Tutoriel TMVA
Machine learning avec ROOT

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CPPM, 25 Janvier 2018

Introduction à TMVA (version ROOT v6.12.04)

- TMVA: Toolkit for MultiVariate Analysis
- ▸ http://tmva.sourceforge.net
- Ecrit par des physiciens
- Intégré dans ROOT
- Manuel assez complet
- Inclut de très nombreuses techniques multivariées
- Pour compiler, ajouter les headers appropriés dans le code (par exemple `#include "TMVA/Factory.h"`) et ceci pour compiler : `‘root-config --cflags --libs --glibs‘ -lTMVA`
- Exemples plus complets de code : `$ROOTSYS/tutorials/tmva`
  - macro `createData.C` pour créer des échantillons de test
  - exemples de classification et régression
  - inclut également des exemples avec Keras
- Mesures parfois utiles:

```
#include "TMVA/ROCCalc.h"
TMVA::ROCCalc(TH1* S,TH1* B).GetROCIntegral();
#include "TMVA/Tools.h"
TMVA::gTools().GetSeparation(TH1* S,TH1* B);
```

Entraînement avec TMVA (`Train.C`)

```
TFile* outputFile = TFile::Open("output.root","RECREATE");
TMVA::Factory *factory = new TMVA::Factory( "TMVAClassification", outputFile,
    "!V:Color:DrawProgressBar:Transformations=I:AnalysisType=Classification");
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TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* sig = (TTree*)inputFile->Get("TreeS");
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double sigWeight = 1.0; double bkgWeight = 1.0;
TMVA::DataLoader *dataloader =
    new TMVA::DataLoader("dataset");
dataloader->AddSignalTree(sig, sigWeight);
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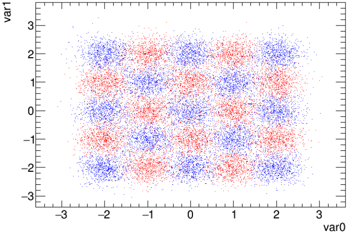

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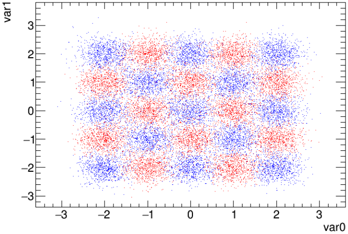

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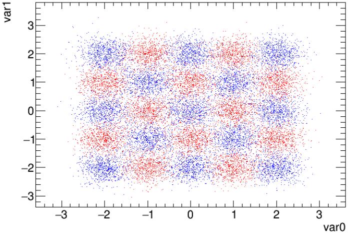

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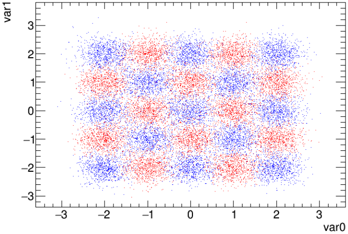
TCut mycut = "";
dataloader->PrepareTrainingAndTestTree(mycut,"SplitMode=Random");
factory->BookMethod(dataloader, TMVA::Types::kBDT, "BDT", "!H:!V:NTrees=400:
    MinNodeSize=4%:MaxDepth=5:BoostType=AdaBoost:AdaBoostBeta=0.15:nCuts=80");
factory->BookMethod(dataloader, TMVA::Types::kFisher, "Fisher", "!H:!V:Fisher");
```



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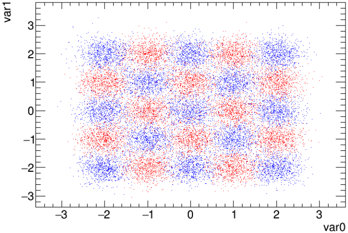
factory->TrainAllMethods(); // Train MVAs using training events
```



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TCut mycut = "";
dataloader->PrepareTrainingAndTestTree(mycut,"SplitMode=Random");
factory->BookMethod(dataloader, TMVA::Types::kBDT, "BDT", "!H:!V:NTrees=400:
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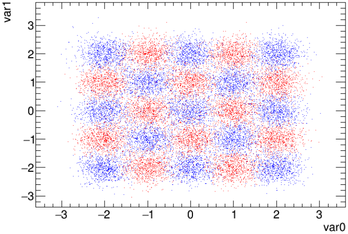
factory->BookMethod(dataloader, TMVA::Types::kFisher, "Fisher", "!H:!V:Fisher");
factory->TrainAllMethods(); // Train MVAs using training events
factory->TestAllMethods(); // Evaluate all MVAs using test events
```



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TCut mycut = "";
dataloader->PrepareTrainingAndTestTree(mycut,"SplitMode=Random");
factory->BookMethod(dataloader, TMVA::Types::kBDT, "BDT", "!H:!V:NTrees=400:
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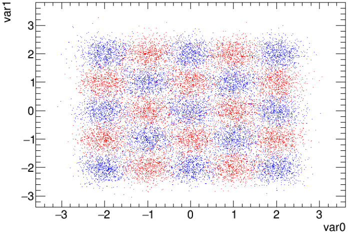
factory->BookMethod(dataloader, TMVA::Types::kFisher, "Fisher", "!H:!V:Fisher");
factory->TrainAllMethods(); // Train MVAs using training events
factory->TestAllMethods(); // Evaluate all MVAs using test events
// ----- Evaluate and compare performance of all configured MVAs
factory->EvaluateAllMethods();
```



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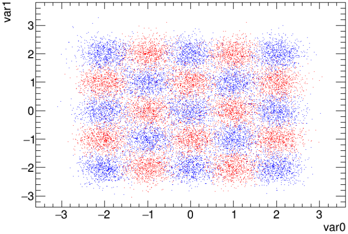
// ----- Evaluate and compare performance of all configured MVAs
factory->EvaluateAllMethods();
outputFile->Close();
delete factory; delete dataloader;
```



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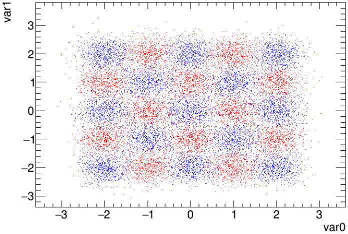

```
TMVA::TMVAGui("output.root");
```

Application avec TMVA (Apply.C)

```
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* data = (TTree*)inputFile->Get("TreeS");
Float_t var0=-99., var1=-99.;
data->SetBranchAddress("var0", &var0);
data->SetBranchAddress("var1", &var1);
```

Application avec TMVA (Apply.C)

```
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* data = (TTree*)inputFile->Get("TreeS");
Float_t var0=-99., var1=-99.;
data->SetBranchAddress("var0", &var0);
data->SetBranchAddress("var1", &var1);
TMVA::Reader *reader = new TMVA::Reader();
reader->AddVariable( "var0", &var0 );
reader->AddVariable( "var1", &var1 );
```

Application avec TMVA (Apply.C)

```
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* data = (TTree*)inputFile->Get("TreeS");
Float_t var0=-99., var1=-99.;
data->SetBranchAddress("var0", &var0);
data->SetBranchAddress("var1", &var1);
TMVA::Reader *reader = new TMVA::Reader();
reader->AddVariable( "var0", &var0 );
reader->AddVariable( "var1", &var1 );
reader->BookMVA( "My BDT", "dataset/weights/TMVAClassification_BDT.weights.xml");
reader->BookMVA( "Fisher discriminant",
  "dataset/weights/TMVAClassification_Fisher.weights.xml");
```

Application avec TMVA (Apply.C)

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TFile* inputFile = new TFile("dataSchachbrett.root");
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data->SetBranchAddress("var0", &var0);
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reader->AddVariable( "var0", &var0 );
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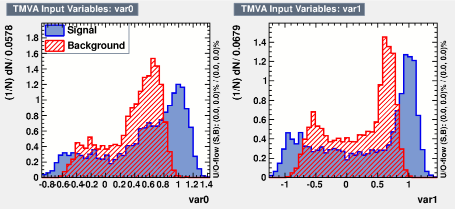
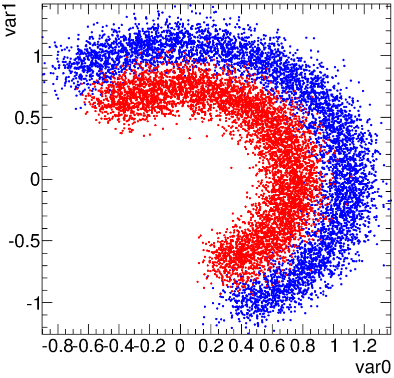
reader->BookMVA( "My BDT", "dataset/weights/TMVAClassification_BDT.weights.xml");
reader->BookMVA( "Fisher discriminant",
  "dataset/weights/TMVAClassification_Fisher.weights.xml");
// ------- start your event loop
for (Long64_t ievt=0; ievt<10; ++ievt) {
  data->GetEntry(ievt);
  double bdt = reader->EvaluateMVA("My BDT");
  double fisher = reader->EvaluateMVA("Fisher discriminant");
  cout<<"var0="<<var0<<" var1="<<var1<<" BDT="<<bdt<<" Fisher="<<fisher<<endl;
}
delete reader;
inputFile->Close();
```

Circular correlation

- Using TMVA and `create_circ` macro from (`$ROOTSYS/tutorials/tmva/createData.C` to generate dataset
- Plots: `TMVA::TMVAGui("filename")`

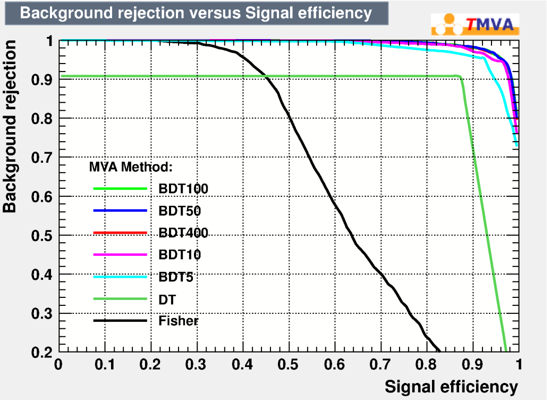




Circular correlation

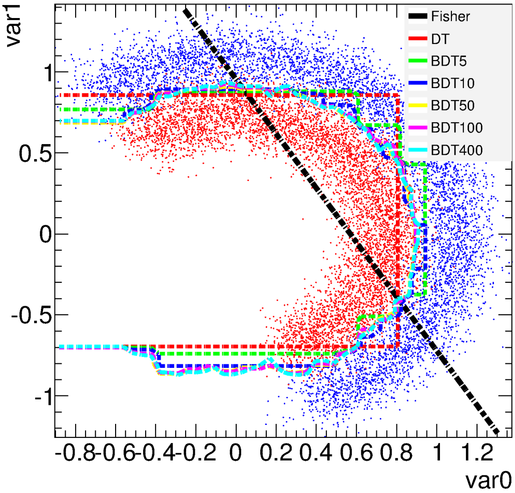
Boosting longer (TMVA: `NTrees`)

- Compare performance of Fisher discriminant, single DT and BDT with more and more trees (5 to 400)
- All other parameters at TMVA default (would be 400 trees)



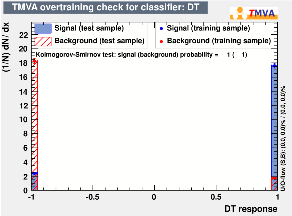
- Fisher bad (expected)
- Single (small) DT: not so good
- More trees ⇒ improve performance until saturation

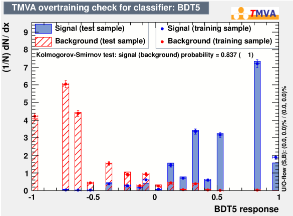
Decision contours

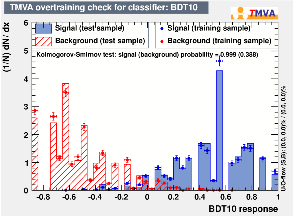


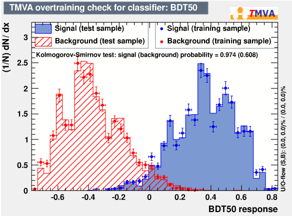
- Fisher bad (expected)
- Note: max tree depth = 3
- Single (small) DT: not so good. Note: a larger tree would solve this problem
- More trees ⇒ improve performance (less step-like, closer to optimal separation) until saturation
- Largest BDTs: wiggle a little around the contour ⇒ picked up features of training sample, that is, overtraining

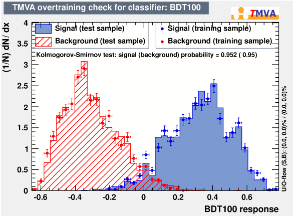
Training/testing output

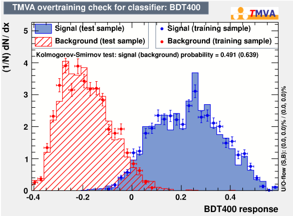






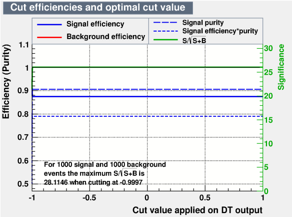




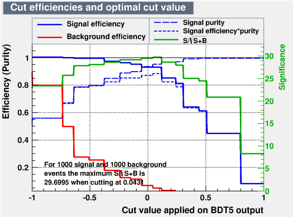


- Better shape with more trees: quasi-continuous
- Overtraining because of disagreement between training and testing? Let's see

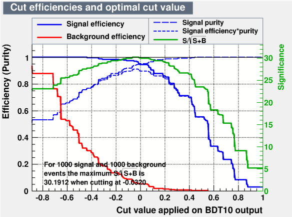
Performance in optimal significance


Cut efficiencies and optimal cut value

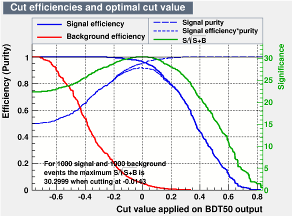
For 1000 signal and 1000 background events the maximum S/\S+B is 28.1146 when cutting at -0.9997


Cut efficiencies and optimal cut value

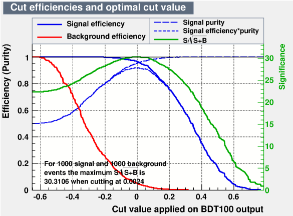
For 1000 signal and 1000 background events the maximum S/\S+B is 29.6995 when cutting at 0.0431


Cut efficiencies and optimal cut value

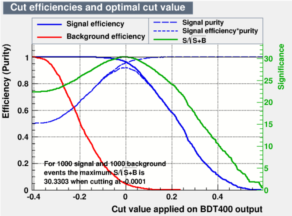
For 1000 signal and 1000 background events the maximum S/\S+B is 30.1912 when cutting at -0.0320


Cut efficiencies and optimal cut value

For 1000 signal and 1000 background events the maximum S/\S+B is 30.2999 when cutting at -0.0143


Cut efficiencies and optimal cut value

For 1000 signal and 1000 background events the maximum S/\S+B is 30.3106 when cutting at 0.0024

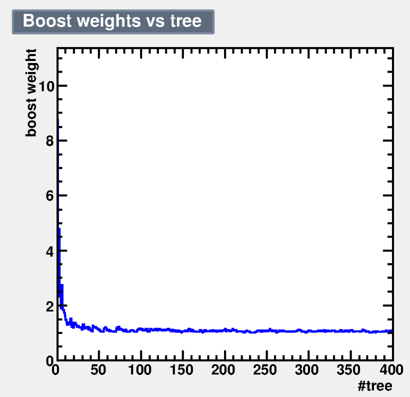

Cut efficiencies and optimal cut value

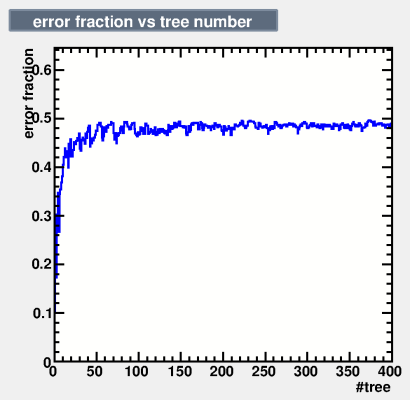
For 1000 signal and 1000 background events the maximum S/\S+B is 30.3303 when cutting at 0.0001

- Best significance actually obtained with last BDT, 400 trees!
- But to be fair, equivalent performance with 10 trees already
- Less "stepped" output desirable? ⇒ maybe 50 is reasonable

Control plots

- Boosting weight decreases fast and stabilises
- First trees have small error fractions, then increases towards 0.5 (random guess)
- ⇒ confirms that best trees are first ones, others are small corrections


Boost weights vs tree
boost weight
#tree


error fraction vs tree number
error fraction
#tree