

INFN-ML

Improving Reaction Identification
With ROOT TMVA

Derek Glazier
University of Glasgow

Overview

Exclusive reactions

JLAB + CLAS + CLAS12

Discriminatory variables

Training variables

TMVA

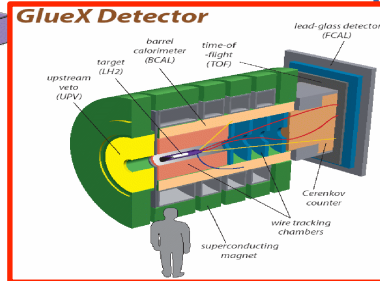
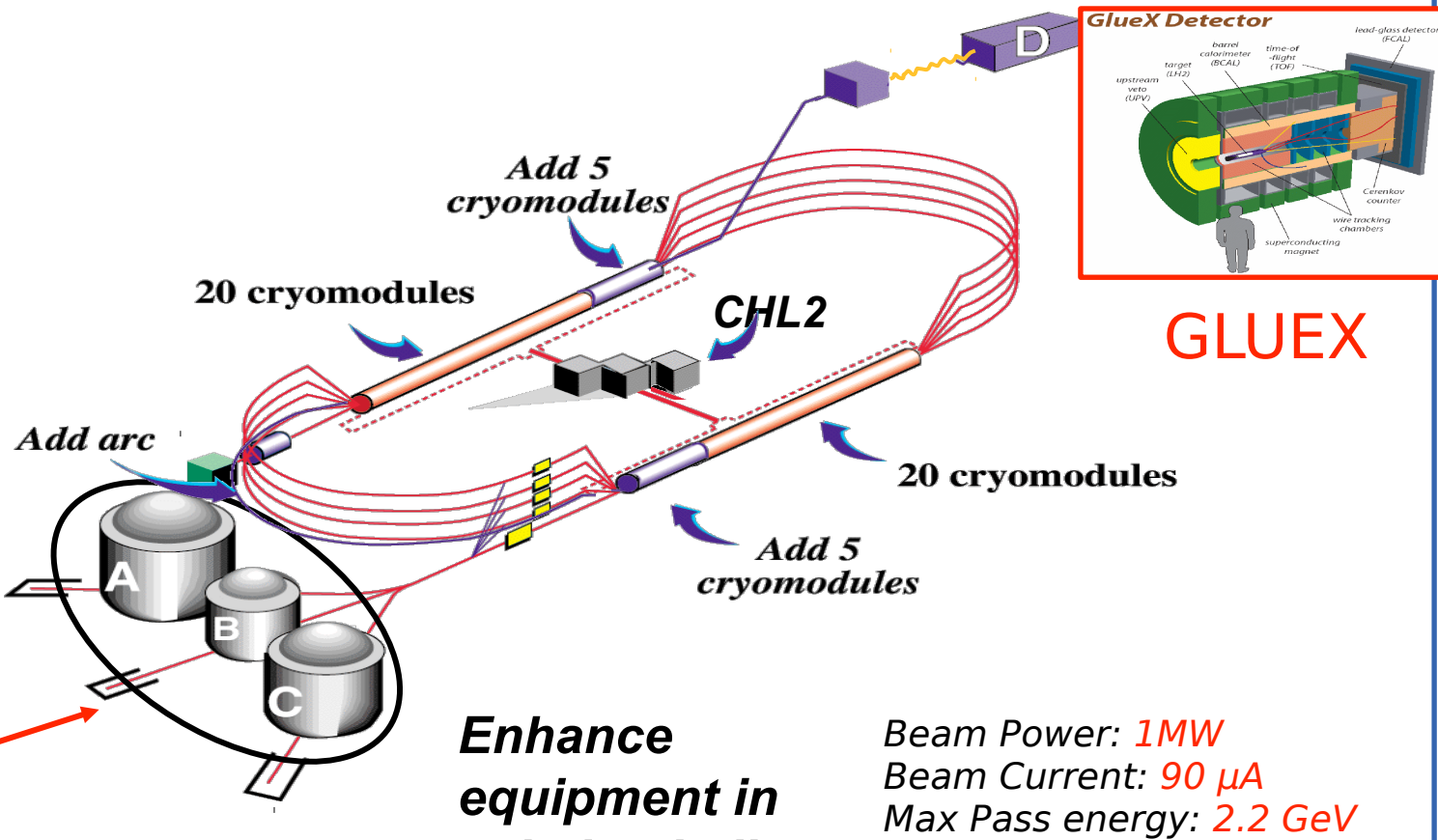
Simulation training

Mixed events training

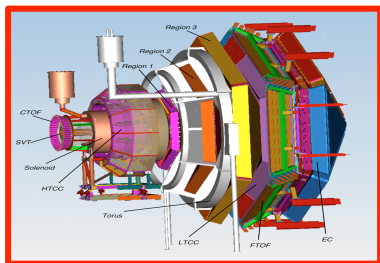
sPlot training

Accelerate BDT->MLP

JLAB at 12GeV



GLUEX



CLAS12

**Enhance
equipment in
existing halls**

Beam Power: **1MW**
Beam Current: **90 μ A**
Max Pass energy: **2.2 GeV**
Max Energy Hall A-C: **10.9 GeV**
Max Energy Hall D: **12 GeV**

Variable classes

Observables

Invariant masses
Production/Decay angles
CoM kinematics

Discriminatory

Exclusive Process
Missing Mass
Missing Energy
Missing Momentum
Decay Processes
+ Invariant masses

Particle Identification

Momentum, Position
Time of Flight
Delta Energy
Cherenkov ...

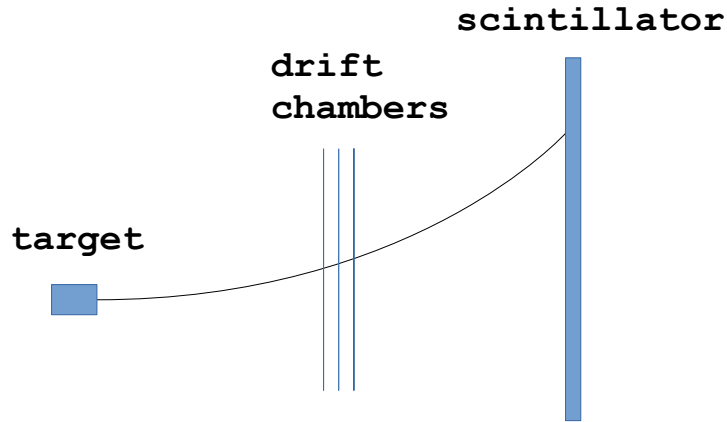
Used to extract physics

Used to remove backgrounds

Used to minimise backgrounds

Focus of this talk

"Standard" CLAS track PID



Measure momentum, charge C , vertex V , from tracking in Toroidal field

Measure Time of Flight T , to scintillator from reaction vertex

"Swim" track in field to reconstruct path length D .

Determine Time of flight T_i , from momentum and path for species hypothesis i e.g. $i = \text{proton}, K^+, \pi^+, \dots$

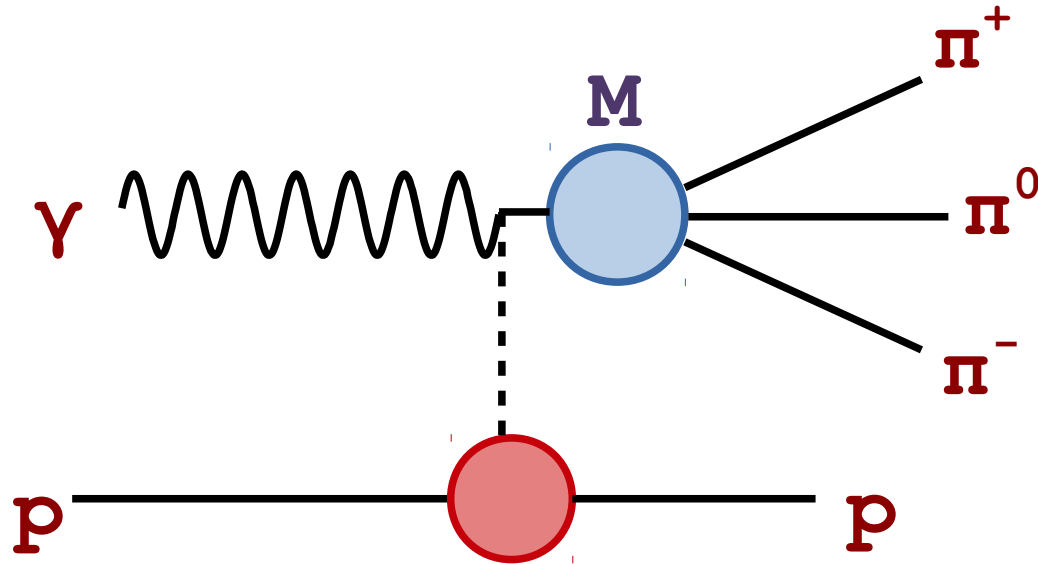
$$T_i = \frac{D}{\beta_i \cdot c} \text{ with } \beta_i = \frac{P}{\sqrt{P^2 + M_i^2}}$$

then

$$\Delta T = T - T_i \sim 0 \text{ for correct hypothesis}$$

Also measure mass, $\Delta\beta$, ... but just the same information

Example Reaction



Focus on CLAS charge
particle detection
- miss π^0

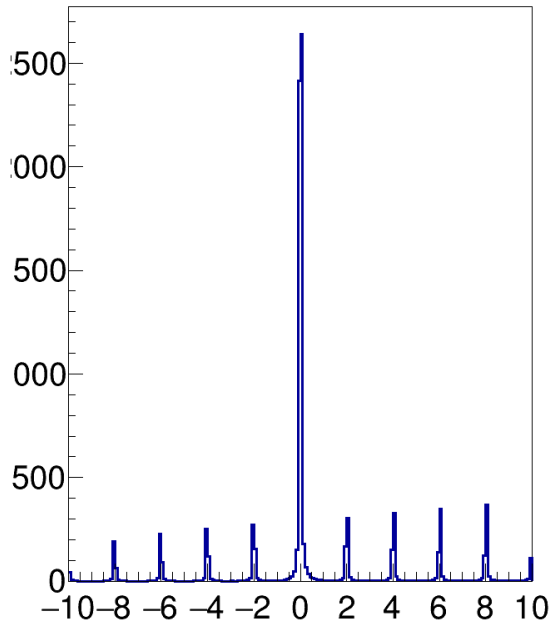
Filter events with 1 -ve , 2 +ve and N tagged photons

assume -ve = π^-

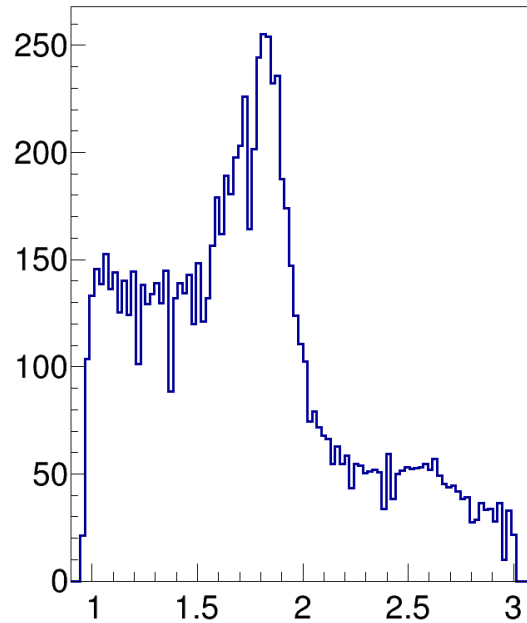
create 2 events for each positive as proton and π^+

Tagged Photon

ΔT Beam (ns)



Beam Energy (GeV)



CEBAF e⁻ beam ~2ns bunches

Photon beam produced from e⁻ bremsstrahlung

Use of diamond radiator gives Coherent peak (polarised)

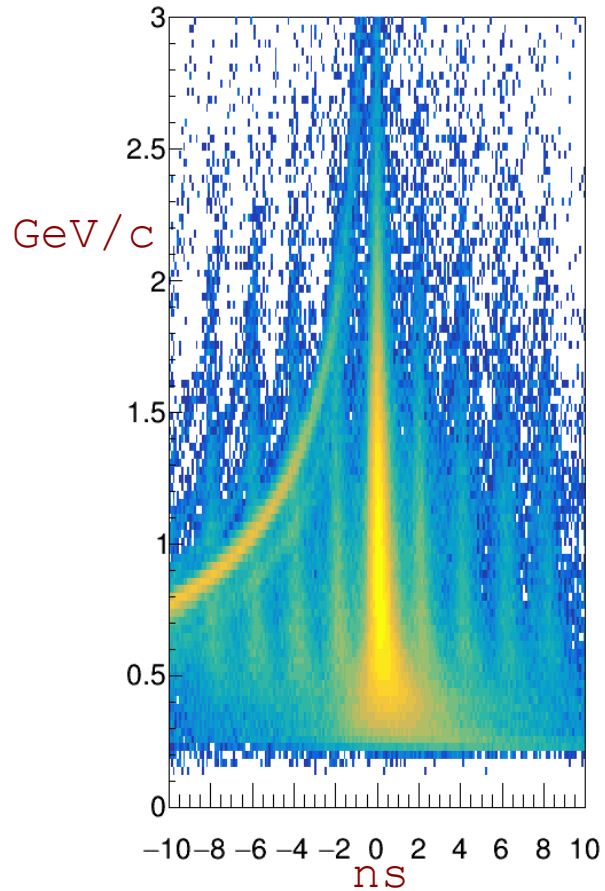
Recoil electron detected in Magnetic spectrometer "tagger" => the photon energy

ΔT Beam gives coincidence of tagger with CLAS and reaction vertex time

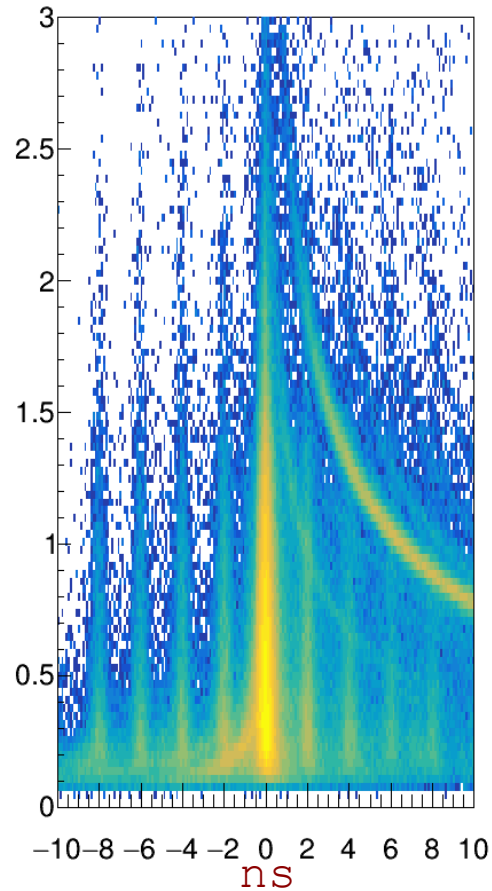
Δ Time PID

*Log scale

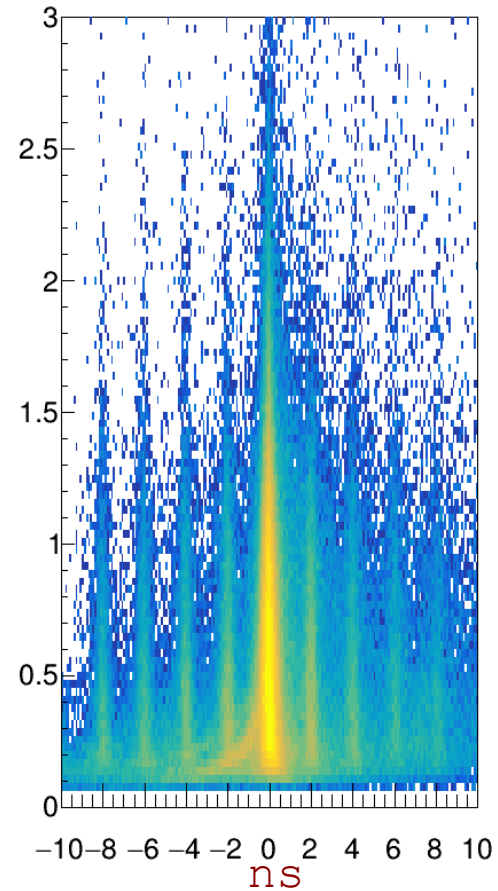
Proton $P \nu \Delta T$



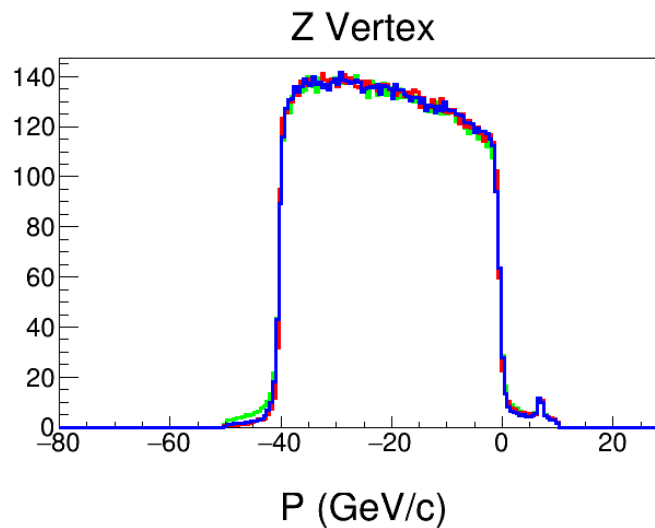
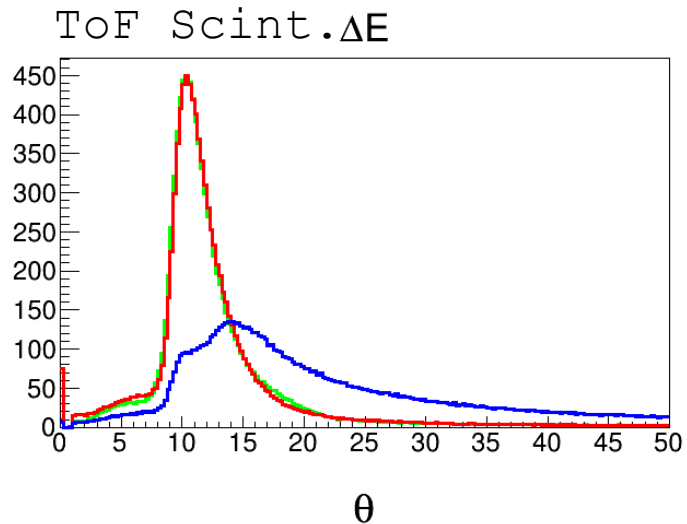
π^+ $P \nu \Delta T$



π^- $P \nu \Delta T$



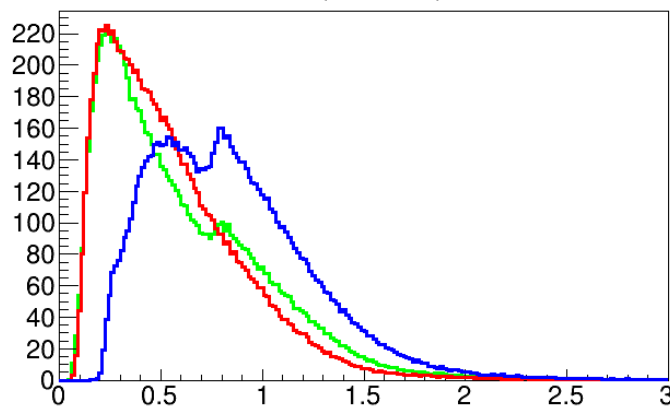
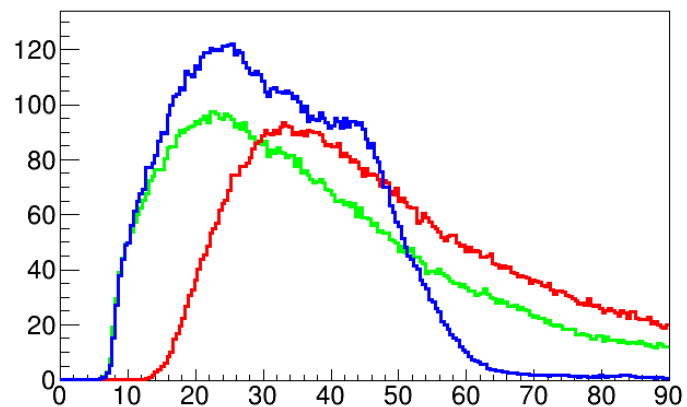
Other Input Variables



Proton

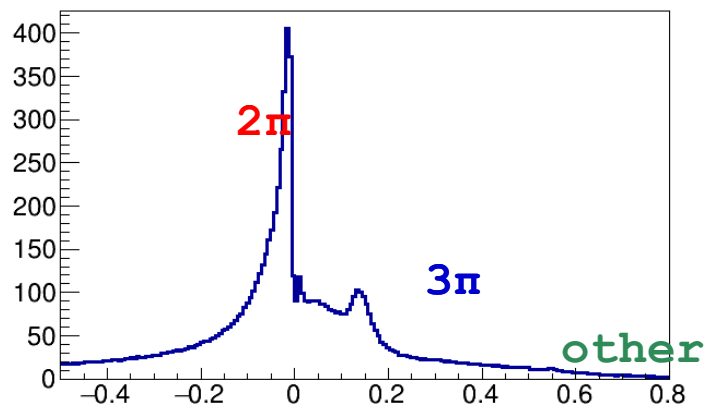
π^+

π^-

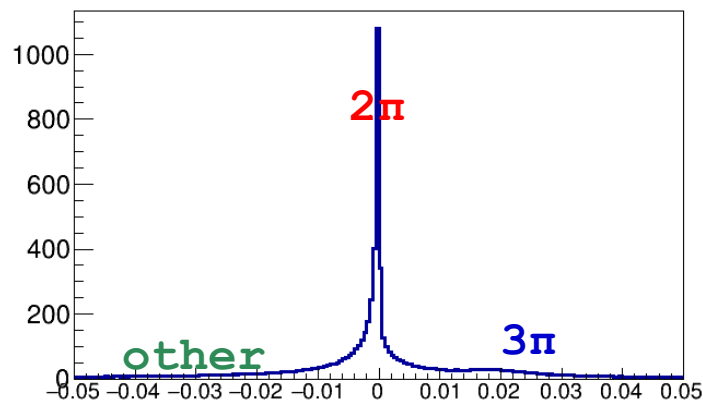


Exclusive variables

Missing Mass ($p\pi+\pi^-$)

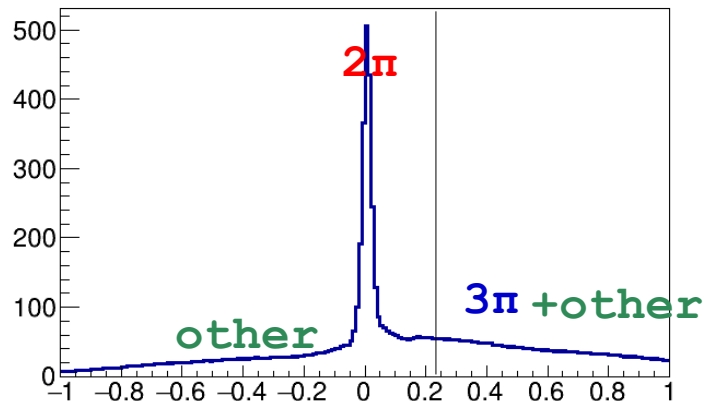


Missing Mass Squared ($p\pi+\pi^-$)

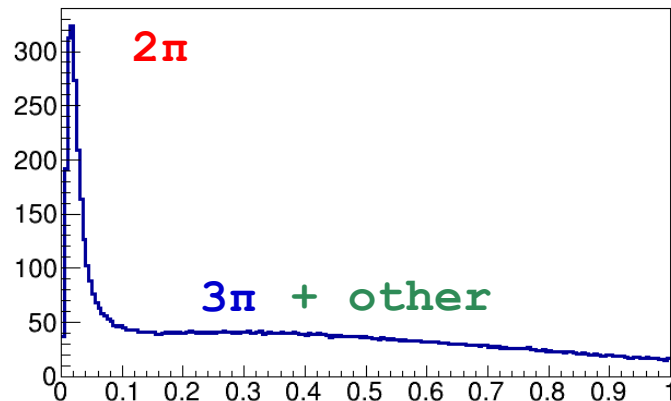


NOT FOR
TRAINING WITH

Missing Energy ($p\pi+\pi^-$)



Missing Momentum ($p\pi+\pi^-$)



GOAL :
Using PID variables
Retain all 3π
Remove backgrounds

ROOT-TMVA

Range of classifiers

- Rectangular cut optimization
- Projective likelihood estimation (PDE approach)
- Multidimensional probability density estimation (PDE - range-search approach)
- Multidimensional k-nearest neighbor classifier
- Linear discriminant analysis (H-Matrix and Fisher discriminants)
- Function discriminant analysis (FDA)
- Predictive learning via rule ensembles (RuleFit)
- Support Vector Machine (SVM)
- Artificial neural networks (MLP)
- Boosted/Bagged decision trees (BDT)
- (Newer) Deep NN, Convolutional NN,...
- Interface for R, Keras,...

+ Jupyter ROOTbooks or PyROOT

Train with Simulation

Signal : **Simulated** 3π (Correct Combitorial)

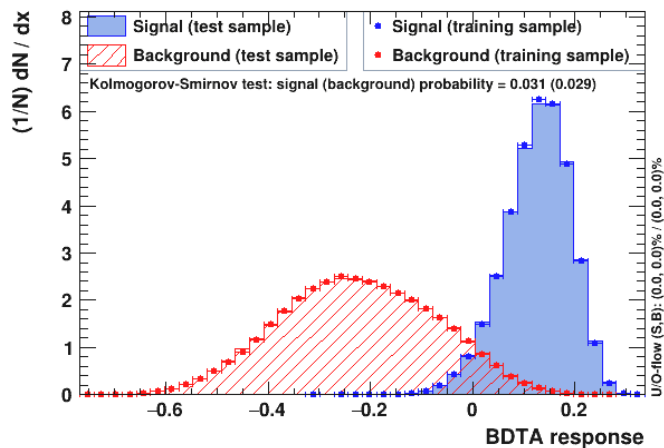
Background : All Experimental Data Events +(Simulated Wrong Combitorial)

Training variables + E_γ

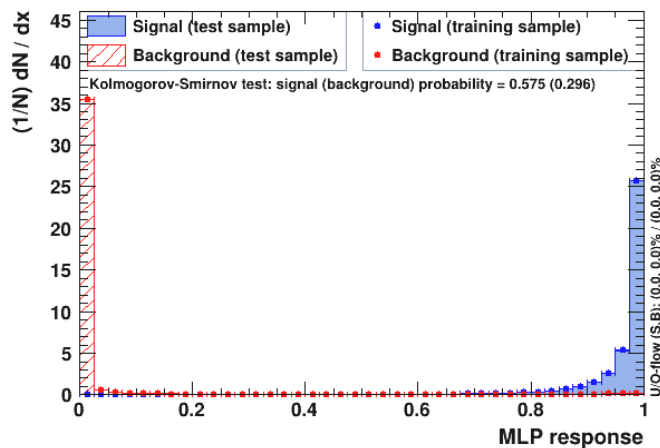
Particle(Δ Time, Δ Energy, P, Vz, θ , φ)

200k Training and Test data

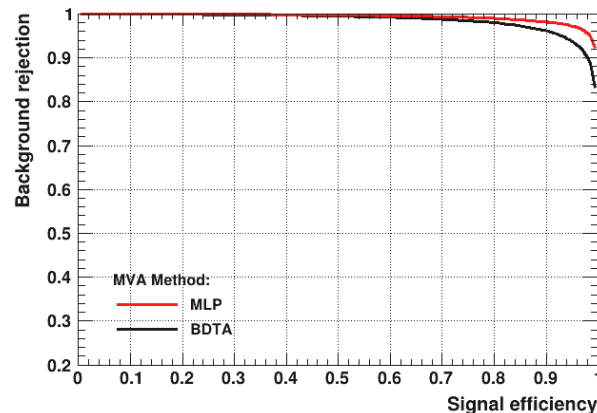
TMVA overtraining check for classifier: BDTA



TMVA overtraining check for classifier: MLP



Background rejection versus Signal efficiency

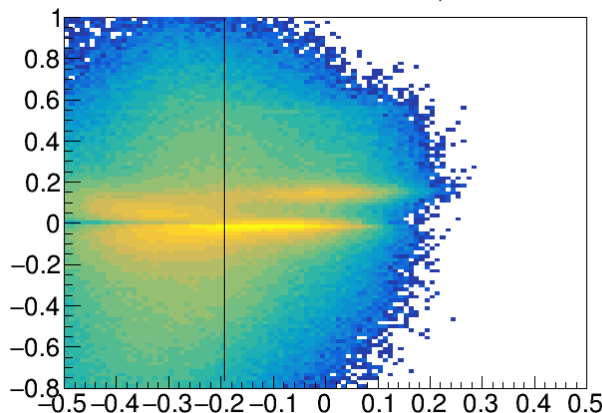
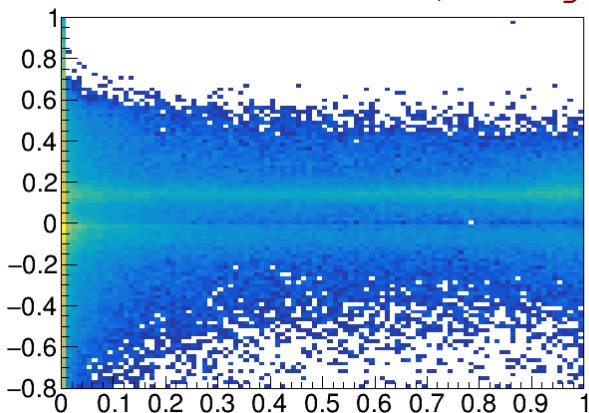


Apply Simulated training

MissMass V MLP (with E_γ)

Log z scale

MissMass V BDT (with E_γ)

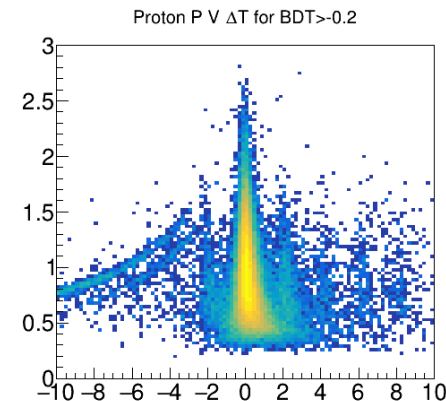
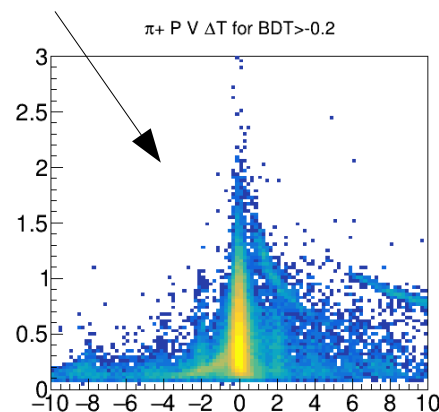


Real Experiment
distributions shifted to
background values
compared to Simulation

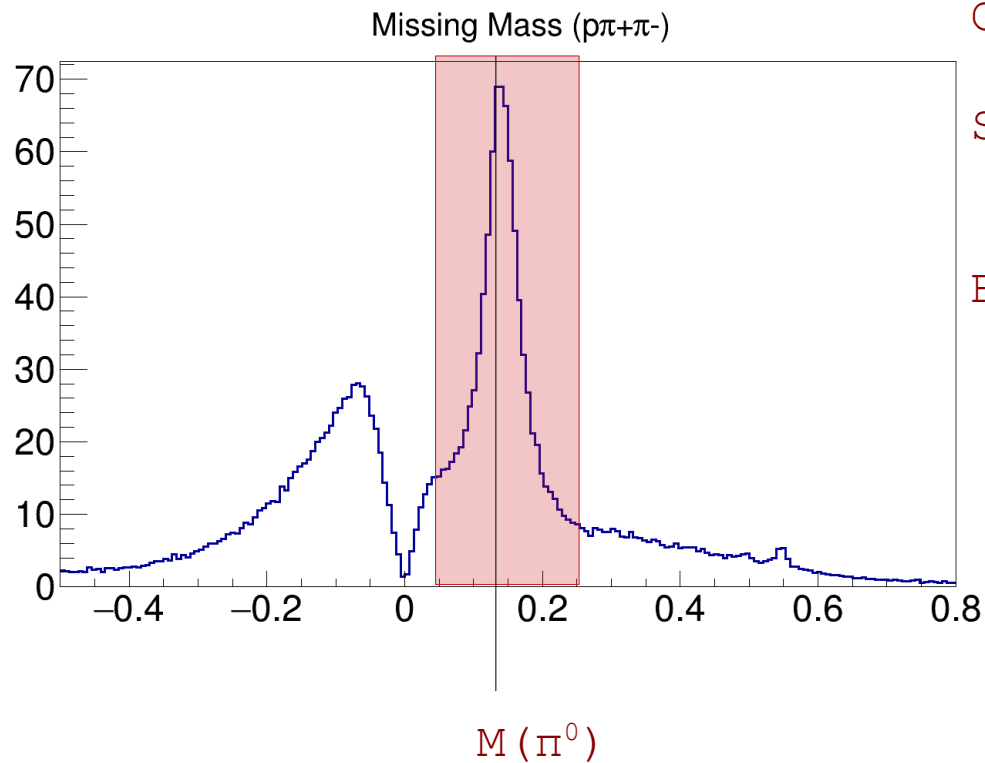
Simulation must be very
Realistic!

Small separation between 2π and 3π
- OK PID variables similar

Cuts still clean up
data, but must use
low BDT value



Mixed events training



Cut on region with high signal density

Signal = (Missing mass peak $\sim \pi^0$)

Background = Everything else

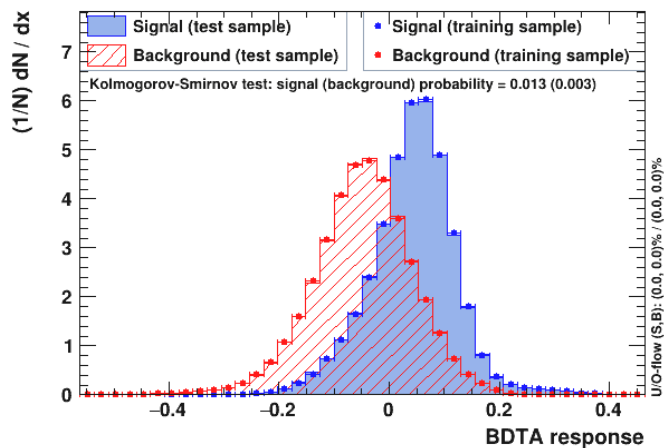
Train with Mixed Events (I)

Signal : $0.1 < \text{MissMass} < 0.2$

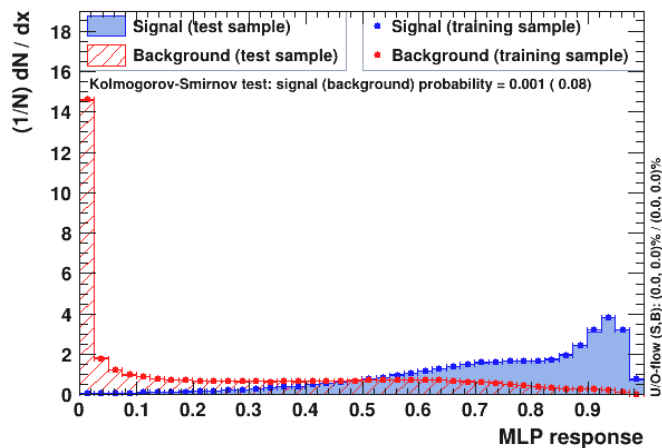
Background : !Signal

Variables + E_γ

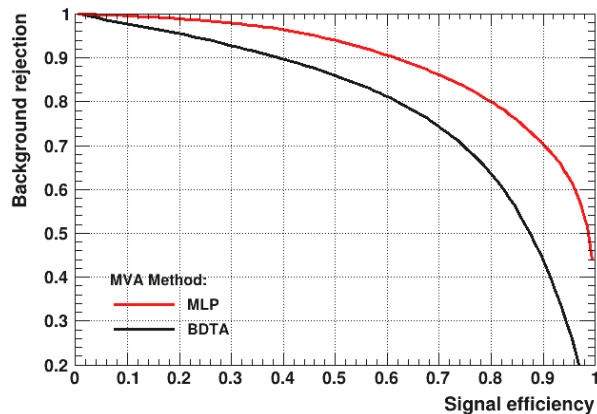
TMVA overtraining check for classifier: BDTA



TMVA overtraining check for classifier: MLP



Background rejection versus Signal efficiency



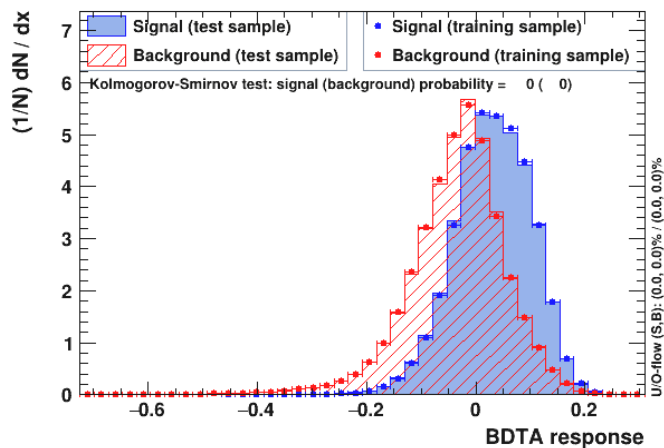
Train with Mixed Events (II)

Signal : $0.1 < \text{MissMass} < 0.2$

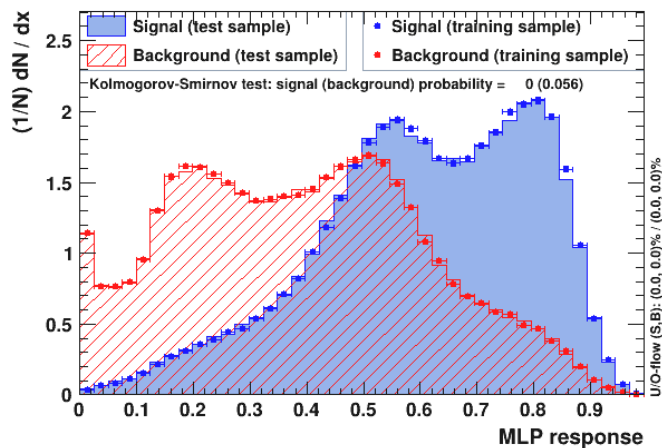
Background : !Signal

Variables - E_Y

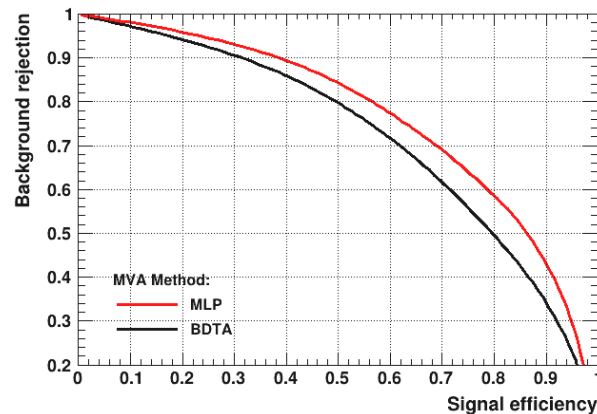
TMVA overtraining check for classifier: BDTA



TMVA overtraining check for classifier: MLP

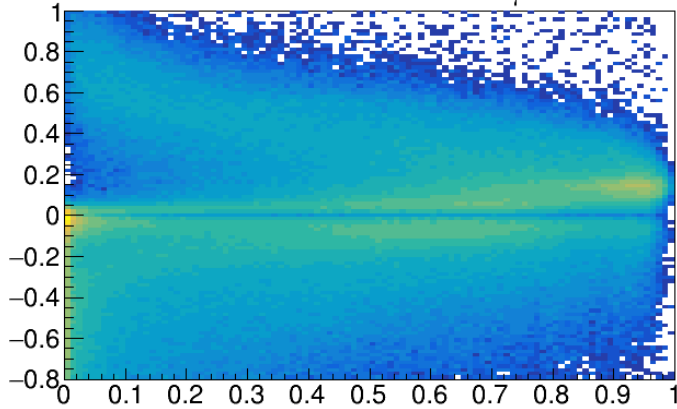


Background rejection versus Signal efficiency

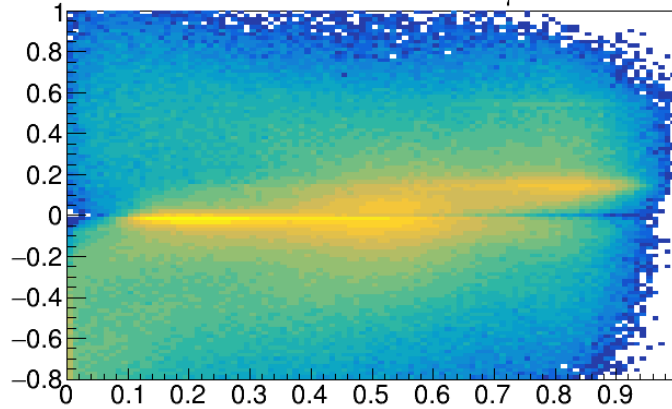


Miss Mass V Responses

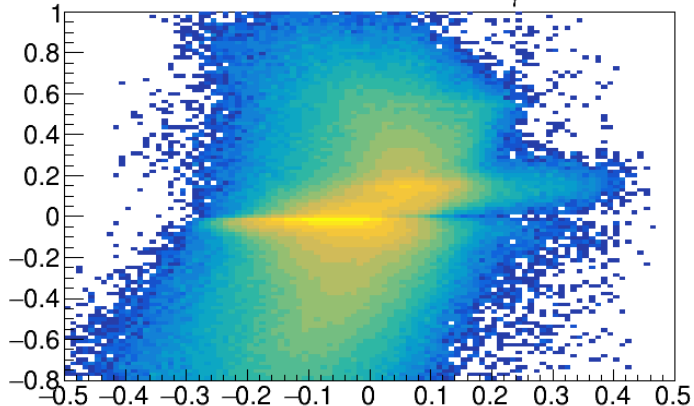
MissMass V MLP (with E_γ)



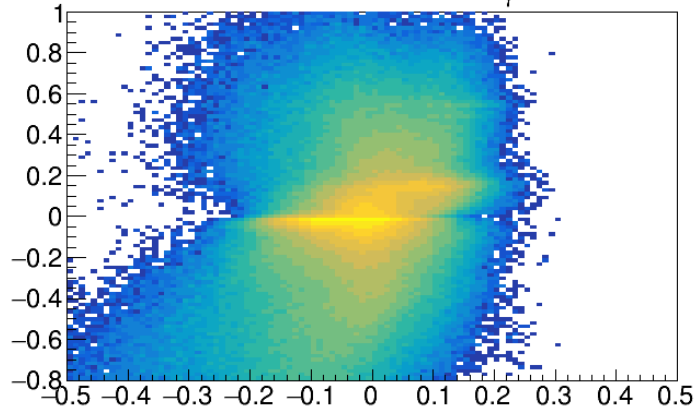
MissMass V MLP (no E_γ)



MissMass V BDT (with E_γ)



MissMass V BDT (no E_γ)

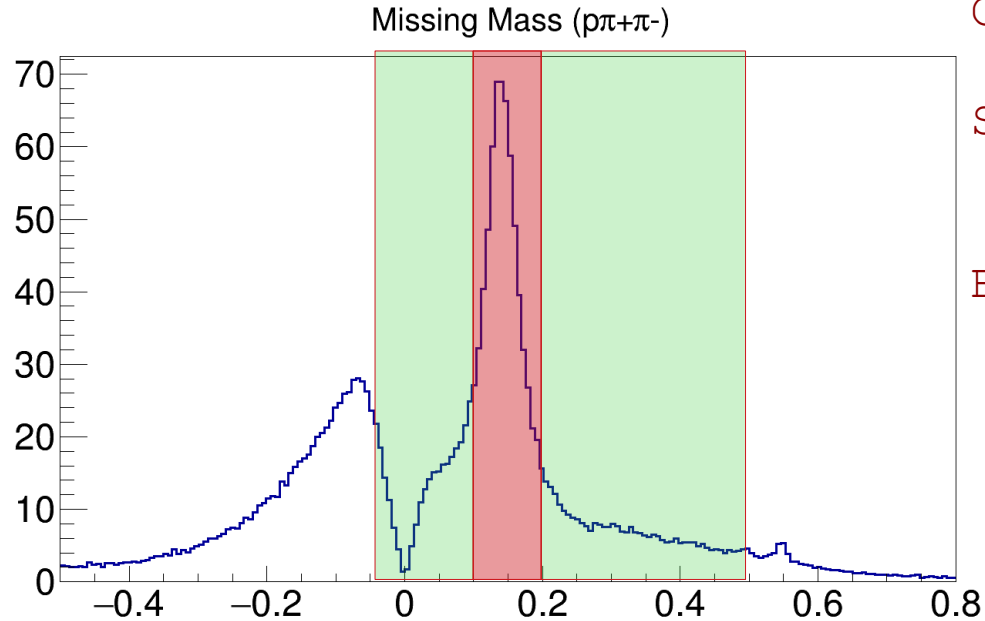


Visually MLP gives
Better separation
(as with ROCs)

E_γ input gives greater
separation of $2\pi - 3\pi$
Particularly for MLP

E_γ input creates
Correlation of
Response with
Exclusivity variable

Mixed events training



Cut on region with high signal density

Signal = (Missing mass peak $\sim \pi^0$)

Background = sidebands inc 2π

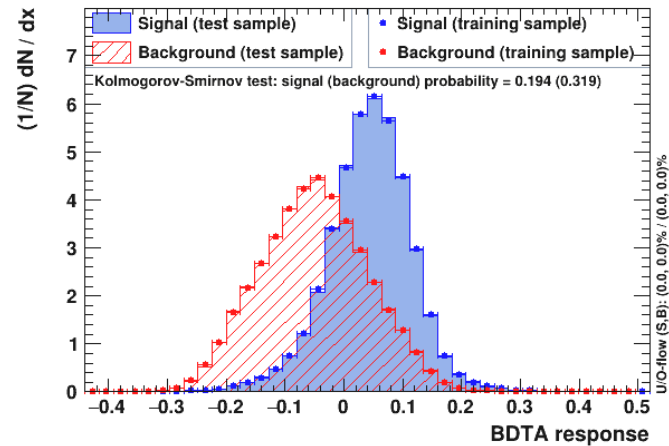
Train with Mixed Events (III)

Signal : $0.1 < \text{MissMass} < 0.2$

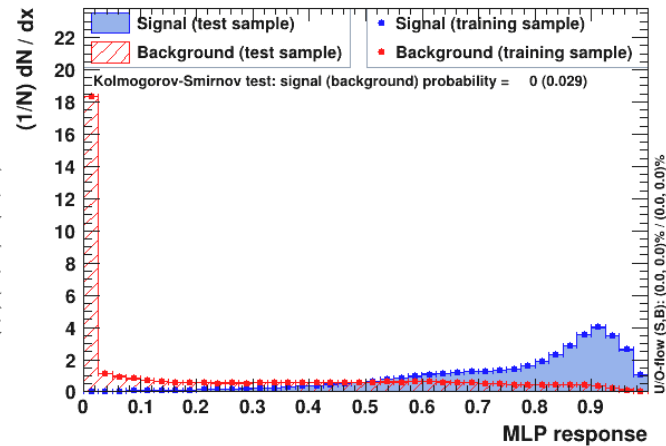
Background : $-0.04 < \text{MissMass} < 0.1$ and $0.2 < \text{MissMass} < 0.5$

Variables + E_γ

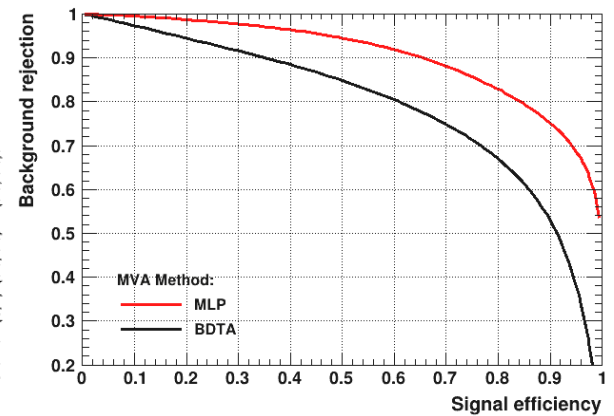
TMVA overtraining check for classifier: BDTA



TMVA overtraining check for classifier: MLP



Background rejection versus Signal efficiency



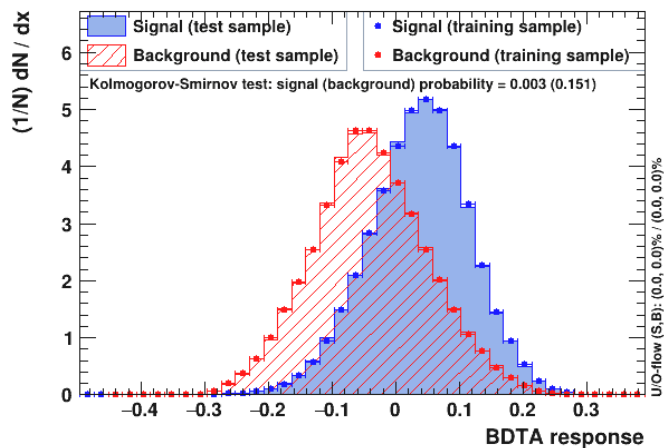
Train with Mixed Events (IV)

Signal : $0.1 < \text{MissMass} < 0.2$

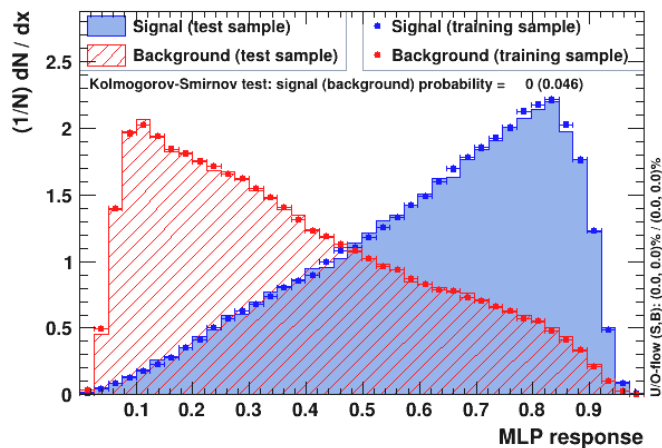
Background : $-0.04 < \text{MissMass} < 0.1$ and $0.2 < \text{MissMass} < 0.5$

Variables - E_γ

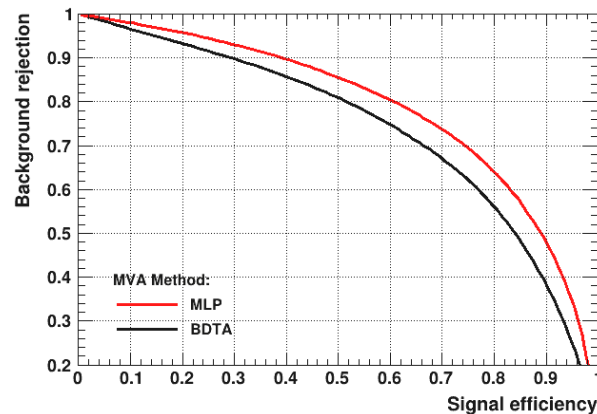
TMVA overtraining check for classifier: BDTA



TMVA overtraining check for classifier: MLP

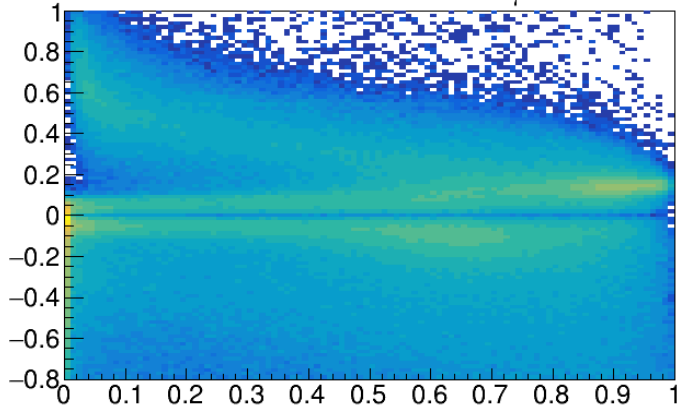


Background rejection versus Signal efficiency

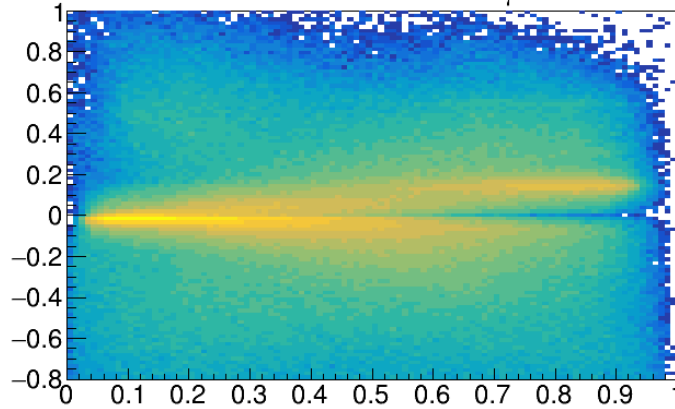


Miss Mass V Responses

MissMass V MLP (with E_γ)

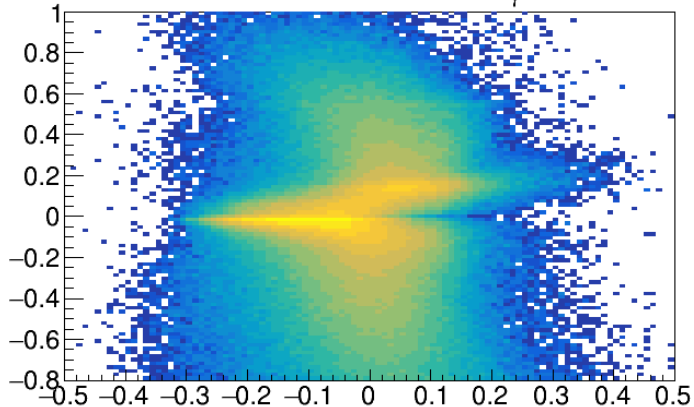


MissMass V MLP (no E_γ)

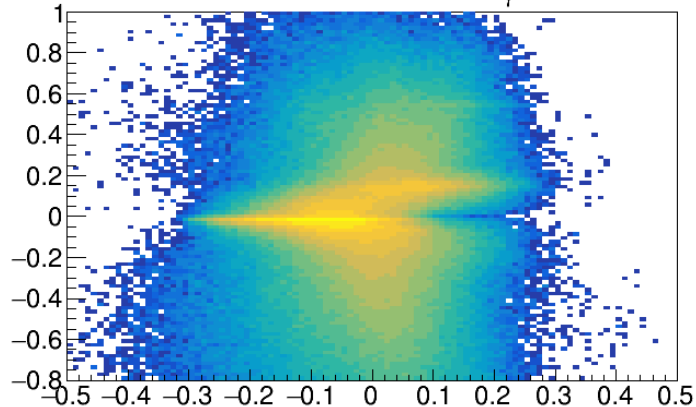


These background events give better discrimination of 2π

MissMass V BDT (with E_γ)

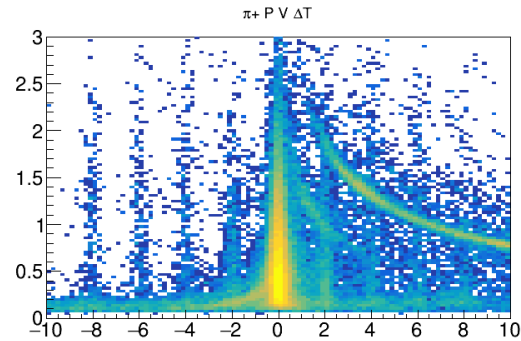
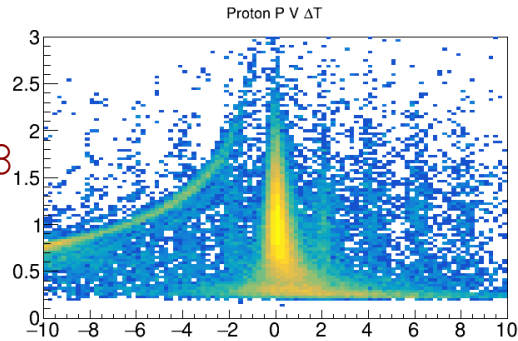


MissMass V BDT (no E_γ)

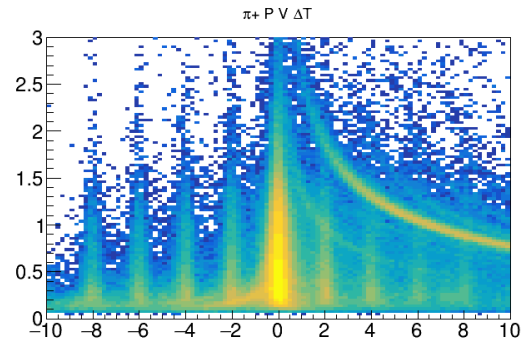
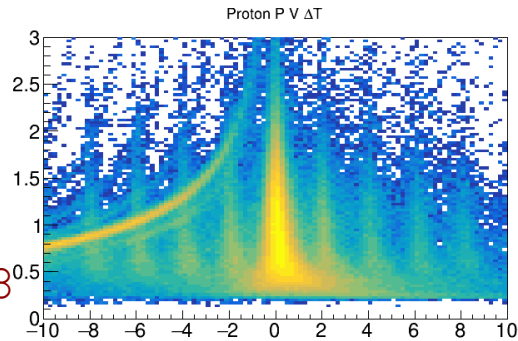


MisIDed particles

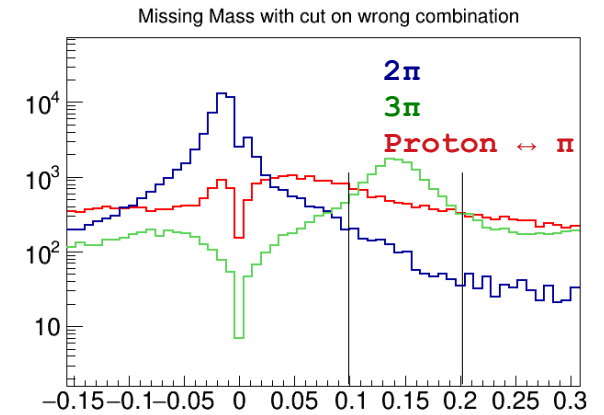
TOP:
MLP>0.8



BOTTOM
MLP<0.8



Still see significant Background from randoms and wrong combinations



Wrong combi can give relatively high contribution to "signal" region 22

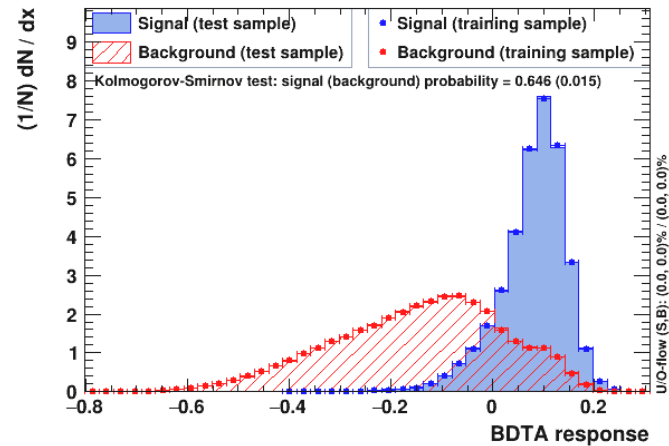
Train with Mixed Events (III)

Signal : $0.1 < \text{MissMass} < 0.2$ && **Simulated BDTA** > -0.2
Background : $-0.04 < \text{MissMass} < 0.1$ and $0.2 < \text{MissMass} < 0.5$

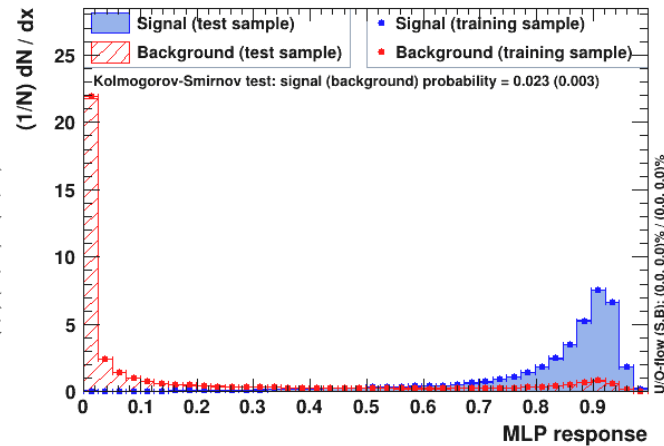
Variables + E_γ

Simulated training was able to remove wrong combinations

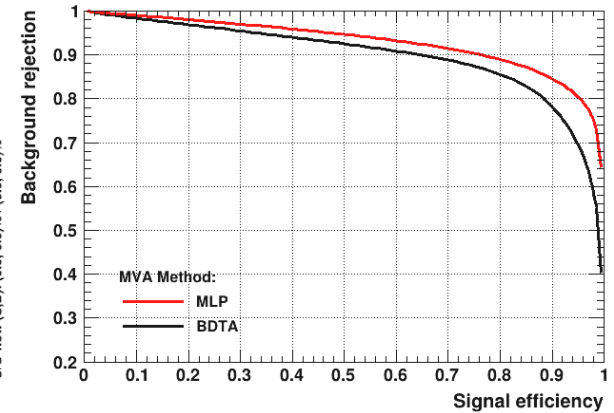
TMVA overtraining check for classifier: BDTA



TMVA overtraining check for classifier: MLP



Background rejection versus Signal efficiency



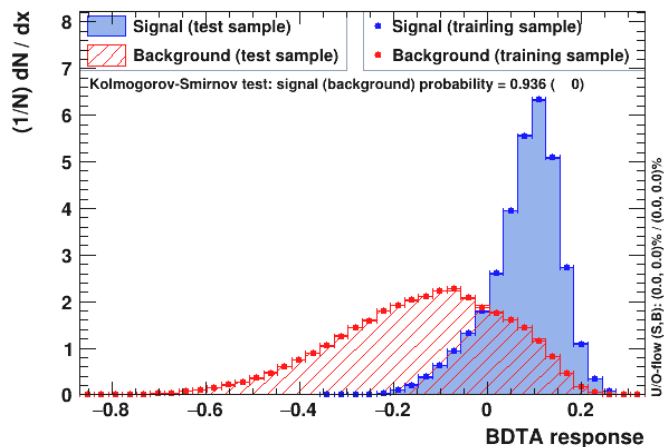
Train with Mixed Events (IV)

Signal : $0.1 < \text{MissMass} < 0.2$ && **Simulated BDTA** > -0.2

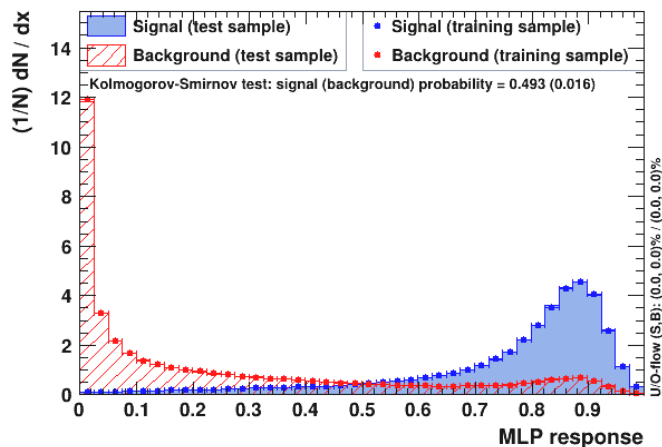
Background : $-0.04 < \text{MissMass} < 0.1$ and $0.2 < \text{MissMass} < 0.5$

Variables - E_Y

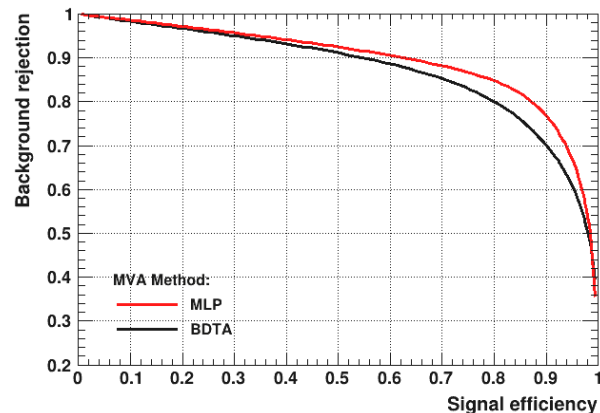
TMVA overtraining check for classifier: BDTA



TMVA overtraining check for classifier: MLP

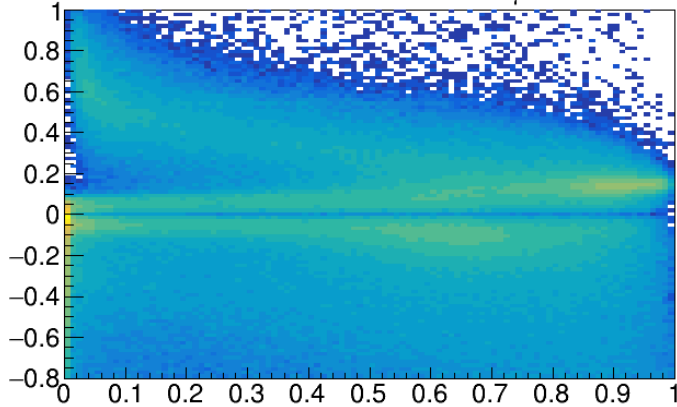


Background rejection versus Signal efficiency

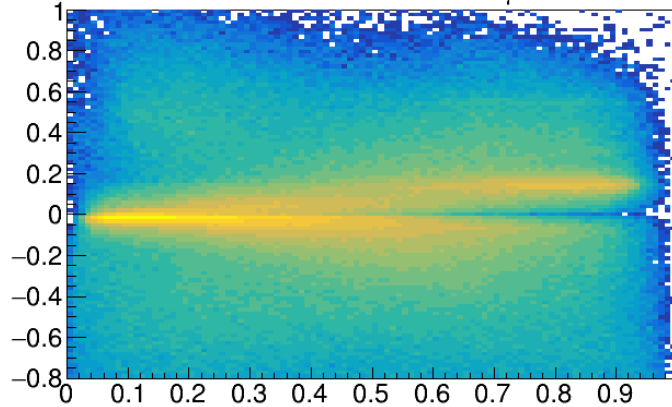


Miss Mass V Responses

MissMass V MLP (with E_γ)

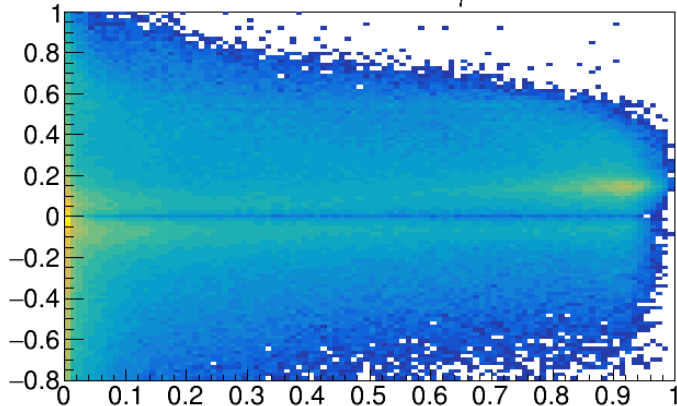


MissMass V MLP (no E_γ)

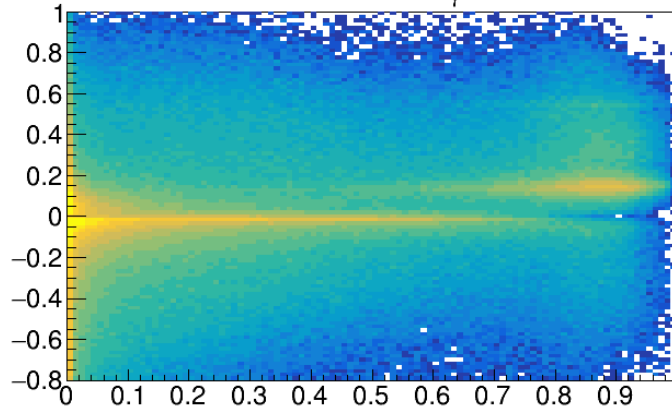


TOP : Mixed Training
with sidebands

MissMass V MLP (with E_γ and Sim)



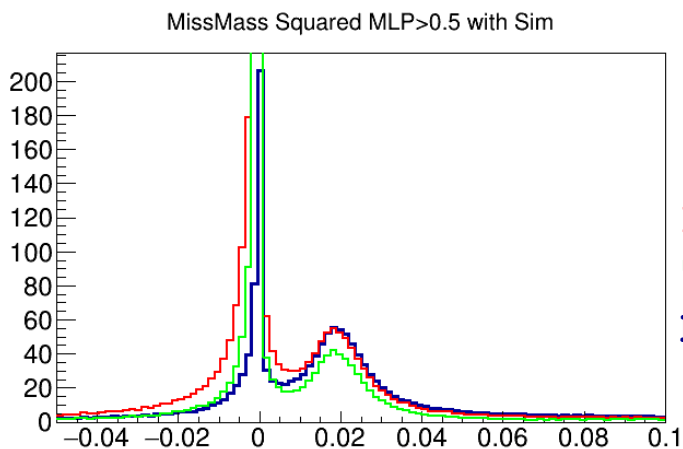
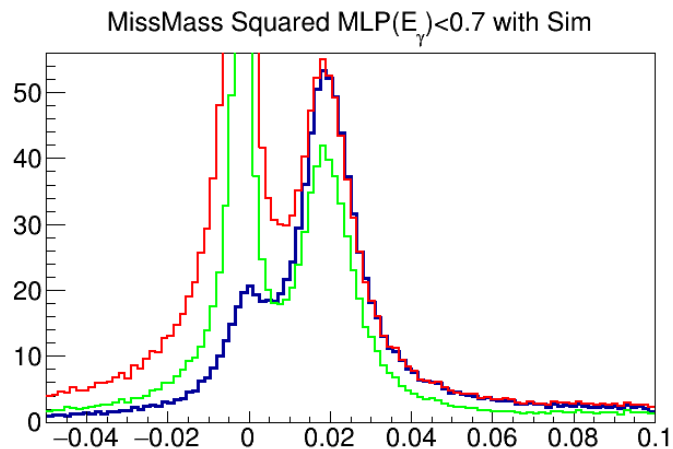
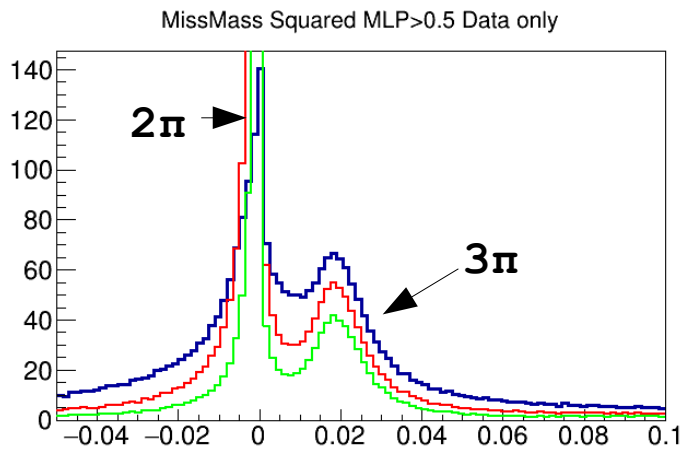
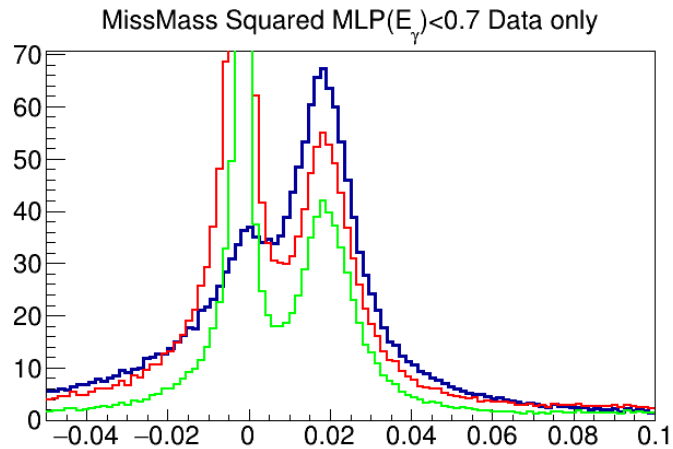
MissMass V MLP (no E_γ and Sim)



BOTTOM : additional
Filter for signal
Training events
 $\text{SimBDTA} > -0.2$

- less "other"
(random, wrong combi)
backgrounds

Effect on Missing Mass Squared



TOP : Mixed Training with sidebands

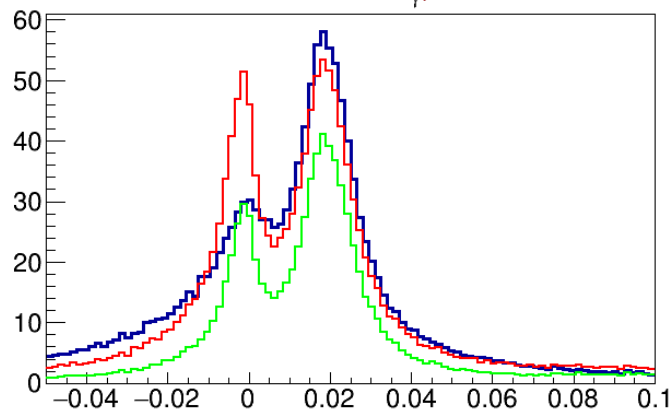
BOTTOM : additional Filter for signal Training events
SimBDTA>-0.2

Only 3π => single peak ~ 0.02

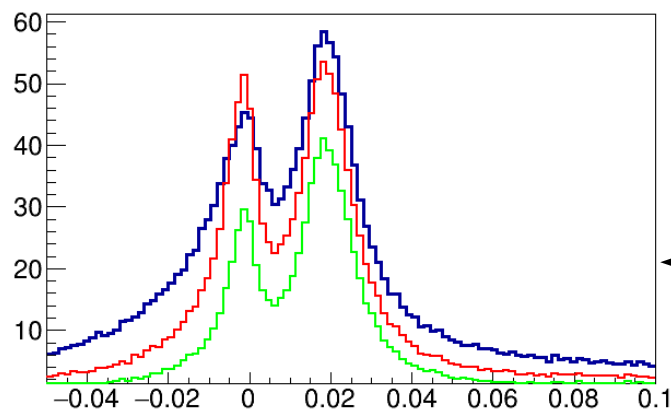
Loose Cuts Based(3ns)
Tight Cuts Based(1ns)
MLP Cut

With extra exclusivity cut

MissMass Squared MLP(E_γ) >0.7 Data only



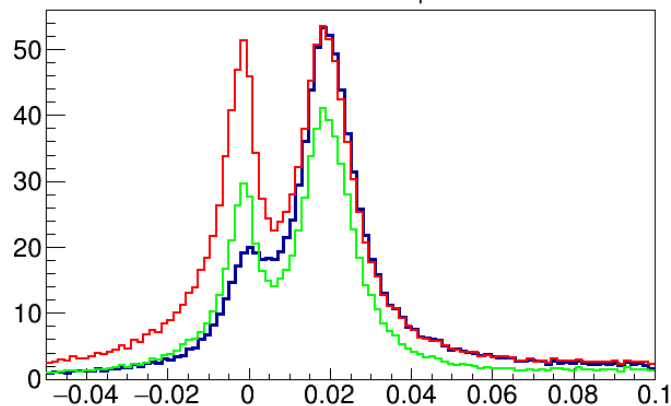
MissMass Squared MLP >0.5 Data only



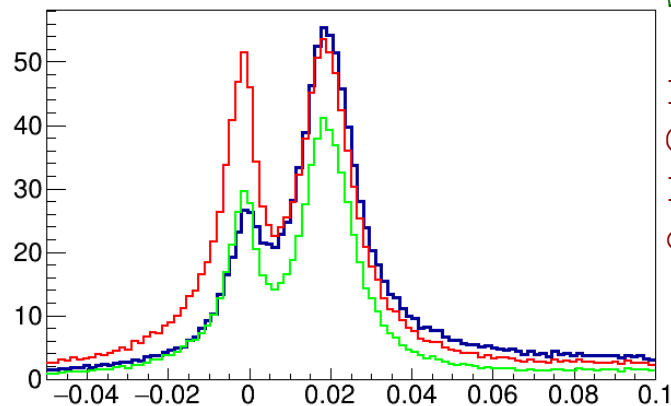
Additional
exclusivity cut
MissEnergy >0.1

Without SimBDT
filter
← Additional BG in
MLP cuts

MissMass Squared MLP(E_γ) >0.7 with Sim



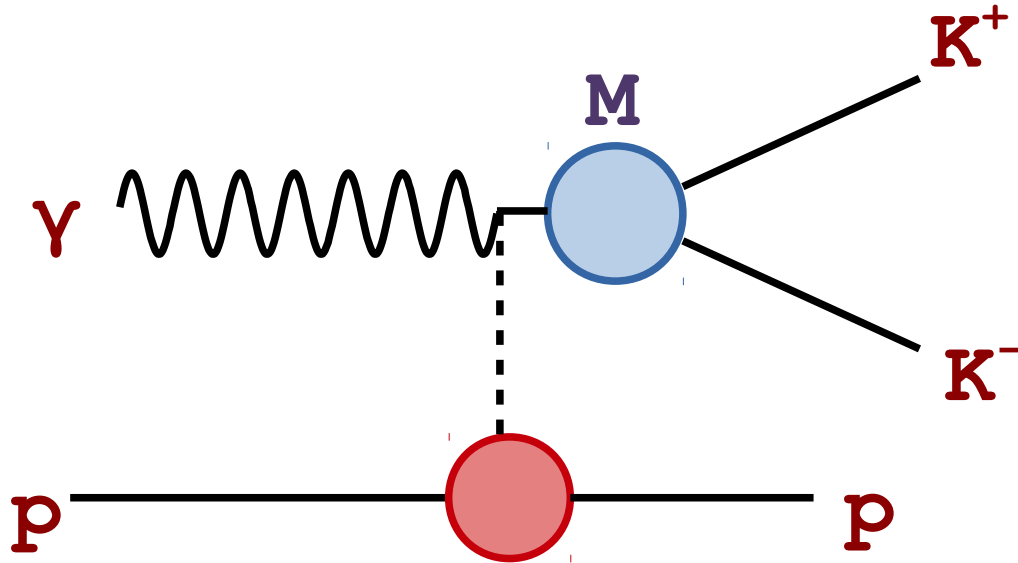
MissMass Squared MLP >0.5 with Sim



Cleaned up
With Sim BDT filter

Improved rejection of 2π
Could also be done with
Improved exclusivity
cuts/kinematic fit,...

Example Reaction

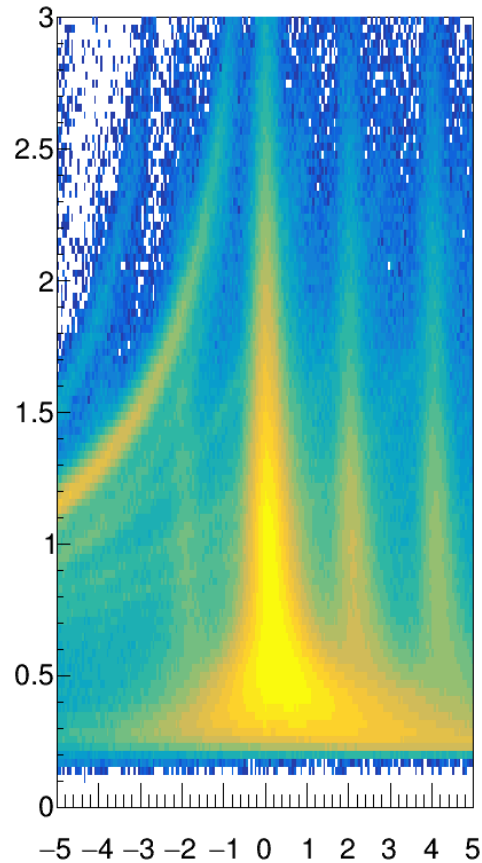


Large background from
Pions IDed as Kaons

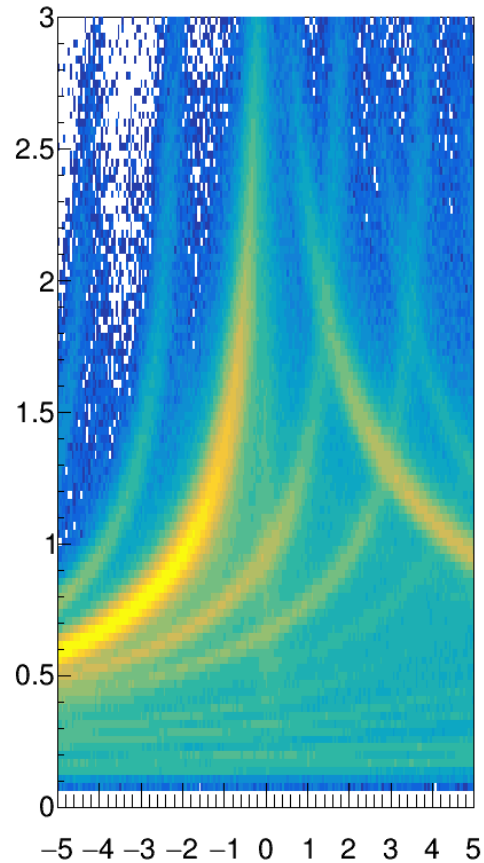
Δ Time PID

*Log scale

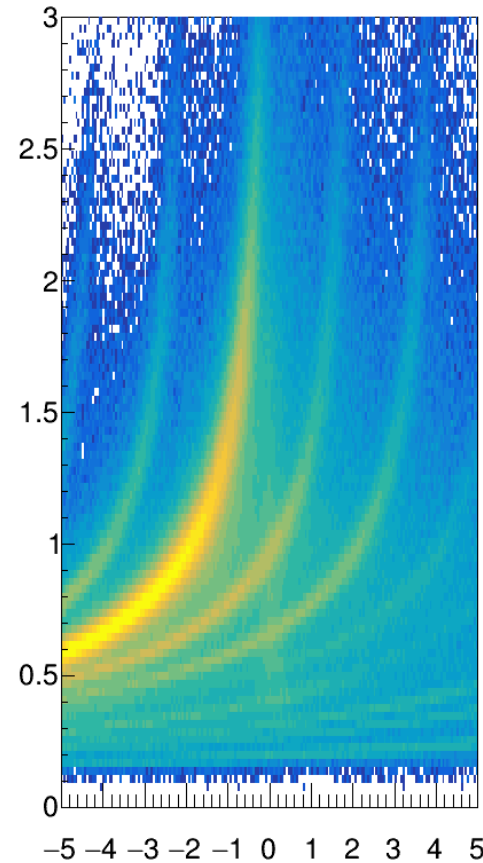
Proton P v Δ T



K+ P v Δ T

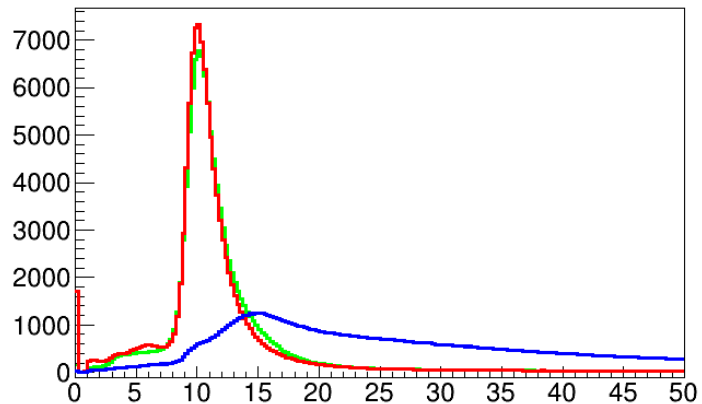


K- P v Δ T



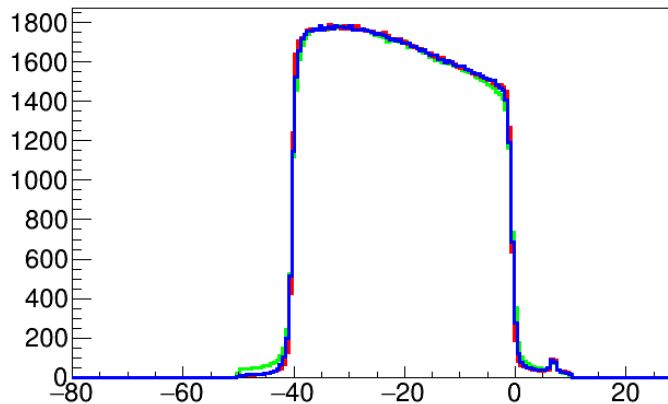
Other Input Variables

ToF Scint. ΔE



θ

Z Vertex

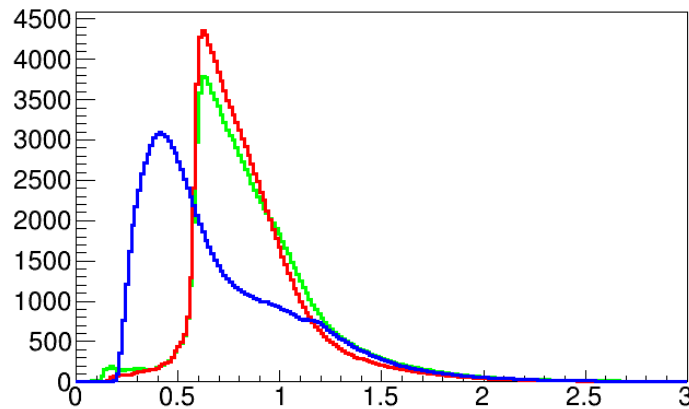
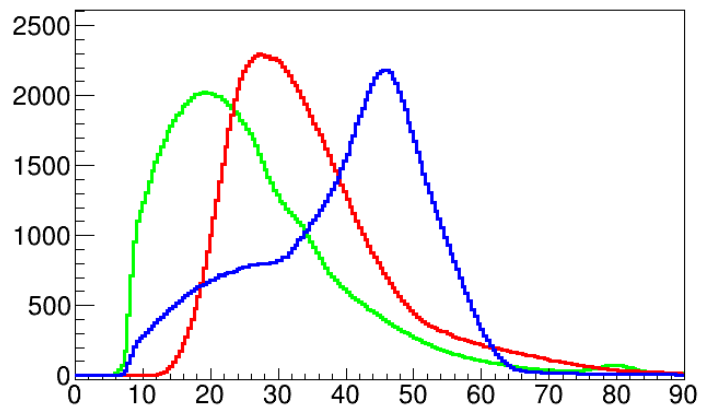


Proton

K^+

K^-

Momentum



Train BDT with sWeights

SPlot - technique for disentangling different event species using a discriminatory variable (generalised side-band subtraction)

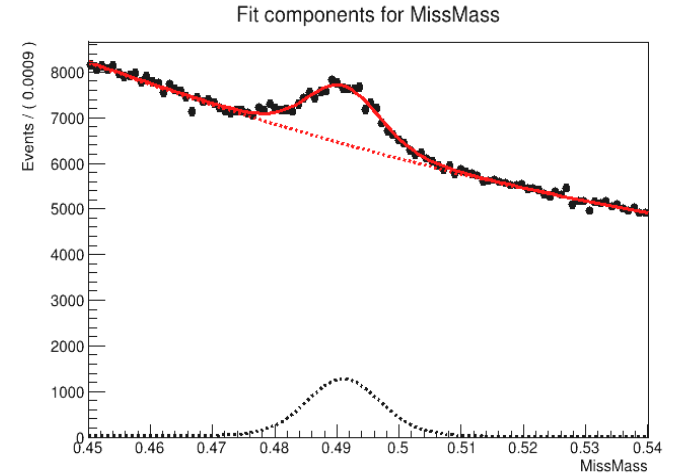
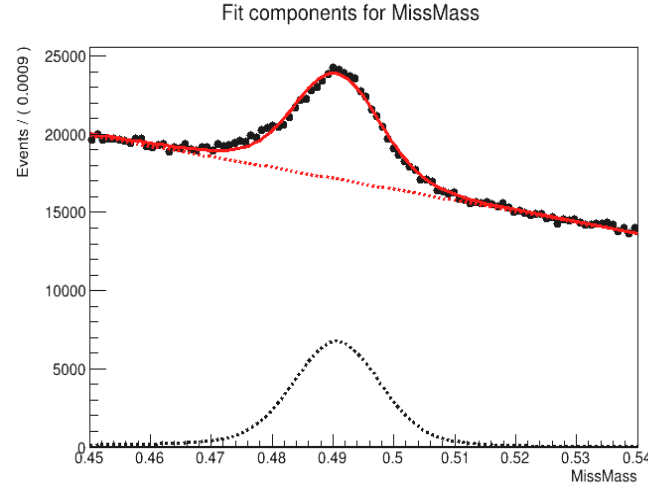
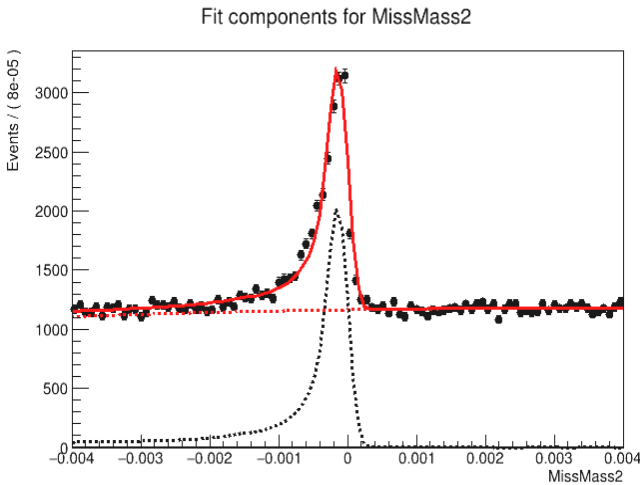
M. Pivk, F.R. Le Diberder, Nucl.Inst.Meth.A 555, 356-369, 2005

Used RooStats implementation

Exclusive

Missing K-

Missing K+



In TMVA BDT accept negative event weights
MLP does not

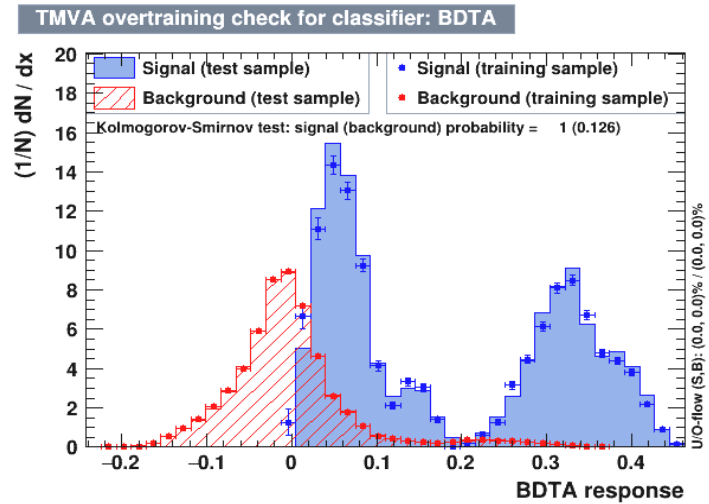
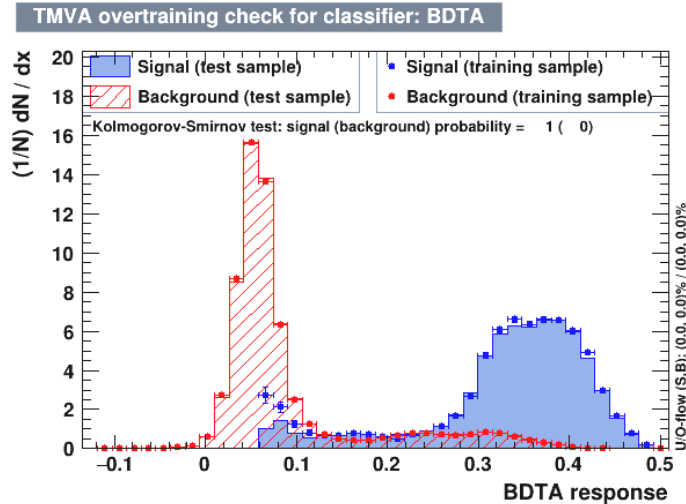
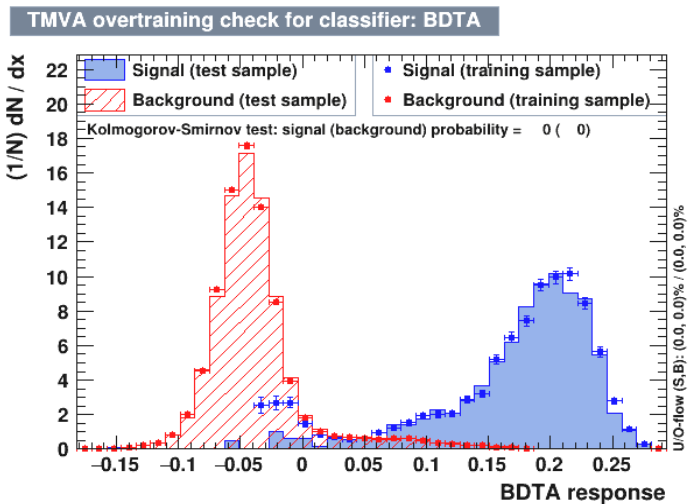
$${}_s\mathcal{P}_n(y_e) = \frac{\sum_{j=1}^{N_s} \mathbf{V}_{nj} f_j(y_e)}{\sum_{k=1}^{N_s} N_k f_k(y_e)}$$

Train BDT with sWeights

80k test and 20k train
Exclusive

300k test and train
Missing K-

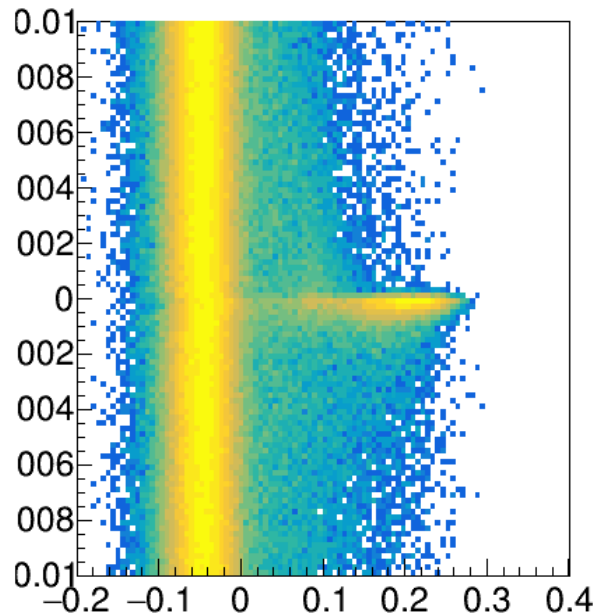
300k test and train
Missing K+



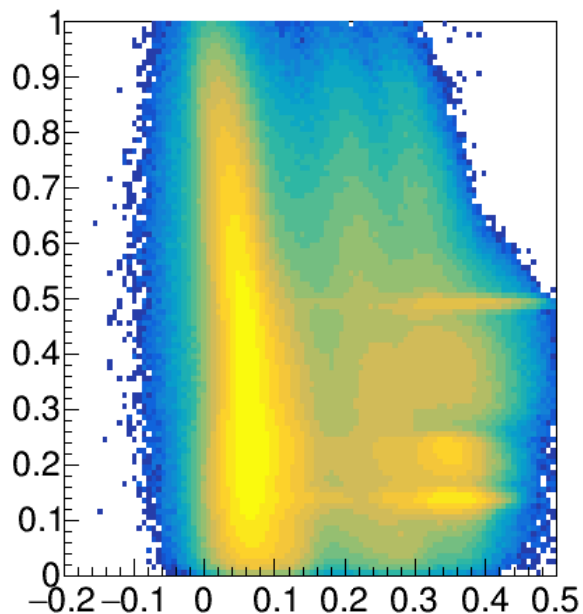
2 types of events
in Missing K+ signal
weights
Separated by training

Exclusivity variables V BDT

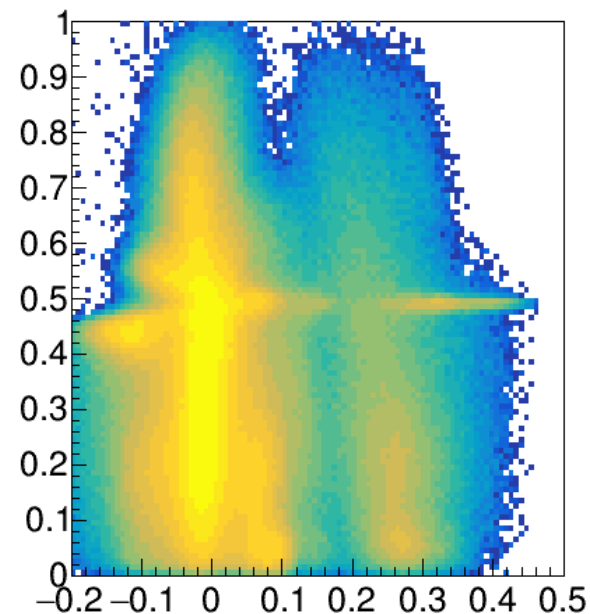
Exclusive MissMass2 V BDT



MissK- MissMass V BDT

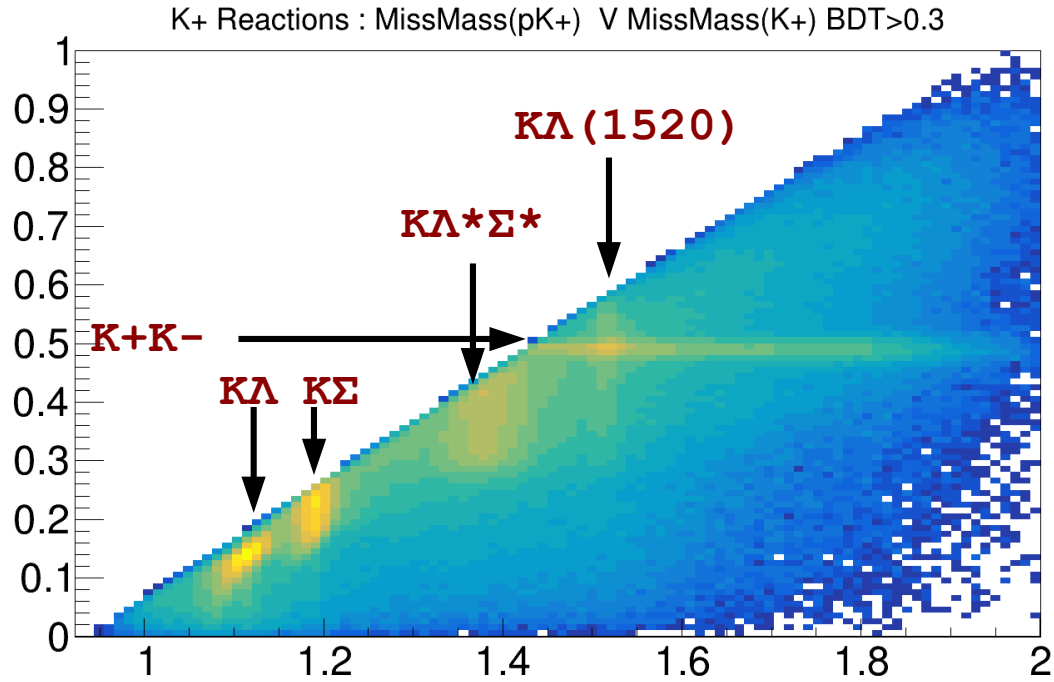


MissK+ MissMass V BDT



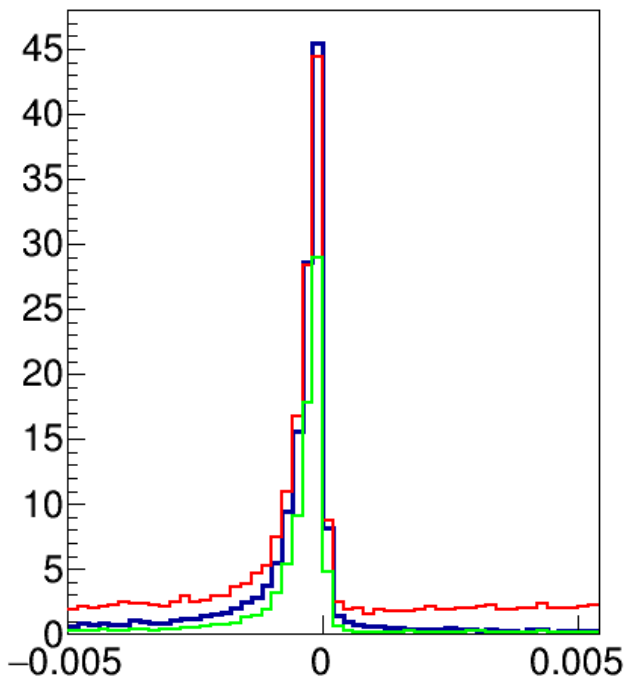
K⁺ production mechanisms

Missing K⁻ Topology

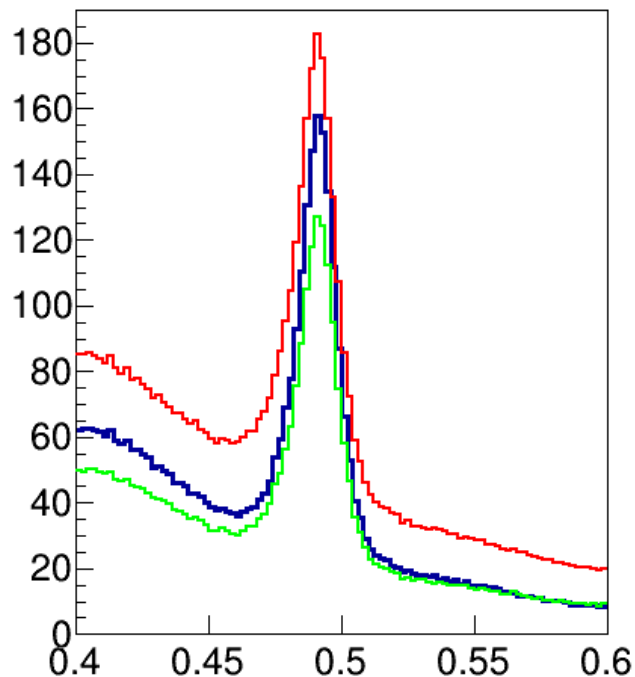


Event exclusivity with BDT cut

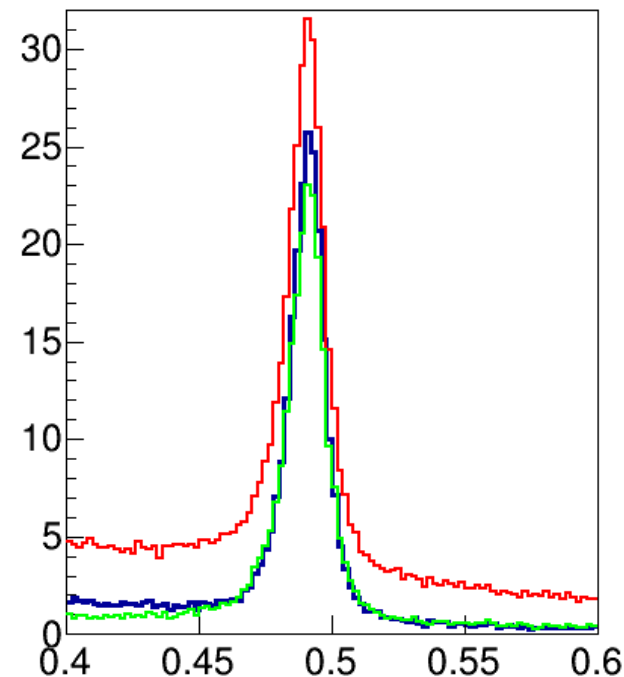
Exclusive MissMass Squared BDT>0.1



MissMass(pK-) BDT>0.28



MissMass(pK+) BDT>0.28



Loose Cuts Based(1ns)

Tight Cuts Based(0.5ns)

BDT Cut

Train MLP with BDT

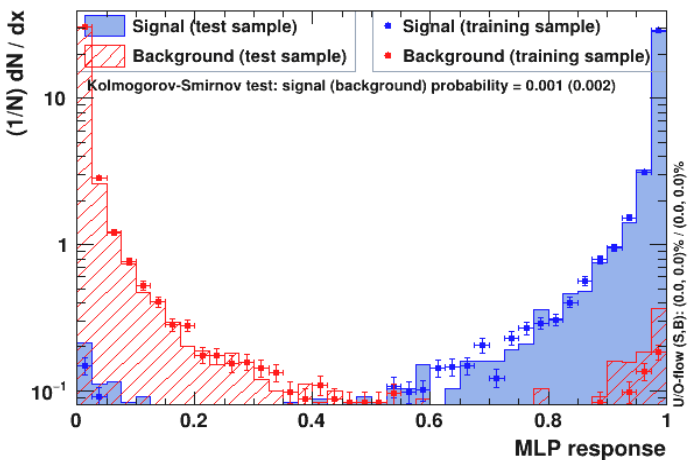
MLP ~ factor 10 faster to apply

Exclusive

Missing K-

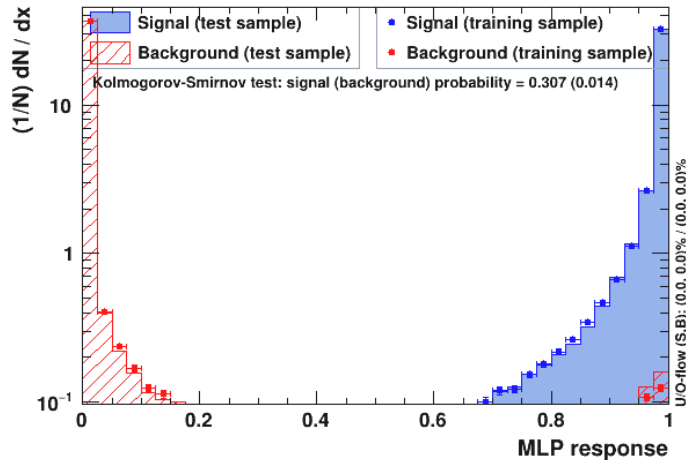
Missing K+

TMVA overtraining check for classifier: MLP



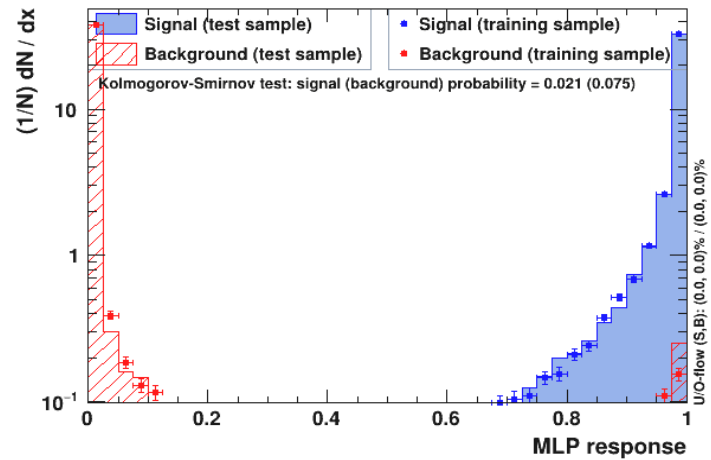
Signal BDT > 0.05
Backgr BDT < 0.05

TMVA overtraining check for classifier: MLP



Signal BDT > 0.3
Backgr BDT < 0.3

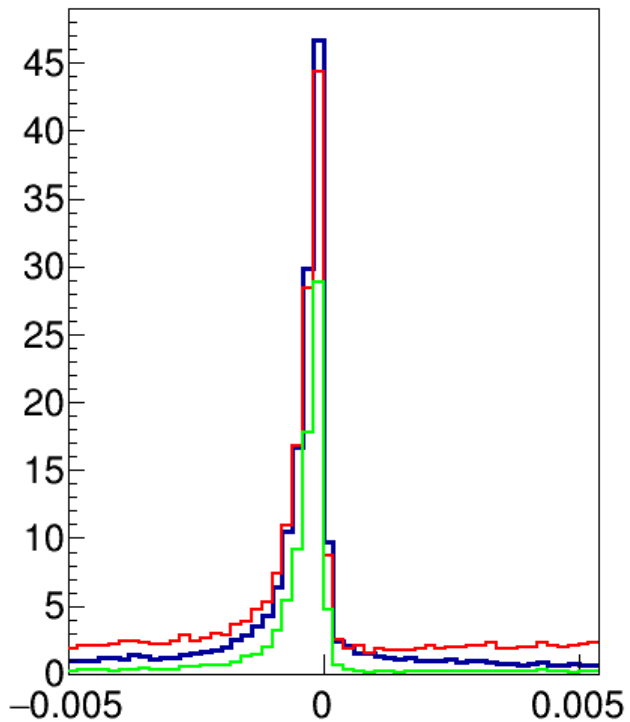
TMVA overtraining check for classifier: MLP



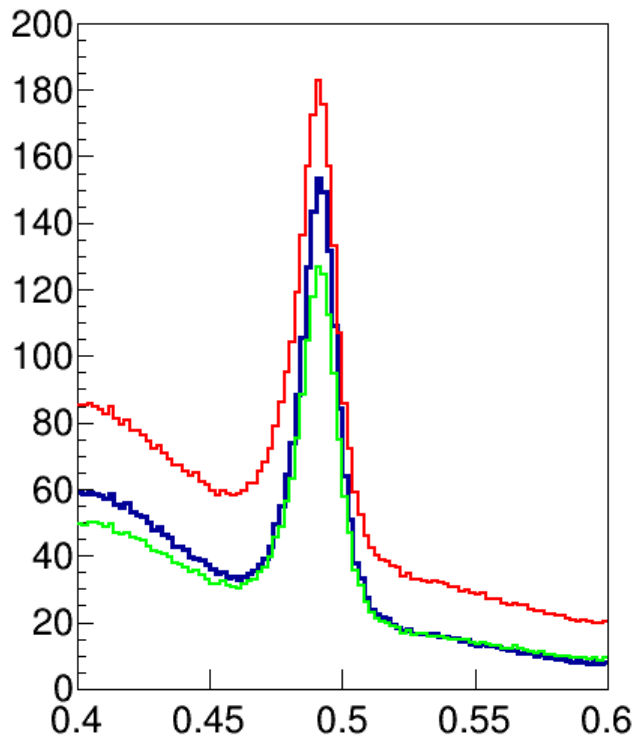
Signal BDT > 0.3
Backgr BDT < 0.3

Event exclusivity with MLP cut

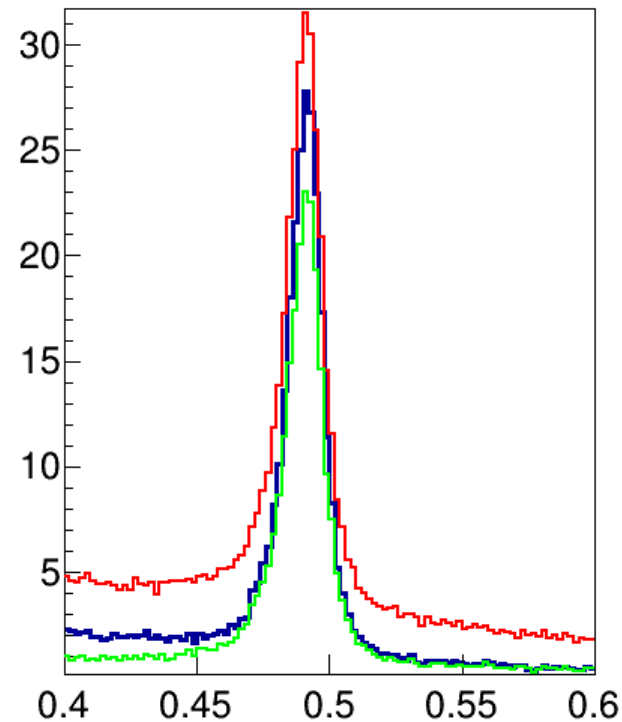
Exclusive MissMass Squared MLP>0.9995



MissMass(pK-) MLP>0.8



MissMass(pK+) MLP>0.8



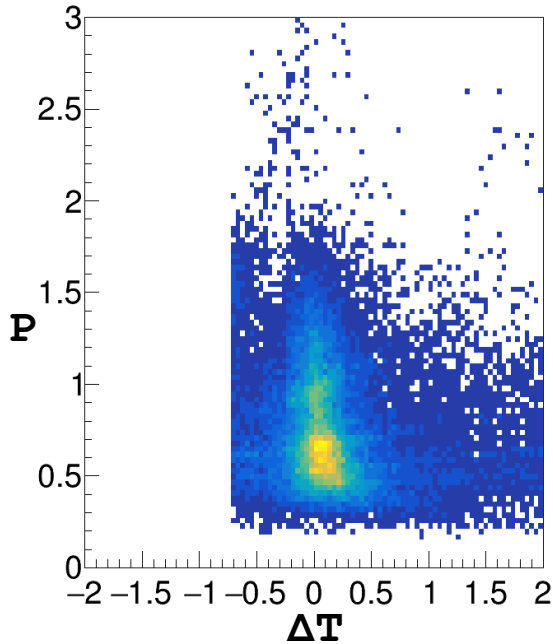
Loose Cuts Based(1ns)

Tight Cuts Based(0.5ns)

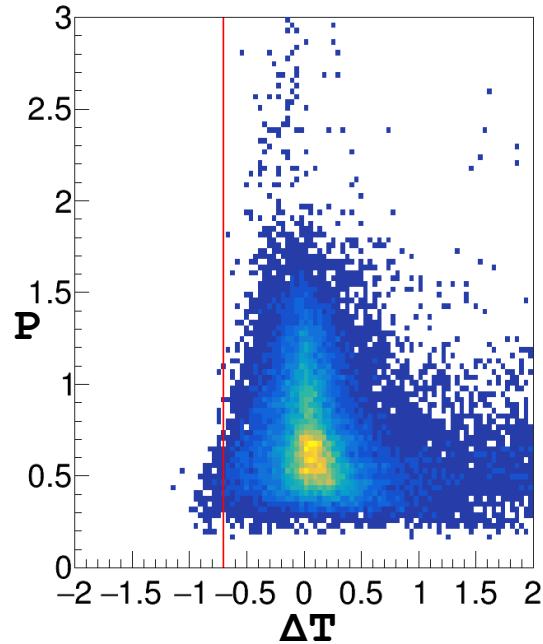
MLP Cut

MLP and correlations

Miss K+ CUT BDTA>0.25

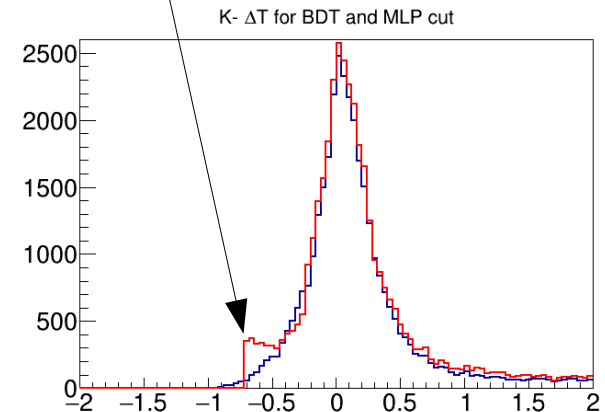


Miss K+ CUT MLP>0.7



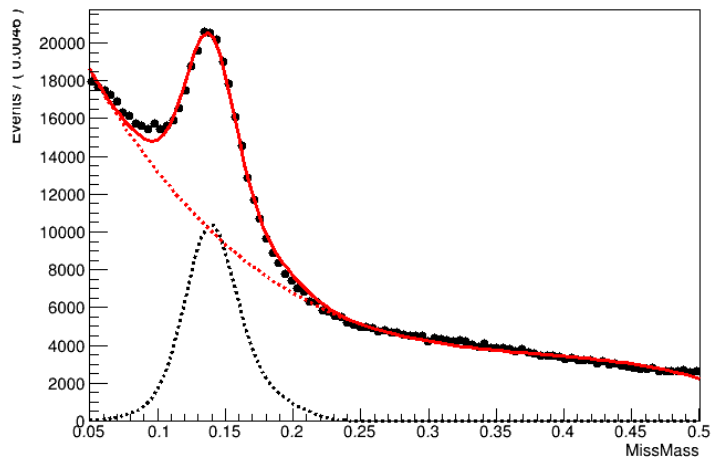
MLP better handles
Correlations
Within inputs

But small improvement
Very few events
Actually removed



Using sPlot training with 3π

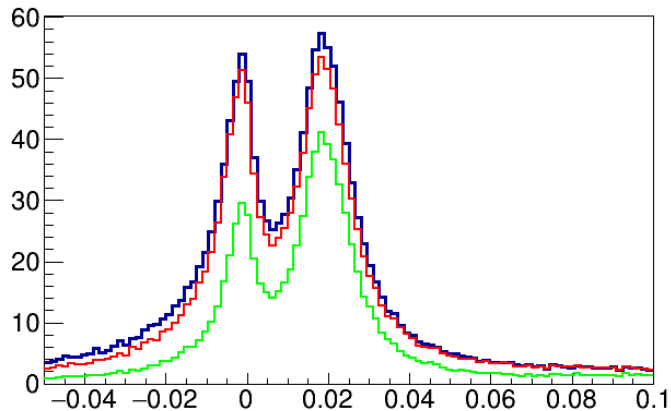
Fit components for MissMass



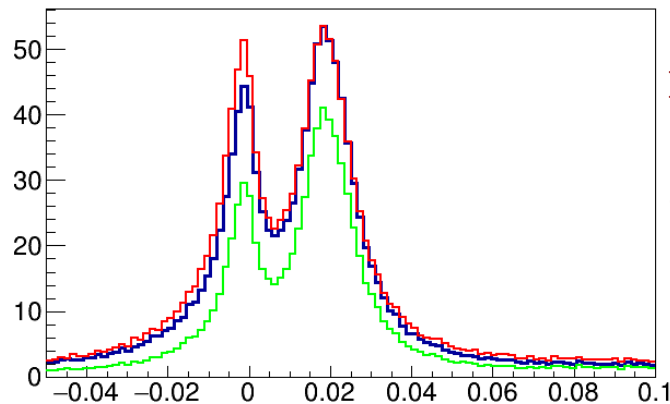
Relatively small sample of 2π background
In fit range

Beam Energy not used as input

MissMass Squared BDT>0.08 Data only



MissMass Squared BDT>0.12

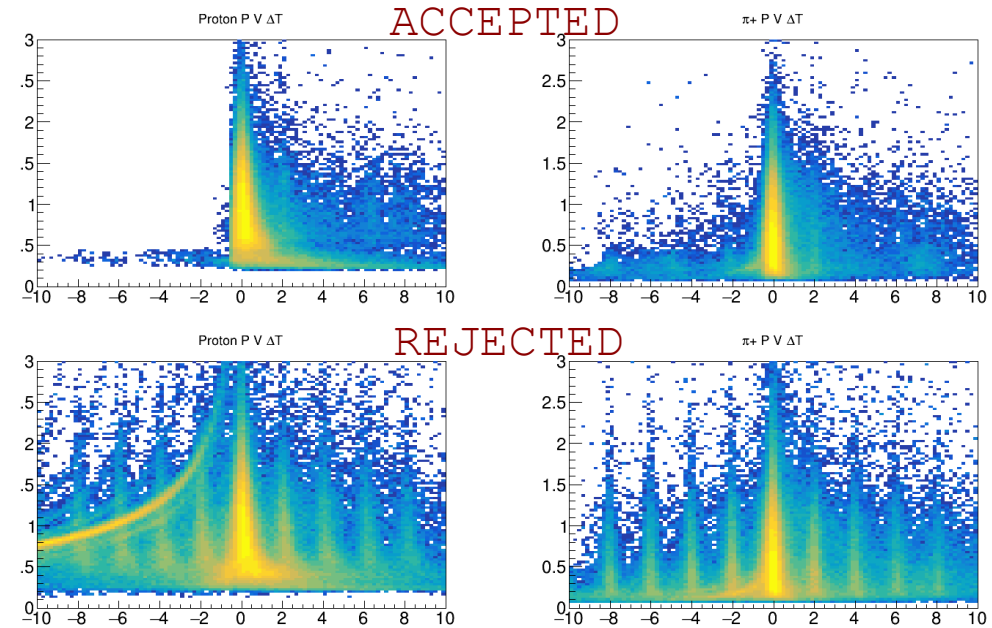
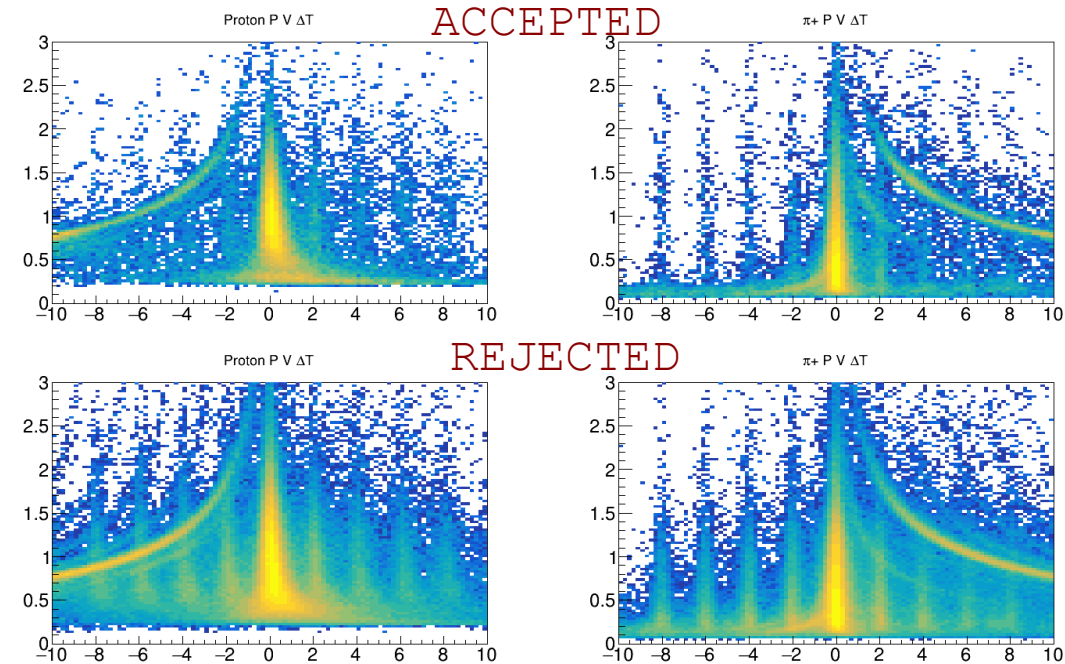


sPlot trained
BDT at
least as good
as straight cuts

sPlot Training for 3π

Mixed Event Training

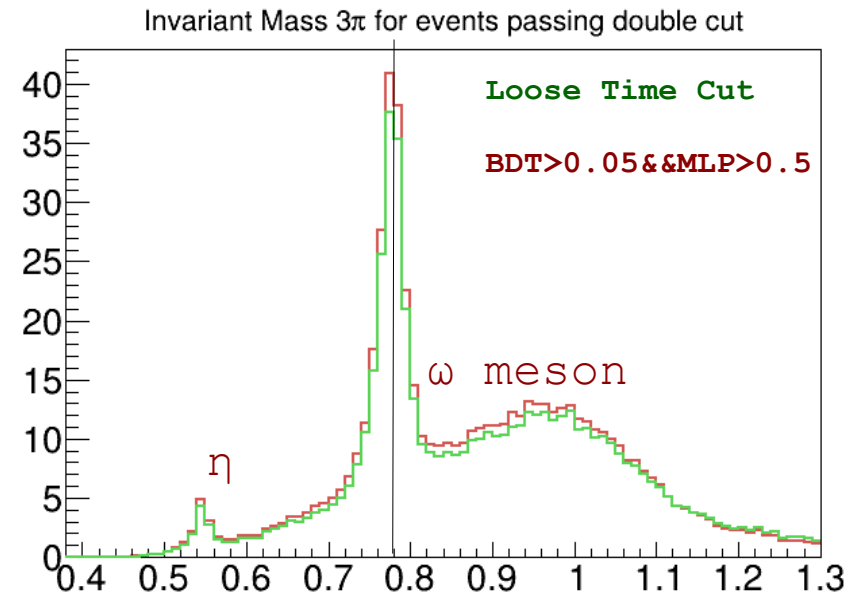
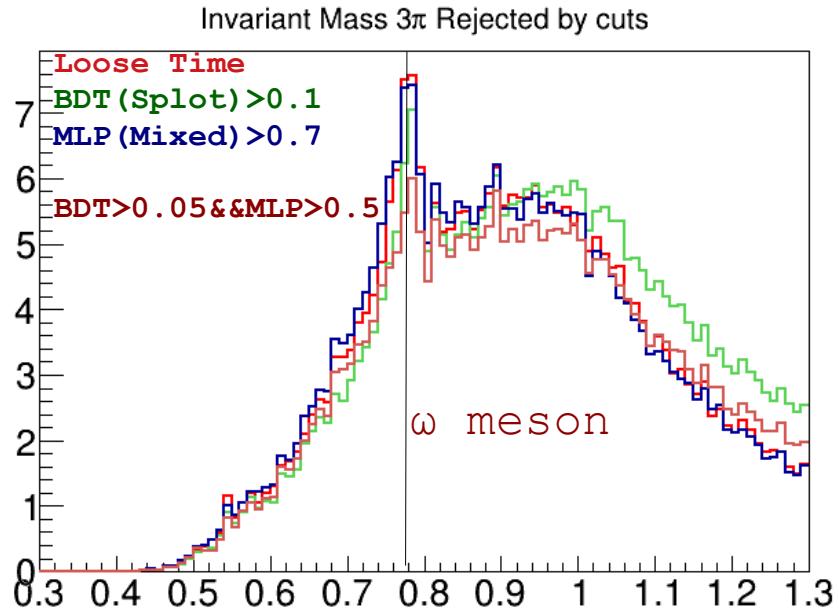
Splot Training



Fixes wrong combination problem
Wrong combination doesn't peak
At π^0 mass

But what about false negatives?

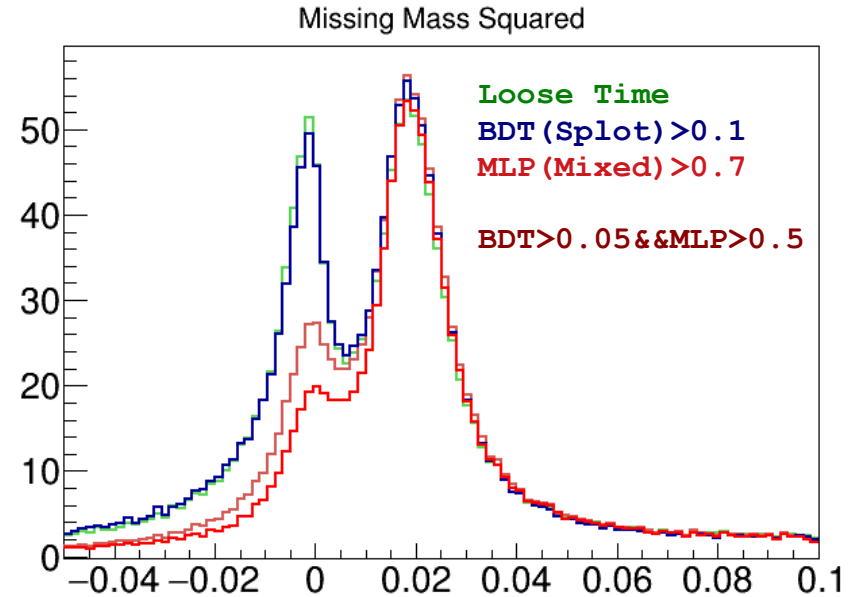
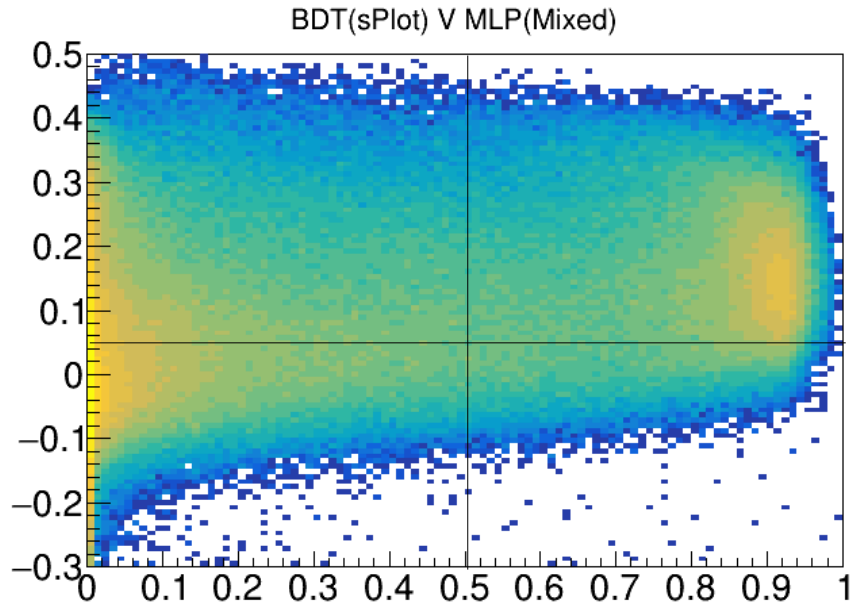
Check with 3π invariant mass, which should peak at ω mass



Judge from ω mass peak, we lose $\sim 5\%$ of events using previous cuts

Can regain these using a combination of classifiers with looser cuts

Double classifier cut



Further Reading

Boosted decision trees, sPlot training, ...

The Full Event Interpretation An Exclusive Tagging Algorithm for the Belle II Experiment
Keck, T., Abudinén, F., Bernlochner, F.U. et al. Comput Softw Big Sci (2019) 3: 6.
<https://doi.org/10.1007/s41781-019-0021-8>

T. Keck. Machine learning algorithms for the Belle II experiment and their validation on Belle data. PhD thesis, KIT, 2017. URL <http://dx.doi.org/10.5445/IR/1000078149>.

FastBDT: A Speed-Optimized Multivariate Classification Algorithm for the Belle II Experiment
Keck, T. Comput Softw Big Sci (2017) 1: 2.

<https://doi.org/10.1007/s41781-017-0002-8>

Removing acceptance artifacts from BDT cuts

Stevens J, Williams M (2013) uboost: a boosting method for producing uniform selection efficiencies from multivariate classifiers. J Instrum 8(12).

<http://stacks.iop.org/1748-0221/8/i=12/a=P12013>

Summary

TMVA can be used in place of standard particle ID cuts

Different methods can be used for creating signal and background samples
Simulation, Mixed events, sPlots, ...

Can benefit from multiple classifiers with different training conditions

Verification very important

Further work :

Train with simulation as signal and sPlot Background
i.e. remove signal events when using data as background

Multiple Classifiers trained with Signal against different sources
of backgrounds

- Wrong combitorial, random, physics, ...
- Backgrounds from mixed events, sPlots, simulation, ...

Timing Benchmarks

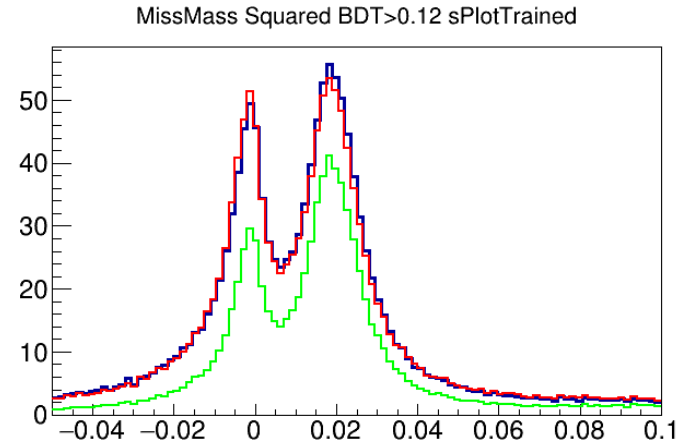
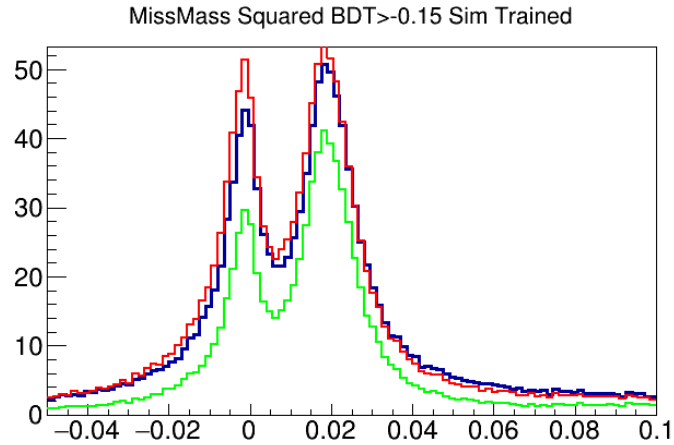
Table 1: Table of training CPU times in seconds.

Method	12-vars
BDT	2.68
Cuts	2.41
CutsD	2.32
FDA_GA	2.40
KNN	1.93
LD	1.16
Likelihood	1.99
LikelihoodPCA	2.02
MLPBNN	19.54
RuleFit	5.33
SVM	2.23

Table 2: Table of evaluation CPU times in seconds.

Method	4-vars	8-vars	12-vars
BDT	29.57	29.33	28.51
Cuts	1.12	1.13	1.16
CutsD	1.12	1.15	1.16
FDA_GA	1.51	1.55	1.53
KNN	24.71	59.75	81.87
LD	1.38	1.47	1.59
Likelihood	2.08	2.40	2.90
LikelihoodPCA	2.92	4.25	6.32
MLPBNN	2.64	3.08	3.77
RuleFit	1.72	2.32	3.10
SVM	1.08	1.07	1.11

MLP

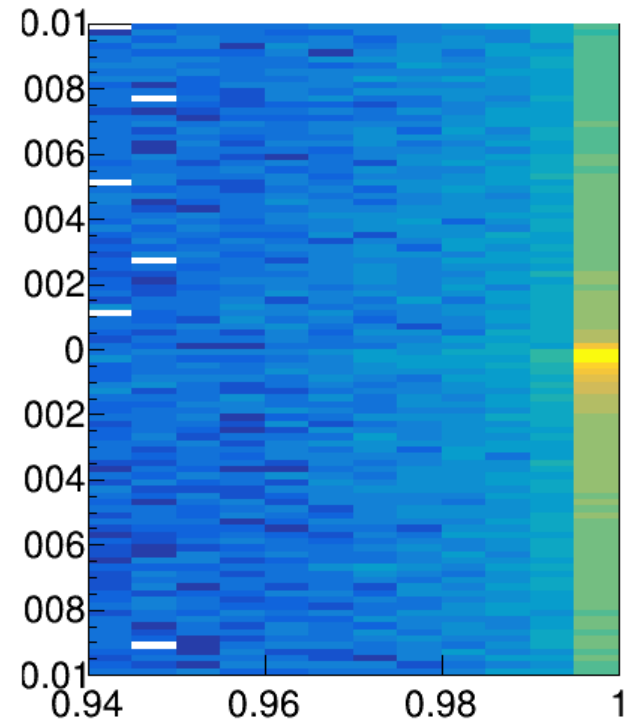


Sim trained BDT
Not quite as good as
Straight cuts
Less signal
Higher "other" background

sPlot trained
BDT only
At least as good
as straight cuts

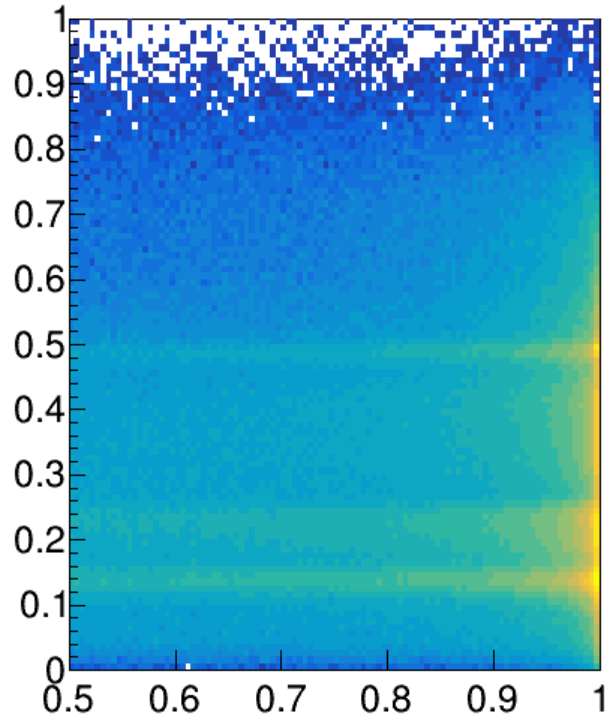
BDT \rightarrow MLP

Exclusive MissMass2 V MLP



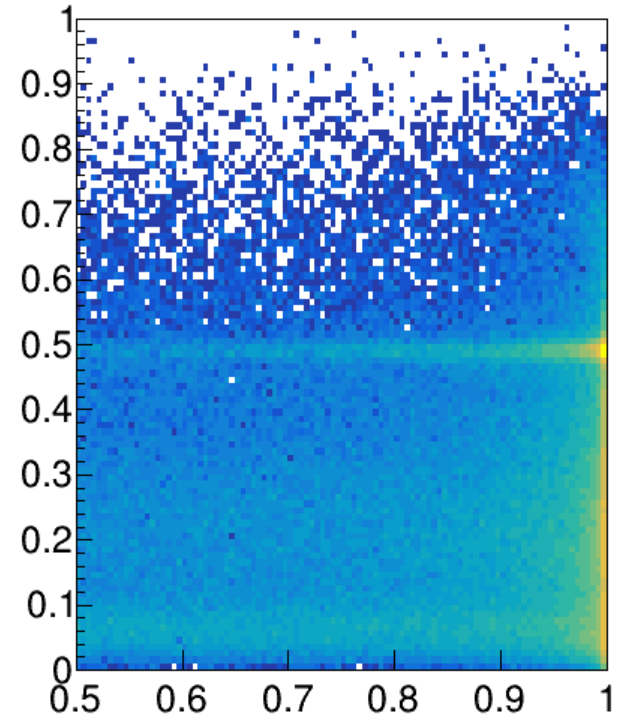
Missing K+

MissMass V MLP



Missing K-

MissMass V MLP



Optimised cuts based analysis

