

Uses of Multivariate Analysis Methods

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on behalf of the CDF and DØ collaborations

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1 Motivation

- Tevatron top groups techniques
- DØ single top group approaches

2 Dataset preparation

3 Cut-based analysis

4 Multivariate analysis methods

- Likelihood discriminants
- Neural networks
- Decision trees

5 Summary and outlook



CDF and DØ top groups techniques

Single variable techniques

- Cut-based  
- Template methods  



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Multivariate approaches

- Matrix elements  
- Kernel density estimation 
- Dynamic likelihood method 
- Neural networks  

Yesterday's talks

- Top pair production cross section (R. Rossin)
- Top decay properties (E. Varnes)
- Top mass in ℓ +jets channel (J. Cammin)
- Top mass in dilepton channel (B. Jayatilaka)
- Search for single top (M. Begel)



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Why multivariate analyses?

Data is multivariate

- Relatively similar signal and background \Rightarrow simple cuts cannot separate them
- Few events \Rightarrow use all information available to keep as many signal events as possible









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Illustration: techniques used in $D\emptyset$ single top group

- Likelihood discriminants
- Decision trees
- Neural networks
- Boosted decision trees

Datasets preparation

Advanced techniques are useless if inputs are not correct

Selection of events

- good object ID and resolution
- use basic criteria that keep events with particular final state

Generate realistic Monte Carlo events

- signal
- all backgrounds not extracted from data

Find discriminating variables (and their correlations)

- key to analysis performance

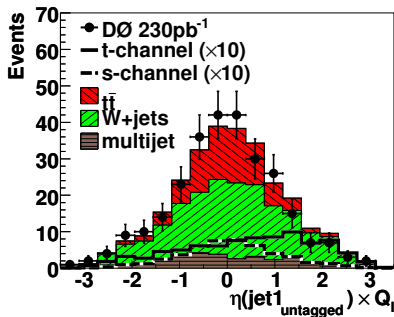
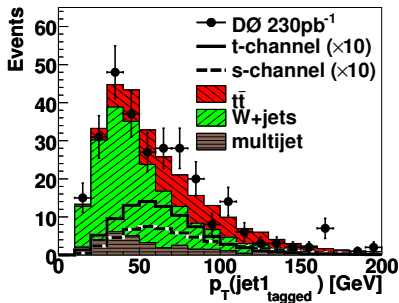
Most important: check models (bkg and/or signal) describe data

- overall normalization
- variables shapes



Cut-based analysis

- Reference for any “advanced” technique
- Example: $D\bar{O}$ single top search



Cut-based analysis

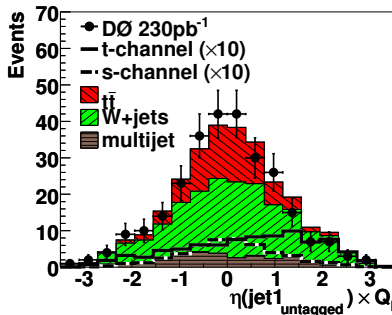
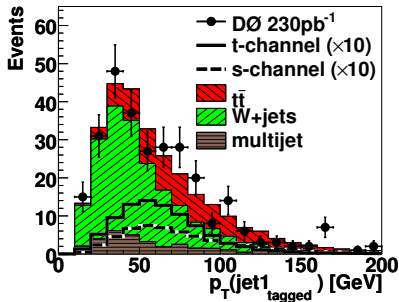
- Reference for any “advanced” technique
- Example: $D\bar{D}$ single top search

Random grid search

- Optimal cut (minimizes expected limit) on all variables
- Combine sets of variables and re-optimize
- Select set yielding lowest expected limit
- Set limits by counting events

Published limits (230 pb^{-1}) [observed (expected)]

	s-channel	t-channel
Preselection	13.0 (14.5) pb	13.6 (16.5) pb
Cut-based	10.6 (9.8) pb	11.3 (12.4) pb



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Likelihood discriminants

Likelihood for a vector of measurements $\vec{x} = x_i$

$$\mathcal{L}(\vec{x}) = \frac{\mathcal{P}_{\text{signal}}(\vec{x})}{\mathcal{P}_{\text{signal}}(\vec{x}) + \mathcal{P}_{\text{background}}(\vec{x})}$$

- \mathcal{L} close to 0 for background and 1 for signal

- Built likelihood for signal/ W +jets and signal/ $t\bar{t}$, with 7 to 10 variables
- Advantage: no training

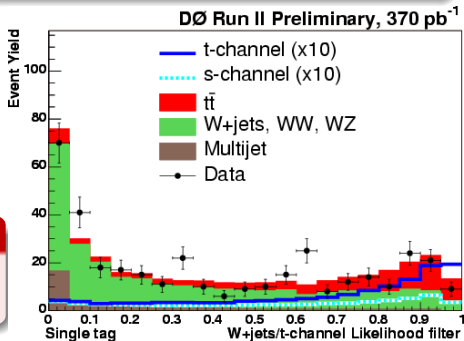
- Probability Density Functions:

$$\mathcal{P}(\vec{x}) = \prod_i^{N_{\text{variables}}} P(x_i)$$

$P(x_i)$ = normalized x_i variable distribution

Prelim. limits (370 pb^{-1}) [observed (expected)]

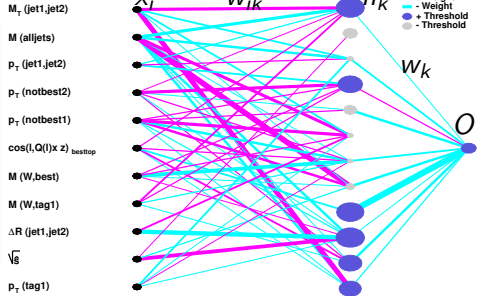
	s-channel	t-channel
Likelihood	5.0 (3.3) pb	4.4 (4.3) pb



Neural networks

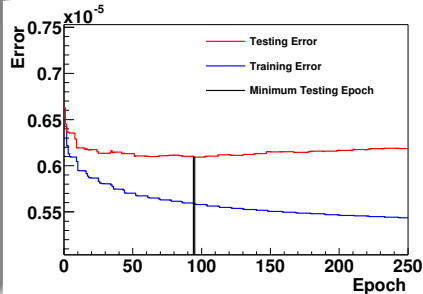
MultiLayer Perceptron

- MLPfit implementation
- Input layer nodes: variables x_i
- Hidden layer nodes:
$$n_k = \frac{1}{1 + \exp^{-\sum w_{ik} x_i}}$$
- Output node: $O = \sum w_k n_k$



Training method

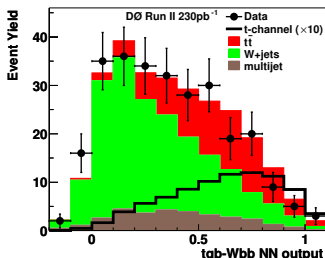
- Initialize weights, minimize error function on training sample, update weights \Rightarrow first epoch
- Repeat procedure. After each epoch, apply NN on independent testing sample. Stop training when testing error increases (avoid overtraining)



Neural networks

Training for single top search

- Train signal/ Wbb and signal/lepton + jets networks
- Train on 60% of events, test on remaining 40%
- Use logarithm of non-angular variables
- Use MLPfit hybrid method for error function minimization



Network optimization

- Optimize choice of input variables, using 11 out of 30 variables
- Optimize number of hidden nodes (found close to 30)
- Optimize number of training epochs (150-250)
- Very powerful technique but:
 - slow to train
 - set of weights sensitive to training events
 - sensitive to extra variables

Published limits (230 pb⁻¹) [obs'd (exp'd)]

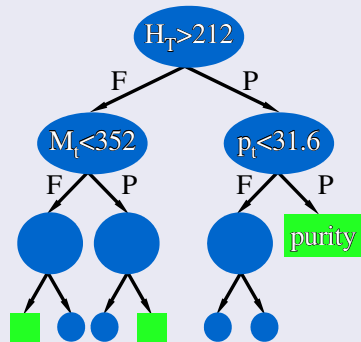
	s-channel	t-channel
Cut-based	10.6 (9.8) pb	11.3 (12.4) pb
Neural net	6.4 (4.5) pb	5.0 (5.8) pb

Decision trees

- Machine learning technique, widely used in social sciences
- Idea: recover events that fail criteria in cut-based analysis

- Start with all events = first node
 - sort all events by each variable
 - for each variable, find splitting value with best separation between two children (mostly signal in one, mostly background in the other)
 - select variable and splitting value with best separation, produce two branches with corresponding events ((F)ailed and (P)assed cut)
- Repeat recursively on each node
- Splitting stops: terminal node = leaf

- Run testing events and data through tree to derive limits
DT output = leaf purity



Ref: Breiman *et al*, "Classification and Regression Trees", Wadsworth (1984)



Tree construction parameters

Normalization of signal and background before training

- same total weight for signal and background events

Selection of splits

- list of questions ($variable_i > cut_i?$)
- goodness of split

Decision to stop splitting (declare a node terminal)

- minimum leaf size
- insufficient improvement from splitting

Assignment of terminal node to a class

- signal leaf if purity > 0.5
- background otherwise



Splitting a node

Impurity $i(t)$

- maximum for equal mix of signal and background
- symmetric in p_{signal} and $p_{background}$
- minimal for node with either signal only or background only
- strictly concave \Rightarrow reward purer nodes

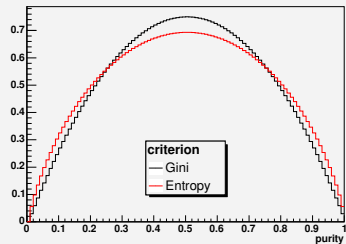
- Decrease of impurity for split s of node t into children t_L and t_R (goodness of split):
$$\Delta i(s, t) = i(t) - p_L \cdot i(t_L) - p_R \cdot i(t_R)$$
- Aim: find split s^* such that:

$$\Delta i(s^*, t) = \max_{s \in \{\text{splits}\}} \Delta i(s, t)$$

- Maximizing $\Delta i(s, t) \equiv$ minimizing overall tree impurity

Examples

$$Gini = 1 - \sum_{i=s,b} p_i^2 = \frac{2sb}{(s+b)^2}$$
$$entropy = - \sum_{i=s,b} p_i \log p_i$$



Decision tree output

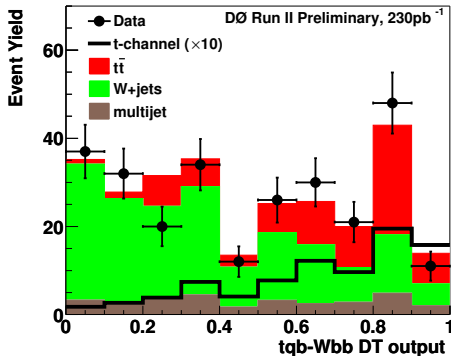
- Followed same training strategy as NN analysis (different trees for different backgrounds)

Advantages

- DT has human readable structure (no black box)
- Training is fast
- Deals with discrete variables
- No need to transform inputs
- Resistant to irrelevant variables

Limitations

- Piecewise nature of output
- Instability of tree structure



Limits (230 pb⁻¹) [observed (expected)]

	s-channel	t-channel
Neural net	6.4 (4.5) pb	5.0 (5.8) pb
Decision tree	8.3 (4.5) pb	8.1 (6.4) pb
Similar sensitivity		



Boosting a decision tree

Boosting

- Recent technique to improve performance of a weak classifier
- Recently used on decision trees in HEP by GLAST and MiniBooNE (Nucl. Instrum. Meth. A 543, 577 (2005) [physics/0408124])
- Basic principal on DT:
 - train a tree T_k
 - minimize error function
 - $T_{k+1} = \text{modify}(T_k)$

AdaBoost algorithm

- Adaptive boosting
- Check which events are misclassified by T_k
- Derive tree weight α_k
- Increase weight of misclassified events
- Train again to build T_{k+1}
- Boosted result of event i :
$$T(i) = \sum_{n=1}^{N_{\text{tree}}} \alpha_k T_k(i)$$

- Averaging \Rightarrow dilutes piecewise nature of DT
- Usually improves performance

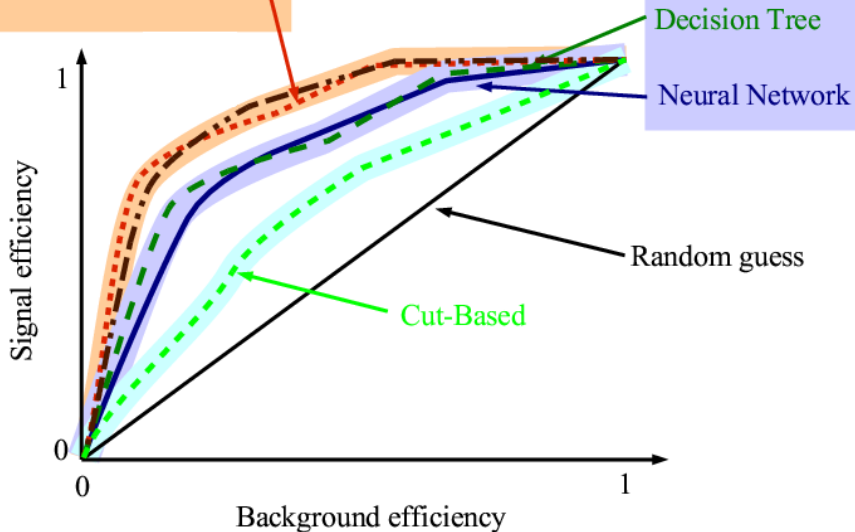
Ref: Freund and Schapire, "Experiments with a new boosting algorithm", in *Machine Learning*

Proceedings of the Thirteenth International Conference, pp 148-156 (1996)



Comparison

Boosted Decision Trees



Summary and outlook

- Many different analysis techniques used by Tevatron top groups
 - single variable methods
 - multivariate approaches
- For all methods: need good inputs first
 - good reconstruction and identification of physics objects
 - realistic Monte Carlo events that describe data
- Advanced techniques useful for precision measurements, searches with small statistics
- Example: different techniques in $D\bar{D}$ single top searches (likelihood discriminants, neural networks, decision trees, boosted decision trees)
- Ongoing:
 - improved results with more statistics and new strategies
 - boosted decision tree results soon
 - superNN: combining results of multiple NN into one

