

# Statistical Methods for Particle Physics

## Lecture 2: multivariate methods

<https://indico.ihep.ac.cn/event/9142/>



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# Outline

## Lecture 1: Introduction and review of fundamentals

Review of probability

Parameter estimation, maximum likelihood

Statistical tests for discovery and limits

## → Lecture 2: Multivariate methods

Neyman-Pearson lemma

Fisher discriminant, neural networks

Boosted decision trees

## Lecture 3: Further topics

Nuisance parameters (Bayesian and frequentist)

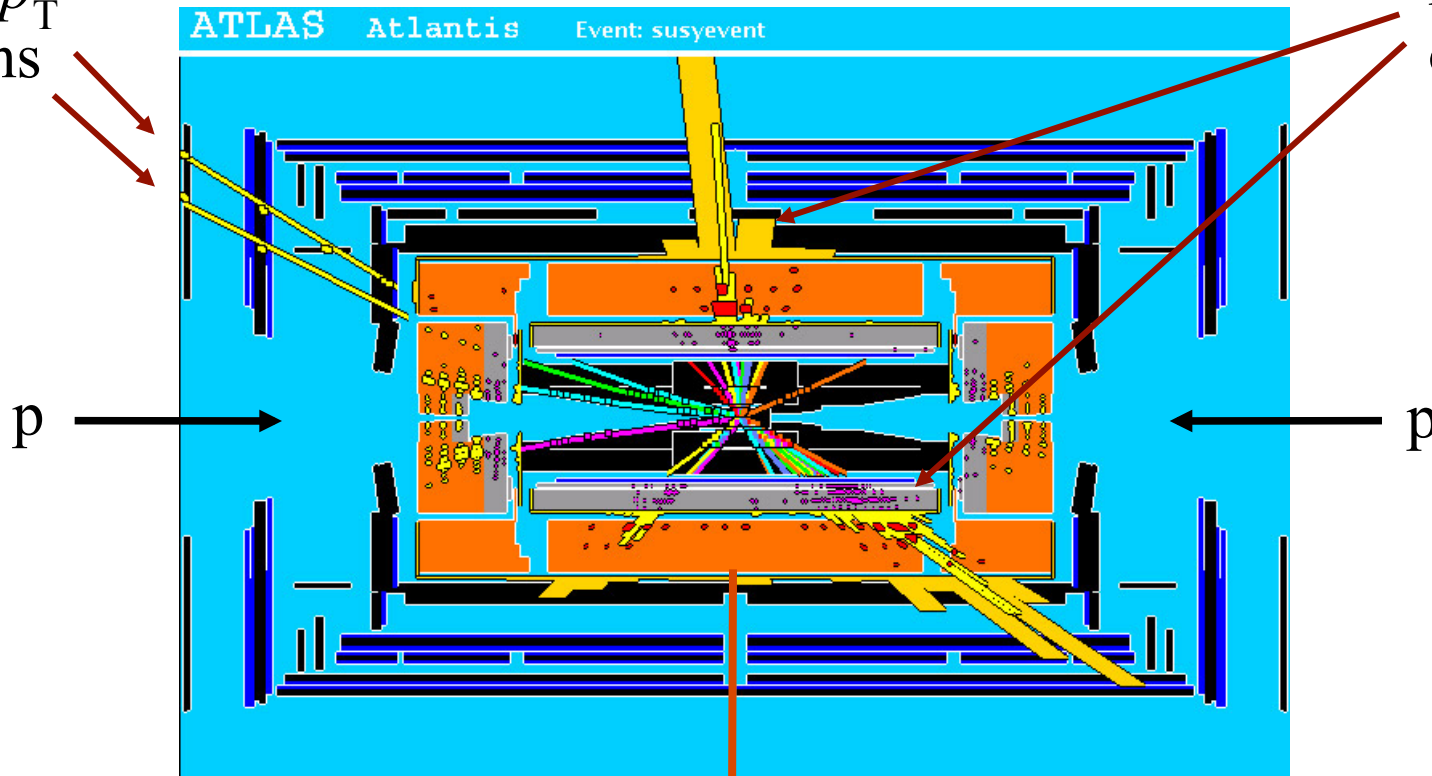
Experimental sensitivity

Revisiting limits

# A simulated SUSY event

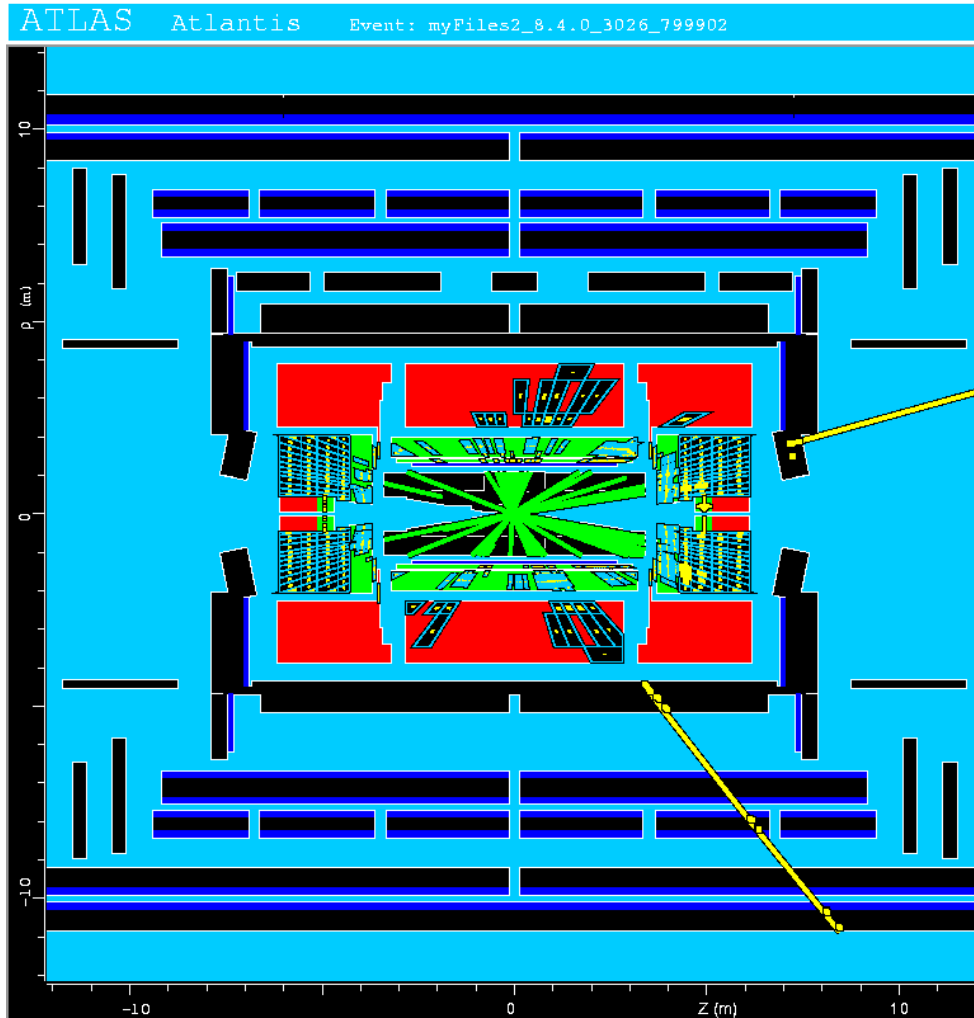
high  $p_T$   
muons

high  $p_T$  jets  
of hadrons



missing transverse energy

# Background events



This event from Standard Model  $t\bar{t}$  production also has high  $p_T$  jets and muons, and some missing transverse energy.

→ can easily mimic a SUSY event.

# Physics context of a statistical test

**Event Selection:** the event types in question are both known to exist.

Example: separation of different particle types (electron vs muon) or known event types (ttbar vs QCD multijet).

E.g. test  $H_0$  : event is background vs.  $H_1$  : event is signal.

Use selected events for further study.

**Search for New Physics:** the null hypothesis is

$H_0$  : all events correspond to Standard Model (background only),

and the alternative is

$H_1$  : events include a type whose existence is not yet established (signal plus background)

Many subtle issues here, mainly related to the high standard of proof required to establish presence of a new phenomenon. The optimal statistical test for a search is closely related to that used for event selection.

# Statistical tests for event selection

Suppose the result of a measurement for an individual event is a collection of numbers  $\vec{x} = (x_1, \dots, x_n)$

$x_1$  = number of muons,

$x_2$  = mean  $p_T$  of jets,

$x_3$  = missing energy, ...

$\vec{x}$  follows some  $n$ -dimensional joint pdf, which depends on the type of event produced, i.e., was it

$$pp \rightarrow t\bar{t}, \quad pp \rightarrow \tilde{g}\tilde{g}, \dots$$

For each reaction we consider we will have a **hypothesis** for the pdf of  $\vec{x}$ , e.g.,  $f(\vec{x}|H_0)$ ,  $f(\vec{x}|H_1)$ , etc.

E.g. call  $H_0$  the **background** hypothesis (the event type we want to reject);  $H_1$  is **signal** hypothesis (the type we want).

# Selecting events

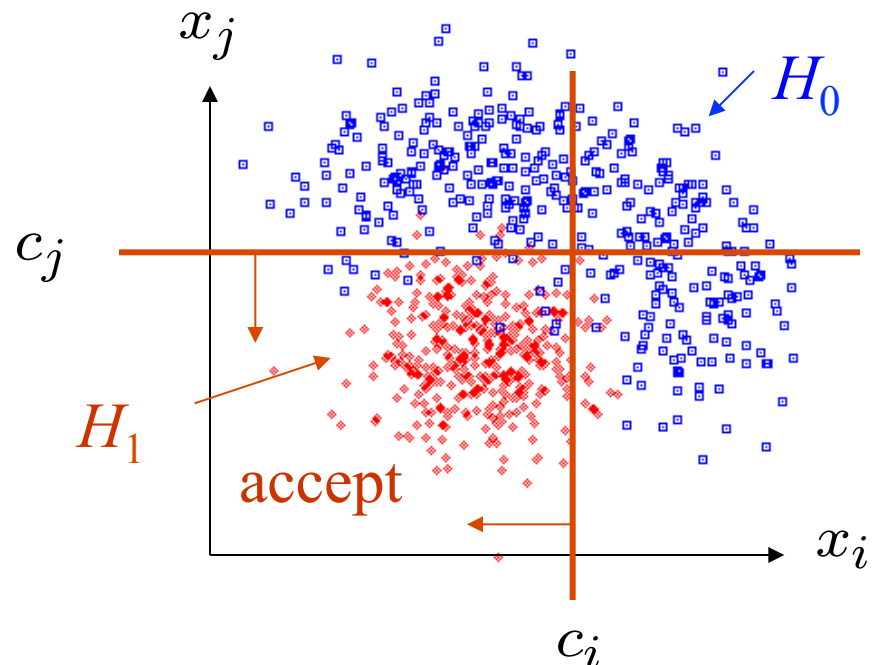
Suppose we have a data sample with two kinds of events, corresponding to hypotheses  $H_0$  and  $H_1$  and we want to select those of type  $H_1$ .

Each event is a point in  $\vec{x}$  space. What ‘decision boundary’ should we use to accept/reject events as belonging to event types  $H_0$  or  $H_1$ ?

Perhaps select events with ‘cuts’:

$$x_i < c_i$$

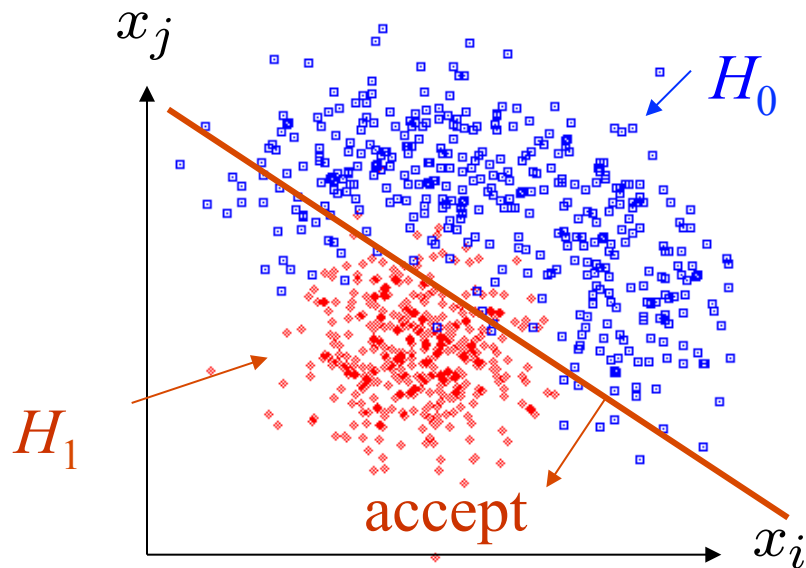
$$x_j < c_j$$



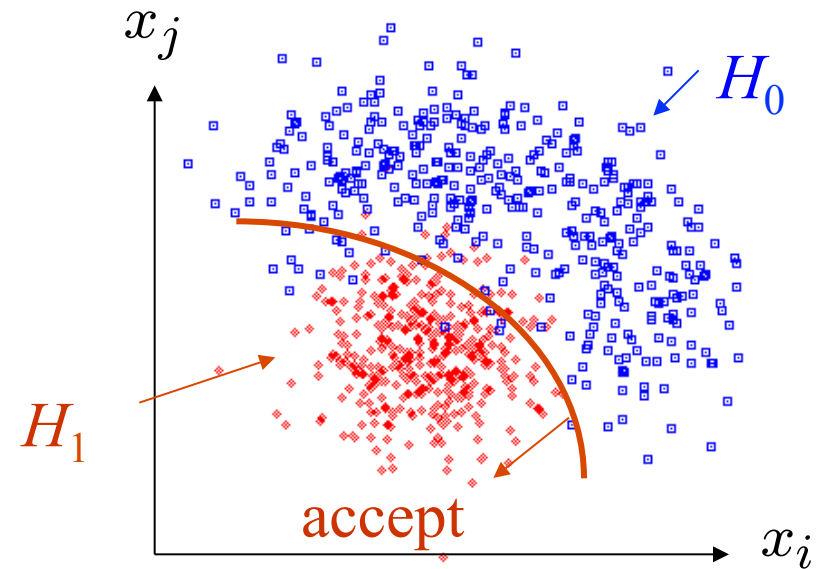
# Other ways to select events

Or maybe use some other sort of decision boundary:

linear



or nonlinear



How can we do this in an ‘optimal’ way?



# Test statistics

The boundary of the critical region for an  $n$ -dimensional data space  $\mathbf{x} = (x_1, \dots, x_n)$  can be defined by an equation of the form

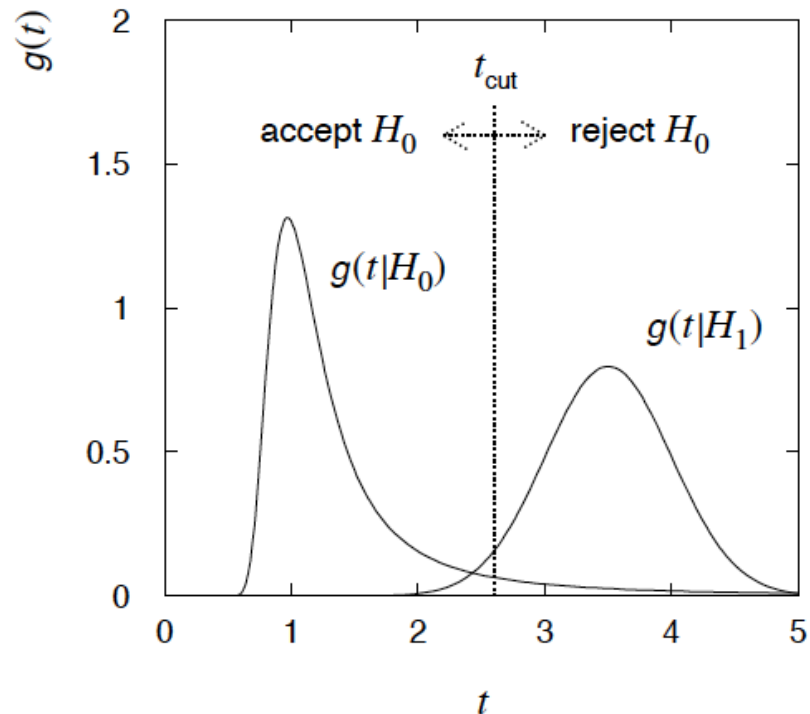
$$t(x_1, \dots, x_n) = t_{\text{cut}}$$

where  $t(x_1, \dots, x_n)$  is a scalar **test statistic**.

We can work out the pdfs  $g(t|H_0)$ ,  $g(t|H_1)$ ,  $\dots$

Decision boundary is now a single ‘cut’ on  $t$ , defining the critical region.

So for an  $n$ -dimensional problem we have a corresponding 1-d problem.



# Test statistic based on likelihood ratio

How can we choose a test's critical region in an 'optimal way'?

Neyman-Pearson lemma states:

To get the highest power for a given significance level in a test of  $H_0$ , (background) versus  $H_1$ , (signal) the critical region should have

$$\frac{f(\mathbf{x}|H_1)}{f(\mathbf{x}|H_0)} > c$$

inside the region, and  $\leq c$  outside, where  $c$  is a constant chosen to give a test of the desired size.

Equivalently, optimal scalar test statistic is

$$t(\mathbf{x}) = \frac{f(\mathbf{x}|H_1)}{f(\mathbf{x}|H_0)}$$

N.B. any monotonic function of this is leads to the same test.

# Classification viewed as a statistical test

Probability to reject  $H_0$  if true (type I error):  $\alpha = \int_W f(\mathbf{x}|H_0) d\mathbf{x}$

$\alpha =$  size of test, significance level, false discovery rate

Probability to accept  $H_0$  if  $H_1$  true (type II error)  $\beta = \int_{\bar{W}} f(\mathbf{x}|H_1) d\mathbf{x}$

$1 - \beta =$  power of test with respect to  $H_1$

Equivalently if e.g.  $H_0 =$  background event,  $H_1 =$  signal event, use efficiencies:

$$\varepsilon_b = P(\mathbf{x} \in W|b) = \int_W f(\mathbf{x}|H_0) d\mathbf{x} = \alpha$$

$$\varepsilon_s = P(\mathbf{x} \in W|s) = \int_W f(\mathbf{x}|H_1) d\mathbf{x} = 1 - \beta = \text{power}$$

# Purity / misclassification rate

Consider the probability that an event of signal ( $s$ ) type classified correctly (i.e., the event selection purity),

Use Bayes' theorem:

Here  $W$  is signal region

$$P(s|\mathbf{x} \in W) = \frac{P(\mathbf{x} \in W|s)P(s)}{P(\mathbf{x} \in W|s)P(s) + P(\mathbf{x} \in W|b)P(b)}$$

posterior probability = signal purity  
= 1 – signal misclassification rate

Note purity depends on the prior probability for an event to be signal or background as well as on s/b efficiencies.

# Neyman-Pearson doesn't usually help

We usually don't have explicit formulae for the pdfs  $f(\mathbf{x}|s)$ ,  $f(\mathbf{x}|b)$ , so for a given  $\mathbf{x}$  we can't evaluate the likelihood ratio

$$t(\mathbf{x}) = \frac{f(\mathbf{x}|s)}{f(\mathbf{x}|b)}$$

Instead we may have Monte Carlo models for signal and background processes, so we can produce simulated data:

generate  $\mathbf{x} \sim f(\mathbf{x}|s)$   $\rightarrow$   $\mathbf{x}_1, \dots, \mathbf{x}_N$

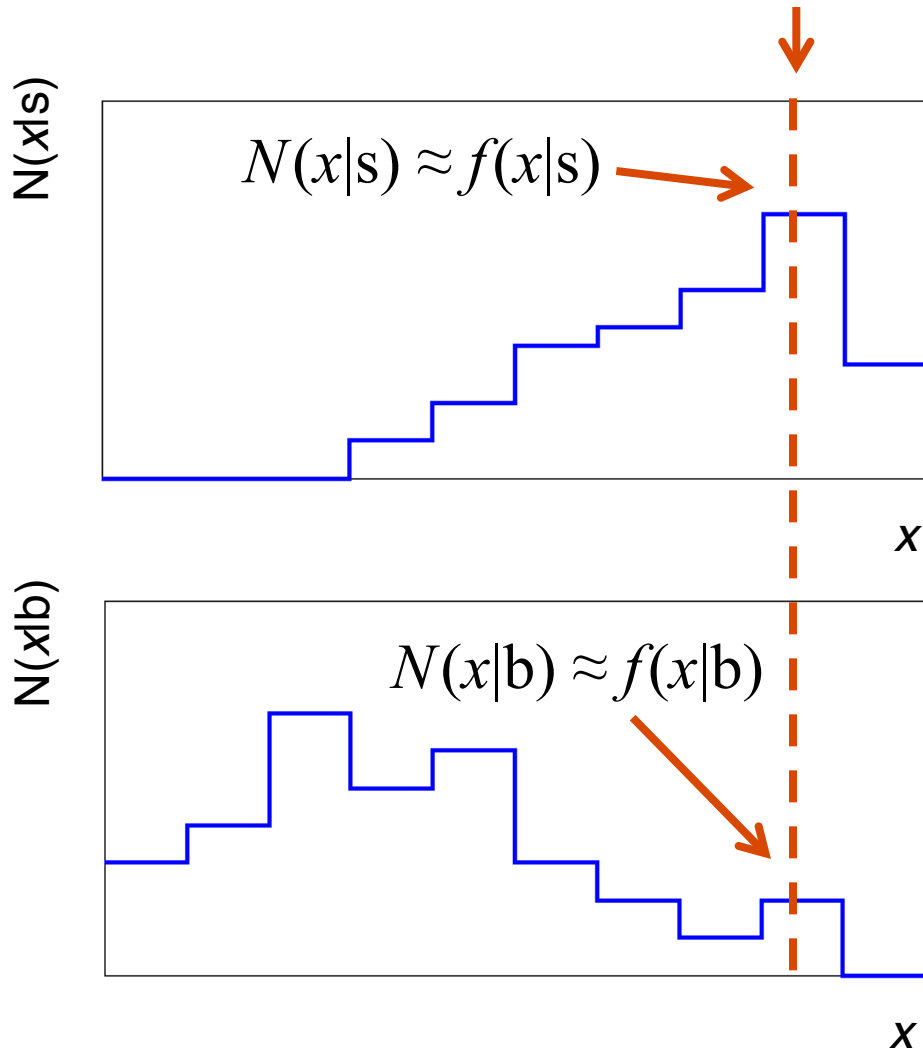
generate  $\mathbf{x} \sim f(\mathbf{x}|b)$   $\rightarrow$   $\mathbf{x}_1, \dots, \mathbf{x}_N$

This gives samples of “training data” with events of known type.

Can be expensive (1 fully simulated LHC event  $\sim$  1 CPU minute).

# Approximate LR from histograms

Want  $t(x) = f(x|s)/f(x|b)$  for  $x$  here



One possibility is to generate MC data and construct histograms for both signal and background.

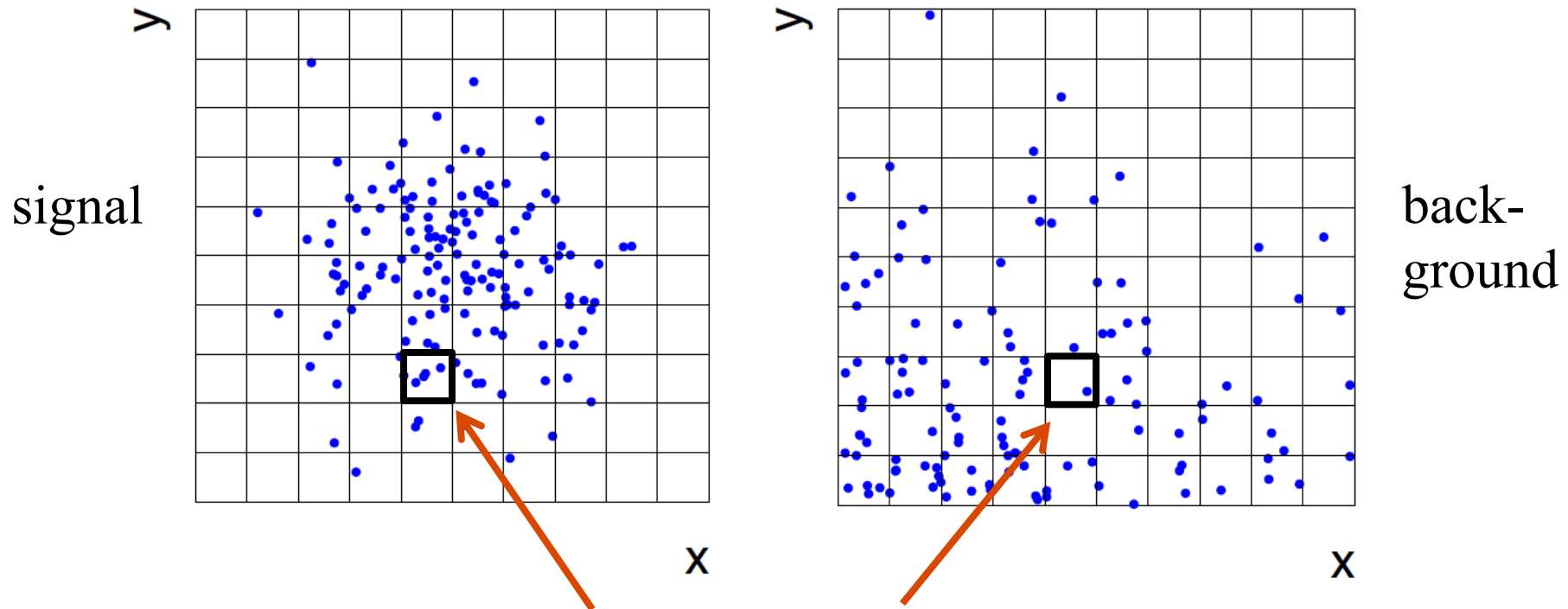
Use (normalized) histogram values to approximate LR:

$$t(x) \approx \frac{N(x|s)}{N(x|b)}$$

Can work well for single variable.

# Approximate LR from 2D-histograms

Suppose problem has 2 variables. Try using 2-D histograms:



Approximate pdfs using  $N(x,y|s)$ ,  $N(x,y|b)$  in corresponding cells.

But if we want  $M$  bins for each variable, then in  $n$ -dimensions we have  $M^n$  cells; can't generate enough training data to populate.

→ Histogram method usually not usable for  $n > 1$  dimension.

# Strategies for multivariate analysis

Neyman-Pearson lemma gives optimal answer, but cannot be used directly, because we usually don't have  $f(\mathbf{x}|\mathbf{s})$ ,  $f(\mathbf{x}|\mathbf{b})$ .

Histogram method with  $M$  bins for  $n$  variables requires that we estimate  $M^n$  parameters (the values of the pdfs in each cell), so this is rarely practical.

A compromise solution is to assume a certain functional form for the test statistic  $t(\mathbf{x})$  with fewer parameters; determine them (using MC) to give best separation between signal and background.

Alternatively, try to estimate the probability densities  $f(\mathbf{x}|\mathbf{s})$  and  $f(\mathbf{x}|\mathbf{b})$  (with something better than histograms) and use the estimated pdfs to construct an approximate likelihood ratio.



# Multivariate methods

Many new (and some old) methods:

Fisher discriminant

(Deep) neural networks

Kernel density methods

Support Vector Machines

Decision trees

    Boosting

    Bagging

# Resources on multivariate methods

C.M. Bishop, Pattern Recognition and Machine Learning, Springer, 2006

T. Hastie, R. Tibshirani, J. Friedman, The Elements of Statistical Learning, 2<sup>nd</sup> ed., Springer, 2009

R. Duda, P. Hart, D. Stork, Pattern Classification, 2<sup>nd</sup> ed., Wiley, 2001

A. Webb, Statistical Pattern Recognition, 2<sup>nd</sup> ed., Wiley, 2002.

Ilya Narsky and Frank C. Porter, *Statistical Analysis Techniques in Particle Physics*, Wiley, 2014.

朱永生 (编著), 实验数据多元统计分析, 科学出版社, 北京, 2009。

# Software

Rapidly growing area of development – two important resources:

**TMVA**, Höcker, Stelzer, Tegenfeldt, Voss, Voss, physics/0703039

From `tmva.sourceforge.net`, also distributed with ROOT

Variety of classifiers

Good manual, widely used in HEP

**scikit-learn**

Python-based tools for Machine Learning

`scikit-learn.org`

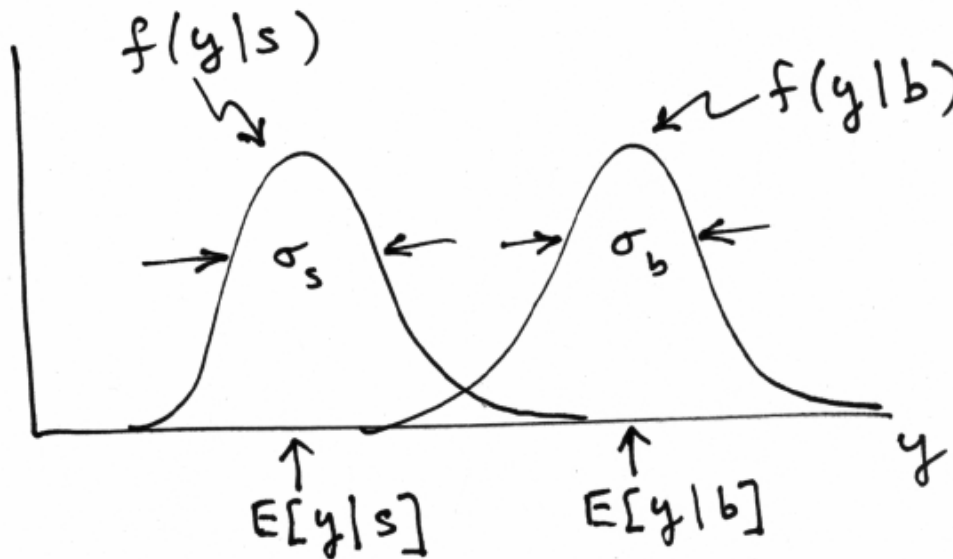
Large user community

# Linear test statistic

Suppose there are  $n$  input variables:  $\mathbf{x} = (x_1, \dots, x_n)$ .

Consider a linear function: 
$$y(\mathbf{x}) = \sum_{i=1}^n w_i x_i$$

For a given choice of the coefficients  $\mathbf{w} = (w_1, \dots, w_n)$  we will get pdfs  $f(y|s)$  and  $f(y|b)$  :



# Linear test statistic

Fisher: to get large difference between means and small widths for  $f(y|s)$  and  $f(y|b)$ , maximize the difference squared of the expectation values divided by the sum of the variances:

$$J(\mathbf{w}) = \frac{(E[y|s] - E[y|b])^2}{V[y|s] + V[y|b]}$$

Setting  $\partial J / \partial w_i = 0$  gives:

$$\mathbf{w} \propto W^{-1}(\boldsymbol{\mu}_b - \boldsymbol{\mu}_s)$$

$$W_{ij} = \text{cov}[x_i, x_j|s] + \text{cov}[x_i, x_j|b]$$

$$\mu_{i,s} = E[x_i|s], \quad \mu_{i,b} = E[x_i|b]$$

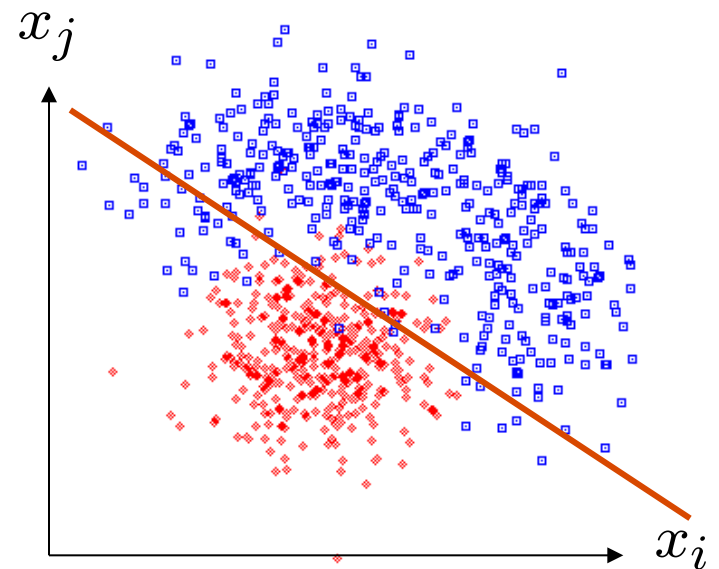
# The Fisher discriminant

The resulting coefficients  $w_i$  define a Fisher discriminant.

Coefficients defined up to multiplicative constant; can also add arbitrary offset, i.e., usually define test statistic as

$$y(\mathbf{x}) = w_0 + \sum_{i=1}^n w_i x_i$$

Boundaries of the test's critical region are surfaces of constant  $y(\mathbf{x})$ , here linear (hyperplanes):



# Fisher discriminant for Gaussian data

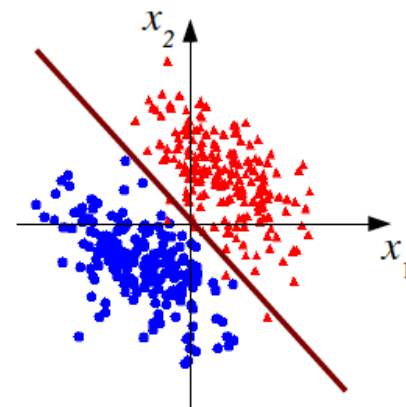
Suppose the pdfs of the input variables,  $f(\mathbf{x}|\mathbf{s})$  and  $f(\mathbf{x}|\mathbf{b})$ , are both multivariate Gaussians with same covariance but different means:

$$f(\mathbf{x}|\mathbf{s}) = \text{Gauss}(\boldsymbol{\mu}_s, V)$$

$$f(\mathbf{x}|\mathbf{b}) = \text{Gauss}(\boldsymbol{\mu}_b, V)$$

← Same covariance

$$V_{ij} = \text{cov}[x_i, x_j]$$



In this case it can be shown that the Fisher discriminant is

$$y(\mathbf{x}) \sim \ln \frac{f(\mathbf{x}|\mathbf{s})}{f(\mathbf{x}|\mathbf{b})}$$

i.e., it is a monotonic function of the likelihood ratio and thus leads to the same critical region. So in this case the Fisher discriminant provides an optimal statistical test.

# Transformation of inputs

If the data are not Gaussian with equal covariance, a linear decision boundary is not optimal. But we can try to subject the data to a transformation

$$\phi_1(\vec{x}), \dots, \phi_m(\vec{x})$$

and then treat the  $\phi_i$  as the new input variables. This is often called “feature space” and the  $\phi_i$  are “basis functions”. The basis functions can be fixed or can contain adjustable parameters which we optimize with training data (cf. neural networks).

In other cases we will see that the basis functions only enter as dot products

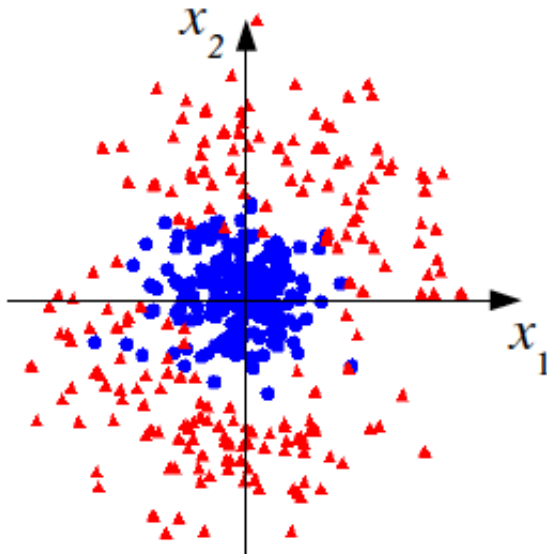
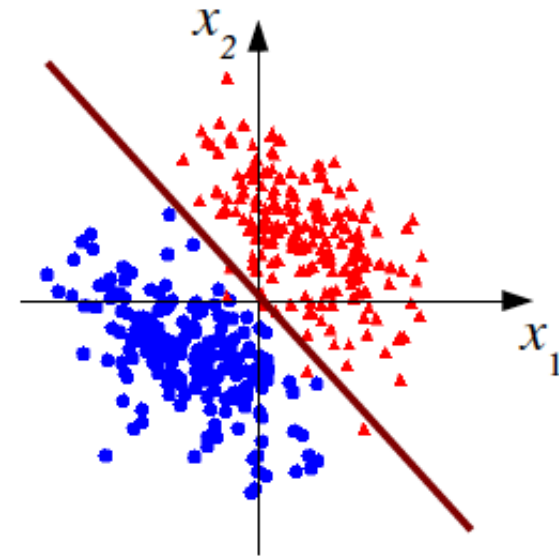
$$\vec{\phi}(\vec{x}_i) \cdot \vec{\phi}(\vec{x}_j) = K(\vec{x}_i, \vec{x}_j)$$

and thus we will only need the “kernel function”  $K(\mathbf{x}_i, \mathbf{x}_j)$



# Linear decision boundaries

A linear decision boundary is only optimal when both classes follow multivariate Gaussians with equal covariances and different means.



For some other cases a linear boundary is almost useless.

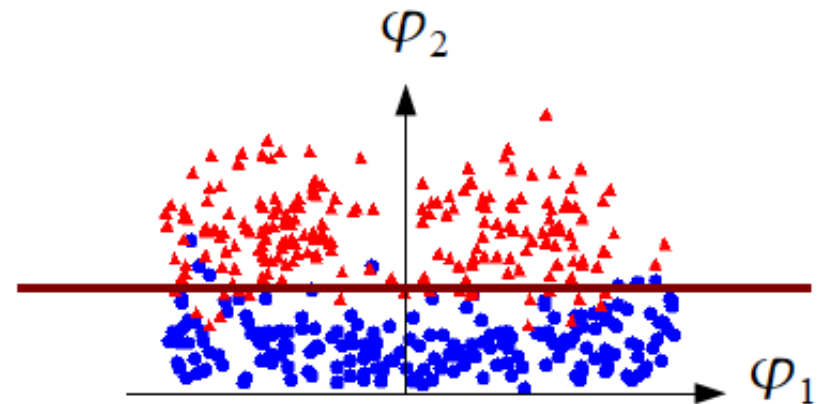
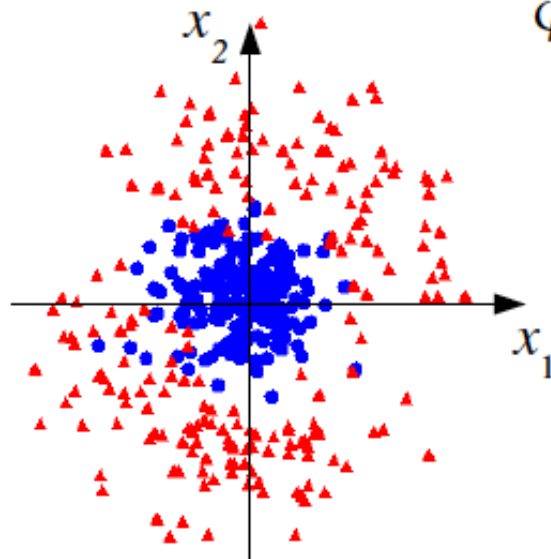
# Nonlinear transformation of inputs

We can try to find a transformation,  $x_1, \dots, x_n \rightarrow \varphi_1(\vec{x}), \dots, \varphi_m(\vec{x})$  so that the transformed “feature space” variables can be separated better by a linear boundary:

$$\varphi_1 = \tan^{-1}(x_2/x_1)$$

$$\varphi_2 = \sqrt{x_1^2 + x_2^2}$$

Here, guess fixed basis functions (no free parameters)



# Neural networks

Neural networks originate from attempts to model neural processes (McCulloch and Pitts, 1943; Rosenblatt, 1962).

Widely used in many fields, and for many years the only “advanced” multivariate method popular in HEP.

We can view a neural network as a specific way of parametrizing the basis functions used to define the feature space transformation.

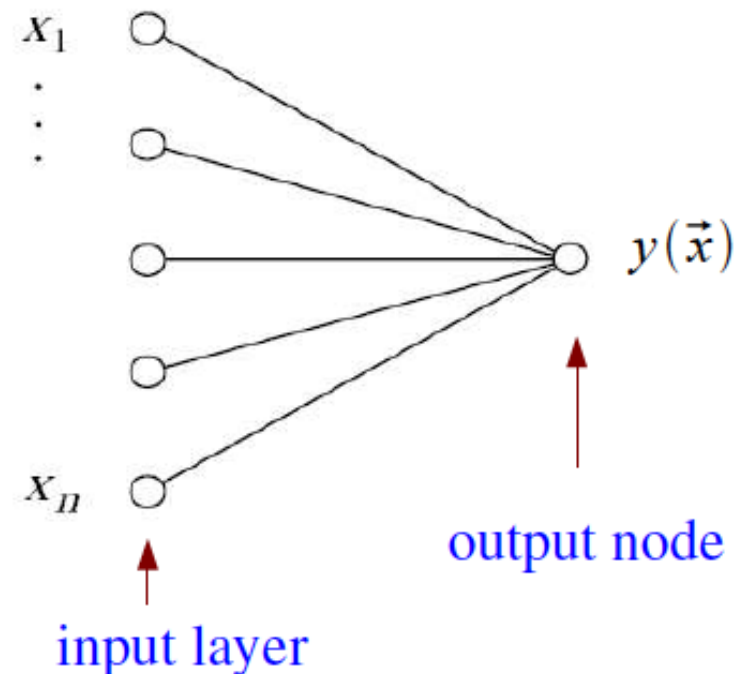
The training data are then used to adjust the parameters so that the resulting discriminant function has the best performance.

# The single layer perceptron

Define the discriminant using  $y(\vec{x}) = h\left(w_0 + \sum_{i=1}^n w_i x_i\right)$

where  $h$  is a nonlinear, monotonic **activation function**; we can use e.g. the logistic sigmoid  $h(x) = (1 + e^{-x})^{-1}$ .

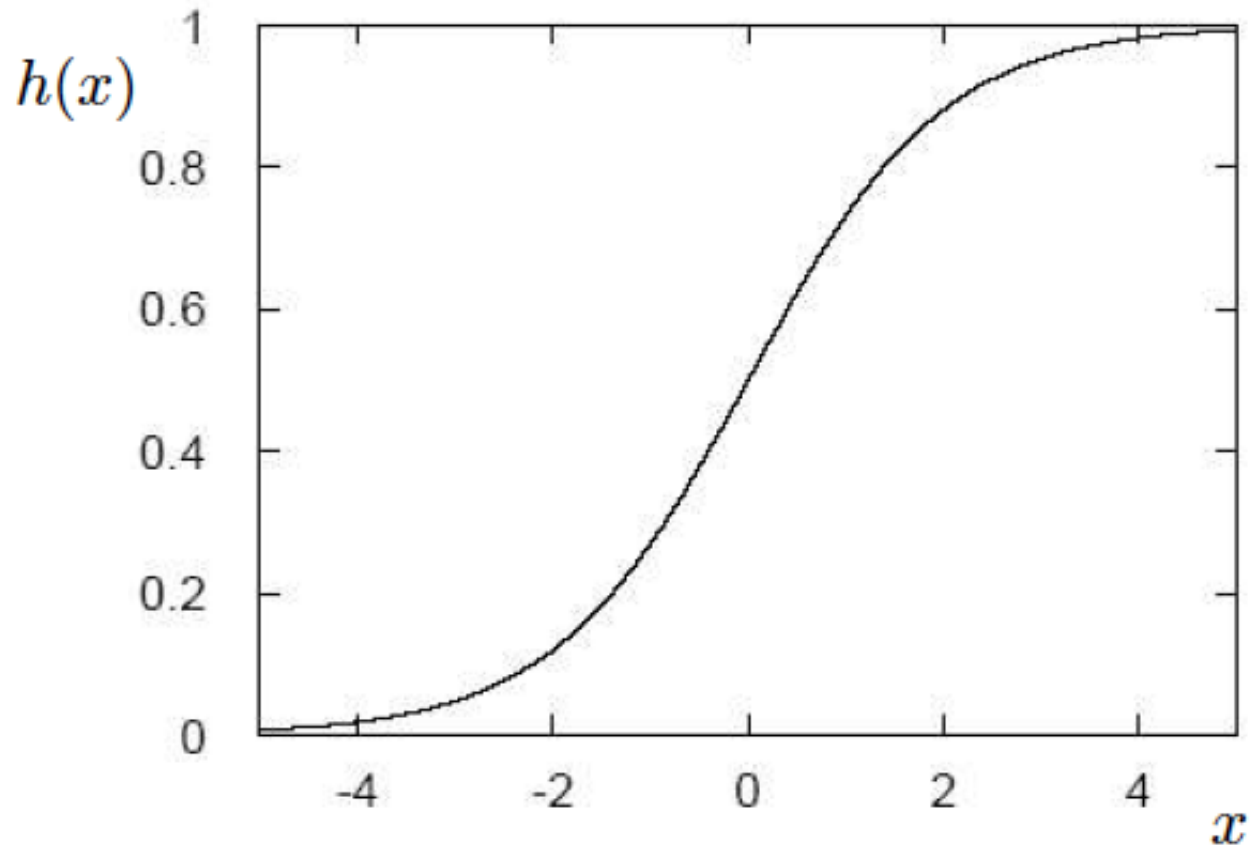
If the activation function is monotonic, the resulting  $y(\mathbf{x})$  is equivalent to the original linear discriminant. This is an example of a “generalized linear model” called the **single layer perceptron**.



# The activation function

For activation function  $h(\cdot)$  often use logistic sigmoid:

$$h(x) = \frac{1}{1 + e^{-x}}$$



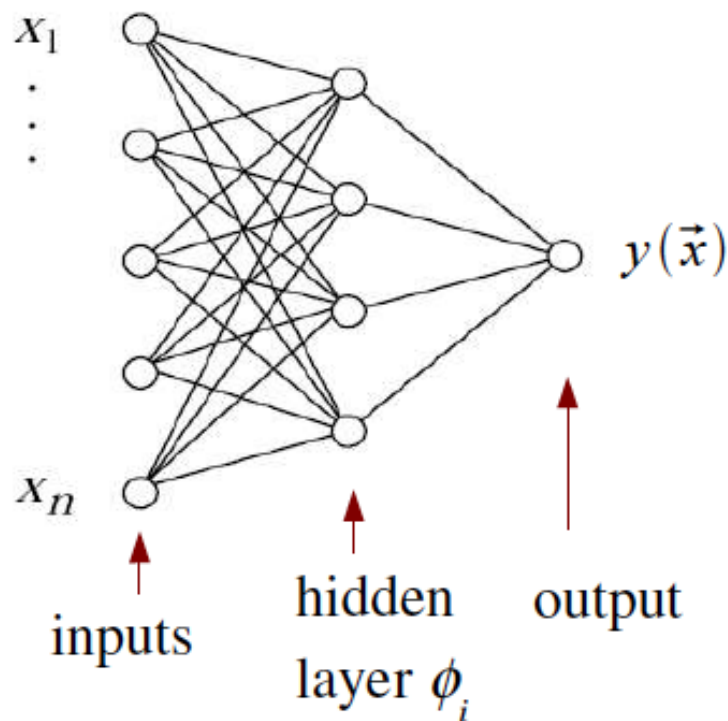
# The multilayer perceptron

Now use this idea to define not only the output  $y(\mathbf{x})$ , but also the set of transformed inputs  $\varphi_1(\vec{x}), \dots, \varphi_m(\vec{x})$  that form a “hidden layer”:

Superscript for weights indicates layer number

$$\varphi_i(\vec{x}) = h\left(w_{i0}^{(1)} + \sum_{j=1}^n w_{ij}^{(1)} x_j\right)$$

$$y(\vec{x}) = h\left(w_{10}^{(2)} + \sum_{j=1}^m w_{1j}^{(2)} \varphi_j(\vec{x})\right)$$



This is the **multilayer perceptron**, our basic neural network model; straightforward to generalize to multiple hidden layers.

# Network training

The type of each training event is known, i.e., for event  $a$  we have:

$$\begin{aligned} \vec{x}_a &= (x_1, \dots, x_n) && \text{the input variables, and} \\ t_a &= 0, 1 && \text{a numerical label for event type (“target value”)} \end{aligned}$$

Let  $\mathbf{w}$  denote the set of all of the weights of the network. We can determine their optimal values by minimizing a sum-of-squares “error function”

$$E(\mathbf{w}) = \frac{1}{2} \sum_{a=1}^N |y(\vec{x}_a, \mathbf{w}) - t_a|^2 = \sum_{a=1}^N E_a(\mathbf{w})$$




Contribution to error function  
from each event

# Numerical minimization of $E(\mathbf{w})$

Consider gradient descent method: from an initial guess in weight space  $\mathbf{w}^{(1)}$  take a small step in the direction of maximum decrease.

I.e. for the step  $\tau$  to  $\tau+1$ ,

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E(\mathbf{w}^{(\tau)})$$

 learning rate ( $\eta > 0$ )

If we do this with the full error function  $E(\mathbf{w})$ , gradient descent does surprisingly poorly; better to use “conjugate gradients”.

But gradient descent turns out to be useful with an online (sequential) method, i.e., where we update  $\mathbf{w}$  for each training event  $a$ , (cycle through all training events):

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_a(\mathbf{w}^{(\tau)})$$



# Error backpropagation

Error backpropagation (“backprop”) is an algorithm for finding the derivatives required for gradient descent minimization.


The network output can be written  $y(\mathbf{x}) = h(u(\mathbf{x}))$  where

$$u(\vec{x}) = \sum_{j=0} w_{1j}^{(2)} \varphi_j(\vec{x}), \quad \varphi_j(\vec{x}) = h\left(\sum_{k=0} w_{jk}^{(1)} x_k\right)$$

where we defined  $\phi_0 = x_0 = 1$  and wrote the sums over the nodes in the preceding layers starting from 0 to include the offsets.

So e.g. for event  $a$  we have  $\frac{\partial E_a}{\partial w_{1j}^{(2)}} = (y_a - t_a) h'(u(\vec{x})) \varphi_j(\vec{x})$

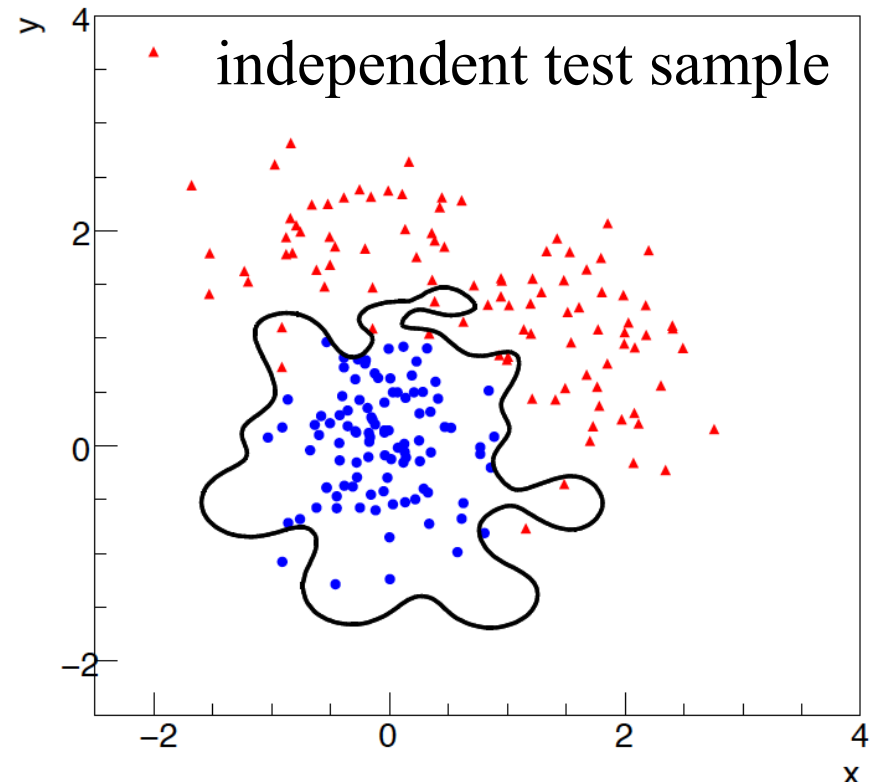
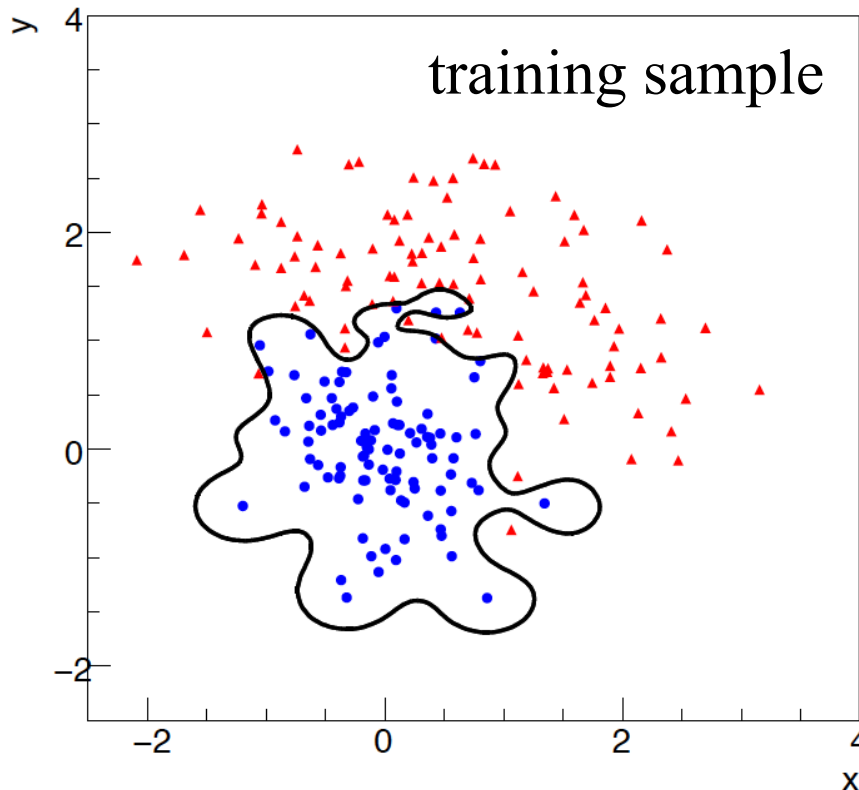
Chain rule gives all the needed derivatives.

 derivative of  
activation function

# Overtraining

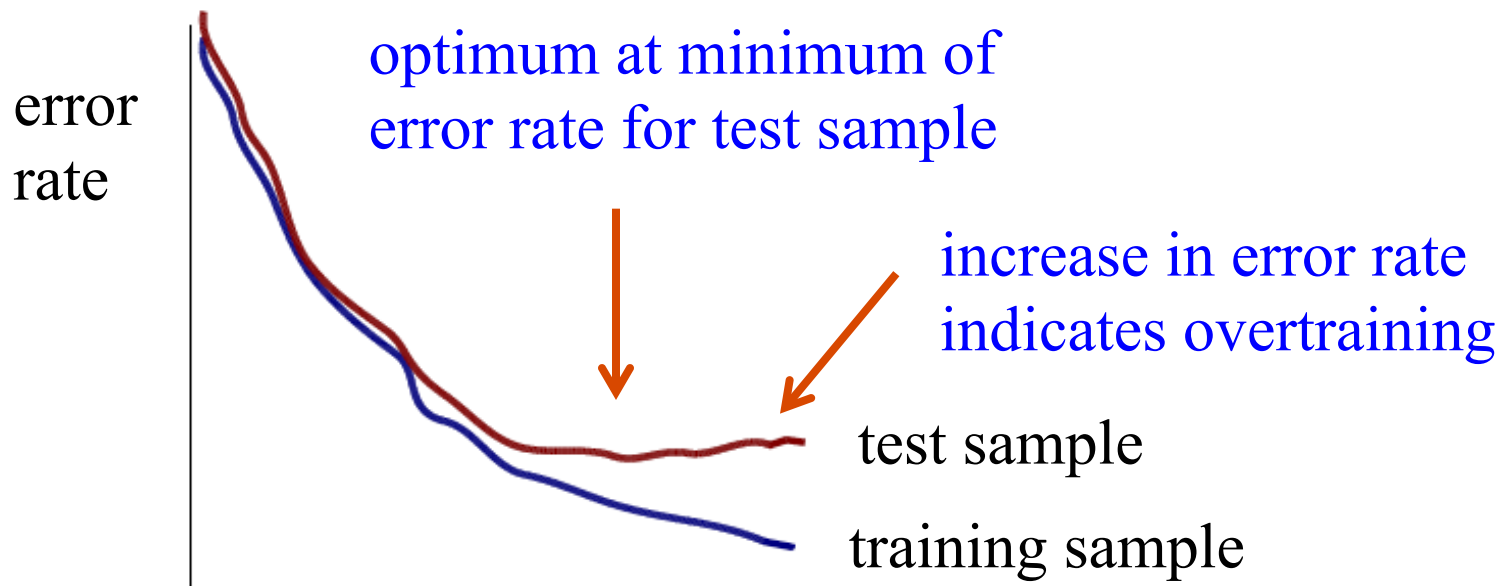
Including more parameters in a classifier makes its decision boundary increasingly flexible, e.g., more nodes/layers for a neural network.

A “flexible” classifier may conform too closely to the training points; the same boundary will not perform well on an independent test data sample (→ “overtraining”).



# Monitoring overtraining

If we monitor the fraction of misclassified events (or similar, e.g., error function  $E(\boldsymbol{w})$ ) for test and training samples, it will usually decrease for both as the boundary is made more flexible:

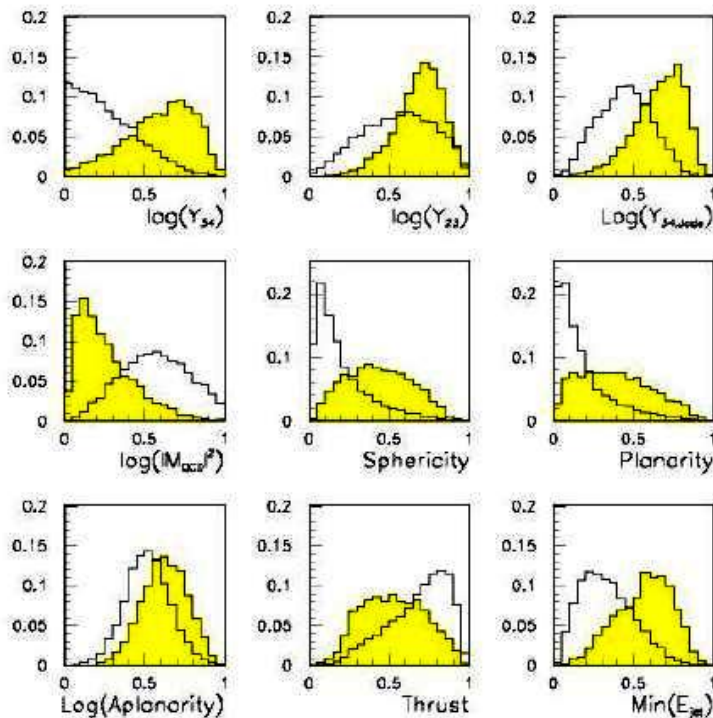


flexibility (e.g., number of nodes/layers in MLP)

# Neural network example from LEP II

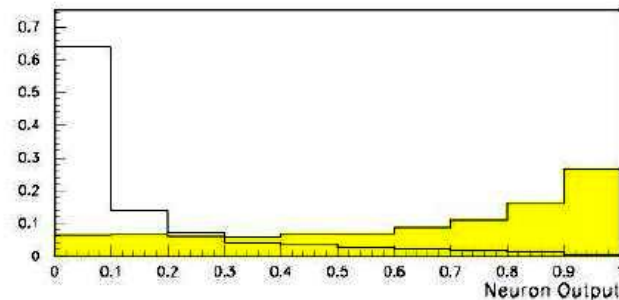
Signal:  $e^+e^- \rightarrow W^+W^-$  (often 4 well separated hadron jets)

Background:  $e^+e^- \rightarrow q\bar{q}g$  (4 less well separated hadron jets)



← input variables based on jet structure, event shape, ...  
none by itself gives much separation.

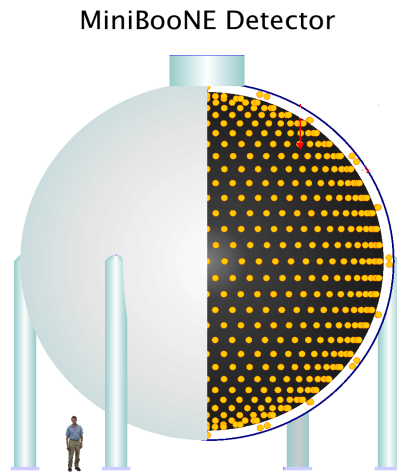
Neural network output:



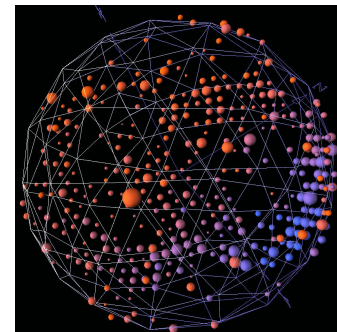
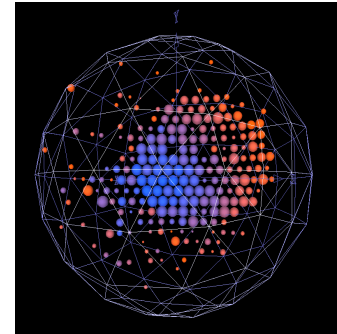
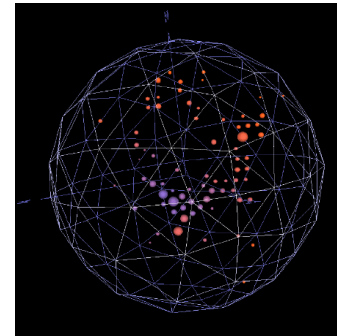
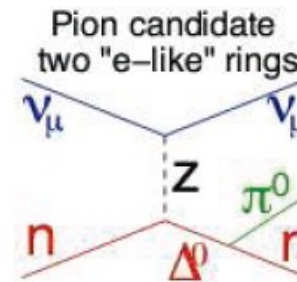
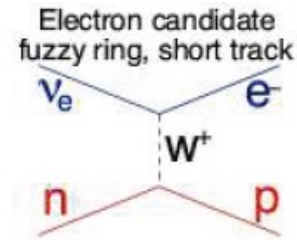
(Garrido, Juste and Martinez, ALEPH 96-144)

# Particle i.d. in MiniBooNE

Detector is a 12-m diameter tank of mineral oil exposed to a beam of neutrinos and viewed by 1520 photomultiplier tubes:



Search for  $n_m$  to  $n_e$  oscillations required particle i.d. using information from the PMTs.



H.J. Yang, MiniBooNE PID, DNP06

# Decision trees

Out of all the input variables, find the one for which with a single cut gives best improvement in signal purity:

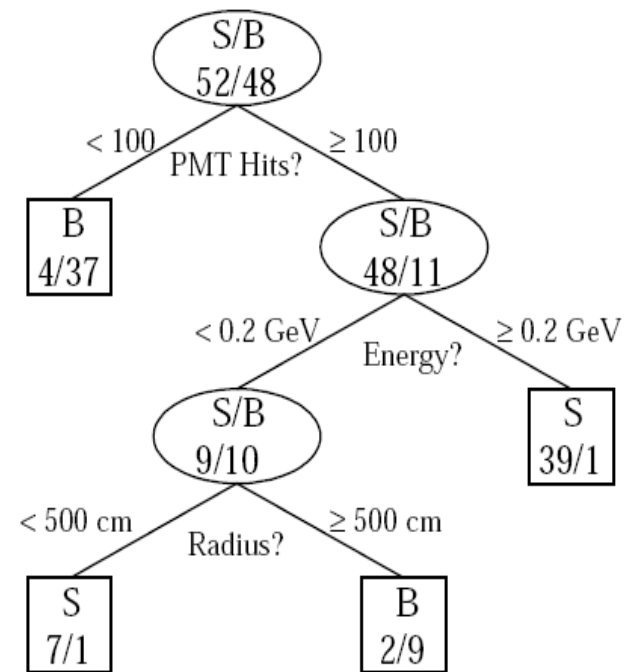
$$P = \frac{\sum_{\text{signal}} w_i}{\sum_{\text{signal}} w_i + \sum_{\text{background}} w_i}$$

where  $w_i$  is the weight of the  $i$ th event.

Resulting nodes classified as either signal/background.

Iterate until stop criterion reached based on e.g. purity or minimum number of events in a node.

The set of cuts defines the decision boundary.



Example by MiniBooNE experiment, B. Roe et al., NIM 543 (2005) 577

# Finding the best single cut

The level of separation within a node can, e.g., be quantified by the *Gini coefficient*, calculated from the (s or b) purity as:

$$G = p(1 - p)$$

For a cut that splits a set of events  $a$  into subsets  $b$  and  $c$ , one can quantify the improvement in separation by the change in weighted Gini coefficients:

$$\Delta = W_a G_a - W_b G_b - W_c G_c \quad \text{where, e.g.,} \quad W_a = \sum_{i \in a} w_i$$

Choose e.g. the cut to maximize  $\Delta$ ; a variant of this scheme can use instead of Gini e.g. the misclassification rate:

$$\varepsilon = 1 - \max(p, 1 - p)$$

## Decision trees (2)

The terminal nodes (**leaves**) are classified a signal or background depending on majority vote (or e.g. signal fraction greater than a specified threshold).

This classifies every point in input-variable space as either signal or background, a **decision tree classifier**, with discriminant function

$$f(\mathbf{x}) = 1 \text{ if } \mathbf{x} \text{ in signal region, } -1 \text{ otherwise}$$

Decision trees tend to be very sensitive to statistical fluctuations in the training sample.

Methods such as **boosting** can be used to stabilize the tree.



# Boosting

Boosting is a general method of creating a set of classifiers which can be combined to achieve a new classifier that is more stable and has a smaller error than any individual one.

Often applied to decision trees but, can be applied to any classifier.

Suppose we have a training sample  $T$  consisting of  $N$  events with

$\mathbf{x}_1, \dots, \mathbf{x}_N$	event data vectors (each $\mathbf{x}$ multivariate)
$y_1, \dots, y_N$	true class labels, +1 for signal, -1 for background
$w_1, \dots, w_N$	event weights

Now define a rule to create from this an ensemble of training samples  $T_1, T_2, \dots$ , derive a classifier from each and average them.

Trick is to create modifications in the training sample that give classifiers with smaller error rates than those of the preceding ones.

A successful example is **AdaBoost** (Freund and Schapire, 1997).

# AdaBoost

First initialize the training sample  $T_1$  using the original

$\mathbf{x}_1, \dots, \mathbf{x}_N$  event data vectors

$y_1, \dots, y_N$  true class labels (+1 or -1)

$w_1^{(1)}, \dots, w_N^{(1)}$  event weights

with the weights equal and normalized such that

$$\sum_{i=1}^N w_i^{(1)} = 1$$

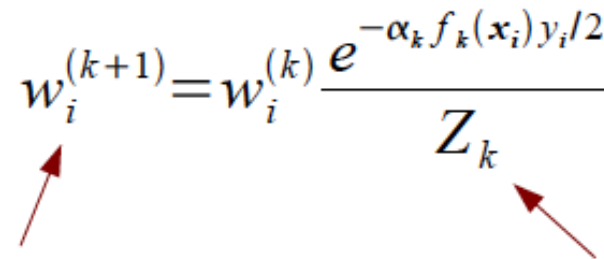
Then train the classifier  $f_1(\mathbf{x})$  (e.g. a decision tree) with a method that incorporates the event weights. For an event with data  $\mathbf{x}_i$ ,

$f_1(\mathbf{x}_i) > 0$  classify as signal

$f_1(\mathbf{x}_i) < 0$  classify as background

# Updating the event weights

Define the training sample for step  $k+1$  from that of  $k$  by updating the event weights according to

$$w_i^{(k+1)} = w_i^{(k)} \frac{e^{-\alpha_k f_k(x_i) y_i / 2}}{Z_k}$$


$i$  = event index

$k$  = training sample index

where  $Z_k$  is a normalization factor defined such that the sum of the weights over all events is equal to one.

Therefore event weight for event  $i$  is **increased** in the  $k+1$  training sample if it was classified **incorrectly** in sample  $k$ .

Idea is that next time around the classifier should pay more attention to this event and try to get it right.

# Error rate of the $k$ th classifier

At each step the classifiers  $f_k(\mathbf{x})$  are defined so as to minimize the error rate  $\varepsilon_k$ ,

$$\varepsilon_k = \sum_{i=1}^N w_i^{(k)} I(y_i f_k(\mathbf{x}_i) \leq 0)$$

where  $I(X) = 1$  if  $X$  is true and is zero otherwise.

# Assigning the classifier score

Assign a score to the  $k$ th classifier based on its error rate,

$$\alpha_k = \ln \frac{1 - \varepsilon_k}{\varepsilon_k}$$

If we define the final classifier as  $f(\mathbf{x}) = \sum_{k=1}^K \alpha_k f_k(\mathbf{x}, T_k)$

then one can show that its error rate on the training data satisfies the bound

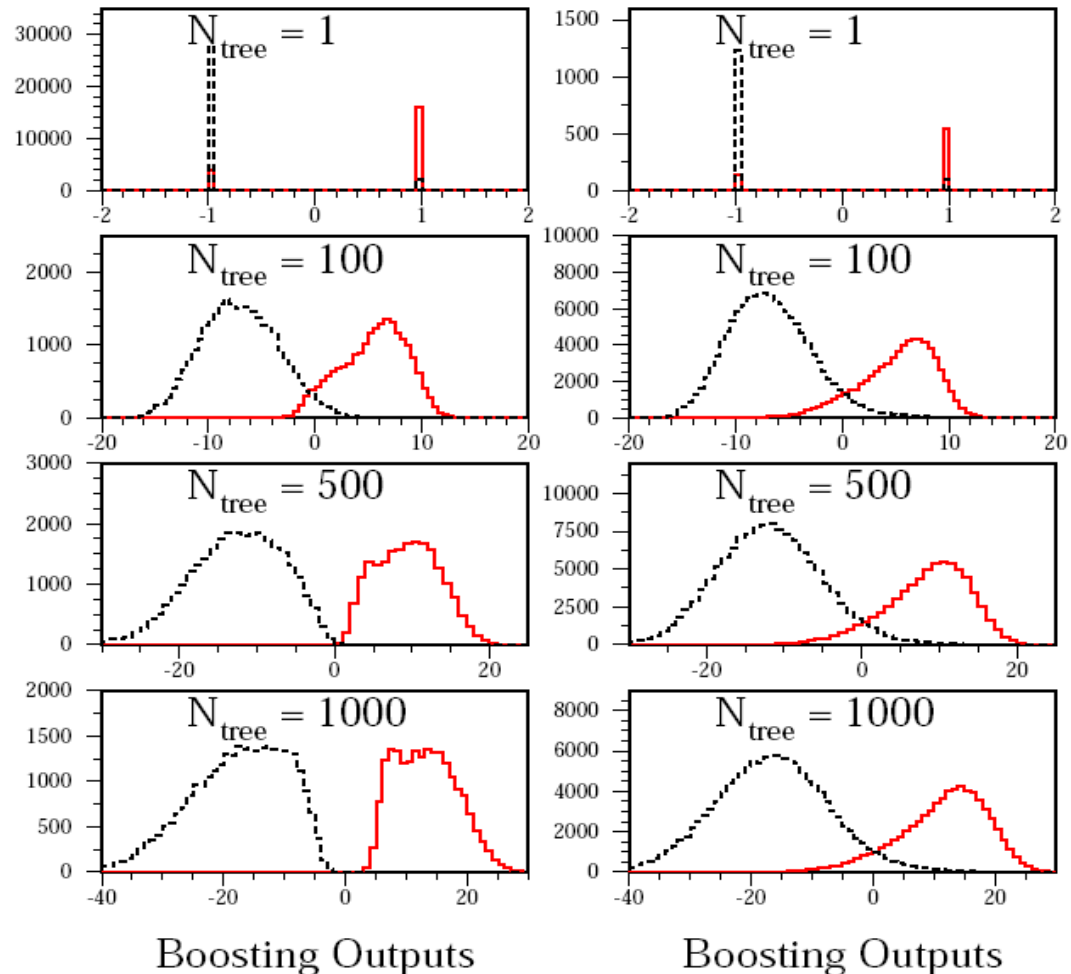
$$\varepsilon \leq \prod_{k=1}^K 2 \sqrt{\varepsilon_k (1 - \varepsilon_k)}$$

# Monitoring overtraining

From MiniBooNE  
example:

Performance stable  
after a few hundred  
trees.

Training MC Samples .VS. Testing MC Samples



# Summary on multivariate methods

Particle physics has used several multivariate methods for many years:

- linear (Fisher) discriminant
- neural networks
- naive Bayes

and has in recent years started to use a few more:

- boosted decision trees
- support vector machines
- kernel density estimation
- $k$ -nearest neighbour

The emphasis is often on controlling systematic uncertainties between the modeled training data and Nature to avoid false discovery.

Although many classifier outputs are "black boxes", a discovery at  $5\sigma$  significance with a sophisticated (opaque) method will win the competition if backed up by, say,  $4\sigma$  evidence from a cut-based method.