*T*MVA

A Multivariate Analysis Toolkit

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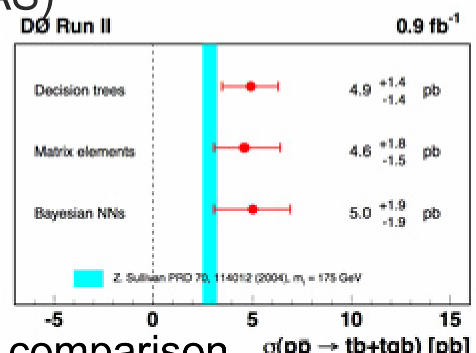
Contributors

– Introduction –

- Event classification is main objective of data mining in HEP
  - Signal vs background event separation, particle ID, flavor-tagging, …
  - Can have many input variables (between ~10 to ~50), often correlated

- Many classification methods exist and are already used in HEP (BABAR almost all analysis use MVA methods)
  - HEP tradition: rectangular cuts (with previous de-correlation) optimization often by hand
  - Also widely accepted: Likelihood (usually in one or two dimensions only)
  - Somewhat new: multidimensional Probability Density Estimators – range search
  - Gaining Trust: Artificial Neural Networks
  - Simple, but can be powerful: Fisher Discriminant (BABAR, BELLE: B selection)
  - Newcomers: Boosted Decision Trees (MiniBoone, D0)
  - Powerful new method from Friedman: Rulefit (Study at ATLAS)
  - Uprising: Support Vector Machines (studies for LEP and Tevatron top analysis)



- Two Problems
  - Skepticism: black box myth, how to evaluate systematics
  - Choice of method: by simplicity, availability, hearsay, limited comparison

– What is *T*MVA –

- Ideally, for a given problem all MVA methods should be tested
  - Systematically chose the best performing classifier
  - Becoming familiar and gaining experience with other MVA methods takes away the mysticism

- *T*MVA – Toolkit for Multivariate Analysis:
  - Framework for parallel training and evaluation of MVA techniques to guide the user to choose of the best signal-background discriminator for his pur
  - TMVA does not seek to promote any particular classifier, the judgmer up to the user

- Currently Supported Methods
  - Cuts (optimizers: MC sampling, Genetic alg, simulated annealing)
  - 1-dimensional Likelihood Estimator
  - Multi-dimensional Probability Density Estimator (range search)
  - Fisher Discriminant (also H-matrix (χ^2-estimator))
  - Artificial Neural Network (3 different implementations)
  - Boosted/bagged Decision Trees
  - Rulefit

- Transformation of input variables: decorrelation, PCA

– What does TMVA do Exactly –

- The analyst provides:
  - Training and testing data for signal and background
    - ROOT tree of text file with events
  - List of variables to be included in the analysis
  - List of MVA methods to be used

- TMVA analysis provides:
  - Training, testing and evaluating all user-selected MVA-methods
    - Graphical and numerical evaluation available → guide user's choice
  - Ranking of input variables
    - Preliminary general ranking
    - Method specific ranking
  - Training results are written to self-contained 'weight'-files
    - Weight files also contain the complete training setup of a method
    - Easy to share an analysis setup with colleagues !
      - no need to send code fragments and explanations back and forth
  - For data analysis (after successful training and selection of MVA) weight file is used by TMVA::Reader class for classification

– TMVA Development and Distribution –

- TMVA is a sourceforge (SF) package to accommodate world-wide access
  - home page ……………………..http://tmva.sourceforge.net/
  - SF project page ………………http://sourceforge.net/projects/tmva
  - view CVS ………………………http://tmva.cvs.sourceforge.net/tmva/TMVA/
  - mailing lists ……………………http://sourceforge.net/mail/?group_id=152074
  - ROOT::TMVA class index…..http://root.cern.ch/root/htmldoc/TMVA_Index.html

- Very active project → fast response time on feature requests (or bug reports)
  - Currently 4 main developers at CERN, ~23 registered contributors at SF

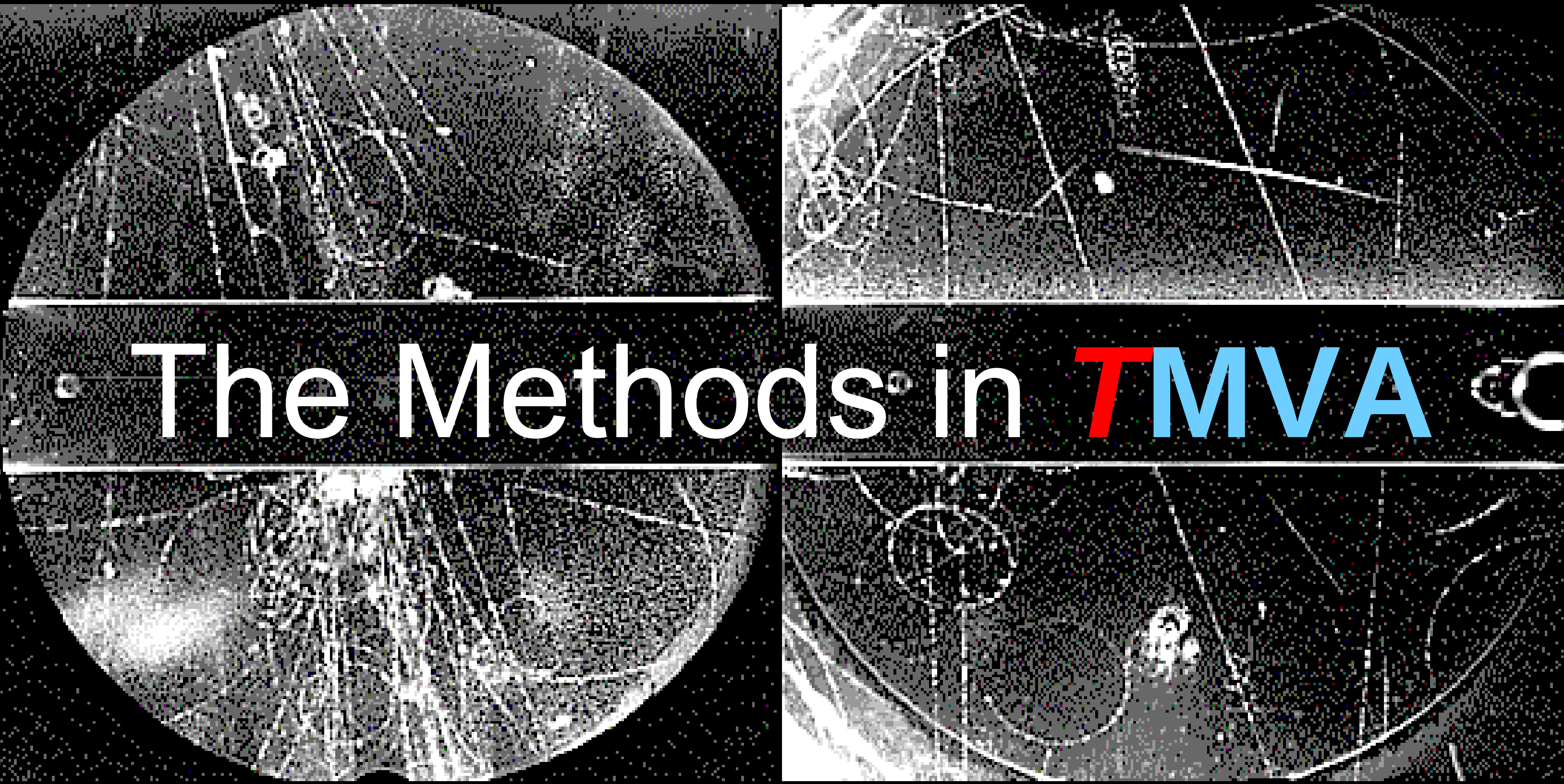
- Written in C++ using core ROOT functionality

- Integrated and distributed with ROOT since ROOT v5.11-03
  - Available out of the box (ROOT is everywhere)
  - Only thoroughly tested TMVA versions in ROOT
  - Always with up-to-date example in $ROOTSYS/tmva/test/

- Documentation currently being written, release date next week

– TMVA Technical Details –

- TMVA can be used
  - C++ executable: (athena), examples SourceForge
  - CINT macros: examples at $ROOTSYS/tmva/test/
  - Python (PyROOT), example only at SourceForge
- Modular
  - Can switch on/off each method
  - Simultaneously train multiple instances of one method with different options
- Flexible
  - Configuration of methods through custom option strings
  - Input variables (can be formulas as in TTree::Draw command)
    - Arrays are handled ("p"), but not array indices at present ("p[0]")
- User friendly
  - Option names easy to interpret
  - Default options are already good choice to start with
  - Graphical training and evaluation output (macros provided)
- Once trained, classification to real data straight forward
  - C++/CINT example at $ROOTSYS/tmva/test/TMVApplication.C



The Methods in *T*MVA

Decorrelation of Input Variables

- Cuts and projective likelihood perform best/optimal if there is no correlation between input variables
  - Remove linear correlations between input variables by rotation of parameter space

$$\mathbf{D} = \mathbf{S}^T \mathbf{C} \mathbf{S}$$

$$\mathbf{C}' = \mathbf{S}\sqrt{\mathbf{D}}\mathbf{S}^T$$

$$\mathbf{x}'(i) = \mathbf{C}'^{-1}\mathbf{x}(i)$$

Diagonalize (S) the covariance matrix C → D

Transform (S^T) the square root of D → C'

Decorrelate input space x with C'^{-1} → x'

- Separate transformation for signal and background

- De-correlation only complete if
  - input variables are Gaussian
  - Correlations are linear
  - In practice the gain is often only modest

Cuts

- Intuitive and most simple method: cut a rectangular volume out of parameter space that defines the signal

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

- Training samples do often not contain realistic signal and background abundance → no direct optimization for significance
  - Instead scan signal efficiency [0,1] and maximize background rejection
  - Straight forward computation of optimal working point (highest significance) given S and B expectation
- Cut optimization:
  - MINUIT fit (simplex) was found not to be reliable
  - Three different (robust) methods

1. **Monte Carlo sampling**:
   - random scanning of parameter space
   - inefficient for large number of input variables
2. **Genetic algorithm**: Preferred method
   - Samples of cut-sets (a *population*) are evaluated and the fittest *individuals* are cross-bred (including mutation) to create the new generation
3. **Simulated annealing**: still need to optimize its performance
   - slow cooling of a metal makes atoms move into lowest energy state, simulated by a energy dependent perturbation probability to recover from local minima

Projected Likelihood Estimator

- Probability density functions for all variables combined (for signal and for background) to form likelihood-ratio estimator

$$y_{\mathrm{Lh}}(i) = \frac{L_S(i)}{L_S(i) + L_B(i)}, \quad L_{S/B}(i) = \prod_{v \in \{\text{variables}\}} p_{S/B,v}\left(x_v(i)\right)$$

Reference PDF

- Optimal MVA approach, **if** variables are uncorrelated
  - In practice rarely the case, solution: **de-correlate input** or use **different method**

- Reference PDFs are automatically generated from training data and represented as histograms (counting) or splines (order 2,3,5) – unbinned kernel estimator in work

- Output of likelihood estimator often strongly peaked at 0 and 1. To ease output parameterization TMVA applies inverse Fermi transformation.

$$y'_{\mathrm{lh}}(i) = -\tau^{-1} \ln\left(y_{\mathrm{lh}}^{-1}(i) - 1\right)$$

Multidimensional PDE

- Extend the one-dimensional approach to *n* dimensions (*n* – number of input variables)
  - Carli-Koblitz *Range-Search:* Searches a volume around event and counts(&weights) signal and background reference events (training sample) this volume ($n_{S/B}$)

$$y_{\mathrm{PDERS}}(i) = \frac{n_S(i)/N_S}{n_S(i)/N_S + n_B(i)/N_B}, \quad n_{S/B}(i) = \prod_{e \in \left\{ \begin{array}{l} \text{reference S/B} \\ \text{events in V(i)} \end{array} \right\}} w_e$$

- Volume:
  - **Size**: can be fixed (defined by the data: % of Max-Min or RMS) or adaptive (define by number of events in search volume)
  - **Shape**: box or ellipsoid

- Weights as function of the (normalized) distance between test- and reference events in volume can be applied (linear or Gaussian)

- Practical challenges:
  - Need very large training sample (**curse of dimensionality** of kernel based methods)
  - Fast training, slow evaluation.
    - Speed up range search by sorting reference sample into binary search trees

Linear Fisher Discriminant

- Well-known, simple and elegant MVA method
  - Linear discriminant analysis determines a axis in the input variable hyperspace ($F_1,\ldots,F_n$, such that a projection of events on this axis pushes signal and background as far away from each other as possible

$$\boxed{y_{\mathrm{Fi}}(i) = F_0 + \sum_{v \in \{\mathrm{variables}\}} F_v x_v(i)}$$

- Optimal for linearly correlated Gaussian variables where S and B have different means
- No separation power from variables *v* with different shapes but the same mean → $F_v=0$

W: sum of S and B covariance matrices

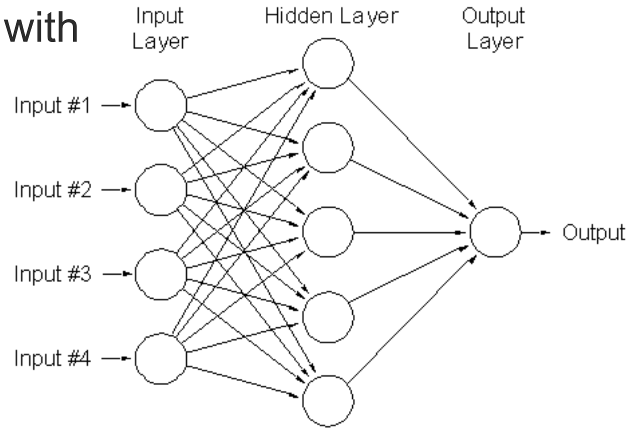
Fisher Coefficient

$$\boxed{F_v = \frac{\sqrt{N_S + N_B}}{N_S N_B} \sum_{l \in \{\mathrm{variables}\}} W_{vl}^{-1}\left(\bar{x}_{S,l} - \bar{x}_{B,l}\right), \quad \mathbf{W} = \mathbf{C}_S + \mathbf{C}_B}$$

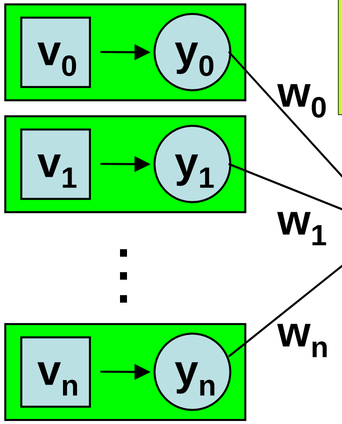
- H-matrix estimator: poor man's variation of Fisher discriminant

Artificial Neural Network (ANN)

- ANNs are non-linear discriminants
  - Non linearity from activation function. (Fisher is an ANN with linear activation function)
- Multilayer perceptron: fully connected, feed forward, $1..N_H$ hidden layers
  - Can approximate every continuous function to arbitrary precision with just one layer and infinite nodes (Weierstrass)

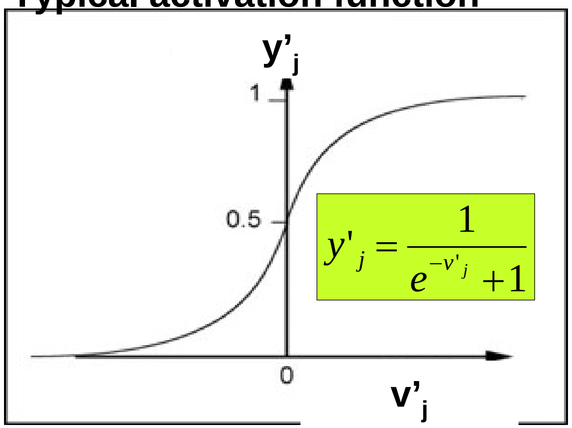


- Training of an MLP: back-propagation method
  - Randomly feed signal and background events to MLP and compare the desired output {0,1} with the received output (0,1): ε = d - r
  - Correct weights, depending on ε and learning rate η



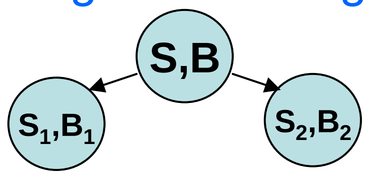
$$v'_j = \sum_{i=0,n} w_i y_i$$

Typical activation function



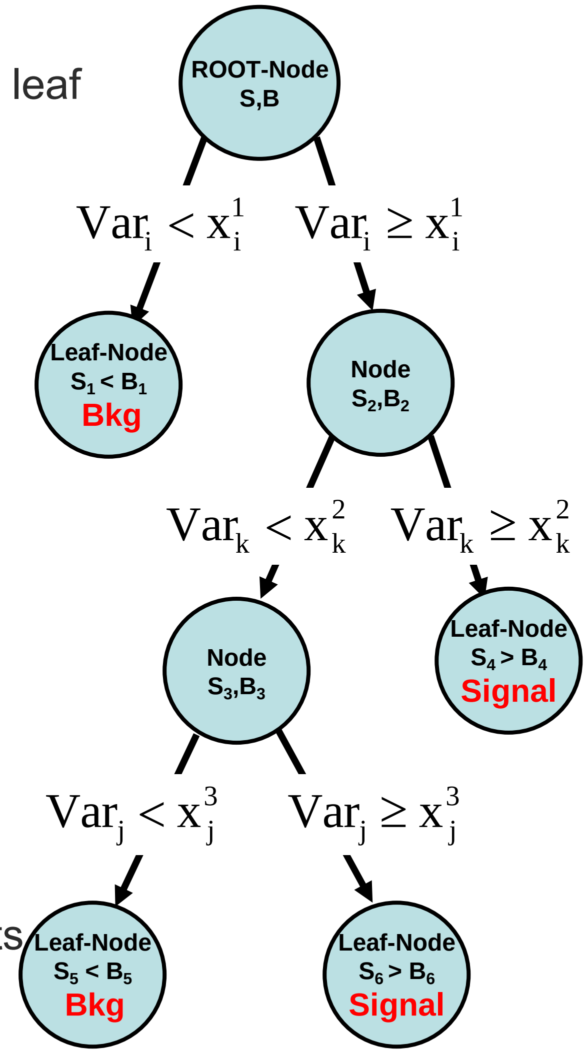
$$y'_j = \frac{1}{e^{-v'_j} + 1}$$

- Tree structure classifier (S and B leafs)
  - Classifies events by following a sequence of decisions depending on the events variable content until a S or B leaf
- Training the tree: e.g. split minimizes Gini-index



$$Gini = \frac{S_1 B_1}{S_1 + B_1} + \frac{S_2 B_2}{S_2 + B_2}$$

  - other splitting criteria: significance, cross-entropy, misclassification error
- Decision trees are robust in many dimensions but by itself not powerful (similar to cuts) → Need to boost
- Method to combine classifiers: boosting (also implemented: bagging)
  - Developed by statisticians in last decade
- Boosting: (Adaboost)
  - Re-weight events, higher weight for misclassified events lower for correctly classified events
  - Retrain and repeat → set of classifiers
  - Classify data by a weighted vote of the classifiers



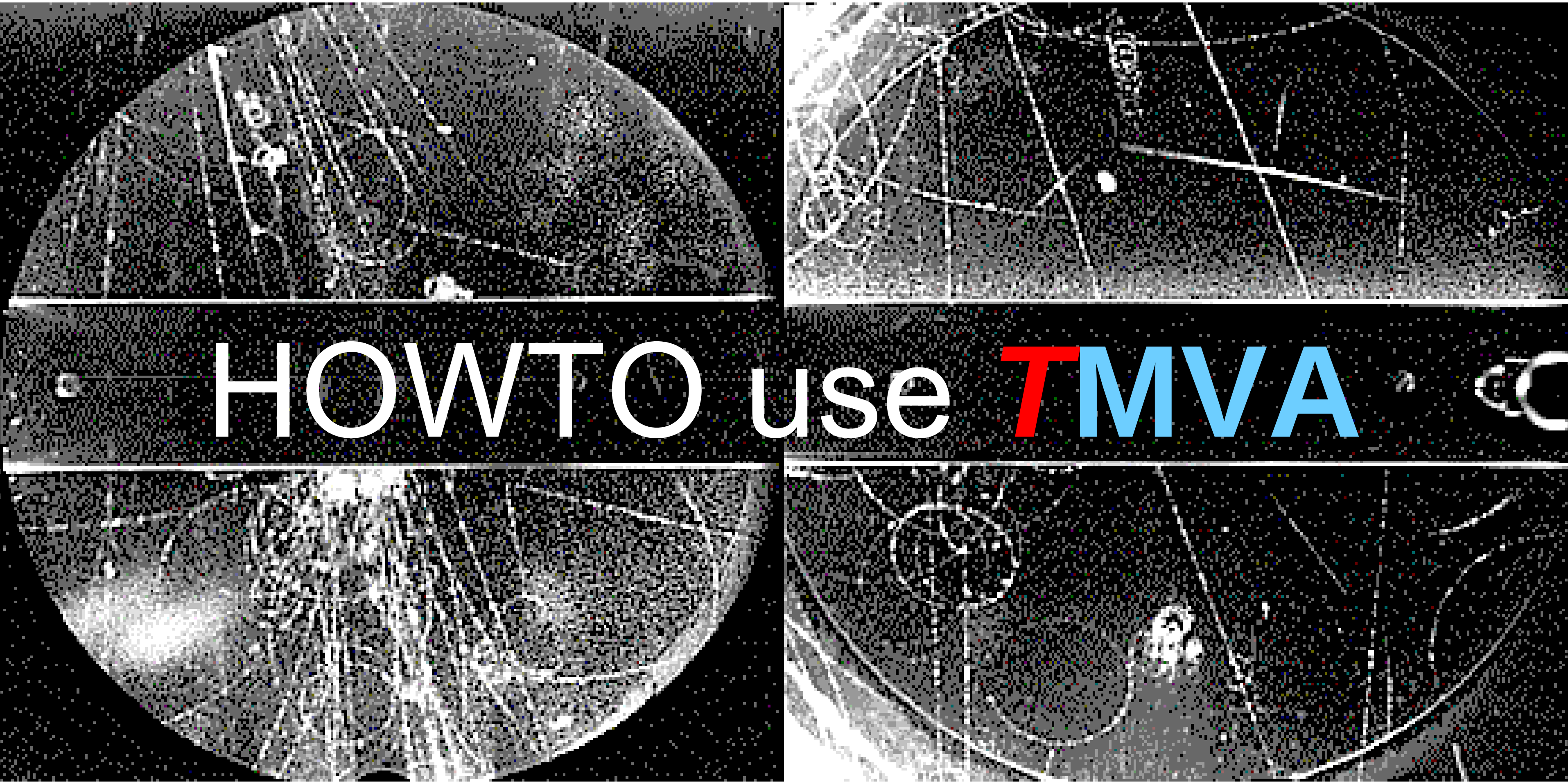
Rulefitter

- New and powerful method of J.Friedman
  - Belongs to the class of combined classifiers
  - This one combines decision trees from a ‘random forest’
  - Also adds a linear discriminant (Fisher) term

$$y_{\mathrm{RF}}(i) = F_0 + \sum_{m \in \{\text{base classifier}\}} a_m y_m\big(x(i)\big) \sum_{v \in \{\text{variables}\}} F_v x_v(i)$$

- Random subsets of training data used to create random forest of decision trees (y_m)
- Coefficients a_m are then fitted
  - Friedman, Popescu, “*Gradient Directed Regularization for Linear Regression and Classification*”, Technical report, statistics department, Stanford University 2003

HOWTO use *T*MVA



– Training (from TMVAnalysis.C) –

```
// create the root output file
TFile* target = TFile::Open( "TMVA.root", "RECREATE" );

// create the factory object
TMVA_Factory *factory = new TMVA_Factory( “Project", target, "" );
```

Create the Factory

```
TFile * input = TFile::Open("tmva_example.root");
TTree *signal = (TTree*)input->Get("TreeS");
TTree *background = (TTree*)input->Get("TreeB");

factory->SetInputTrees( signal, background, sWeight, bWeight);
factory->AddVariable("var1+var2",'F');factory->AddVariable(“var1-var2",'F');
factory->AddVariable("var3", 'F'); factory->AddVariable("var4", 'F');
```

Tell the Factory about your data

```
factory->BookMethod( TMVA::Types::kCuts, "CutsD",
   "!V:MC:EffSel:MC_NRandCuts=200000:VarTranform=Decorrelate" );

factory->BookMethod( TMVA::Types::kLikelihood, "LikelihoodPCA",
   "!V:!TransformOutput:Spline=2:NSmooth=5:VarTransform=PCA");
```

Book desired methods/options

```
// Train all configured MVAs using the set of training events
factory->TrainAllMethods();

// Evaluate all configured MVAs using the set of test events
factory->TestAllMethods();

// Evaluate and compare performance of all configured MVAs
factory->EvaluateAllMethods();
```

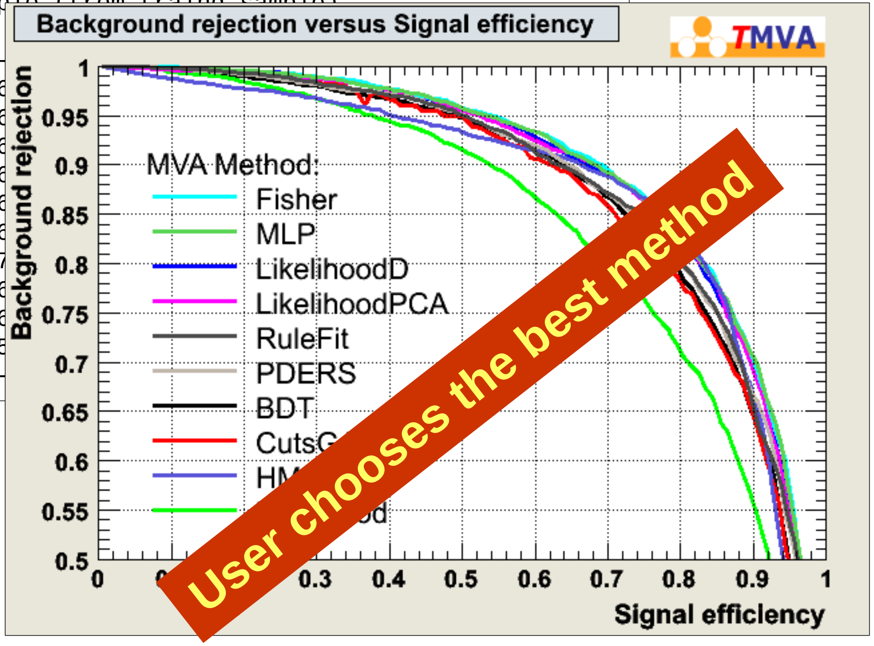
Perform training and evaluation

```
// open the GUI for the root macros
TMVAGui();
```

Open the GUI for performance plots

– Training (from TMVAnalysis.C) –

```
--- Factory       : Evaluation results ranked by best 'signal eff @B=0.10'
--- Factory       : -----------------------------------------------------------------------------
--- Factory       : MVA              Signal efficiency (error):       Signifi- Sepa-    mu-Trans-
--- Factory       : Methods:         @B=0.01    @B=0.10    @B=0.30    cance:   ration:  form:
--- Factory       : -----------------------------------------------------------------------------
--- Factory       : Fisher         : 0.292(07)  0.690(07)  0.900(04)  1.261    0.484    0.991
--- Factory       : LikelihoodPCA  : 0.245(06)  0.684(07)  0.896(04)  1.330    0.477    0.867
--- Factory       : MLP            : 0.287(07)  0.682(07)  0.903(04)  1.328    0.483    0.991
--- Factory       : LikelihoodD    : 0.287(07)  0.673(07)  0.898(04)  1.331    0.480    0.861
--- Factory       : HMatrix        : 0.075(04)  0.663(07)  0.884(05)  1.179    0.451    0.991
--- Factory       : PDERS          : 0.225(06)  0.646(07)  0.878(05)  1.258    0.449    0.911
--- Factory       : BDT            : 0.200(06)  0.641(07)  0.872(05)  1.219    0.432    0.991
--- Factory       : RuleFit        : 0.245(06)  0.632(07)  0.882(05)  1.246    0.451    0.901
--- Factory       : CutsGA         : 0.262(06)  0.622(07)  0.868(05)  0.000    0.000    0.000
--- Factory       : Likelihood     : 0.155(05)  0.538(07)  0.810(06)  0.983    0.353    0.767
--- Factory       : -----------------------------------------------------------------------------
--- Factory       :
--- Factory       : Testing efficiency compared to training efficiency (overtraining check)
--- Factory       : -----------------------------------------------------------------------------
--- Factory       : MVA           Signal efficiency: from test sample (from traing sample)
--- Factory       : Methods:         @B=0.01             @B=0.10
--- Factory       : ---------------------------------------------------
--- Factory       : Fisher         : 0.292 (0.235)       0.690 (0.6
--- Factory       : LikelihoodPCA  : 0.245 (0.222)       0.684 (0.6
--- Factory       : MLP            : 0.287 (0.232)       0.682 (0.6
--- Factory       : LikelihoodD    : 0.287 (0.245)       0.673 (0.6
--- Factory       : HMatrix        : 0.075 (0.058)       0.663 (0.6
--- Factory       : PDERS          : 0.225 (0.335)       0.646 (0.6
--- Factory       : BDT            : 0.200 (0.240)       0.641 (0.7
--- Factory       : RuleFit        : 0.245 (0.242)       0.632 (0.6
--- Factory       : CutsGA         : 0.262 (0.183)       0.622 (0.6
--- Factory       : Likelihood     : 0.155 (0.137)       0.538 (0.5
--- Factory       : ---------------------------------------------------
```



– Application (from TMVApplication.C) –

```
// create the Reader object
TMVA::Reader *reader = new TMVA::Reader();
```

Create the Reader

```
// create a set of variables and declare them to the reader
Float_t var1, var2, var3, var4;
reader->AddVariable( "var1+var2", &var1 );
reader->AddVariable( "var1-var2", &var2 );
reader->AddVariable( "var3", &var3 );
reader->AddVariable( "var4", &var4 );
```

Declare the variables that will hold your data

```
reader->BookMVA( "BDT method",
                 “weigths/Project_BDT.weights.txt"  );
```

Chose the MVA method you like best

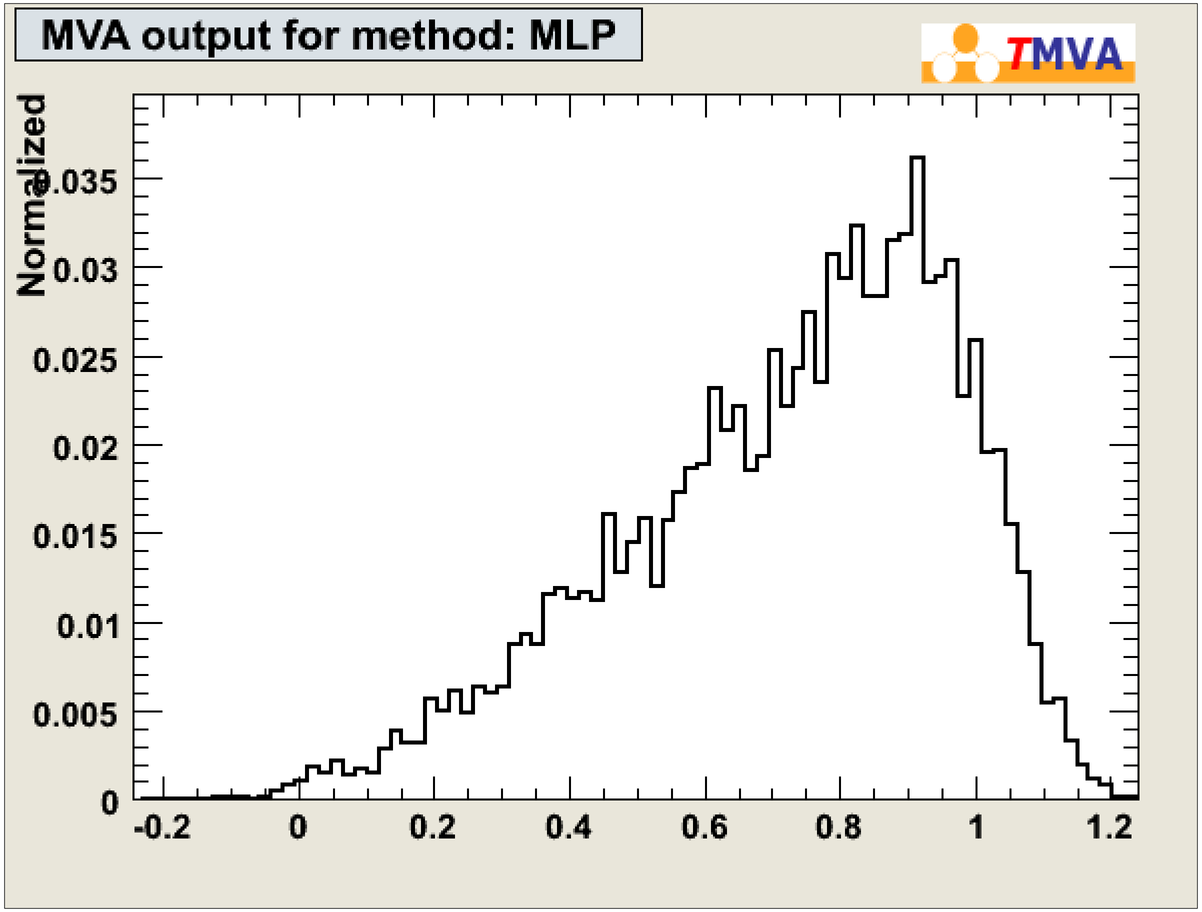
```
TTree* theTree = (TTree*)input->Get("TreeS");
Float_t userVar1, userVar2;
theTree->SetBranchAddress( "var1", &userVar1 );
theTree->SetBranchAddress( "var2", &userVar2 );
theTree->SetBranchAddress( "var3", &var3 );
theTree->SetBranchAddress( "var4", &var4 );
```

Prepare the user data

```
// loop over user data
for (Long64_t ievt=0; ievt<theTree->GetEntries();ievt++) {
  theTree->GetEntry(ievt);
  var1 = userVar1 + userVar2;
  var2 = userVar1 - userVar2;
  histBdt   ->Fill( reader->EvaluateMVA( "BDT method") );
}
```

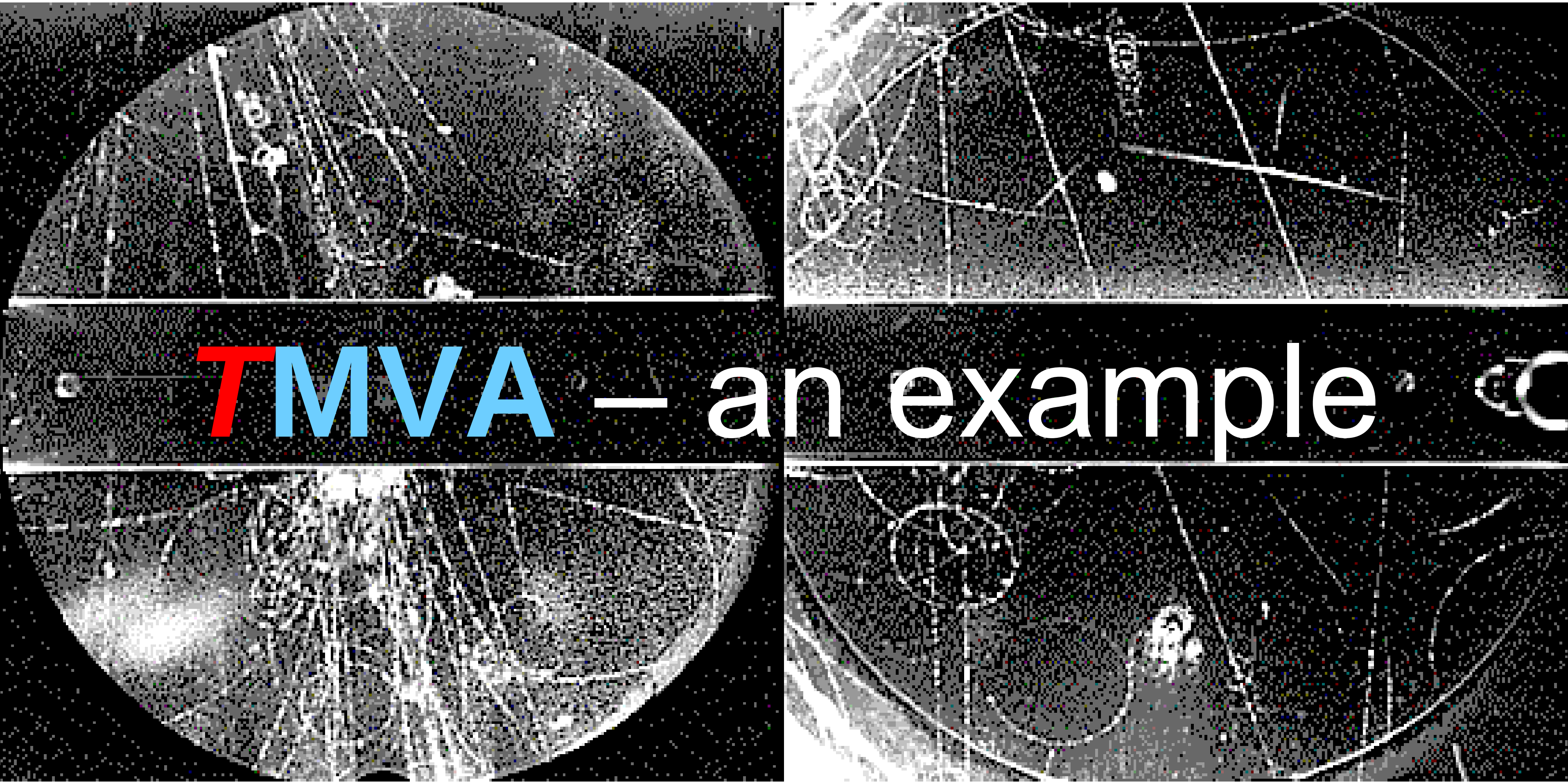
Analyze the user data, fill histogram, etc.

– Application (from TMVApplication.C) –



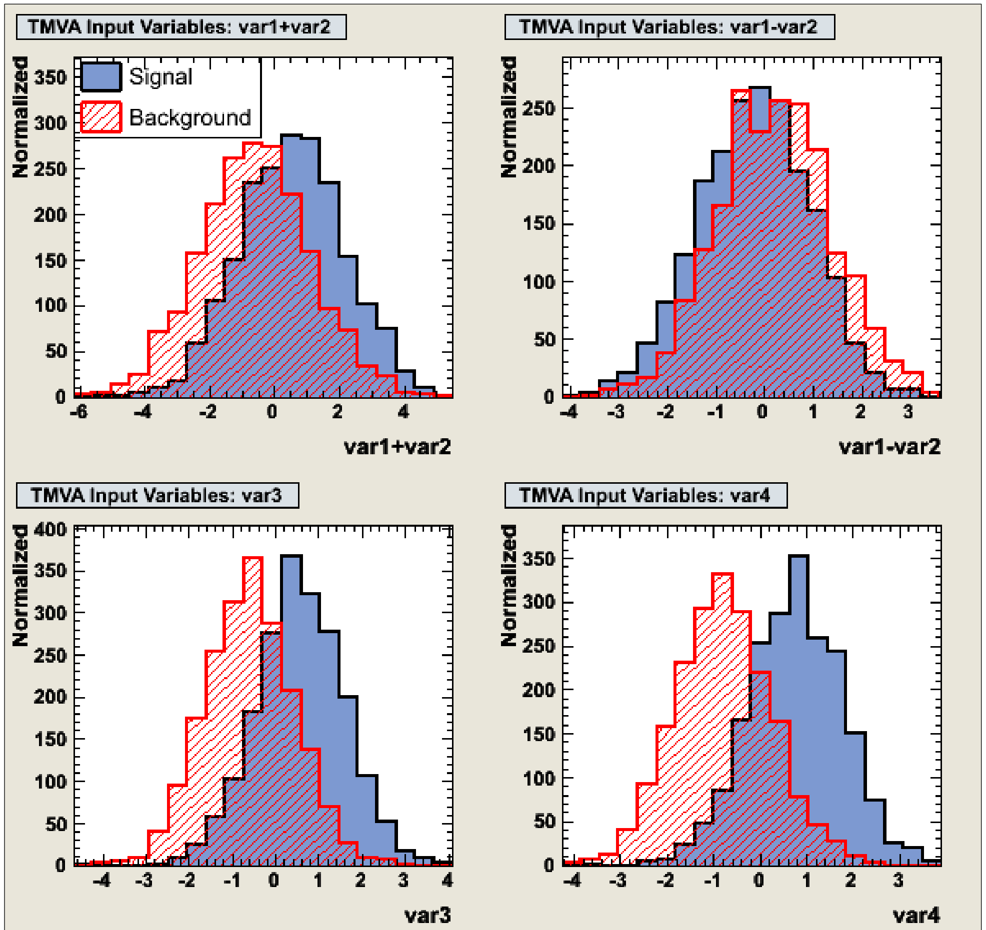
Use for further analysis
(Fit for signal yield, systematic studies, etc.)

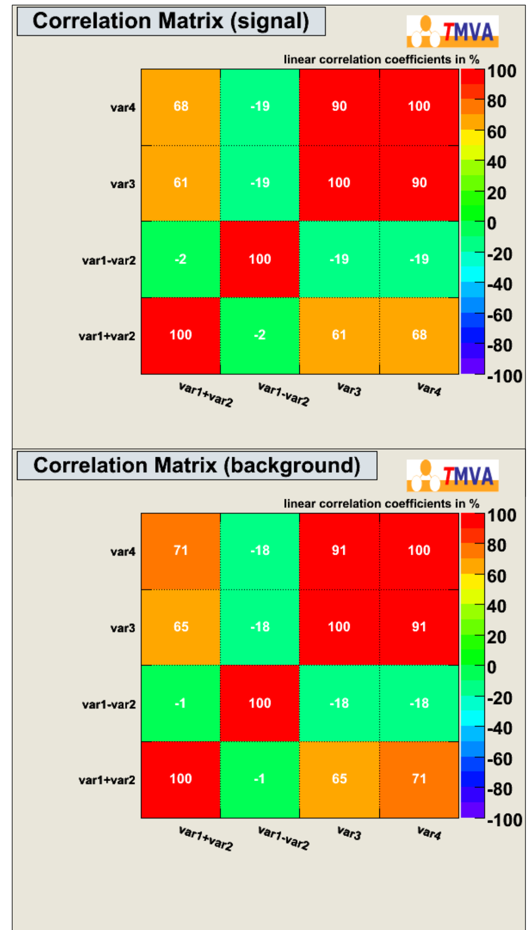
TMVA – an example

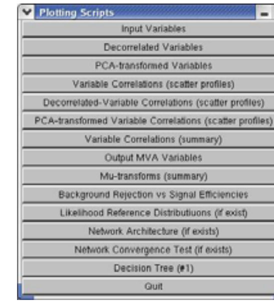


– Toy Example – Also with SF and ROOT –

- Simple toy to illustrate the strength of the de-correlation technique
  - 4 linearly correlated Gaussians, with equal RMS and shifted means between signal and background

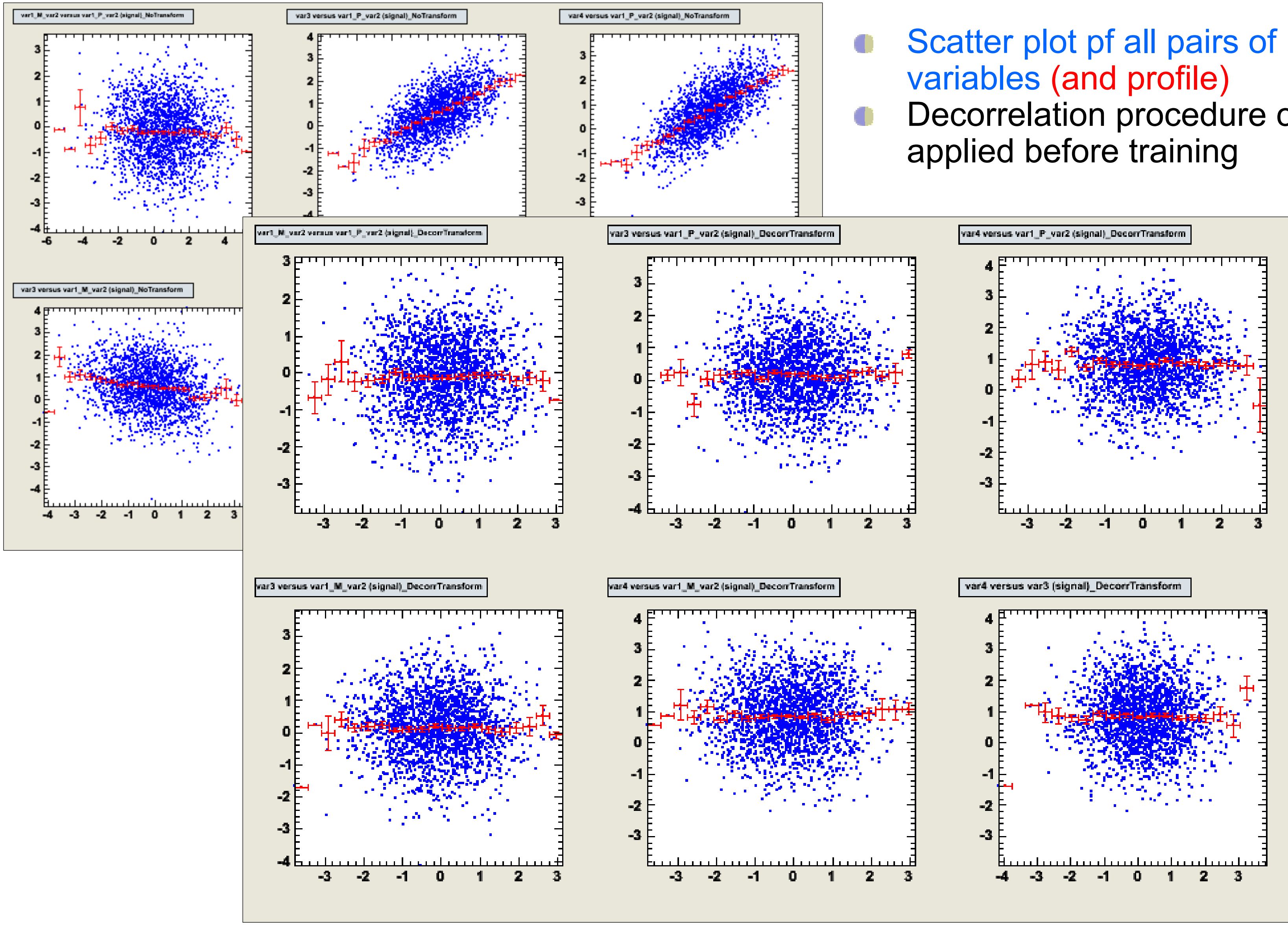






All plots from GUI

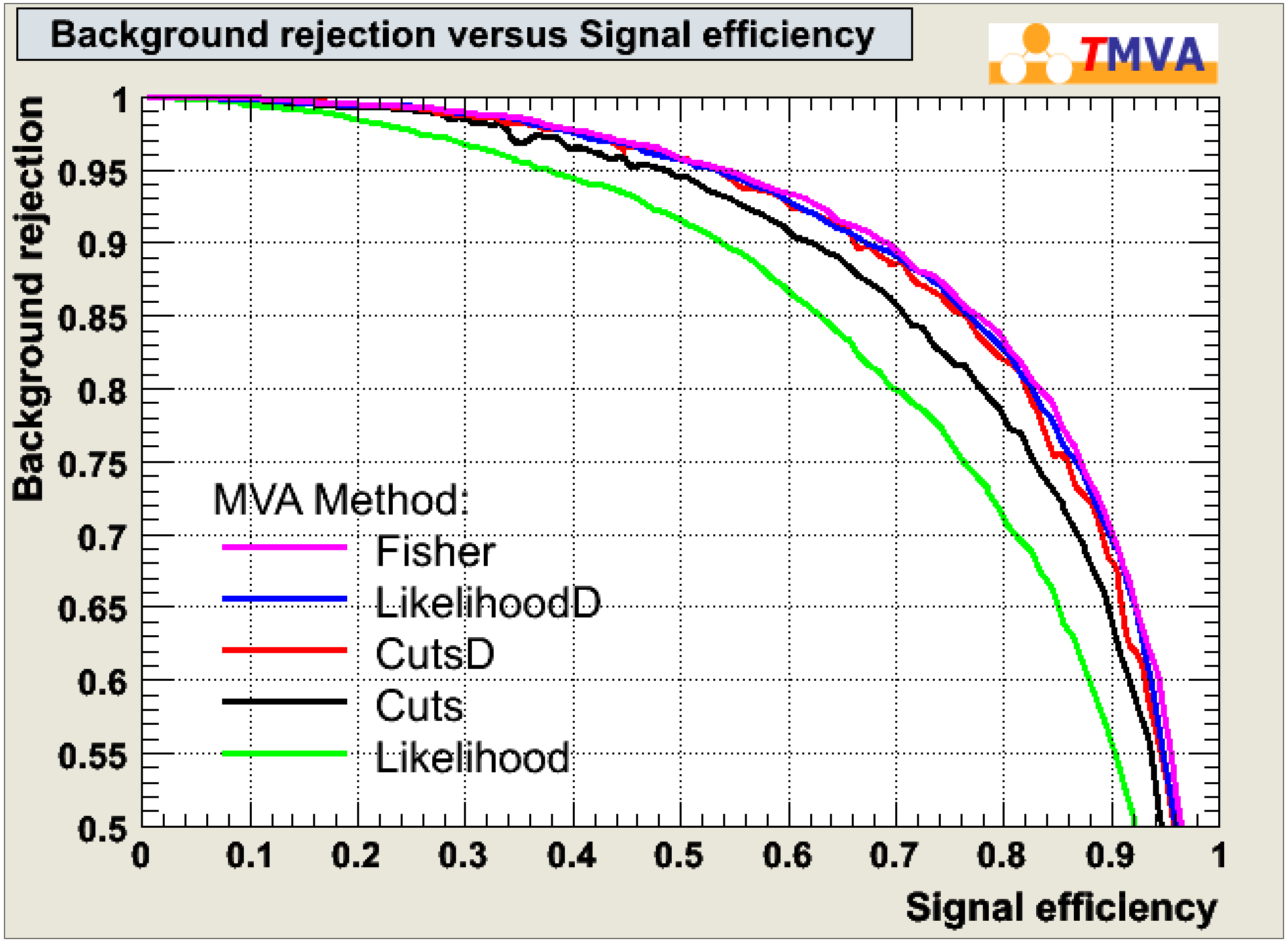
Decorrelation of Training Input



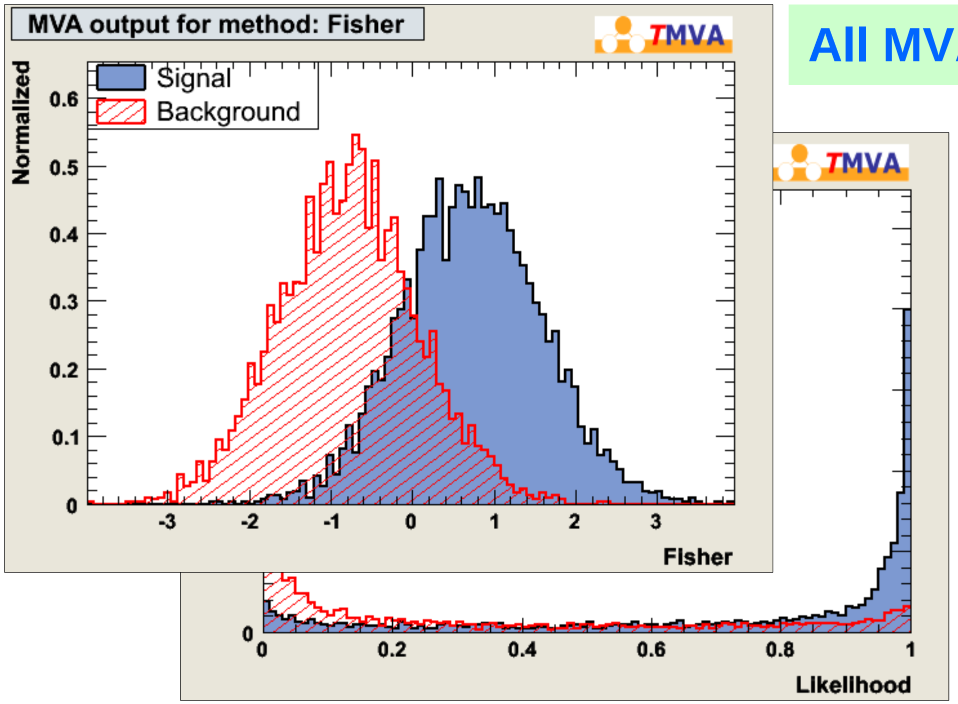
- Scatter plot pf all pairs of input variables (and profile)
- Decorrelation procedure can be applied before training

Likelihood and Cuts Improvement

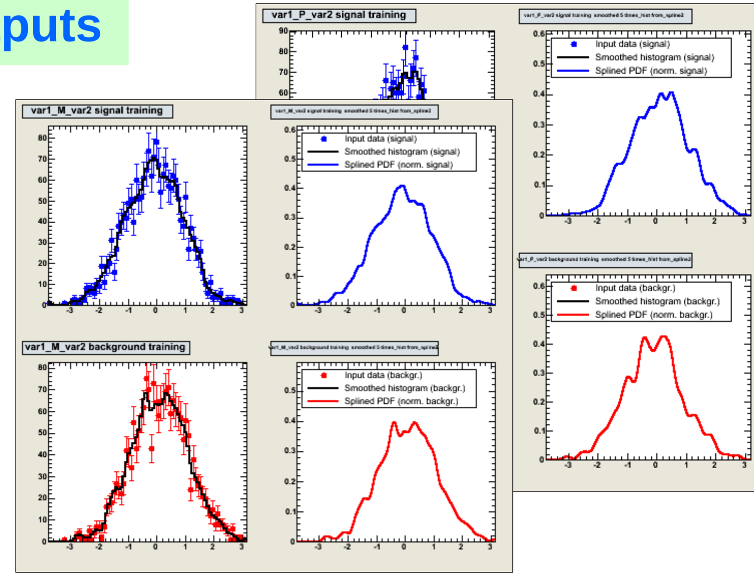
- On linearly correlated variables Fisher is already the optimum
- Decorrelation of input: LH and Cuts comparable with Fisher



More Information

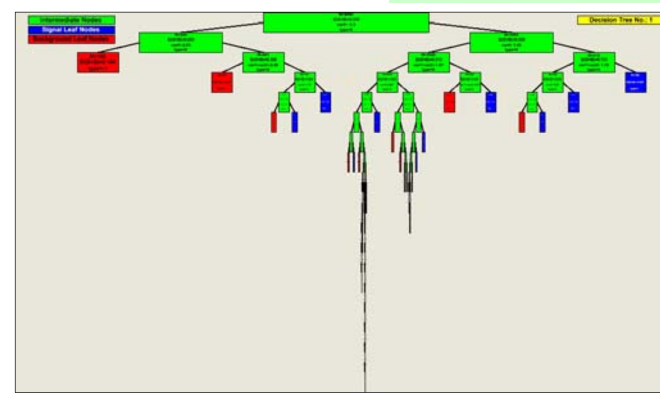


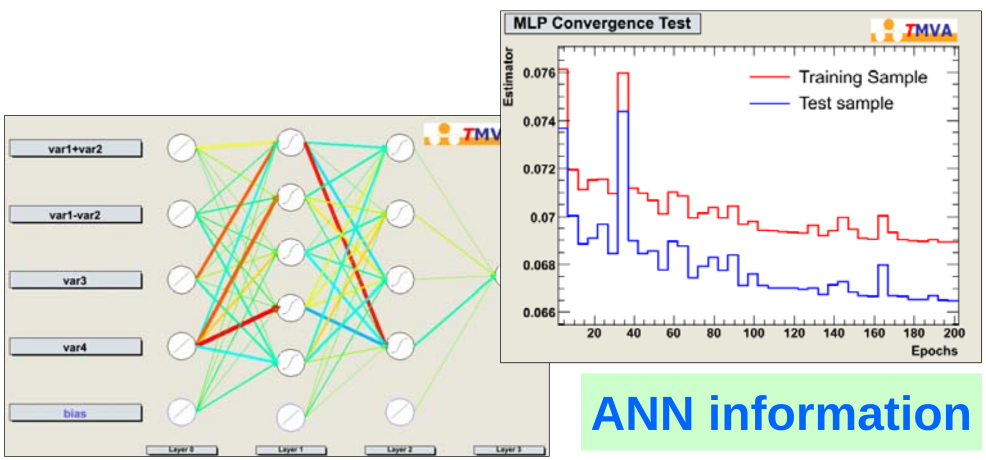
All MVA outputs



LH reference distributions

BDT visual





ANN information

Summary

- TMVA is now a mature package
  - User feedback from many HEP collaborations (including neutrino physics)
- Integration into ROOT essential
- Emphasis on consolidating and improving current methods as well as the TMVA framework
  - Providing user interface to Athena (AOD, EventView analyses)
  - Standalone application of methods
- New methods are being developed
  - Support vector machine
  - Bayesian Classifier
  - Committee method
    - Optimizes arbitrary combinations of MVA methods