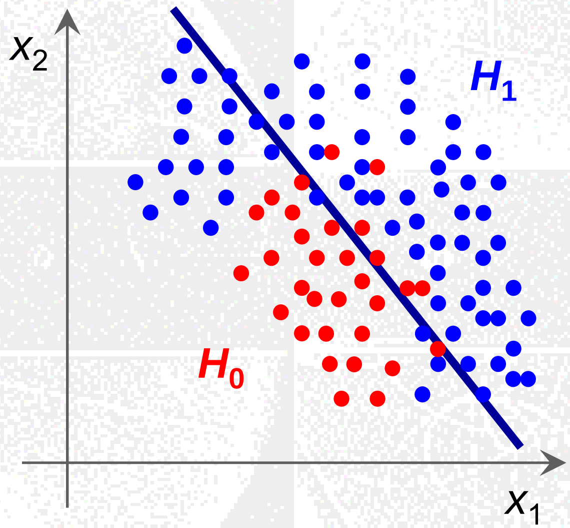


- Suppose data sample with two types of events: H_0, H_1
  - We have found discriminating input variables x_1, x_2, …
  - What decision boundary should we use to select events of type H_1 ?

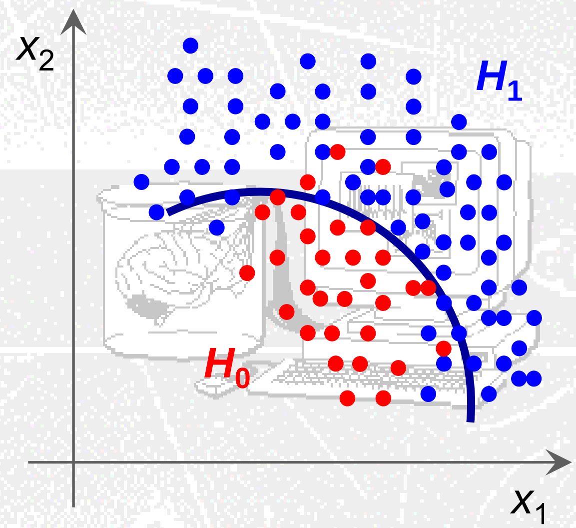
Rectangular cuts?



A linear boundary?



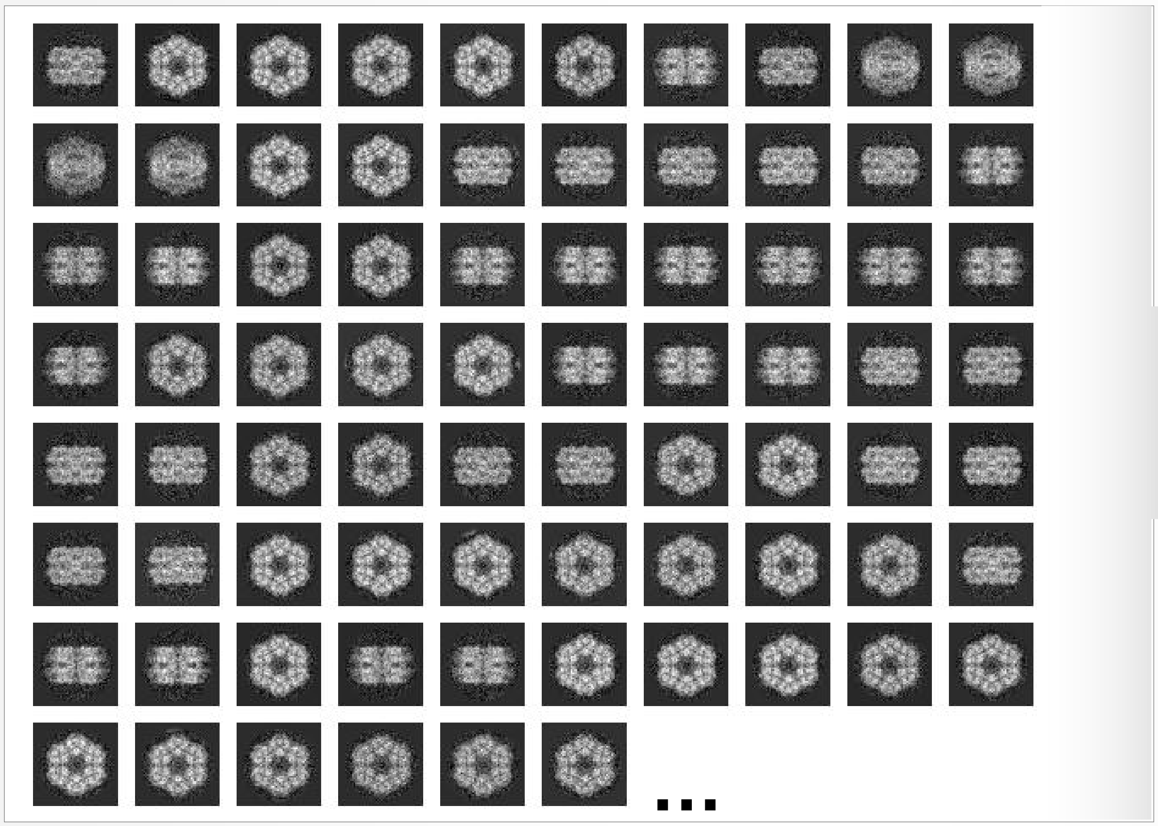
A nonlinear one?



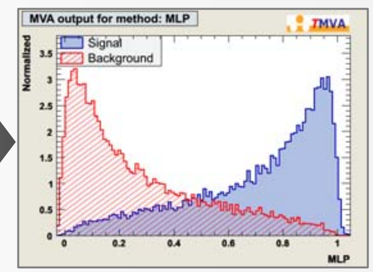
- How can we decide this in an optimal way ? → Let the machine learn it !

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*



$y(H_0) \rightarrow 0$, $y(H_1) \rightarrow 1$



Event Classification in High-Energy Physics (HEP)

- Most HEP analyses require discrimination of signal from background:
  - Event level (Higgs searches, …)
  - Cone level (Tau-vs-jet reconstruction, …)
  - Track level (particle identification, …)
  - Lifetime and flavour tagging (*b*-tagging, …)
  - Parameter estimation (*CP* violation in *B* system, …)
  - etc.

- The multivariate input information used for this has various sources
  - Kinematic variables (masses, momenta, decay angles, …)
  - Event properties (jet/lepton multiplicity, sum of charges, …)
  - Event shape (sphericity, Fox-Wolfram moments, …)
  - Detector response (silicon hits, dE/dx, Cherenkov angle, shower profiles, muon hits, …)
  - etc.

- Traditionally few powerful input variables were combined; new methods allow to use up to 100 and more variables w/o loss of classification power

Multivariate Classification Algorithms

- A large variety of multivariate classifiers (MVAs) exists

Traditional

- Rectangular cuts (optimisation often “by hand”)
- Projective likelihood (up to 2D)
- Linear discriminants (χ^2 estimators, Fisher, …)
- Nonlinear discriminants (Neural nets, …)

Variants

- Prior decorrelation of input variables (input to cuts and likelihood)
- Function discriminants
- Multidimensional likelihood (k-nearest neighbor methods)

New

- Decision trees with boosting and bagging, Random forests
- Rule-based learning machines
- Support vector machines
- Bayesian neural nets, and more general *Committee* classifiers

Multivariate Classification Algorithms

- How to dissipate (often diffuse) skepticism against the use of MVAs

➡ black boxes !

Certainly, cuts are transparent, so
- if cuts are competitive (rarely the case) → use them
- in presence of correlations, cuts loose transparency
- "we should stop calling MVAs black boxes and understand how they behave"

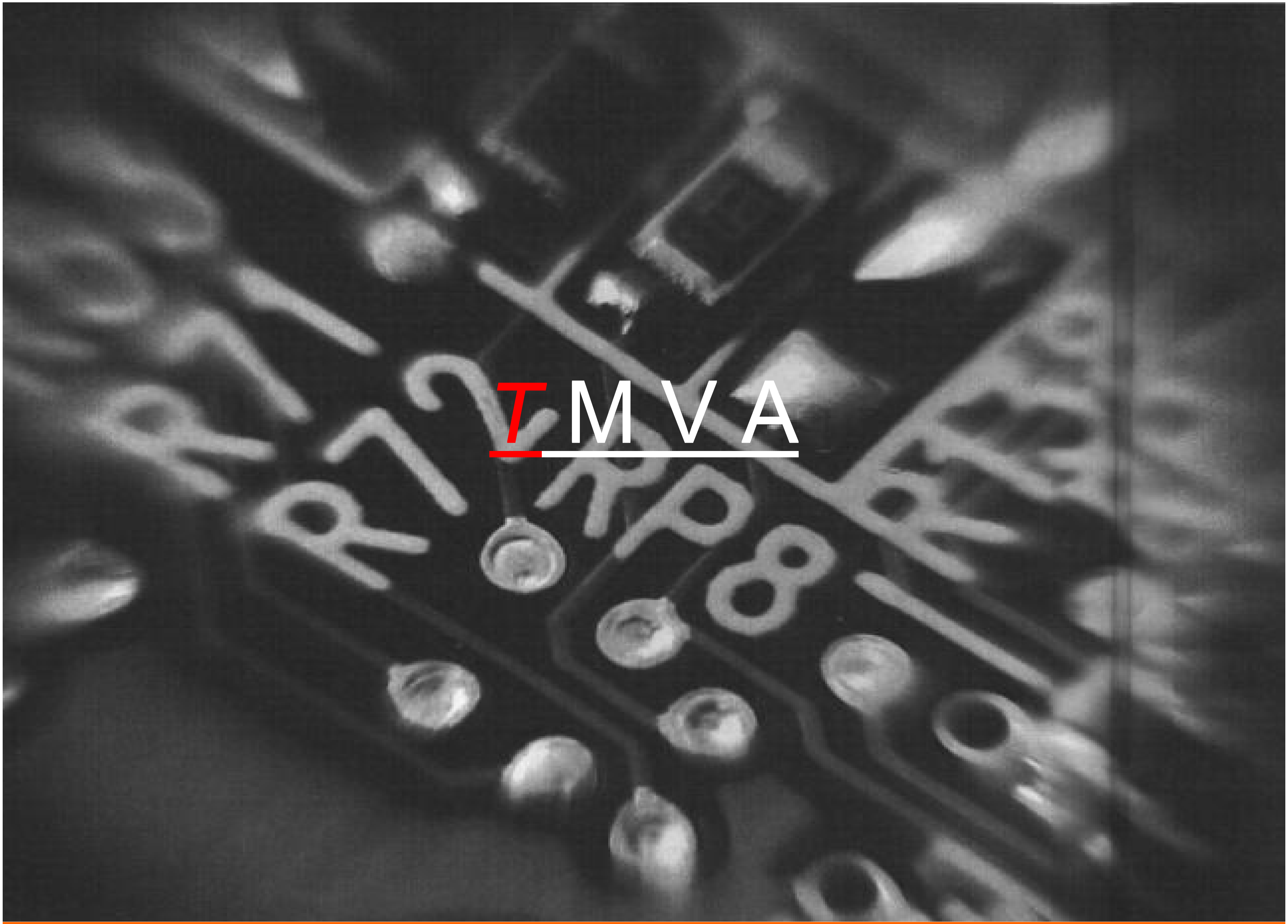
➡ what if the training samples incorrectly de-scribe the data ?

Not good, but not necessarily a huge problem:
- performance on real data will be worse than training results
- however: bad training does not create a bias !
- only if the training efficiencies are used in data analysis → bias
- optimized cuts are <u>not</u> in general less vulnerable to systematics (on the contrary !)

➡ how can one evaluate systematics ?

There is no principle difference in systematics evaluation between single variables and MVAs
- need control sample for MVA output (not necessarily for each input variable)

TMVA



What is *T*MVA

- The various classifiers have very different properties
  - Ideally, all should be tested for a given problem
  - Systematically choose the best performing and simplest classifier
  - Comparisons between classifiers improves the understanding and takes away mysticism
- *T*MVA — Toolkit for multivariate data analysis
  - Framework for *parallel* **training**, **testing**, **evaluation** and **application** of MV classifiers
  - Training events can have weights
  - A large number of linear, nonlinear, likelihood and rule-based classifiers implemented
  - The classifiers rank the input variables
  - The input variables can be decorrelated or projected upon their principal components
  - Training results and full configuration are written to weight files
  - ➡ Application to data classification using a **Reader** or standalone C++ classes

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 6 main developers, and 27 registered contributors at SF
  - >1200 downloads since March 2006 (not accounting cvs checkouts and ROOT users)
- Written in C++, relying on core ROOT functionality
  - Full examples distributed with TMVA, including analysis macros and GUI
  - Scripts are provided for TMVA use in ROOT macro, as C++ executable or with python
- Integrated and distributed with ROOT since ROOT v5.11/03

The *T*MVA Classifiers

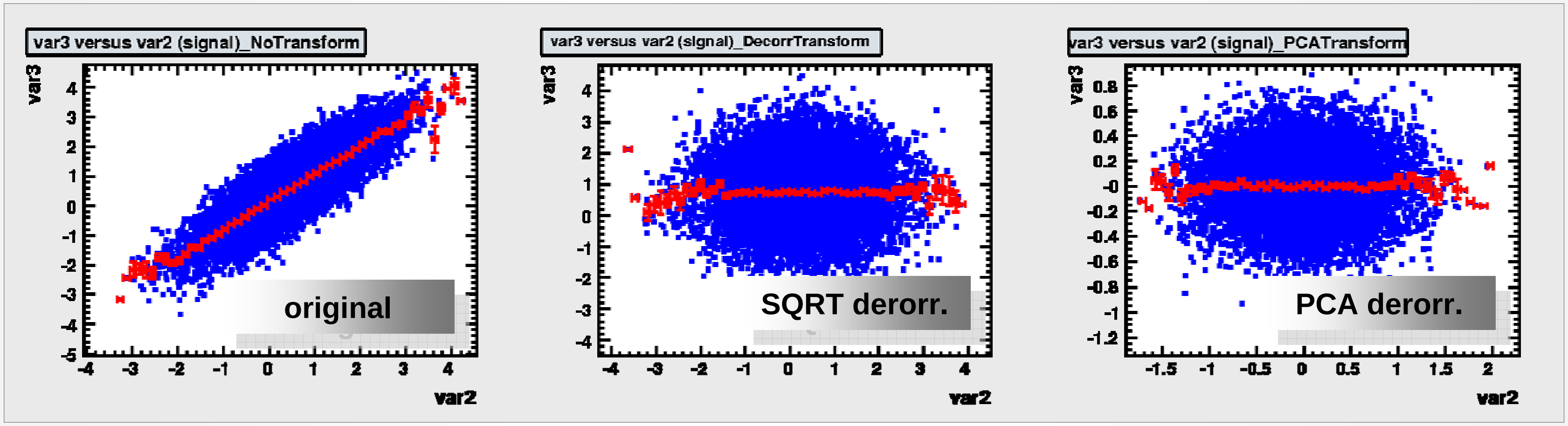
- Currently implemented classifiers :
  - Rectangular cut optimisation
  - Projective and multidimensional likelihood estimator
  - k-Nearest Neighbor algorithm
  - Fisher and H-Matrix discriminants
  - Function discriminant
  - Artificial neural networks (3 different *multilayer perceptrons*)
  - Boosted/bagged decision trees with automatic node pruning
  - RuleFit
  - Support Vector Machine

Data Preprocessing: Decorrelation

- Commonly realised for all methods in *T*MVA (centrally in **`DataSet`** class)

- Removal of linear correlations by rotating input variables
  - Determine *square-root* C' of covariance matrix C, *i.e.*, $C = C'C'$
  - Transform original (x) into decorrelated variable space (x') by: $x' = C'^{-1}x$

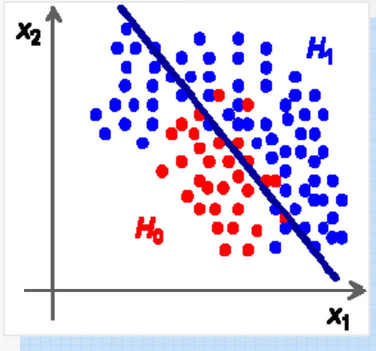
- Various ways to choose basis for decorrelation (also implemented PCA)



Rectangular Cut Optimisation

- Simplest method: cut in rectangular variable volume

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

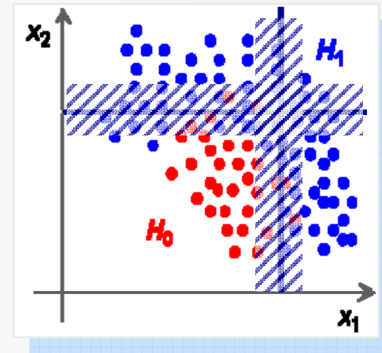


- Technical challenge: how to find optimal cuts ?
  - MINUIT fails due to non-unique solution space
  - *T*MVA uses: **Monte Carlo sampling**, **<u>Genetic Algorithm</u>**, **Simulated Annealing**
  - Huge speed improvement of volume search by sorting events in binary tree

- 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

Likelihood ratio for event i_{event}

PDFs

discriminating variables

$$y_L(i_{\text{event}}) = \frac{\prod\limits_{k\in\{\text{variables}\}} p_k^{\text{signal}}\left(x_k(i_{\text{event}})\right)}{\sum\limits_{U\in\{\text{species}\}}\left(\prod\limits_{k\in\{\text{variables}\}} p_k^{U}\left(x_k(i_{\text{event}})\right)\right)}$$

Species: signal, background types

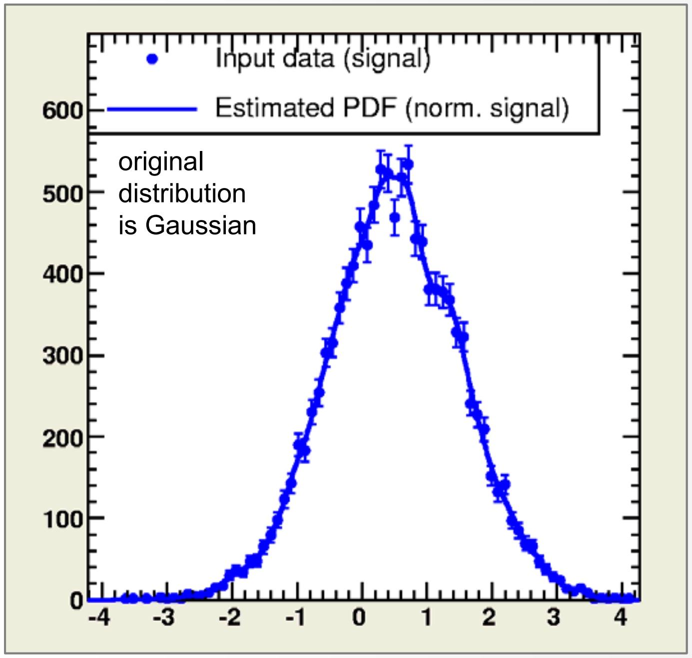
- Ignores correlations between input variables
  - Optimal approach if correlations are zero (or linear → decorrelation)
  - Otherwise: significant performance loss

PDE Approach: Estimating PDF Kernels

- Technical challenge: how to estimate the PDF shapes
  - 3 ways: **parametric fitting (function)** | **nonparametric fitting** | **event counting**

parametric fitting (function)	nonparametric fitting	event counting
Difficult to automate for arbitrary PDFs	Easy to automate, can create artefacts/suppress information	Automatic, unbiased, but suboptimal

- We have chosen to implement nonparametric fitting in *T*MVA
  - Binned shape interpolation using spline functions (orders: 1, 2, 3, 5)
  - Unbinned kernel density estimation (KDE) with Gaussian smearing
  - *T*MVA 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)

  - The signal estimator is then given by (simplified, full formula accounts for event weights and training population)

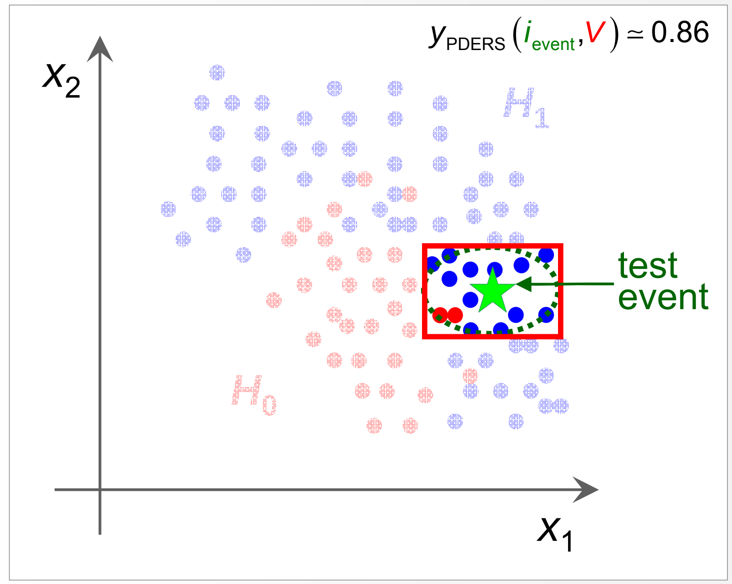
PDE-RS ratio for event i_{event}

chosen volume

#signal events in V

$$y_{PDERS}\left(i_{event}, V\right) = \frac{n_S\left(i_{event}, V\right)}{n_S\left(i_{event}, V\right) + n_B\left(i_{event}, V\right)}$$

#background events in V



- 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

Multidimensional PDE Approach

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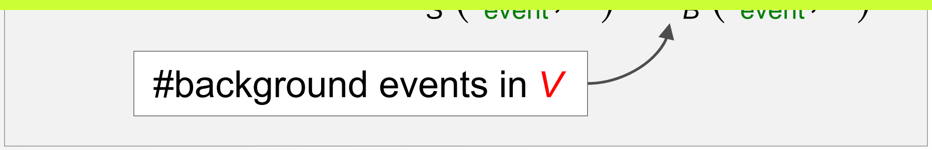
  - PDE Range-Search: count number of signal and background events in "vicinity" of test event → preset or **adaptive** volume defines "vicinity"

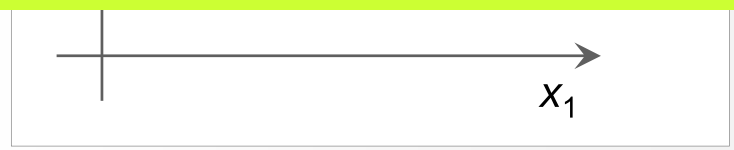
Carli-Koblitz, NIM A501, 576 (2003)

New classifier: **k-Nearest Neighbor** – implemented by R. Ospanov (Texas U.):

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

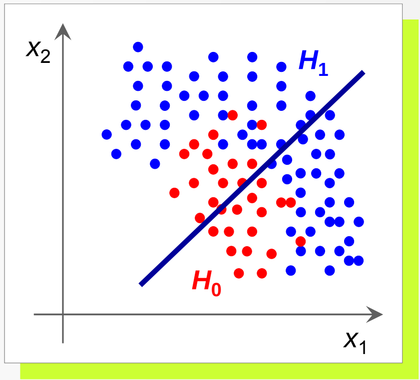




- Improve y_{PDERS} estimate within V by using various N_{var}-D kernel estimators
- Enhance speed of event counting in volume by binary tree search

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:

"Fisher coefficients"

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

  - 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

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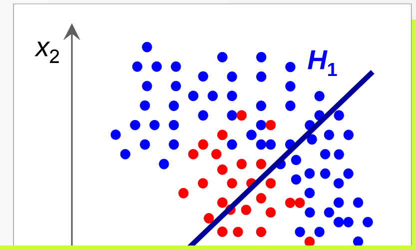


New classifier: **Function discriminant analysis (FDA)**

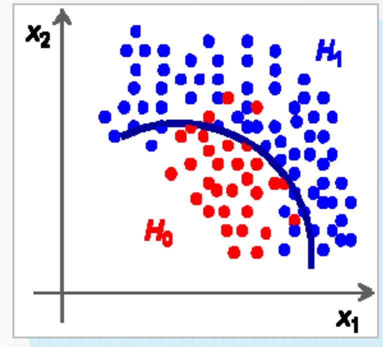
Fit any user-defined function of input variables requiring that signal events return →1 and background →0

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

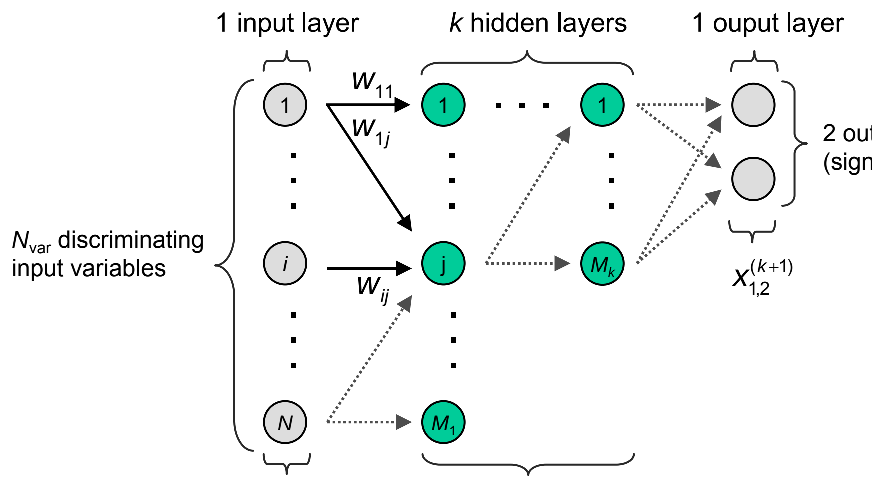
  - Compute Fisher coefficients from signal and background covariance matrices
- Fisher requires distinct sample means between signal and background
- Optimal classifier for linearly correlated Gaussian-distributed variables

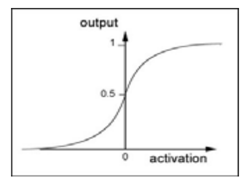
Nonlinear Analysis: Artificial Neural Networks

- Achieve nonlinear classifier response by “activating” output nodes using nonlinear weights
- Call nodes “neurons” and arrange them in series:



Feed-forward Multilayer Perceptron





(“Activation” function)

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

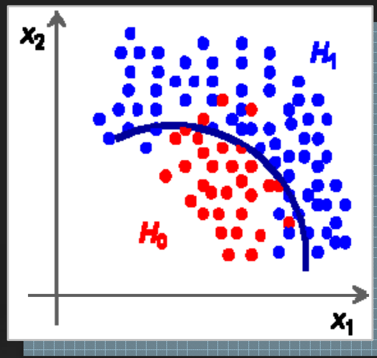
Weierstrass theorem: can approximate any continuous functions to arbitrary precision with a single hidden layer and an infinite number of neurons

Three different multilayer perceptrons available in TMVA

- Adjust weights (=training) using “back-propagation”

Decision Trees

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



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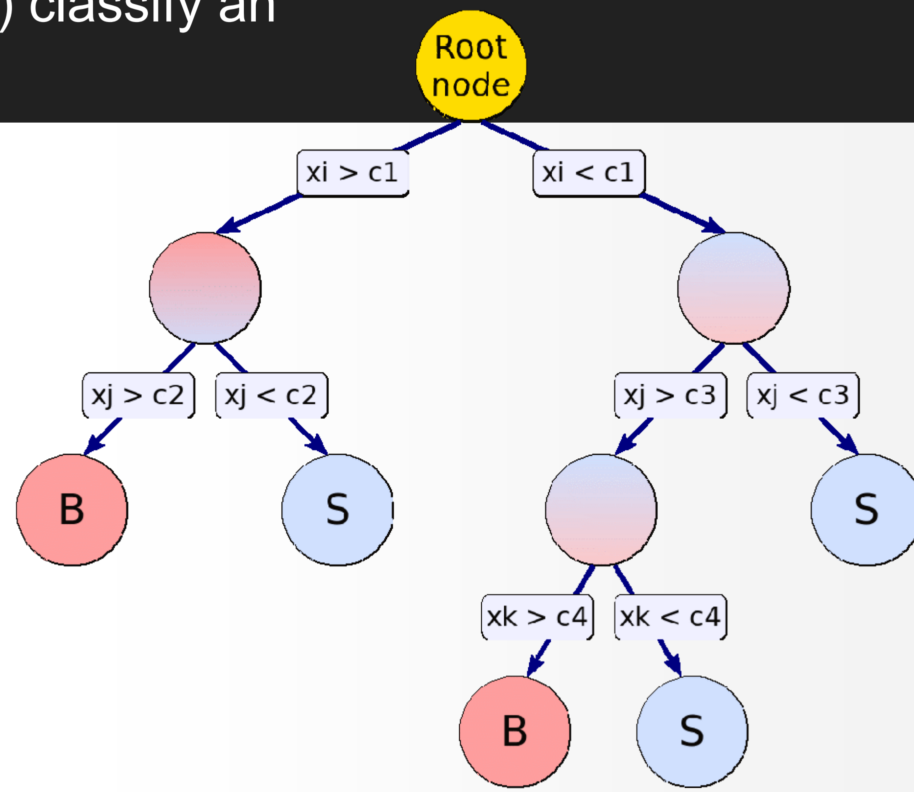
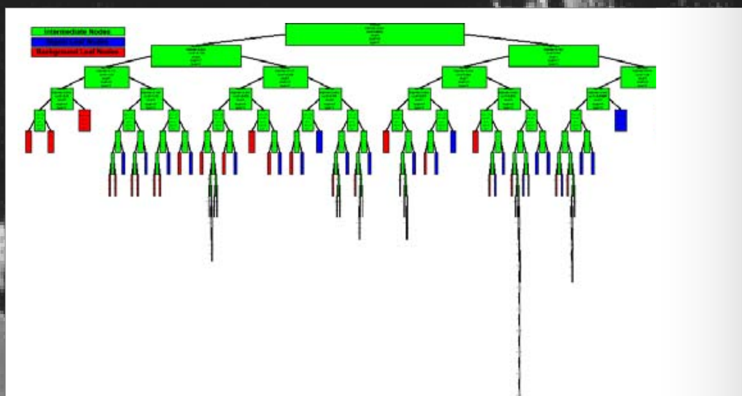
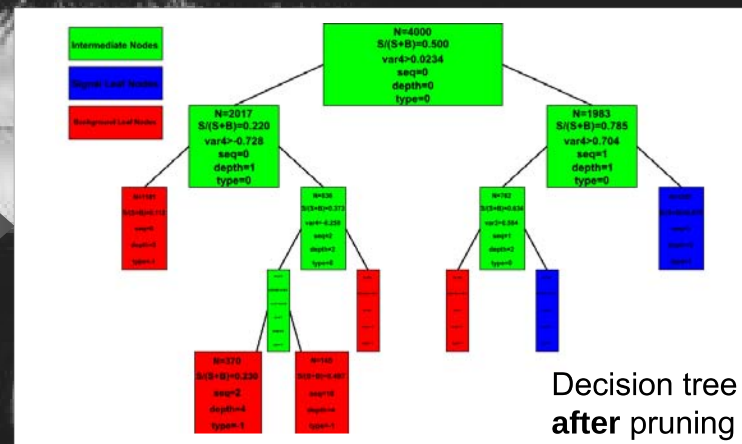


- Growing a decision tree:
  - Start with Root node
  - Split training sample according to cut on best variable at this node
  - Splitting criterion: e.g., maximum "Gini-index": purity $\times$ (1– purity)
  - Continue splitting until min. number of events or max. purity reached
  - Classify leaf node according to majority of events, or give weight; unknown test events are classified accordingly

Decision Trees



Decision tree **before** pruning



Decision tree **after** pruning

- Bottom-up "pruning" of a decision tree
  - Remove statistically insignificant nodes to reduce tree overtraining → automatic in *T*MVA

Boosted Decision Trees (BDT)

- Data mining with decision trees is popular in science (so far mostly outside of HEP)
  - Advantages:
    - Easy interpretation – can always be represented in 2D tree
    - 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 (→ 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

RuleFit classifier

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

normalised discriminating event variables

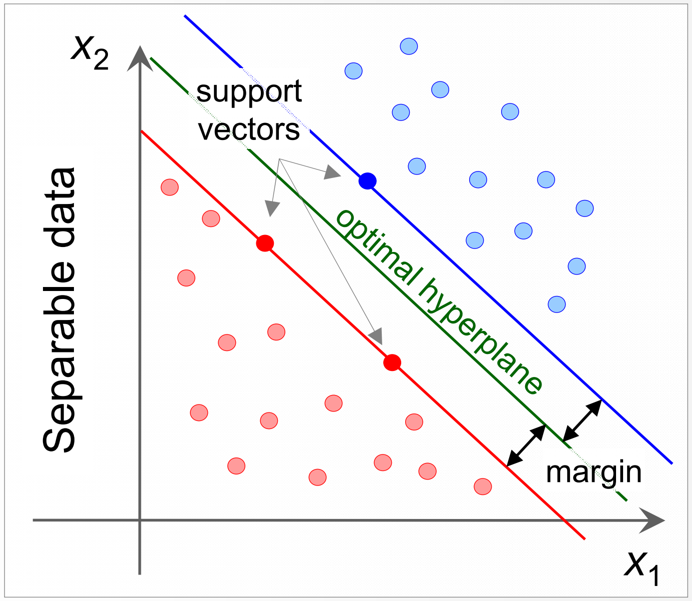
$$y_{RF}(\vec{x}) = a_0 + \underbrace{\sum_{m=1}^{M_R} a_m r_m(\hat{\vec{x}})}_{\text{Sum of rules}} + \underbrace{\sum_{k=1}^{n_R} b_k \hat{x}_k}_{\text{Linear Fisher term}}$$

- 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)

- 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



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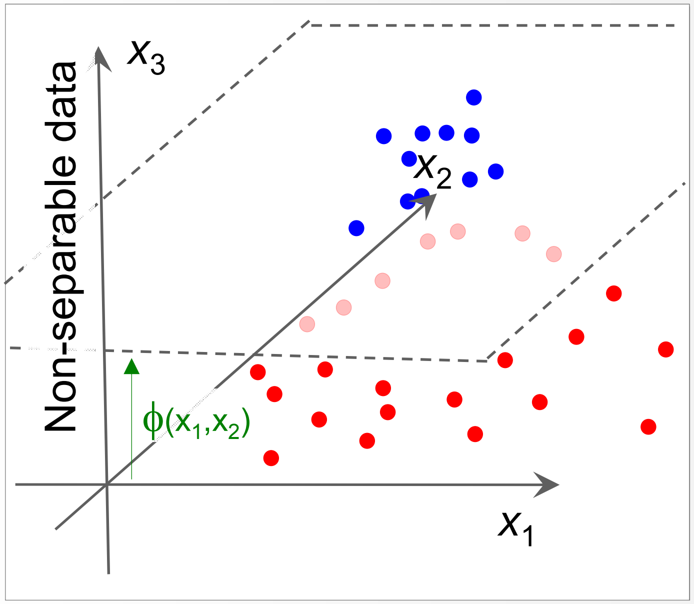


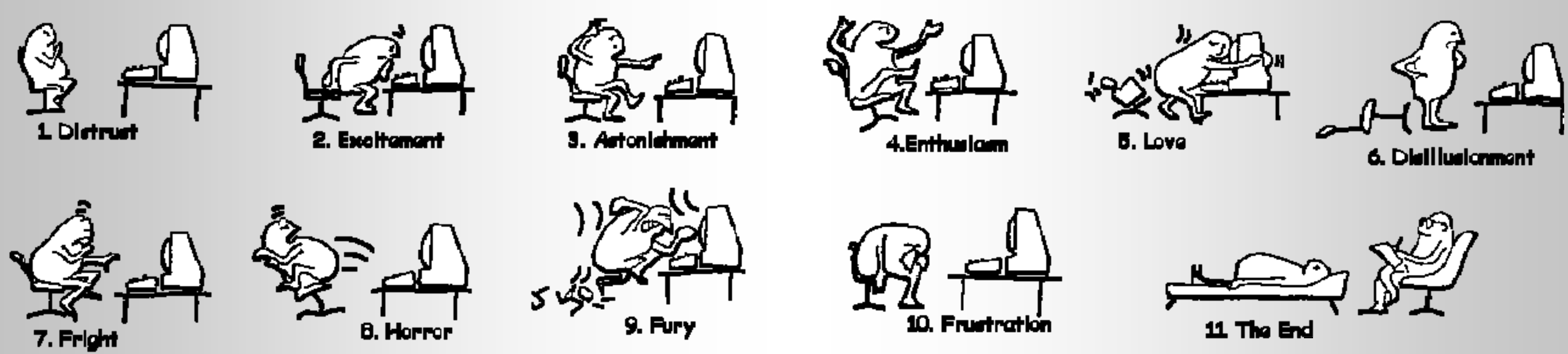
- Non-linear cases:
  - Transform variables into higher dimensional space where again a linear boundary (hyperplane) can separate the data
  - Explicit transformation form not required: use Kernel Functions to approximate scalar products between transformed vectors in the higher dimensional space
  - Choose Kernel and fit the hyperplane using the linear techniques developed above
  - ➡ Available Kernels: Gaussian, Polynomial, Sigmoid

Using *T*MVA

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

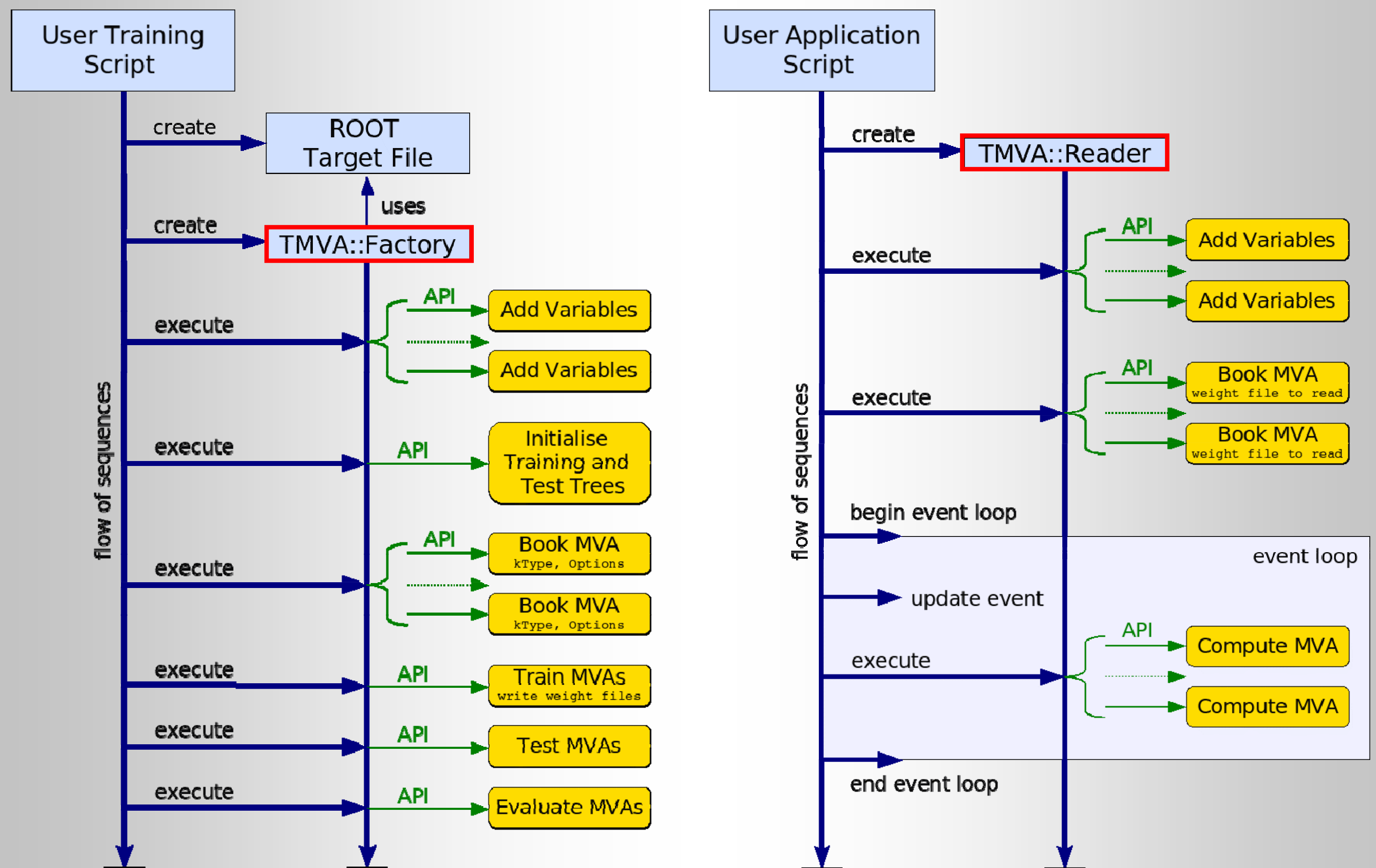
1. *Training phase*: training, testing and evaluation of classifiers using data samples with known signal and background composition
2. *Application phase*: using selected trained classifiers to classify unknown data samples

➧ Illustration of these steps with toy data samples



→ *T*MVA tutorial

Code Flow for *Training* and *Application* Phases



→ *TMVA* tutorial

Code Flow for *Training* and *Application* Phases

User Training Script

User Application Script

Can be ROOT scripts, C++ executables or python scripts (via PyROOT),
or any other high-level language that interfaces with ROOT

→ *T*MVA 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');

  factory->PrepareTrainingAndTestTree("", "NSigTrain=3000:NBkgTrain=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

← train, test and evaluate

→ *TMVA* tutorial

A Simple Example for an *Application*

```
void TMVApplication( )
{
   TMVA::Reader *reader = new TMVA::Reader("!Color");

   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/MVAnalysis_MLP.weights.txt" );

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

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

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

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

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

← create *Reader*

← register the variables

← book classifier(s)

← prepare event loop

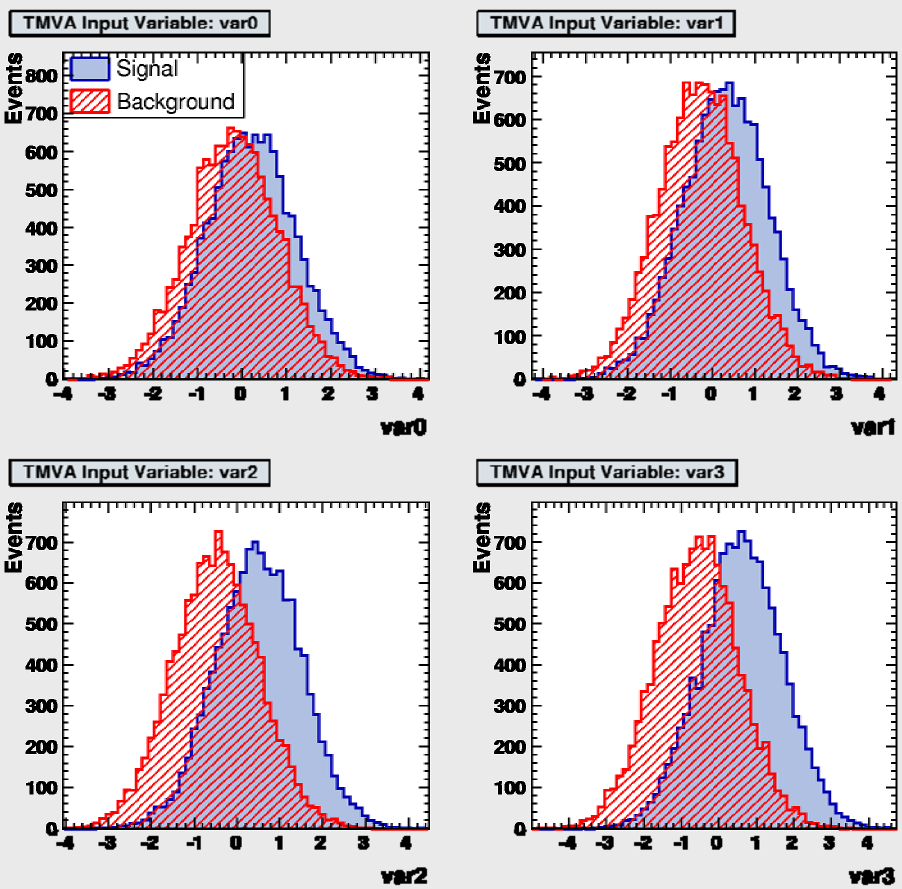
← compute input variables

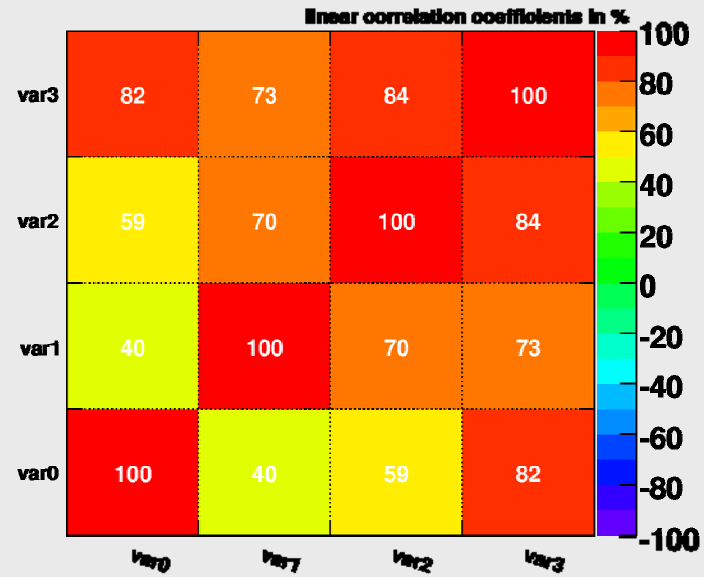
← calculate classifier output

→ *T*MVA tutorial

A Toy Example (idealized)

- Use data set with 4 linearly correlated Gaussian distributed variables:

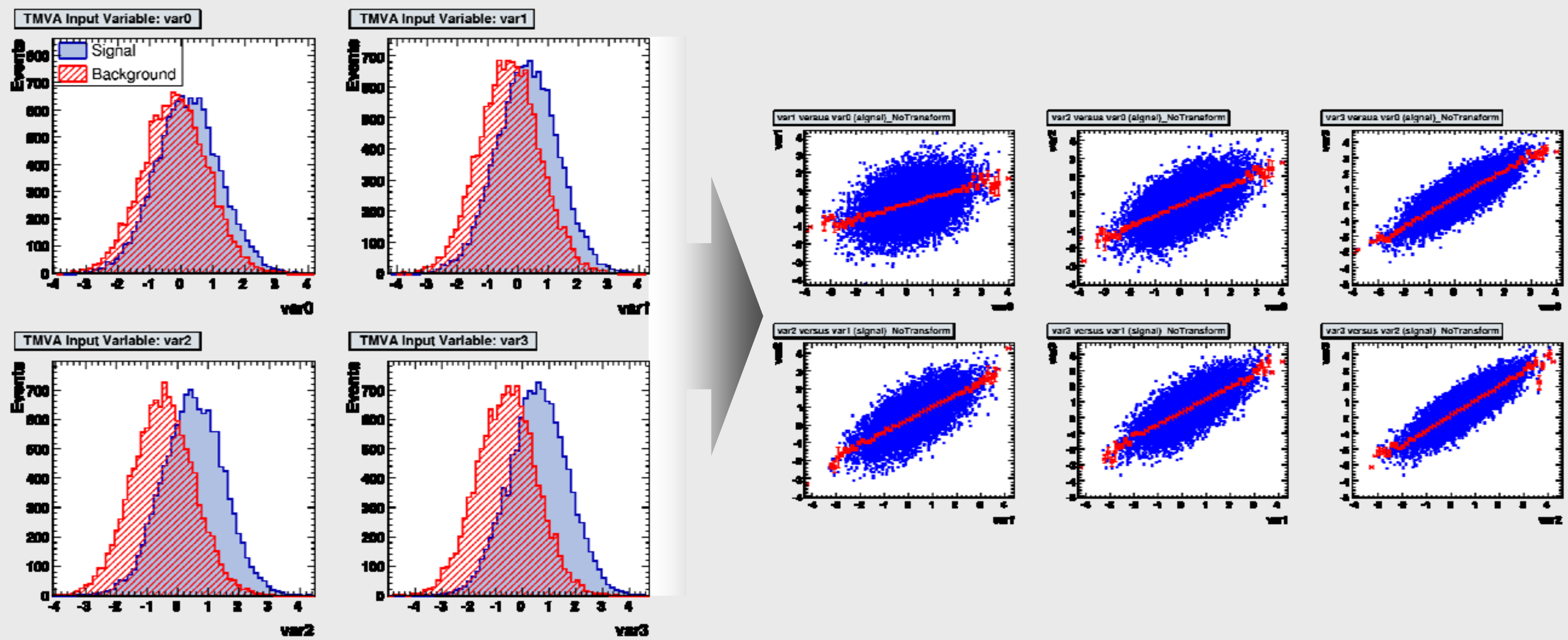




Rank	Variable	Separation
1	var3	3.834e+02
2	var2	3.062e+02
3	var1	1.097e+02
4	var0	5.818e+01

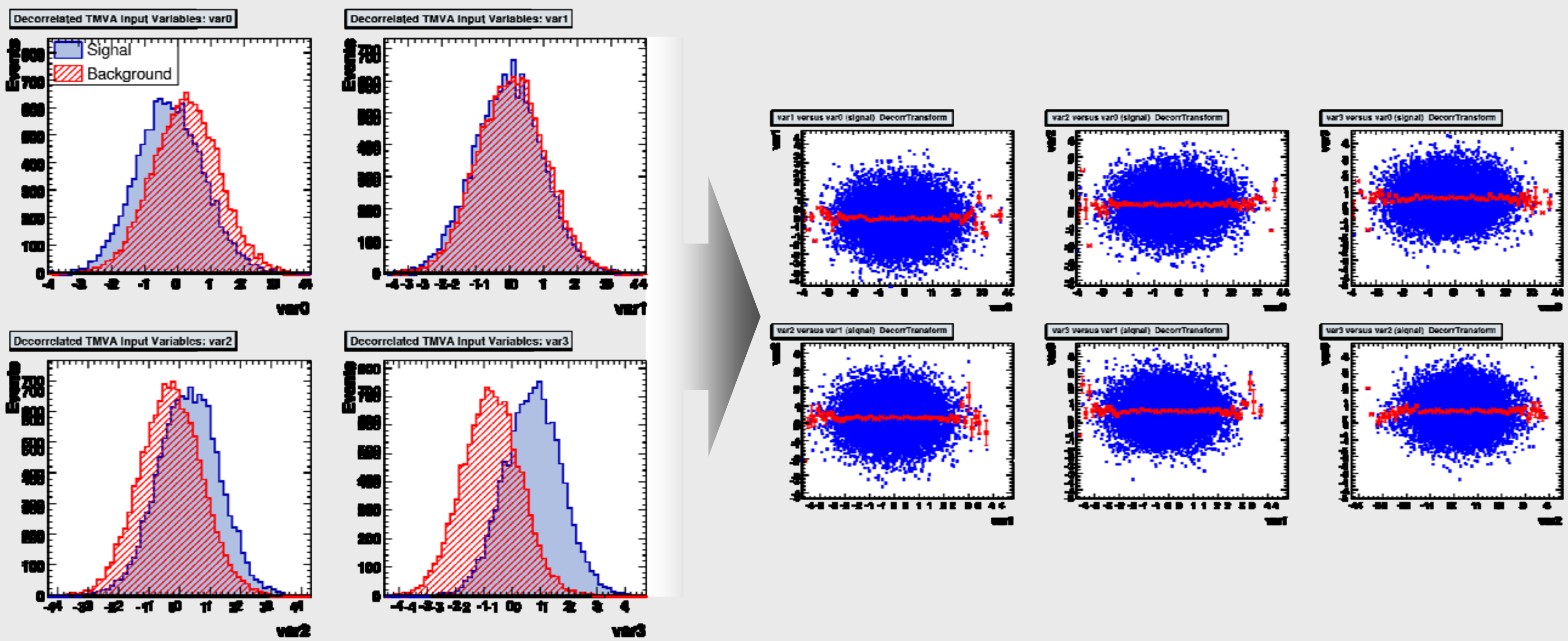
Preprocessing the Input Variables

- Decorrelation of variables before training is useful for *this* example



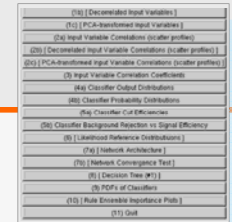
Preprocessing the Input Variables

- Decorrelation of variables before training is useful for *this* example



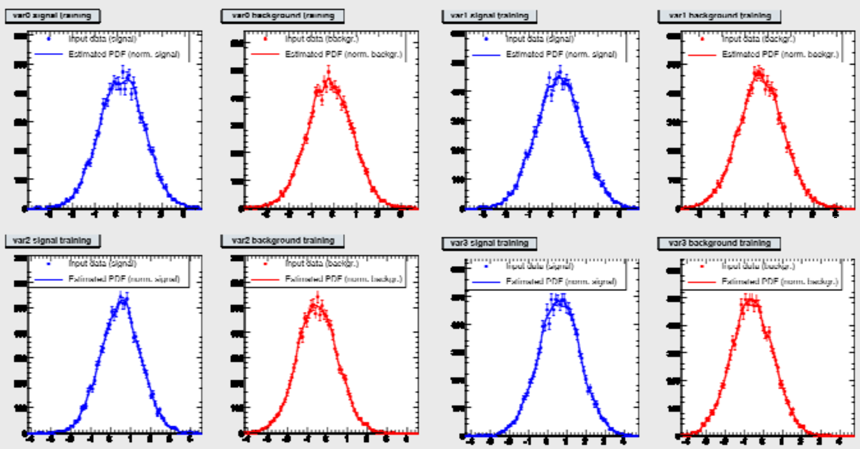
- Note that in cases with non-Gaussian distributions and/or nonlinear correlations decorrelation may do more harm than any good

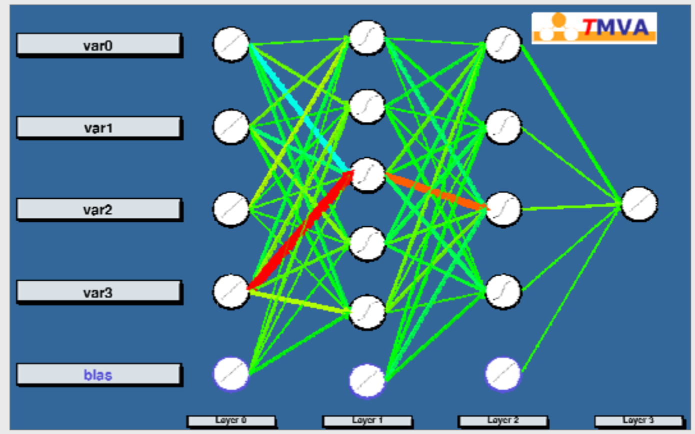
Validating the Classifier Training

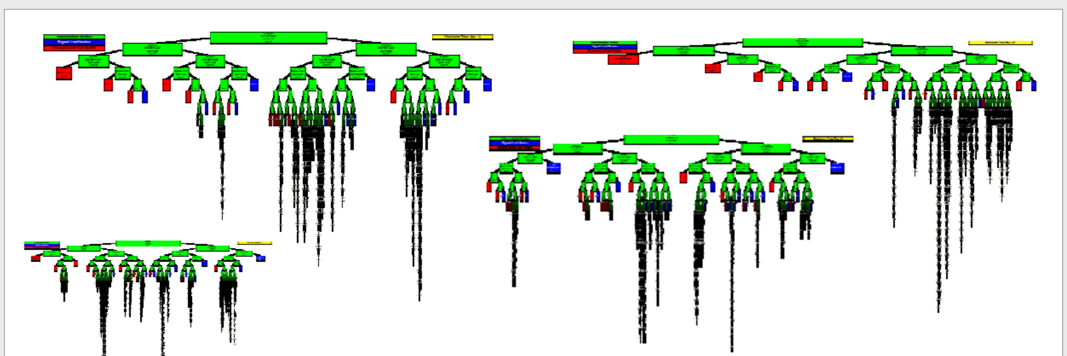


*T*MVA GUI

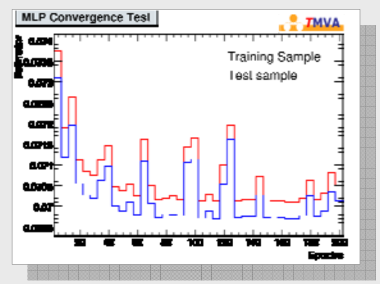
- Projective likelihood PDFs, MLP training, BDTs, …





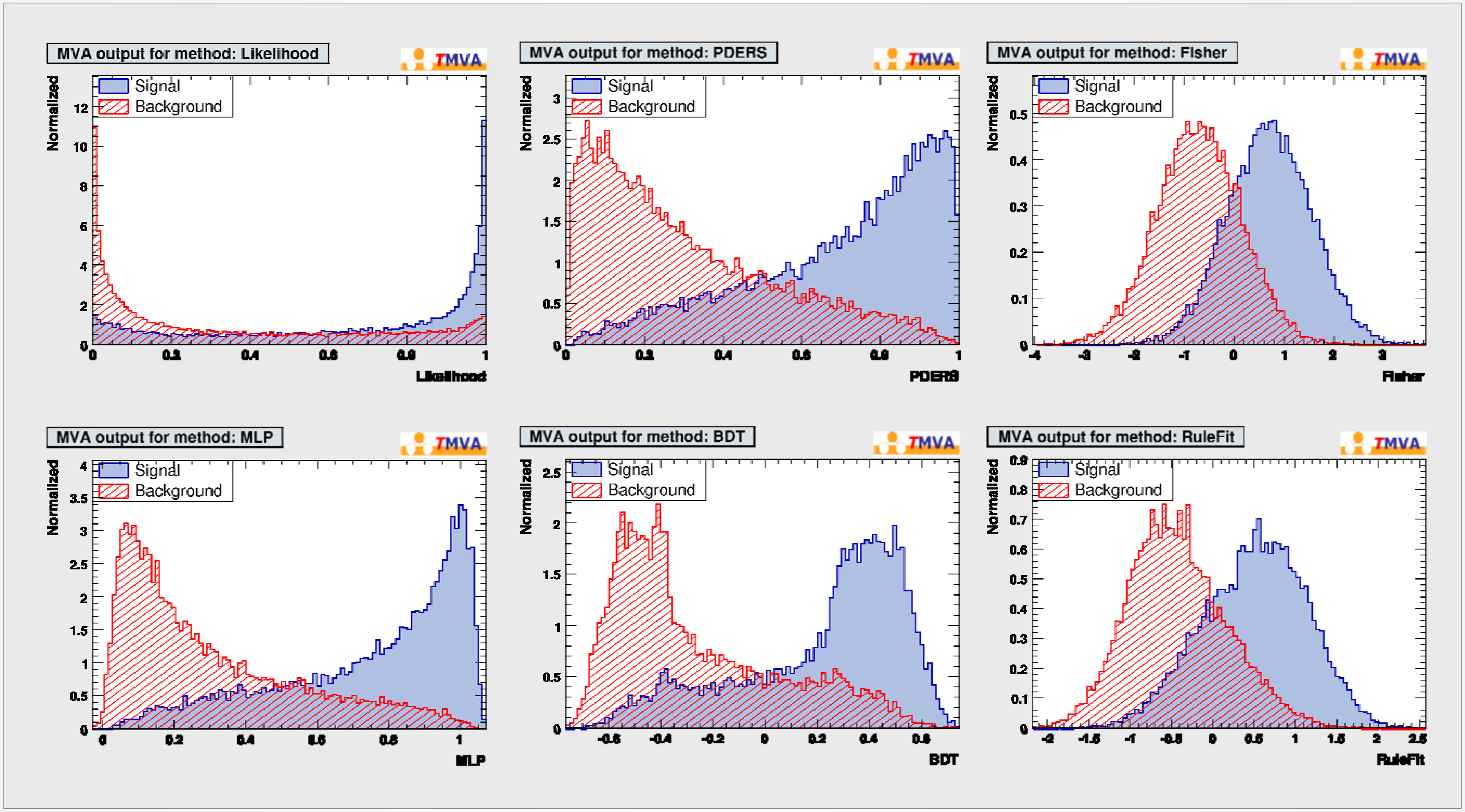


average no. of nodes before/after pruning: 4193 / 968



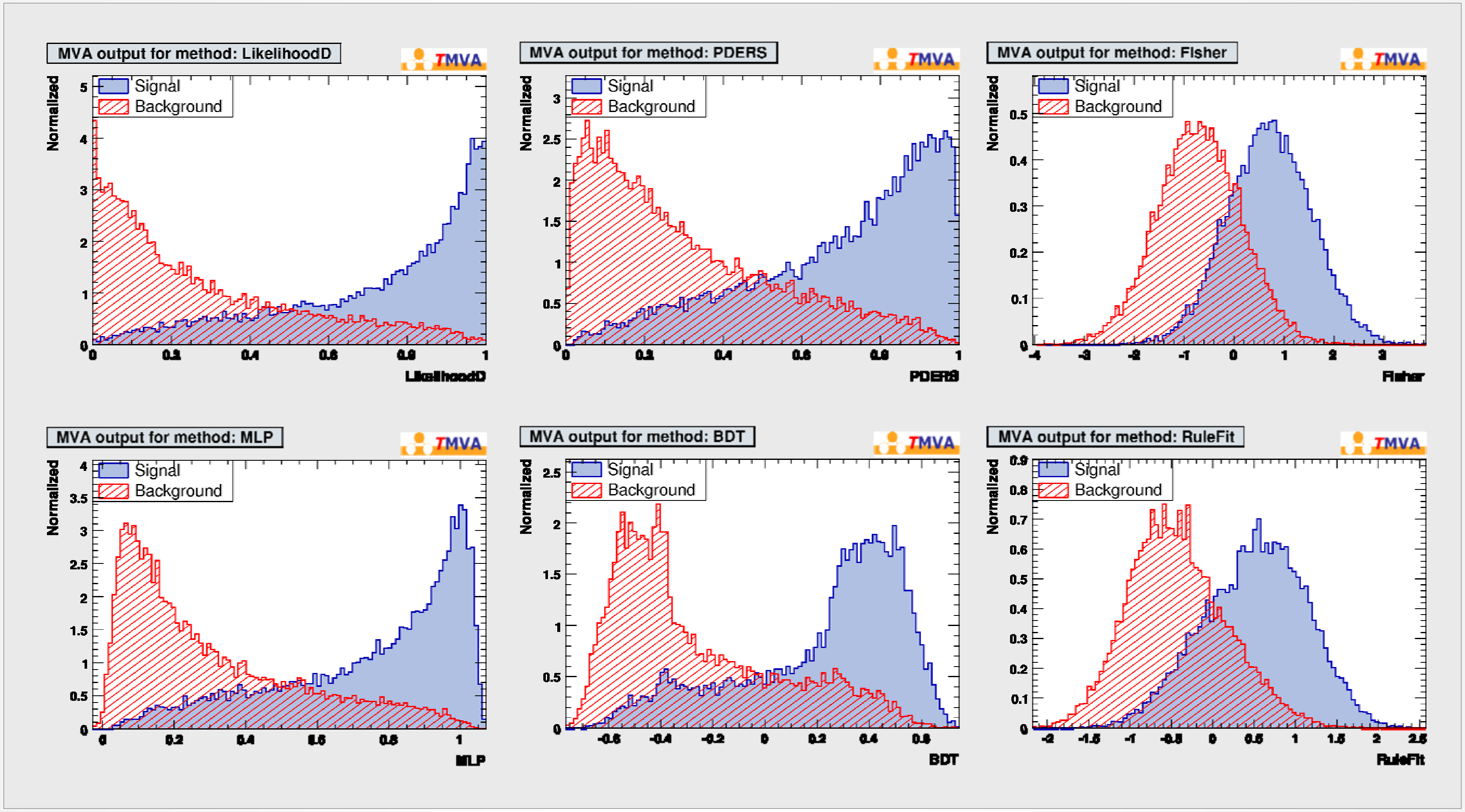
Testing the Classifiers

- Classifier output distributions for independent test sample:



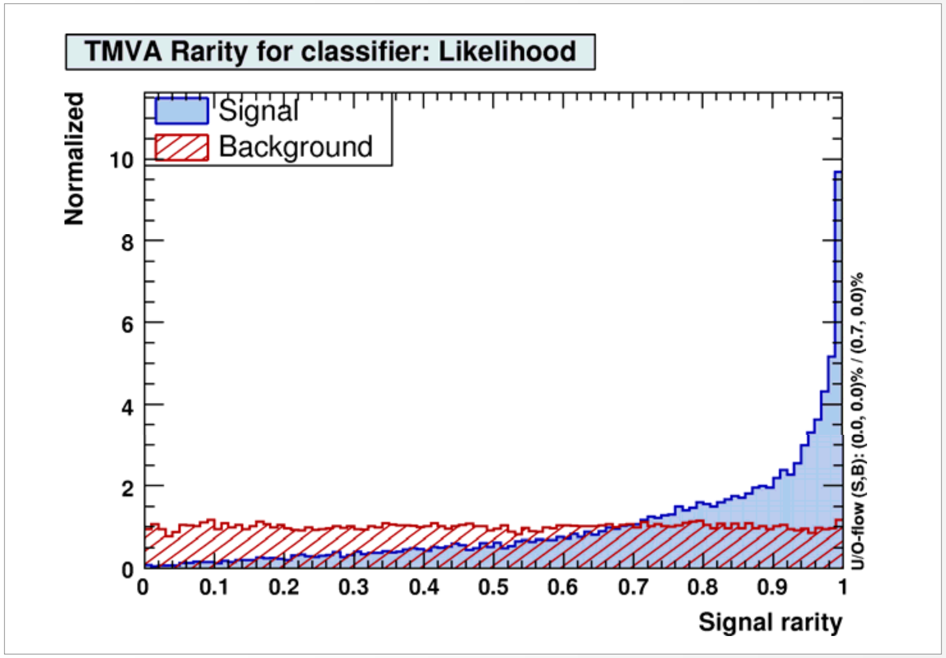
Testing the Classifiers

- Classifier output distributions for independent test sample:



Evaluating the Classifiers

- There is no unique way to express the performance of a classifier → several benchmark quantities computed by *T*MVA
  - Signal eff. at various background effs. (= 1 – rejection) when cutting on classifier output
  - The *Separation*: $\frac{1}{2}\int \frac{(\hat{y}_S(y)-\hat{y}_B(y))^2}{\hat{y}_S(y)+\hat{y}_B(y)}dy$
  - "Rarity" implemented (background flat): $R(y)=\int_{-\infty}^{y}\hat{y}(y')dy'$
  - Other quantities … see Users Guide



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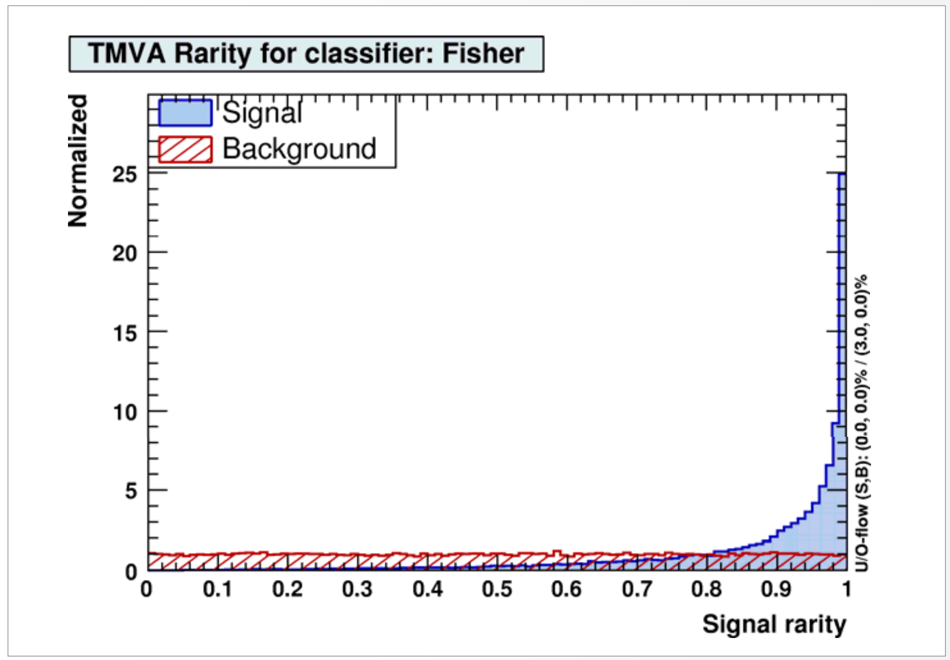

Evaluating the Classifiers

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  - "Rarity" implemented (background flat): $R(y)=\int_{-\infty}^{y}\hat{y}(y')dy'$
  - Other quantities … see Users Guide

- Remark on **overtraining**
  - Occurs when classifier training has too few degrees of freedom because the classifier has too many adjustable parameters for too few training events
  - Sensitivity to overtraining depends on classifier: e.g., Fisher weak, BDT strong
  - Compare performance between training and test sample to detect overtraining
  - Actively counteract overtraining: e.g., smooth likelihood PDFs, prune decision trees, …

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	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

Better classifier

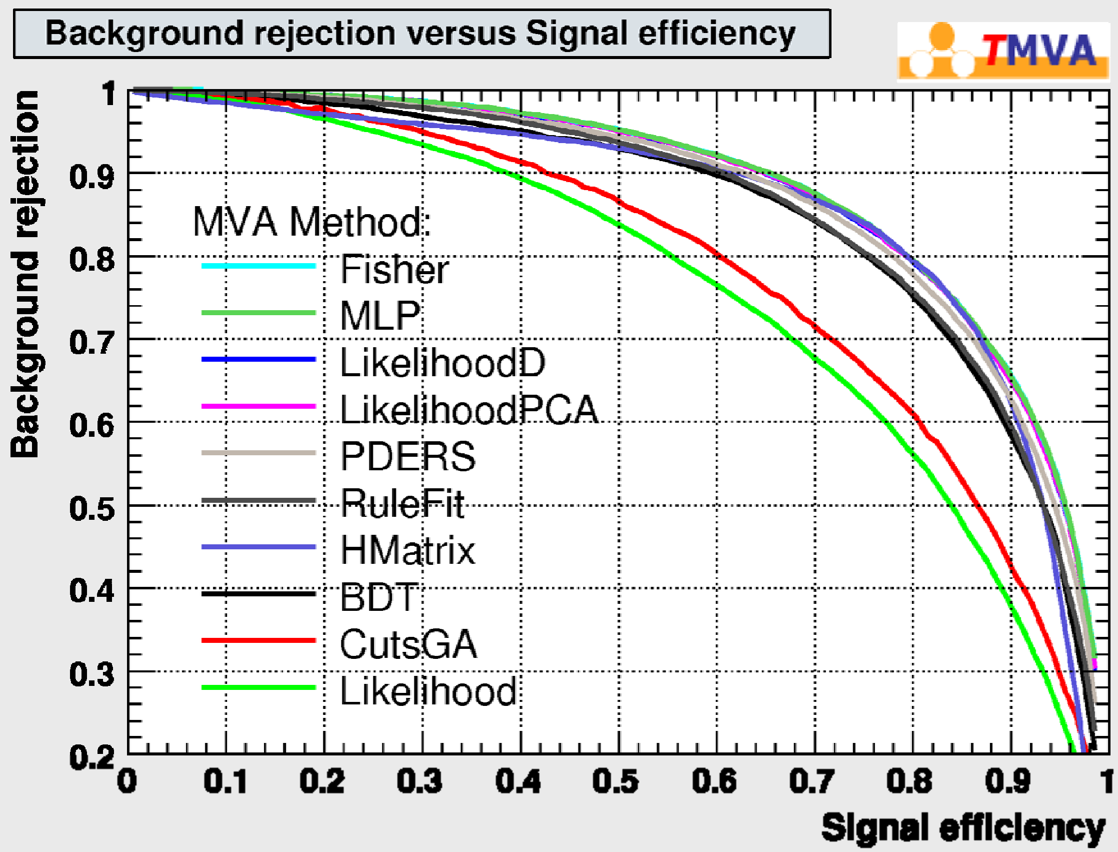
Testing efficiency compared to training efficiency (overtraining check)

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

Evaluating the Classifiers (with a single plot…)

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



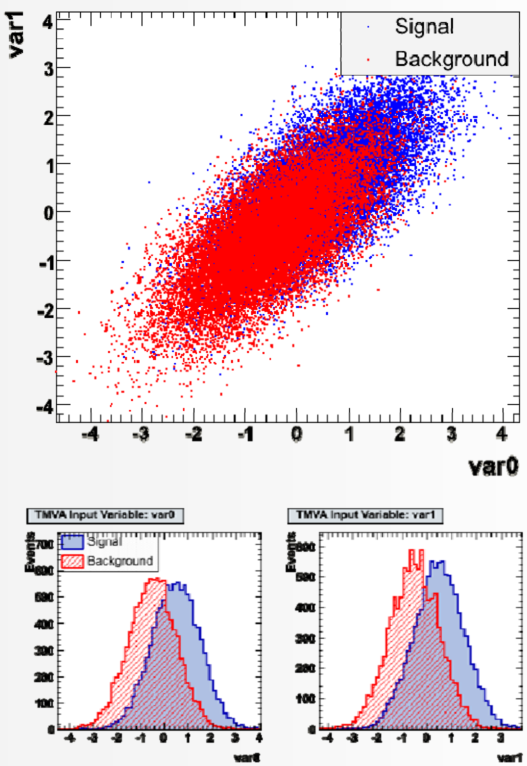
Note: Nearly All Realistic Use Cases are Much More Difficult Than This One

More Toy Examples

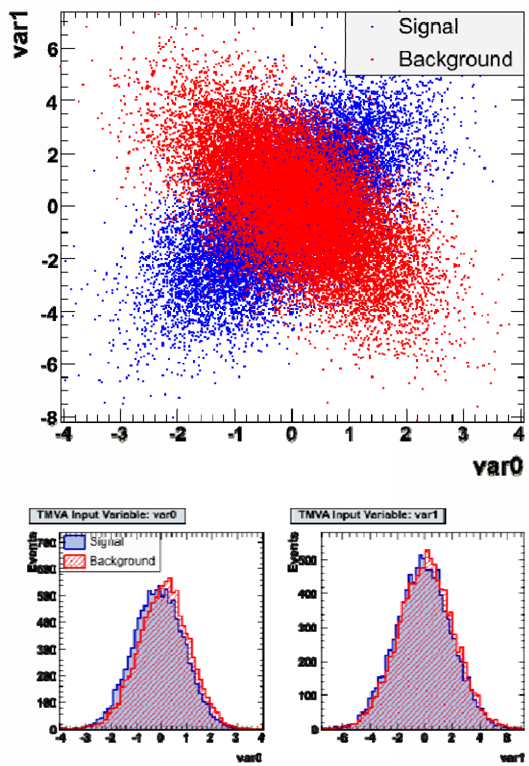
More Toys: Linear-, Cross-, Circular Correlations

- Illustrate the behaviour of linear and nonlinear classifiers

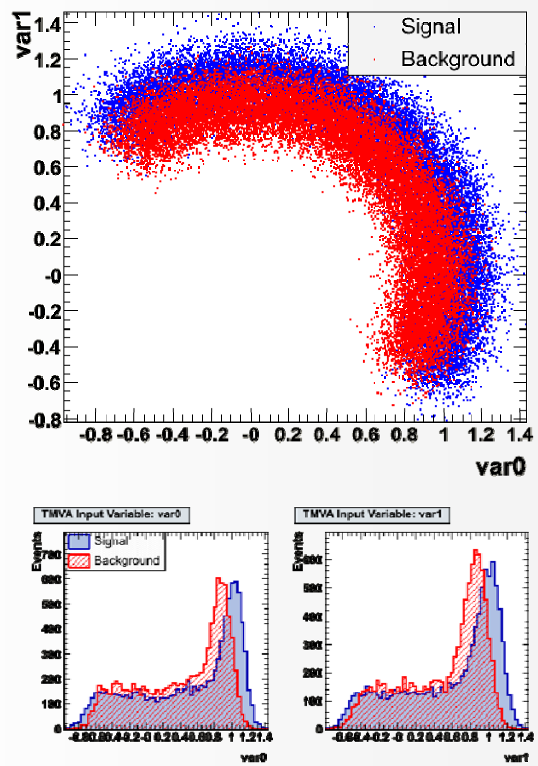
Linear correlations
(same for signal and background)



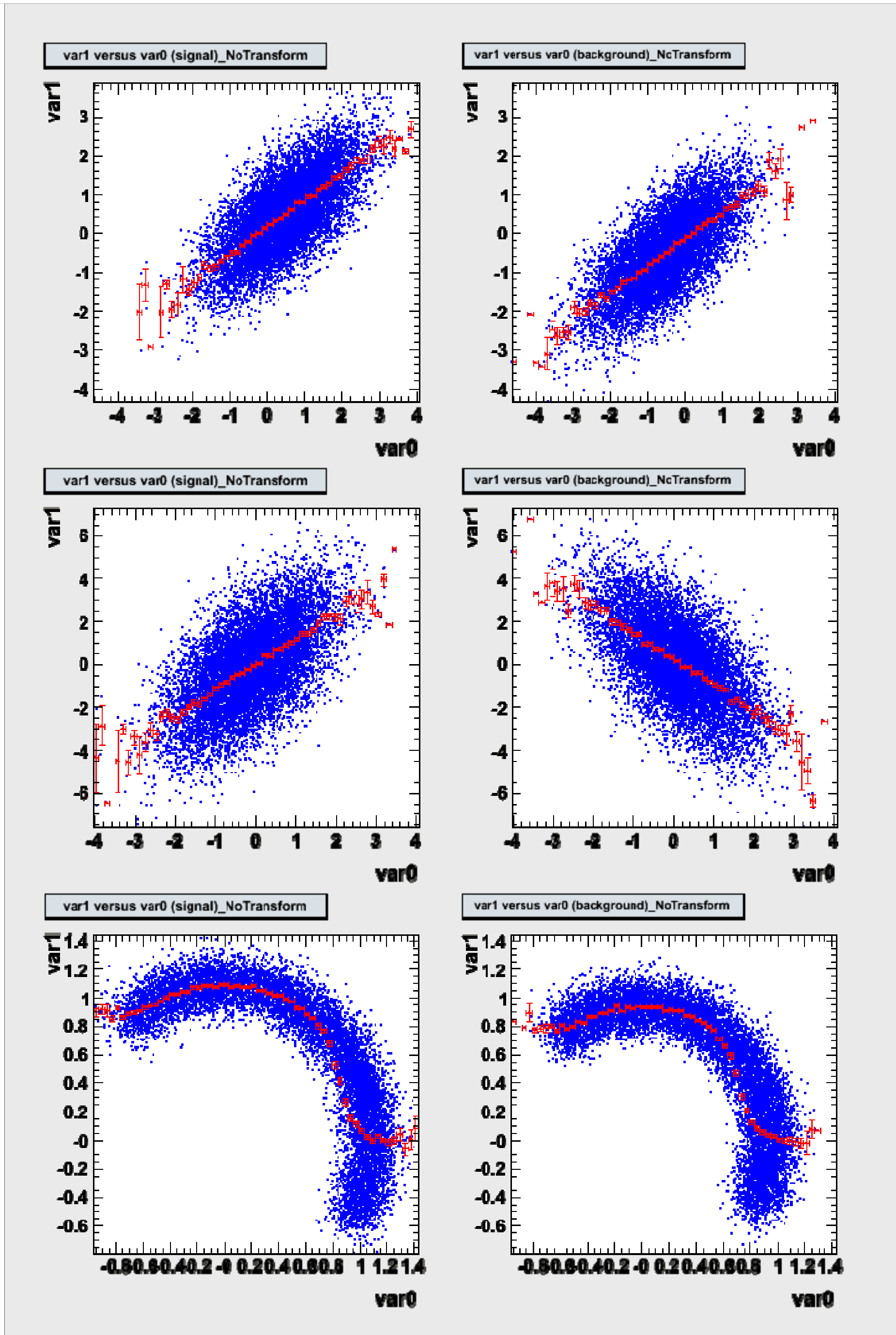
Linear correlations
(opposite for signal and background)



Circular correlations
(same for signal and background)

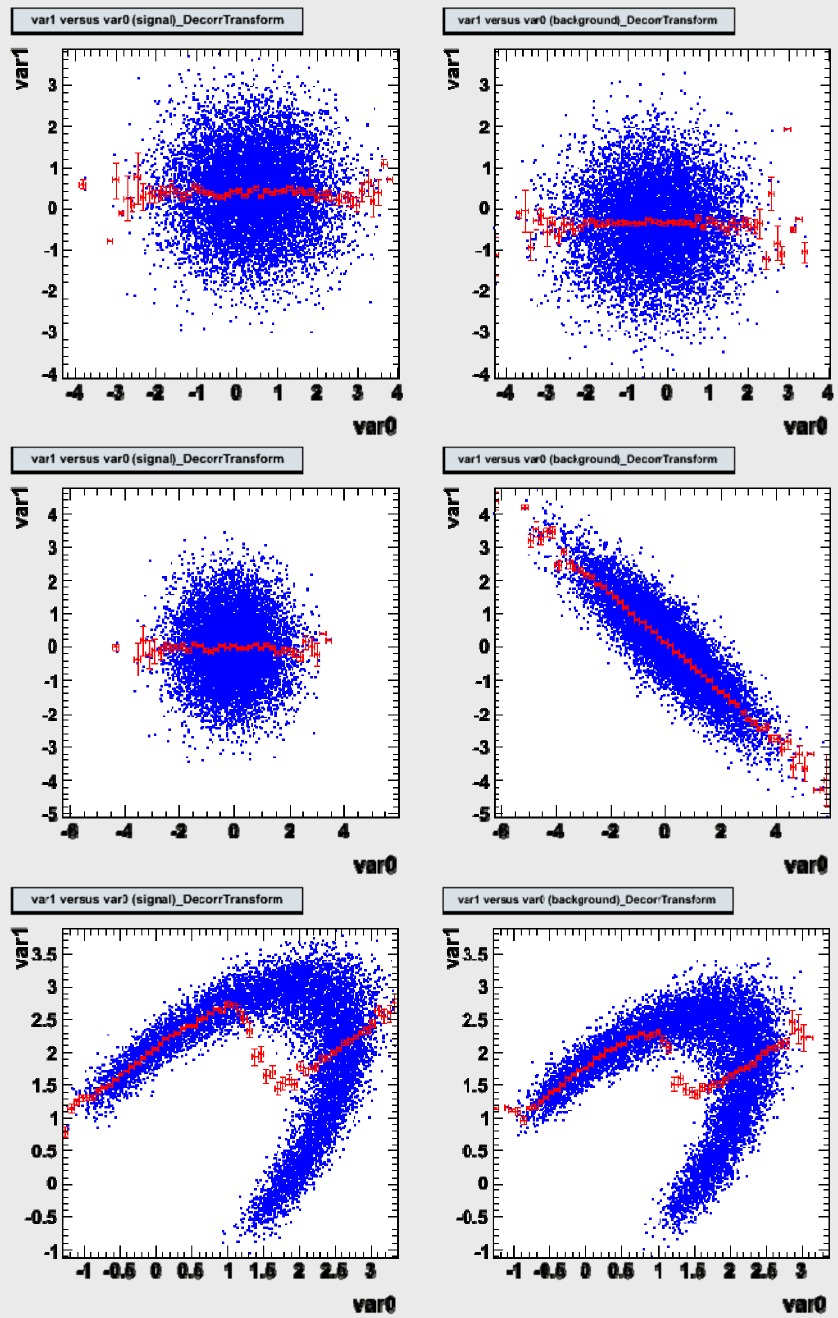


- How does linear decorrelation affect strongly nonlinear cases ?



Original correlations

- How does linear decorrelation affect strongly nonlinear cases ?

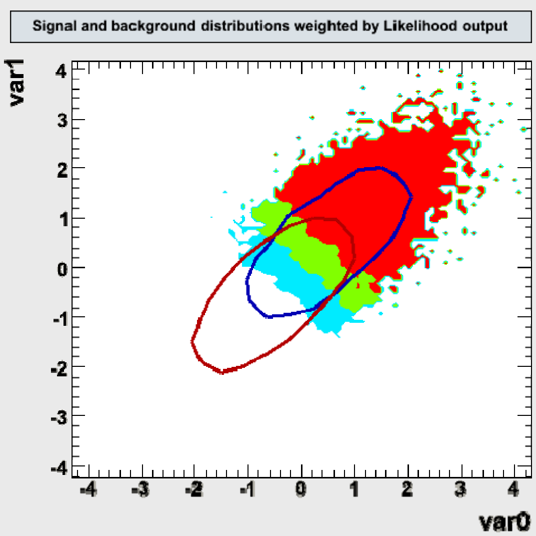


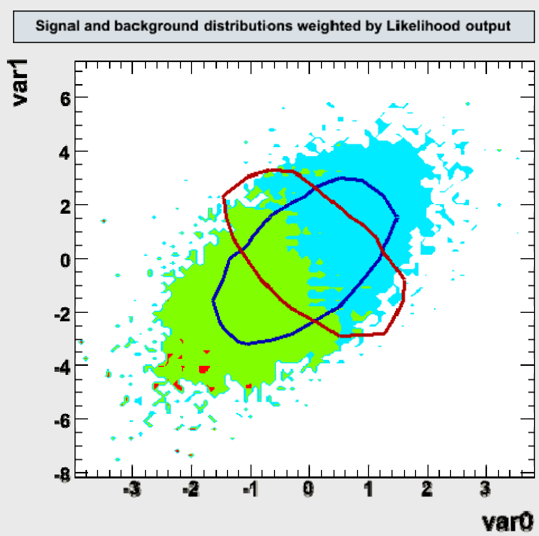
SQRT decorrelation

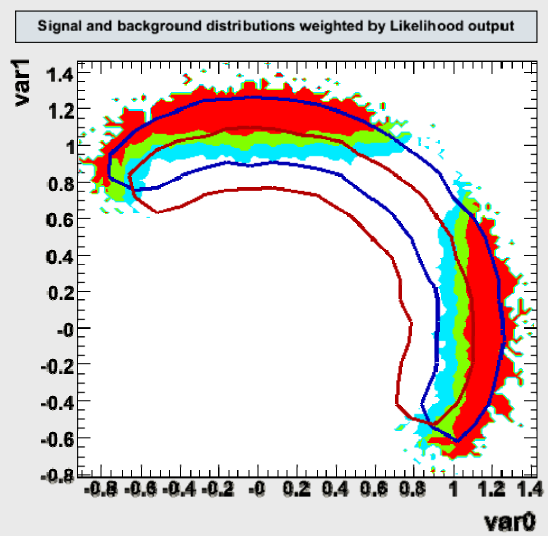
Weight Variables by Classifier Output

- 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)





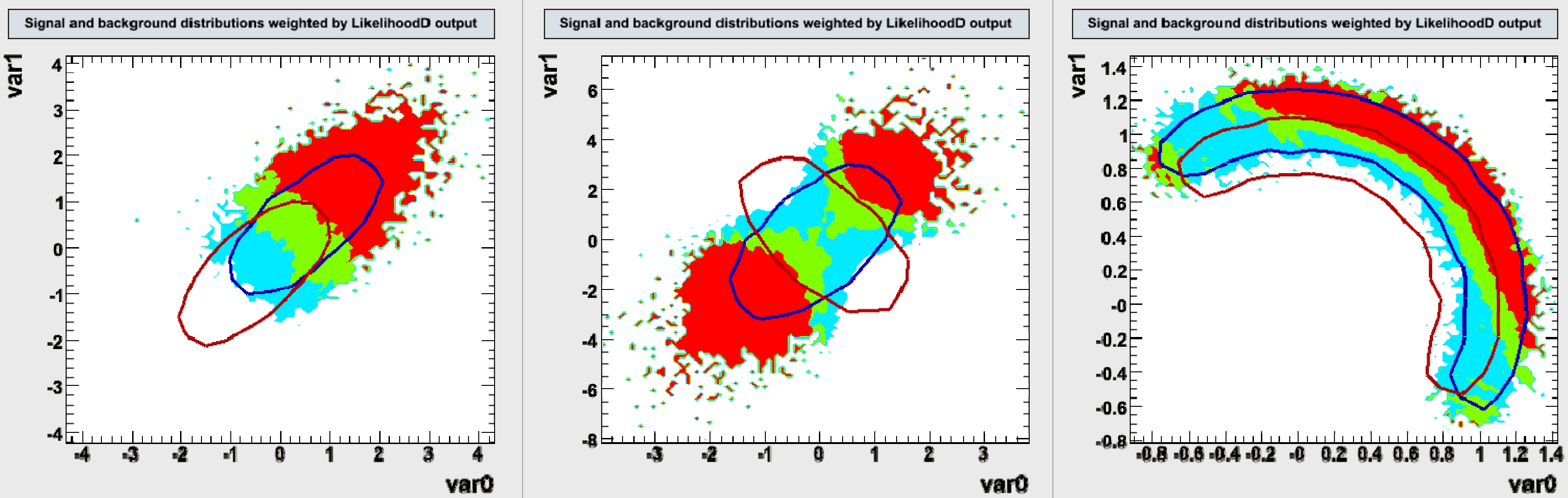


Likelihood

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)

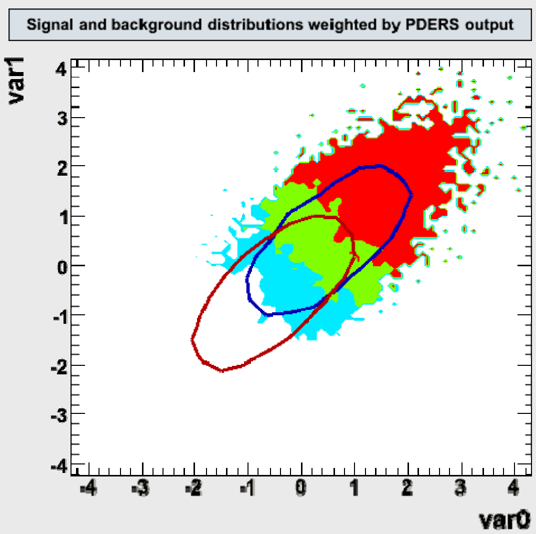


Likelihood - D

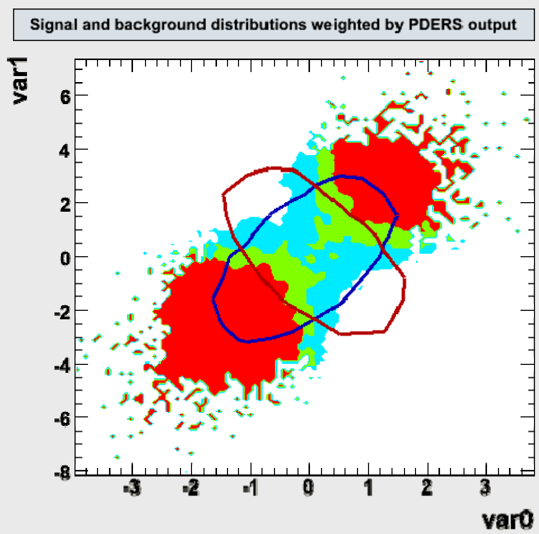
Weight Variables by Classifier Output

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

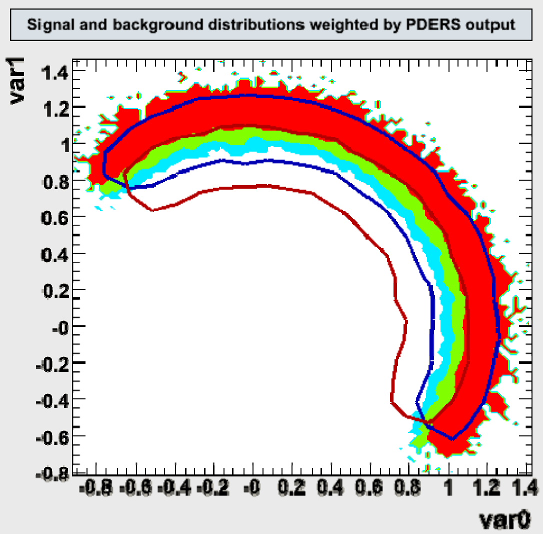
Linear correlations
(same for signal and background)



Cross-linear correlations
(opposite for signal and background)



Circular correlations
(same for signal and background)

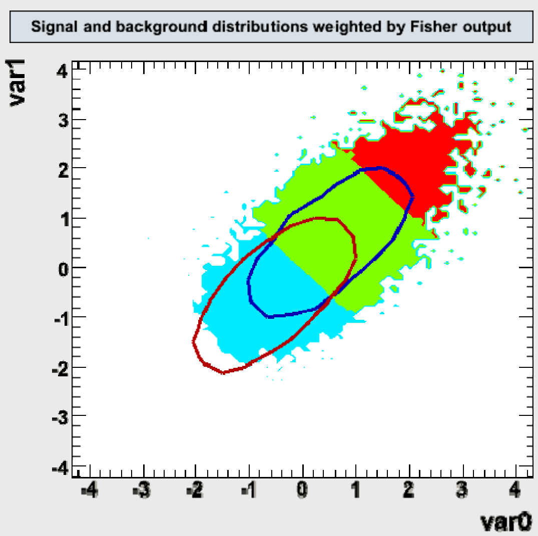


PDERS

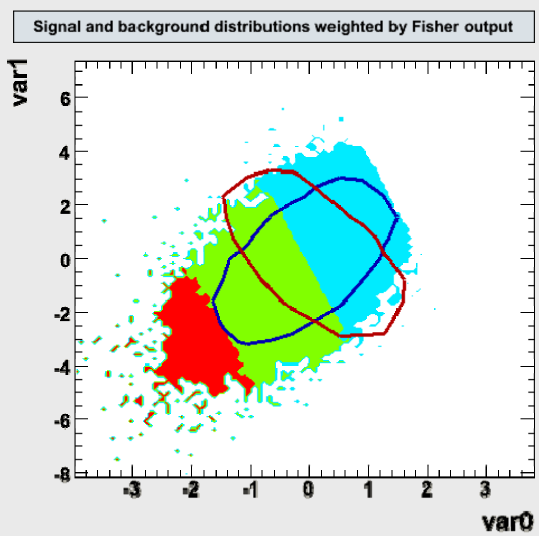
Weight Variables by Classifier Output

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

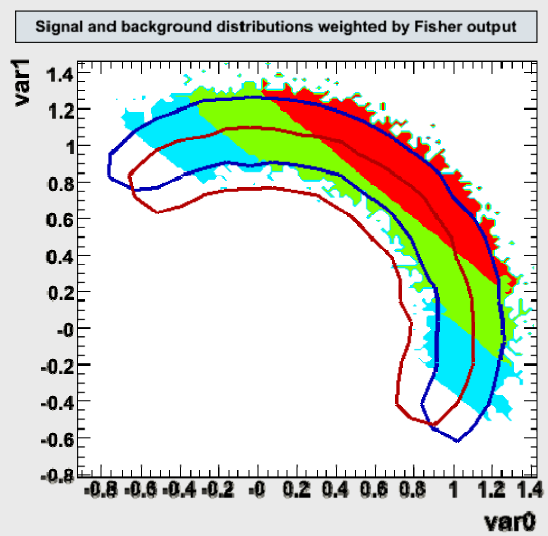
Linear correlations
(same for signal and background)



Cross-linear correlations
(opposite for signal and background)



Circular correlations
(same for signal and background)

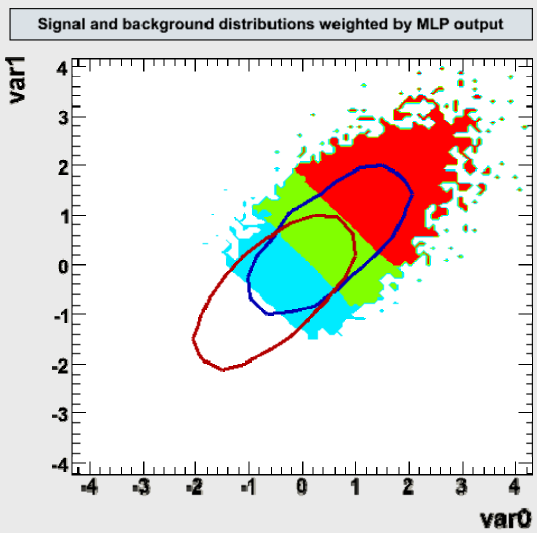


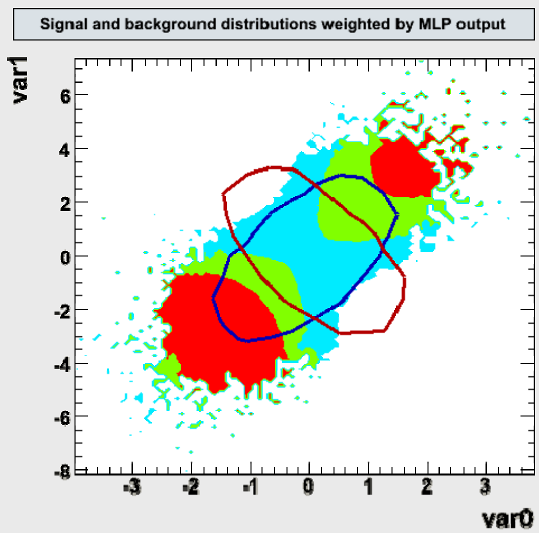
Fisher

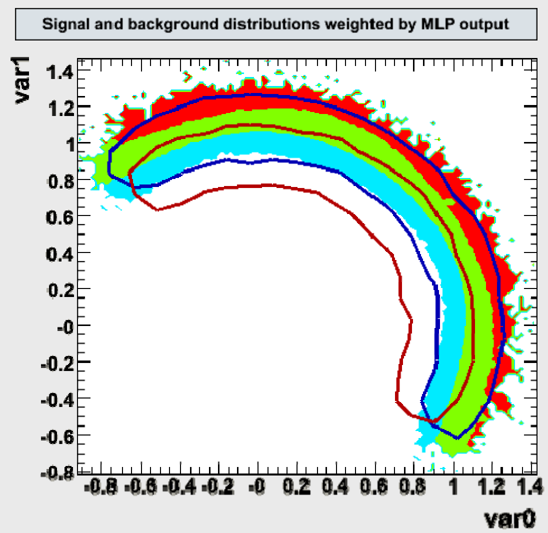
Weight Variables by Classifier Output

- 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)





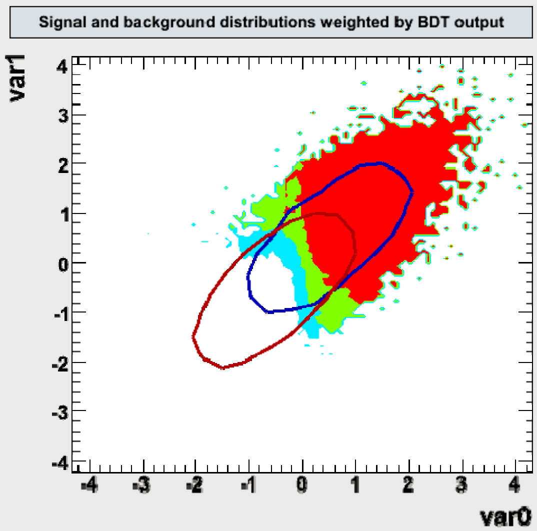


MLP

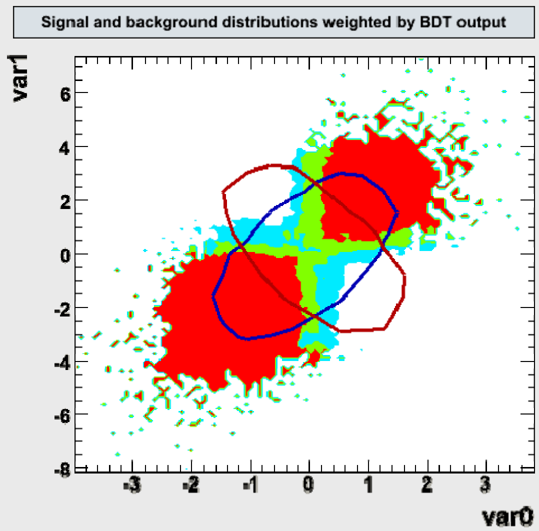
Weight Variables by Classifier Output

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

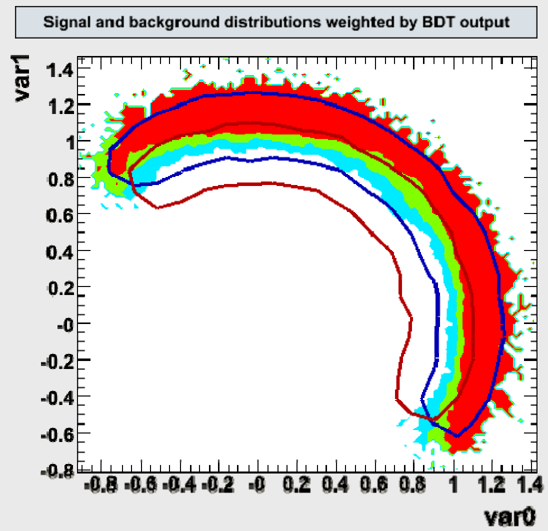
Linear correlations
(same for signal and background)



Cross-linear correlations
(opposite for signal and background)



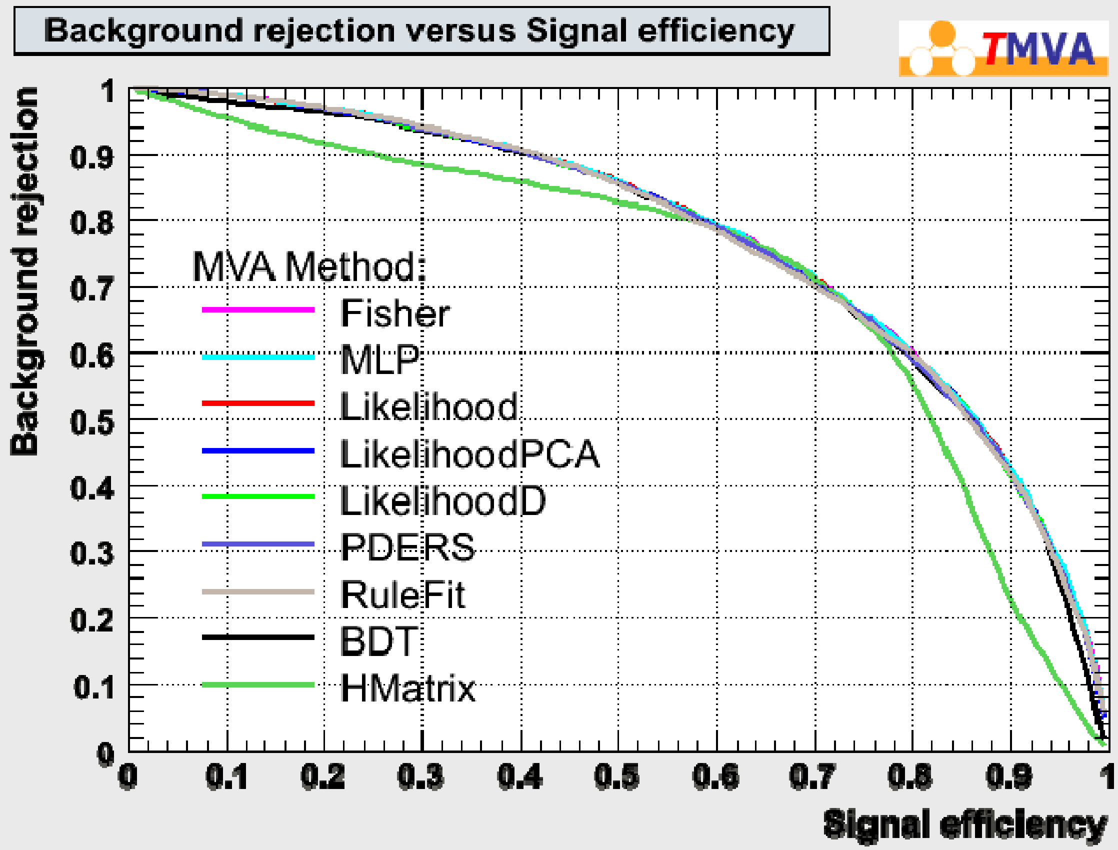
Circular correlations
(same for signal and background)



BDT

Final Classifier Performance

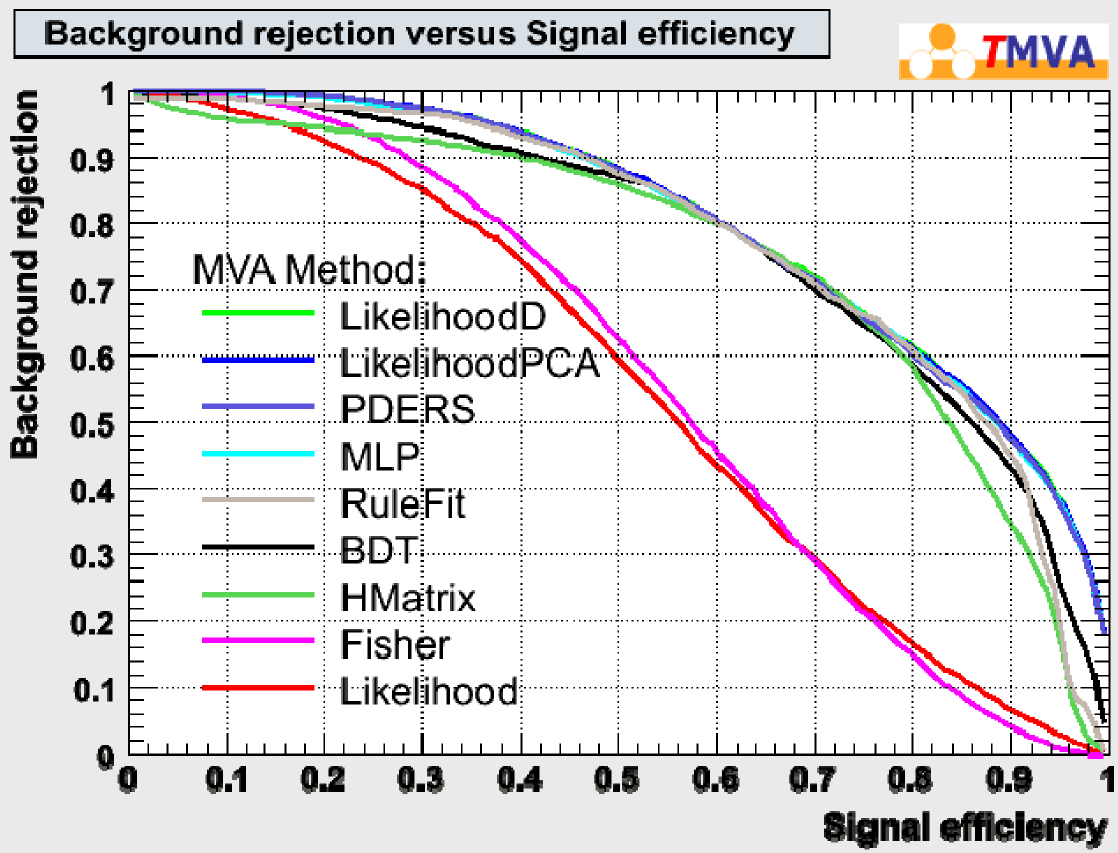
- Background rejection versus signal efficiency curve:



Circular Example

Final Classifier Performance

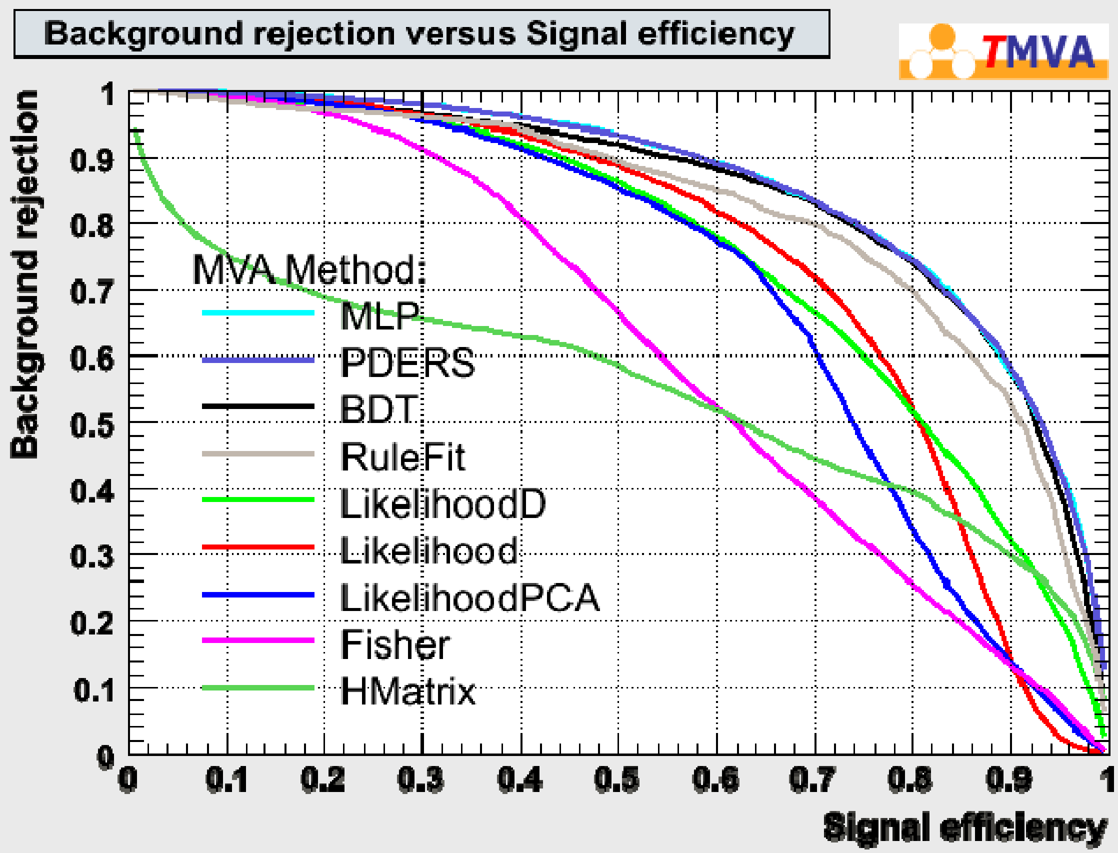
- Background rejection versus signal efficiency curve:



Circular Example

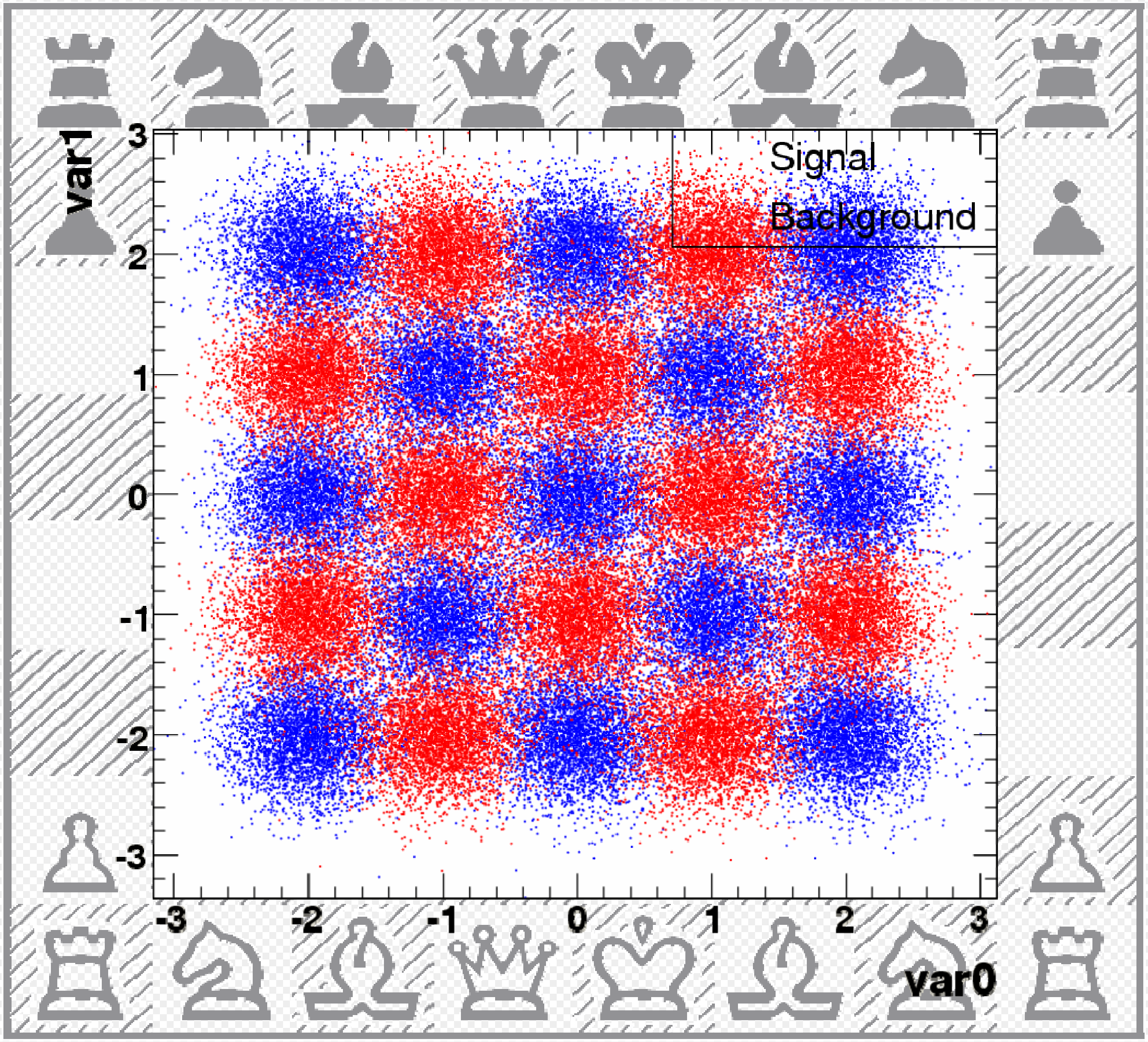
Final Classifier Performance

- Background rejection versus signal efficiency curve:

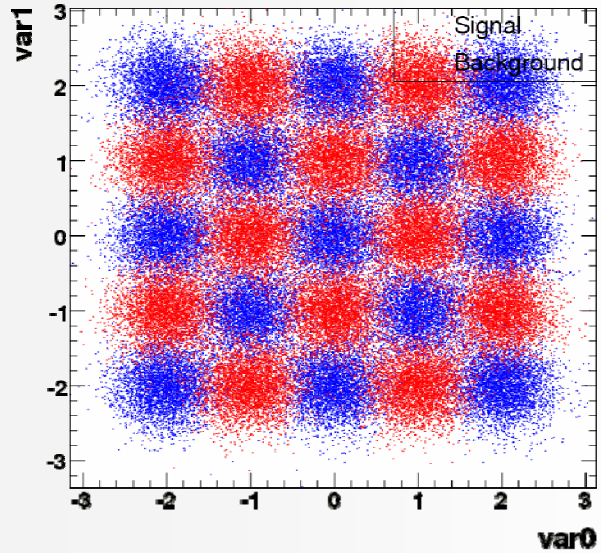


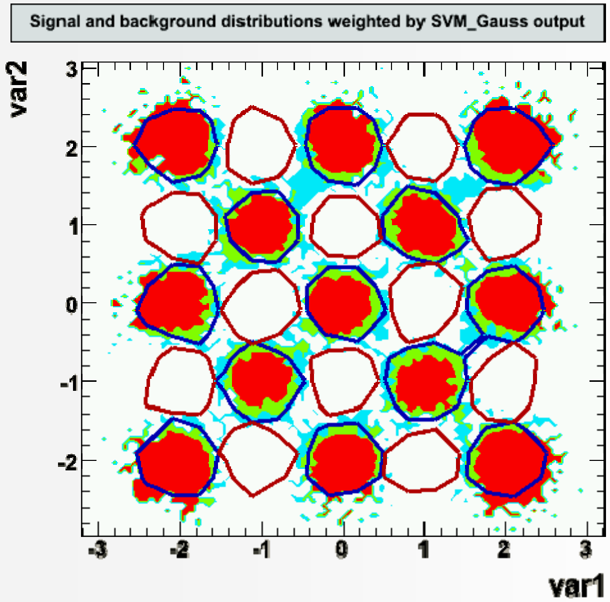
Circular Example

The “Schachbrett” Toy

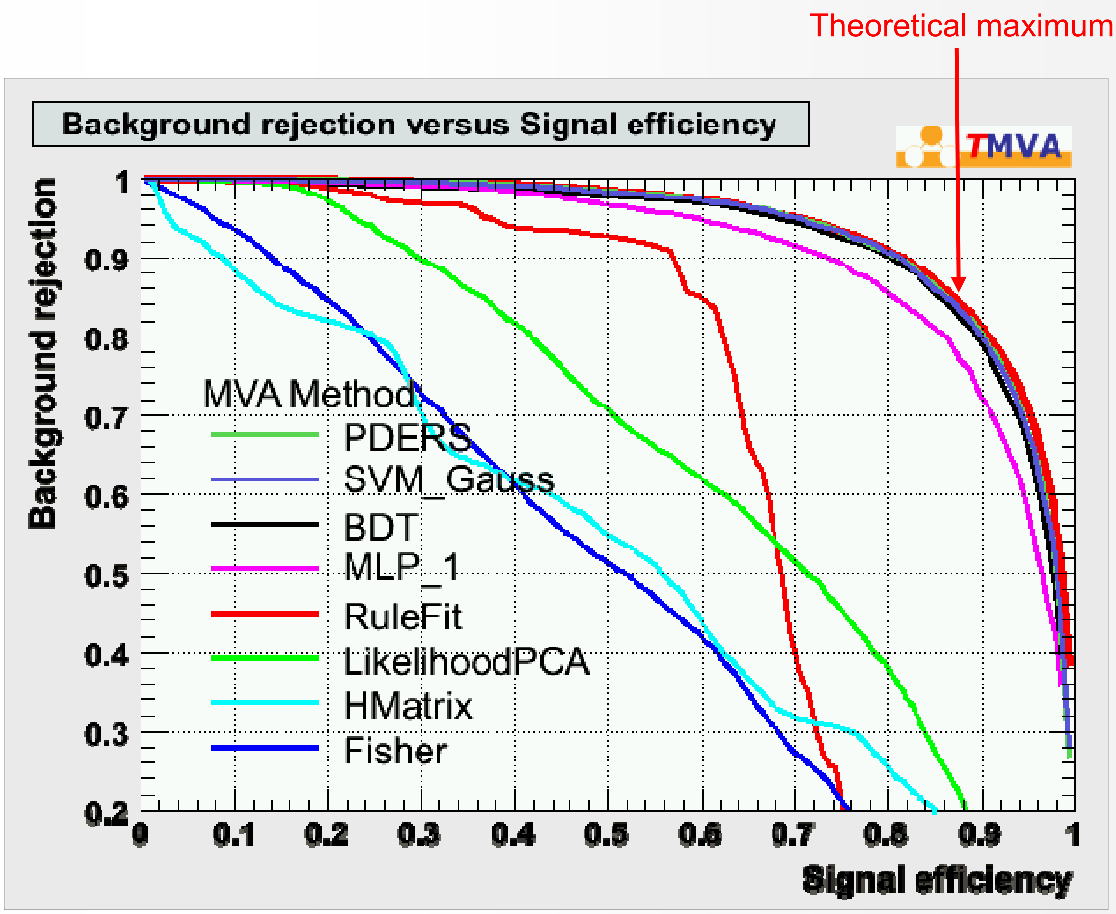


The "Schachbrett" Toy





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



Summary & Plans

Summary of the Classifiers and their Properties

Criteria		Cuts	Likeli-hood	PDERS / k-NN	H-Matrix	Fisher	MLP	BDT	RuleFit	SVM
Perfor-mance	no / linear correlations	😐	🙂	🙂	😐	🙂	🙂	😐	🙂	🙂
	nonlinear correlations	😐	🙁	🙂	🙁	🙁	🙂	🙂	😐	🙂
Speed	Training	🙁	🙂	🙂	🙂	🙂	😐	🙁	😐	🙁
	Response	🙂	🙂	🙁/😐	🙂	🙂	🙂	😐	😐	😐
Robust -ness	Overtraining	🙂	😐	😐	🙂	🙂	🙁	🙁	😐	😐
	Weak input variables	🙂	🙂	🙁	🙂	🙂	😐	😐	😐	😐
Curse of dimensionality		🙁	🙂	🙁	🙂	🙂	😐	😐	😐	😐
Clarity		🙂	🙂	😐	🙂	🙂	🙁	🙁	🙁	🙁

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

Plans

Primary goal for this Summer: Generalised ***Committee*** classifier

- Combine *any* classifier with *any other* classifier using *any* combination of input variables in *any* phase space region

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

Copyrights & Credits

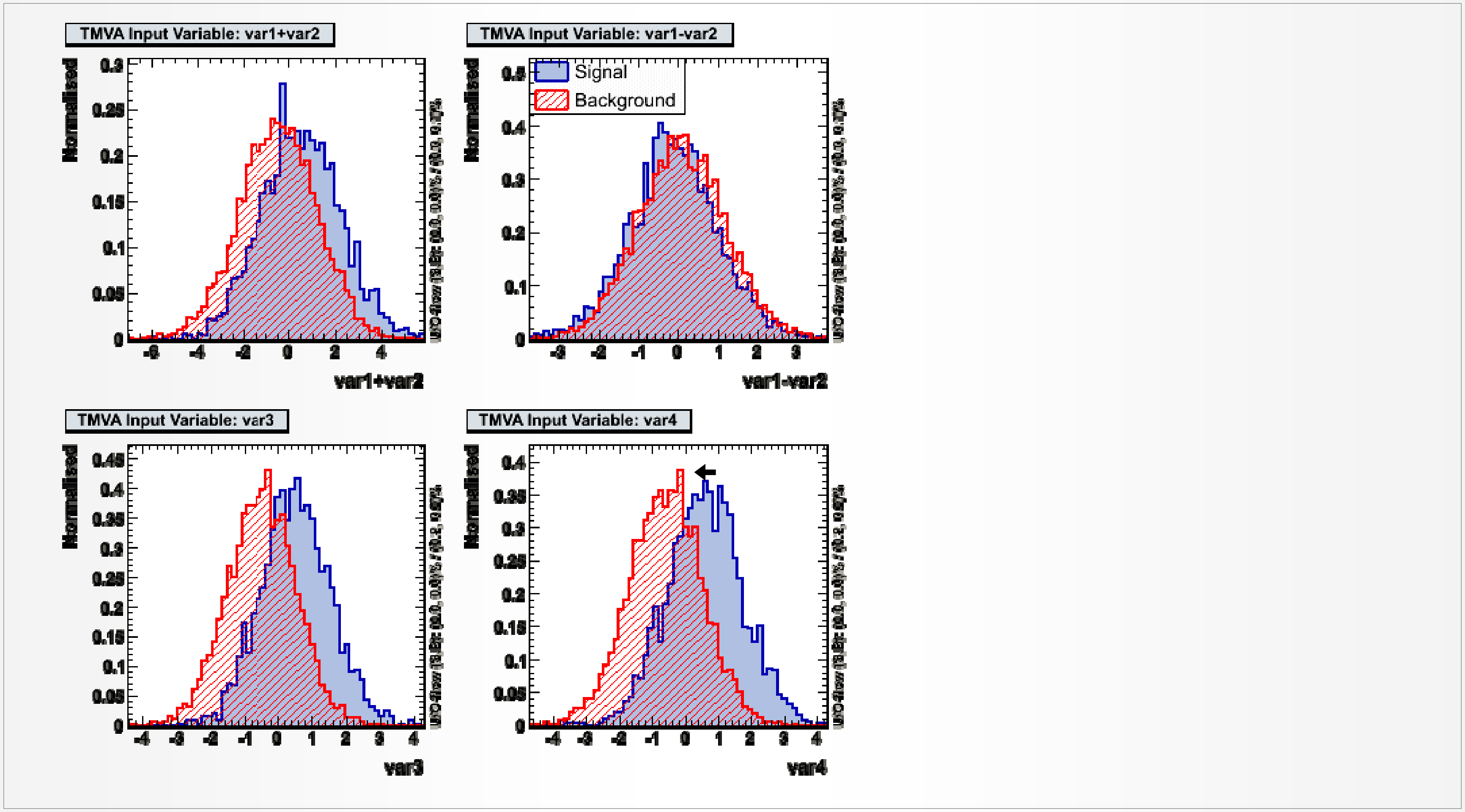
- *T*MVA is open source software
- Use & redistribution of source permitted according to terms in BSD license
- Several similar data mining efforts with rising importance in most fields of science and industry
- Important for HEP:
  - Parallelised MVA training and evaluation pioneered by *Cornelius* 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, and Yair Mahalalel (Tel Aviv) for a significant improvement 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.

b a c k u p   s l i d e s

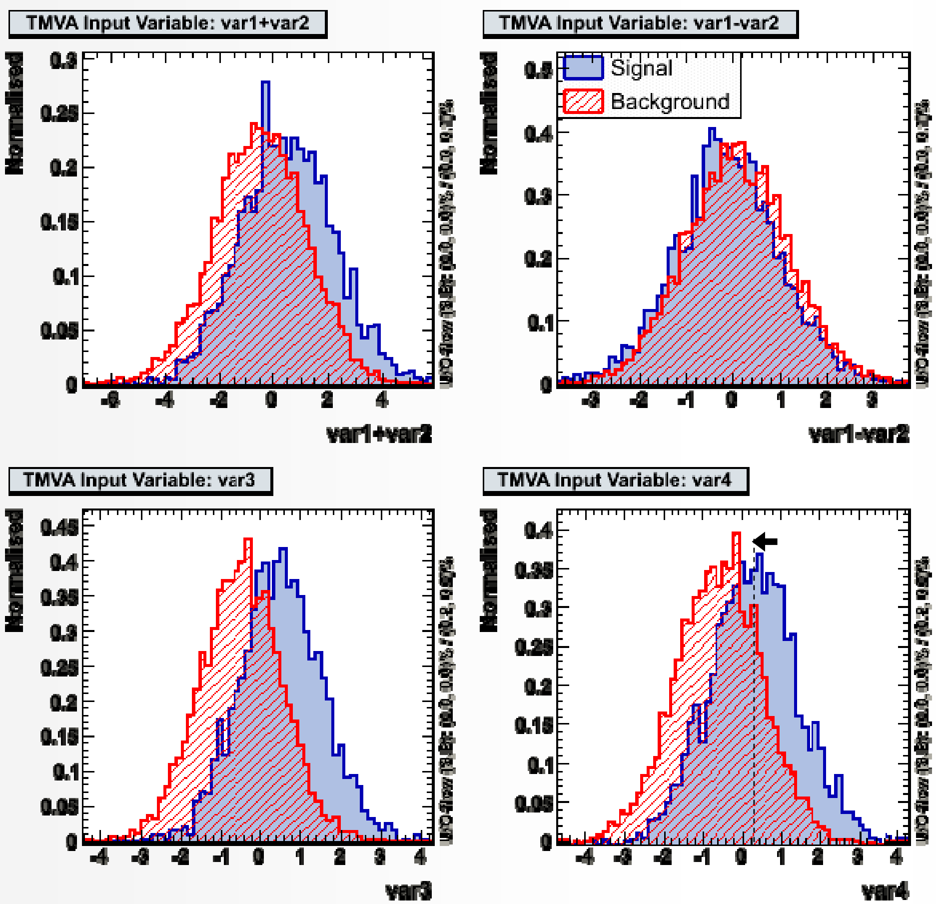
Treatment of Systematic Uncertainties

- Assume strongest variable "var4" suffers from systematic uncertainty



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

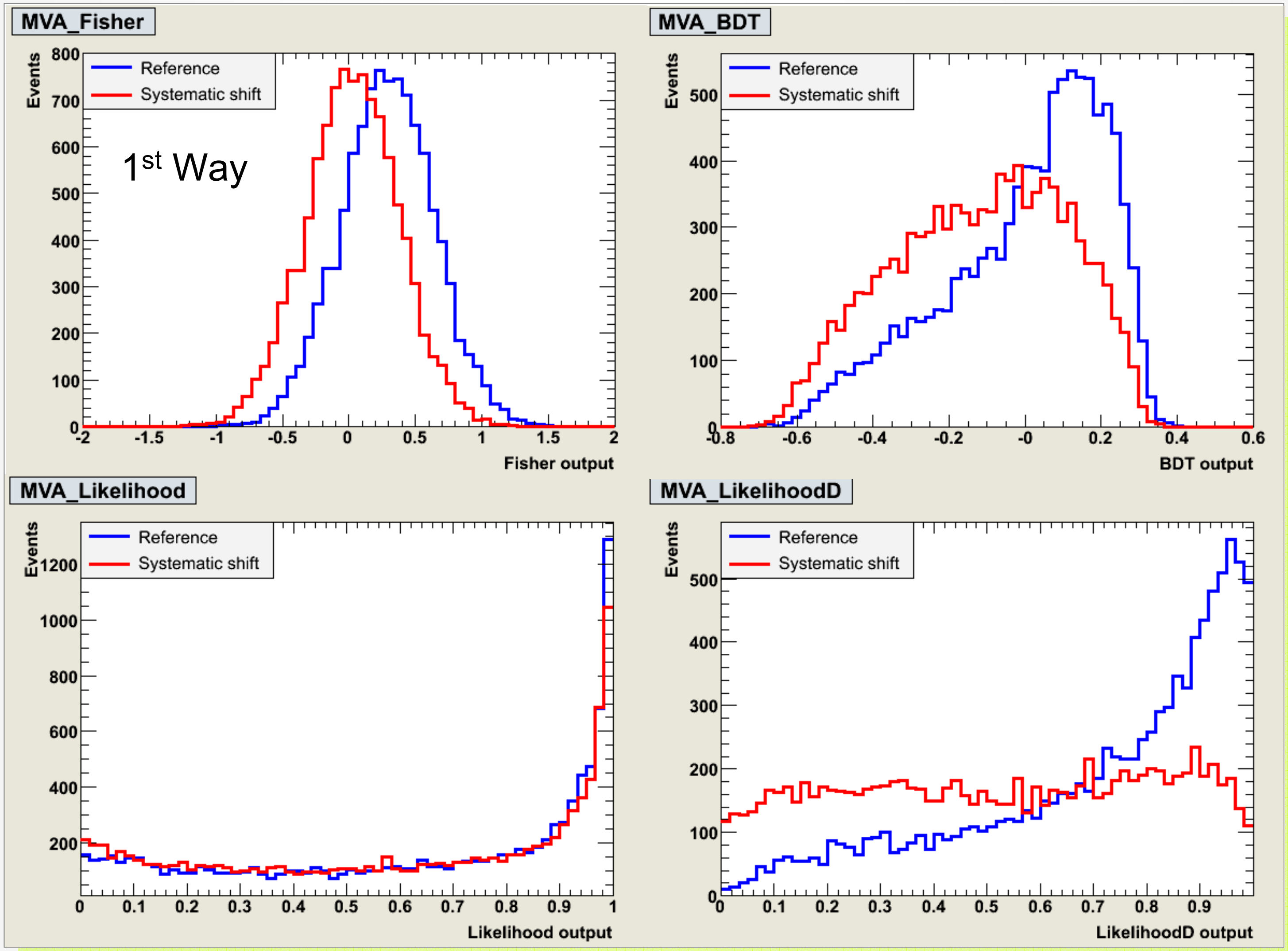
- Assume strongest variable “var4” suffers from systematic uncertainty
- (at least) Two ways to deal with it:

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



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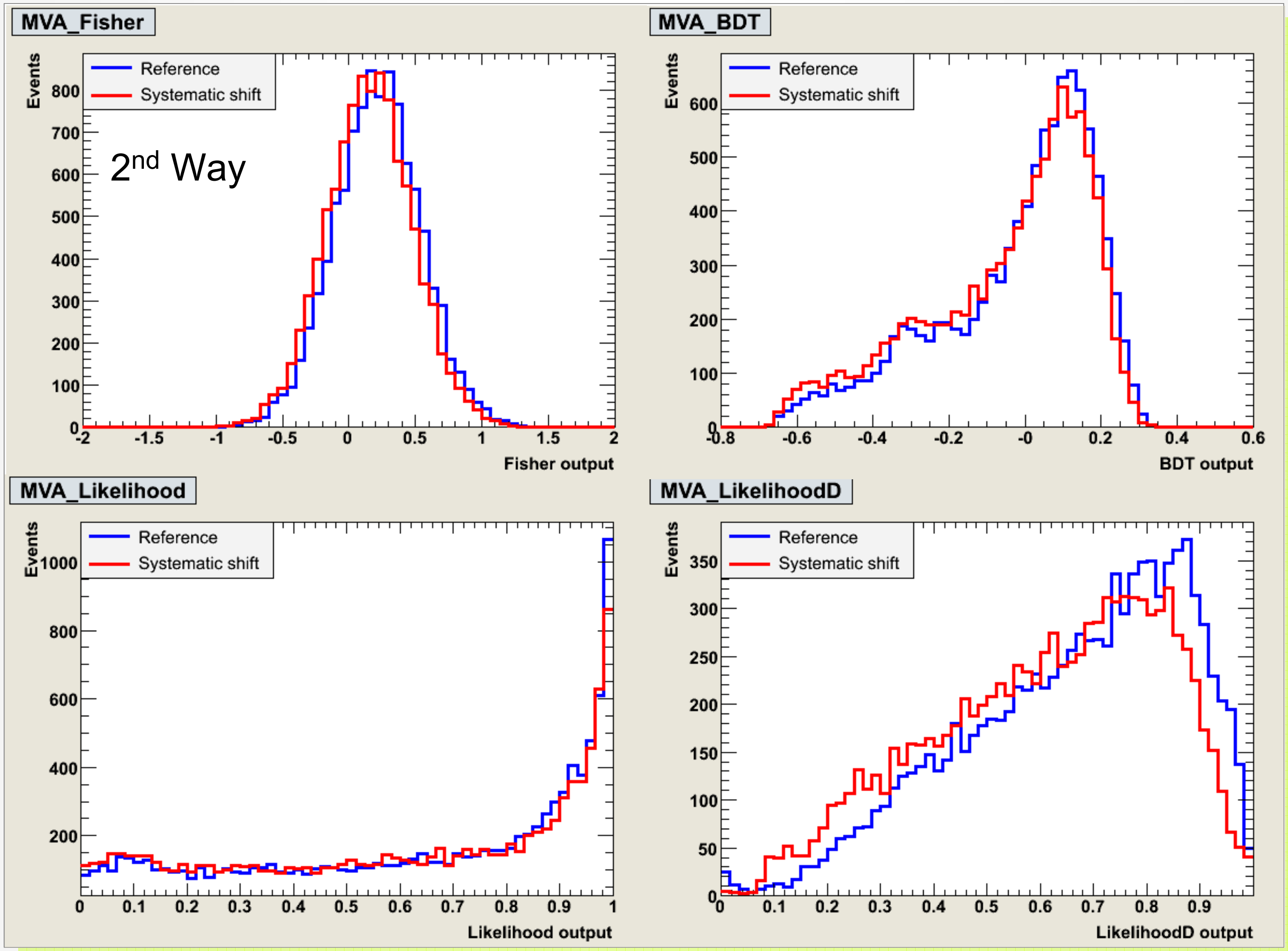
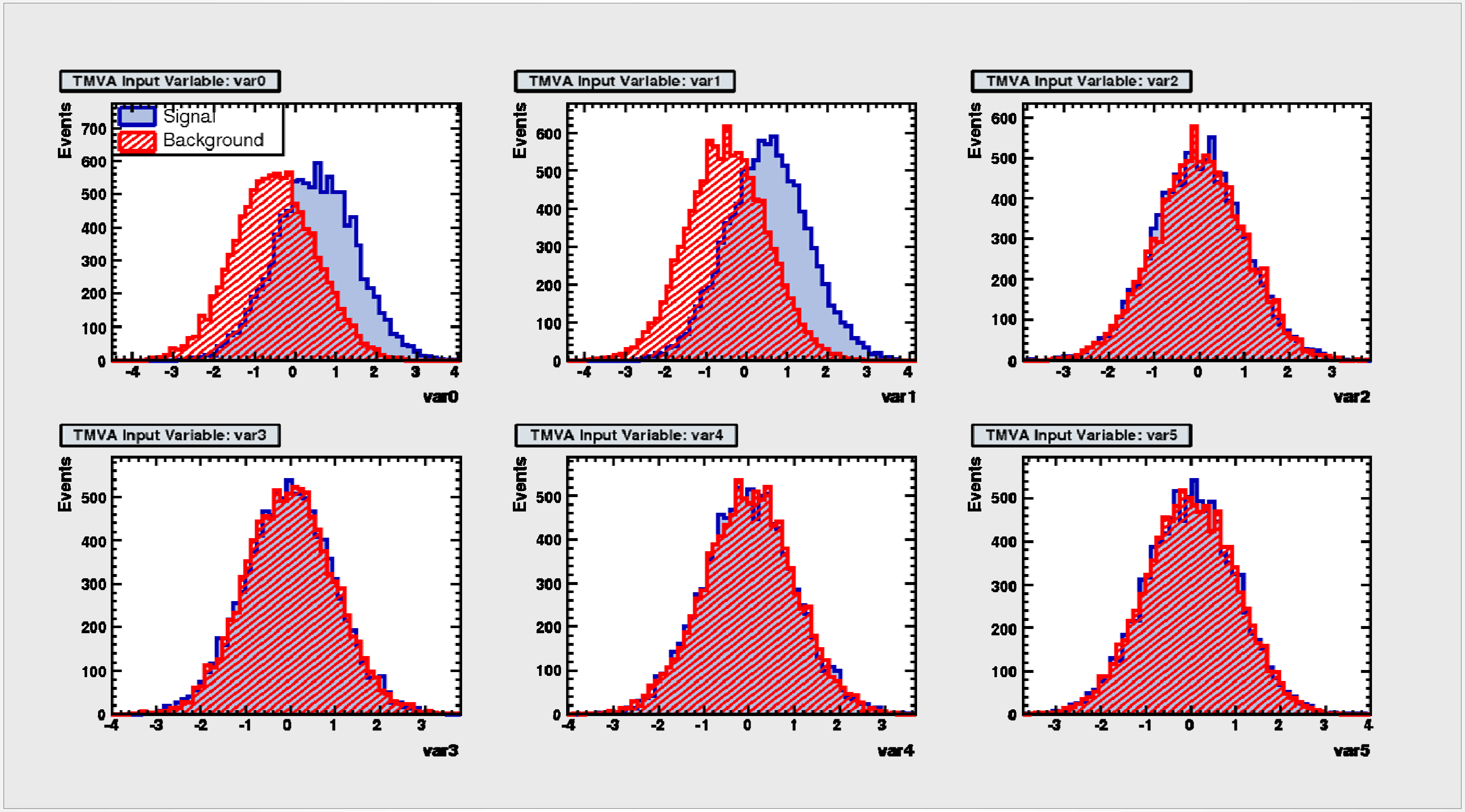


Stability with Respect to Irrelevant Variables

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



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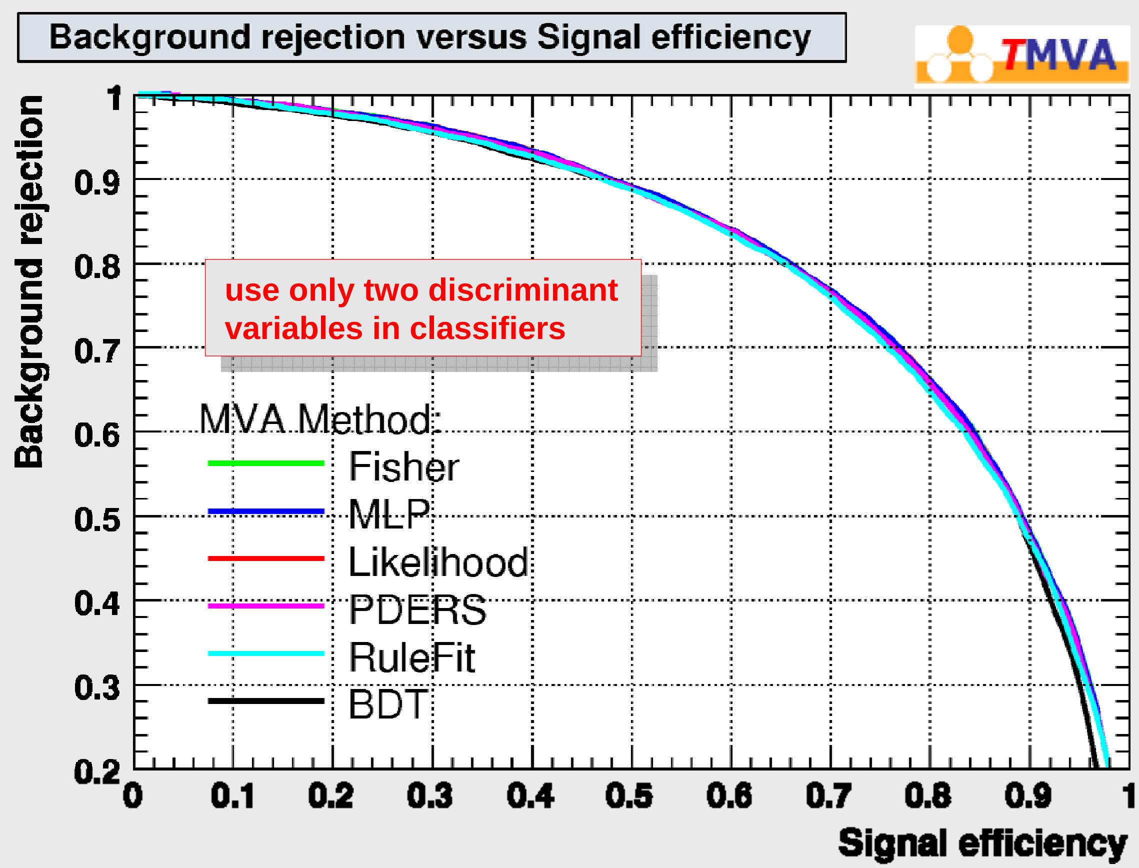

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