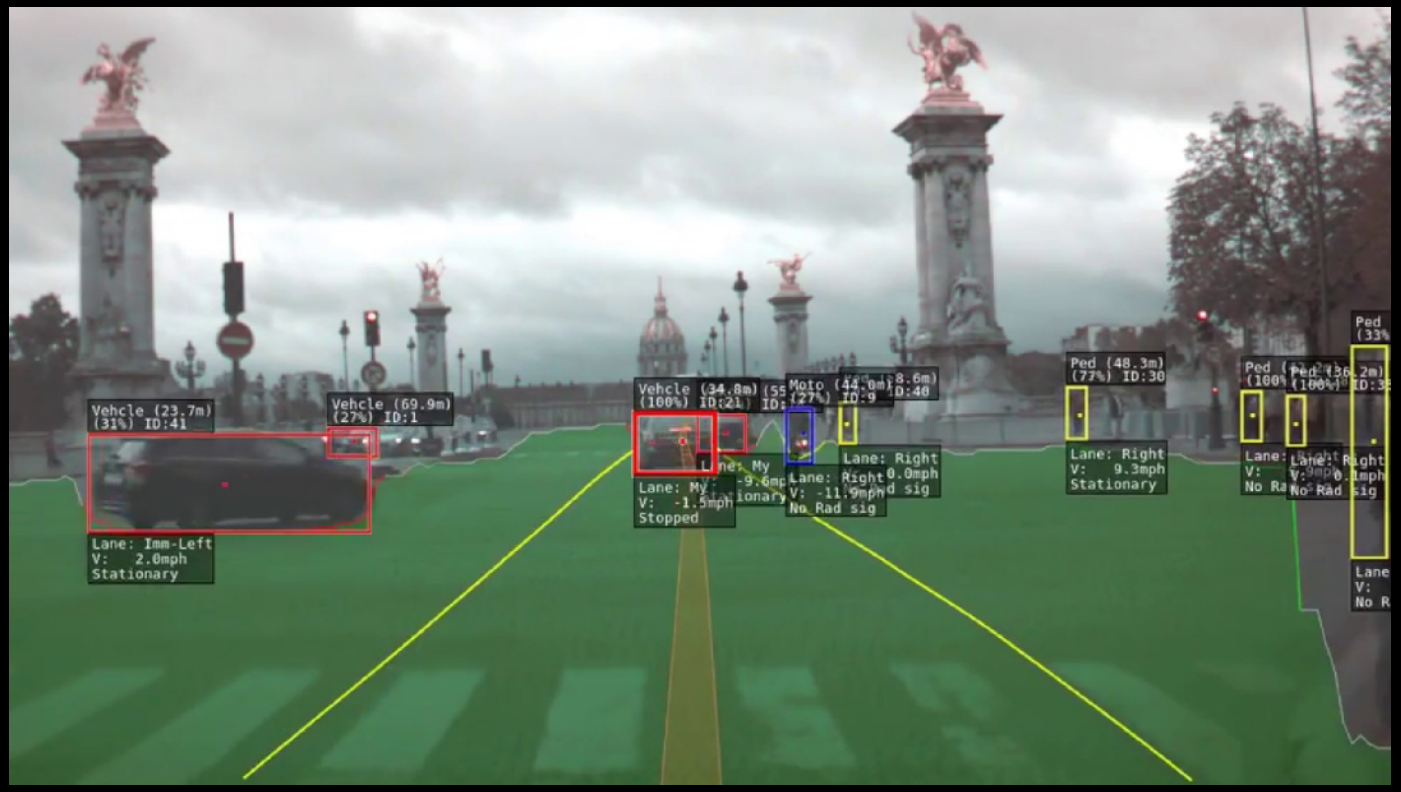
Multivariate Analysis and Machine Learning: Basic Ideas

Lecture 5
Apr 5 2024

Multivariate Analysis and Machine Learning: Basic Ideas



Multivariate Analysis: Classification and Regression

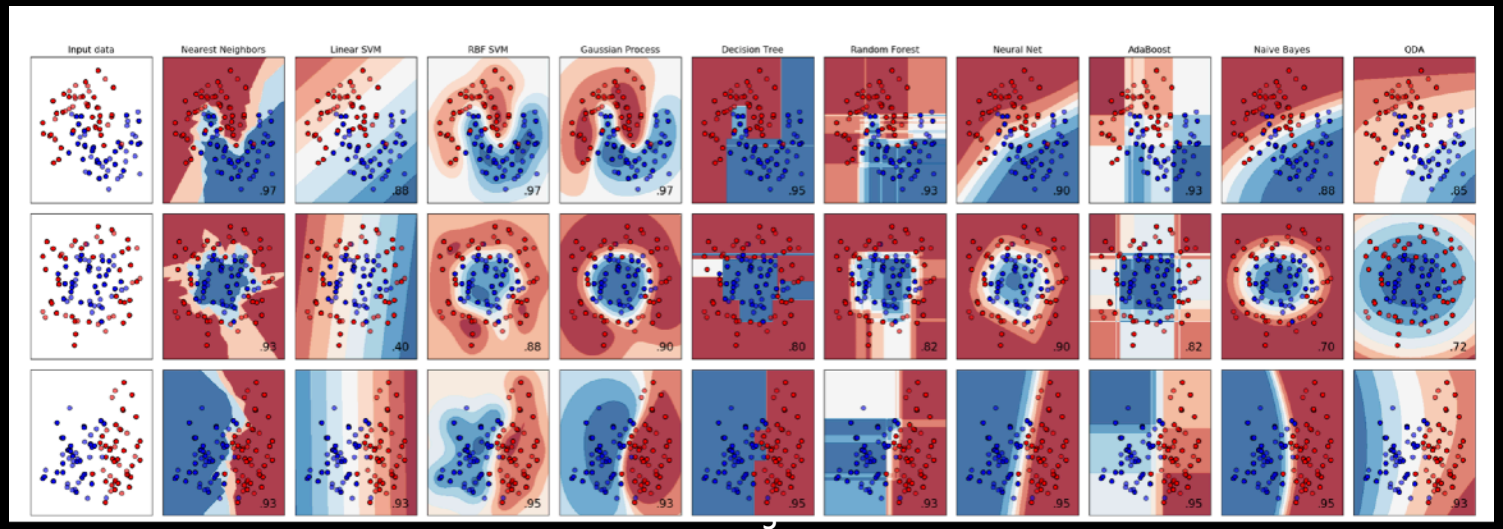
- Related, common problems in data analysis
- **Multivariate analysis:** Multiple features (input variables)
- **Classification**: Which *class* does a particular object belong to, based on features?
- **Regression**: Predict output for a set of features (e.g., interpolation/extrapolation)

Supervised machine learning

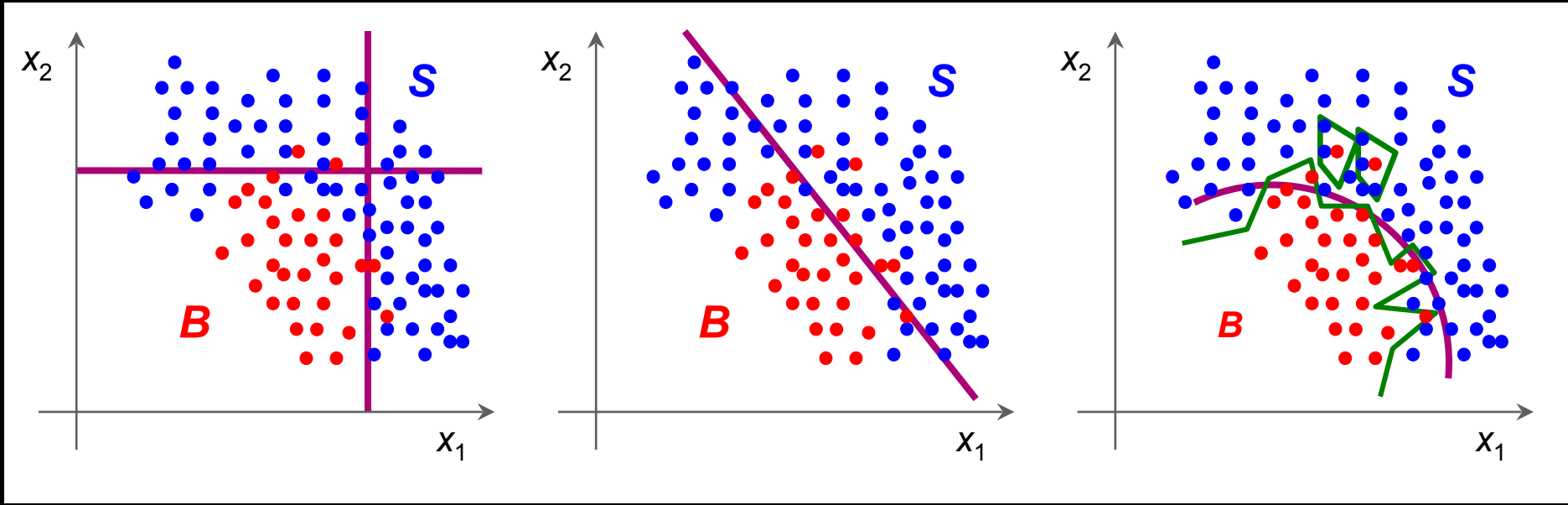
- **Machine learning (ML):** Build ***model*** for classification or regression automatically
- **Supervised ML**: Model “learns” from training sample for which correct answer is known
- **Model**: “function” determined by ML algorithm and used for classification or regression
  - Model provides output value for any valid input
  - Model has to generalize from the training sample to test sample

Methods for MVA

- There are MANY MVA methods
  - e.g., 10 methods from scikit-learn shown below
- We will focus on 2…
  - Boosted Decision Trees (BDTs)
  - Artificial Neural Networks (ANNs)
- …unless we need to try something different
- Many ideas apply to several/all methods

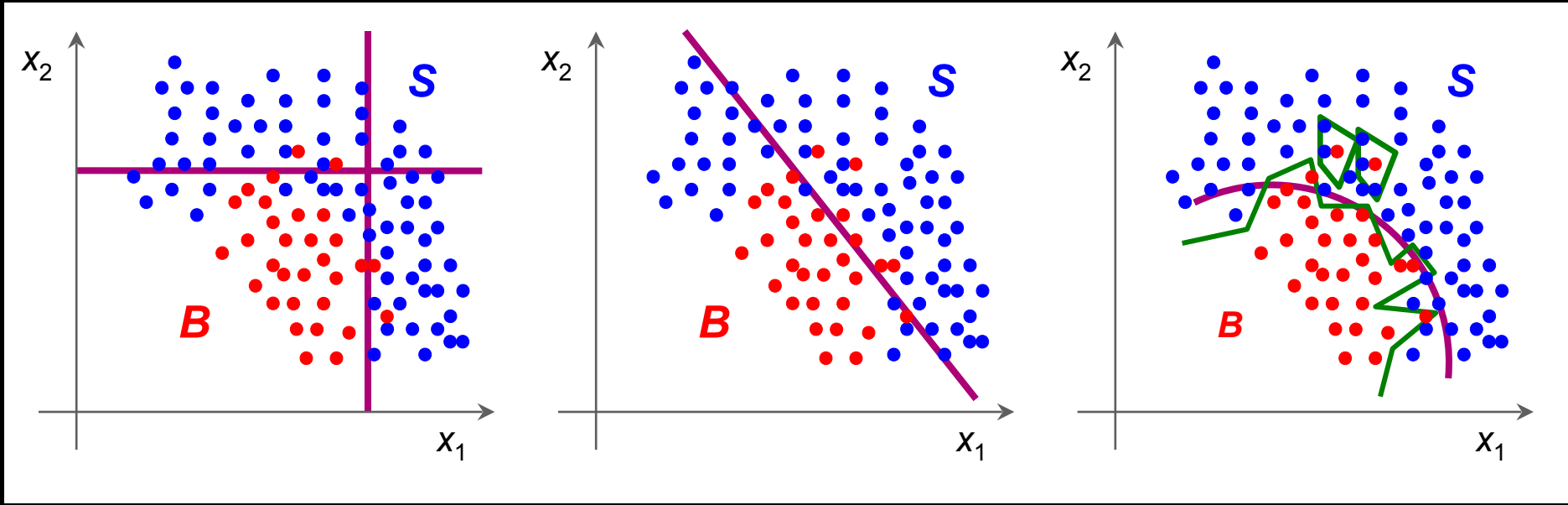


Classification



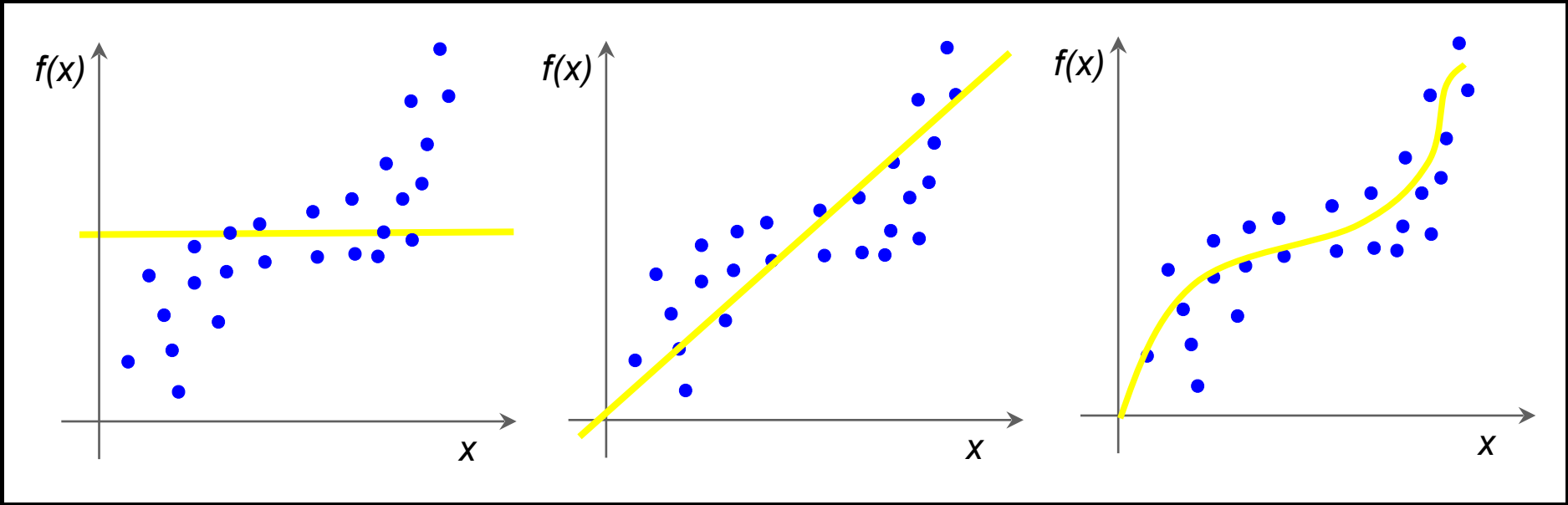
- Classification: Find “decision boundary” to separate different event classes (in physics, often “signal” and “background”)
- Boundary: D-1 dimensional hypersurface in D-dimensional feature space

Classification



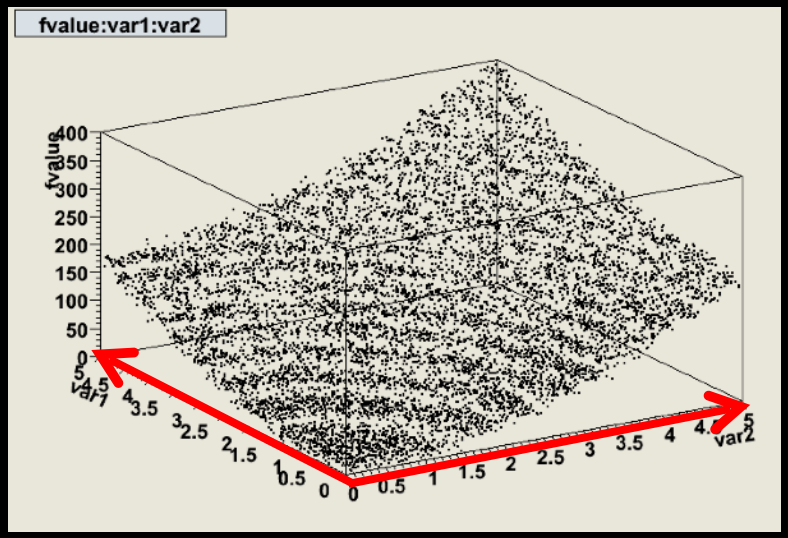
Q: Which of these four boundaries would you pick?

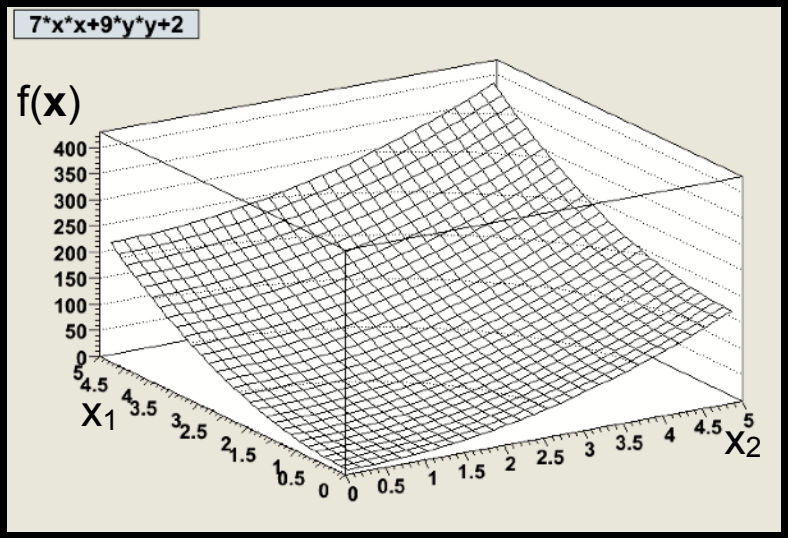
Regression



- Regression: Find “model” to predict f(**x**) for every point x in feature space
  - in general, x is D-dimensional vector
- Model: D-dimensional “hypersurface” in (D+1)-dimensional space (**x**,f(**x**))

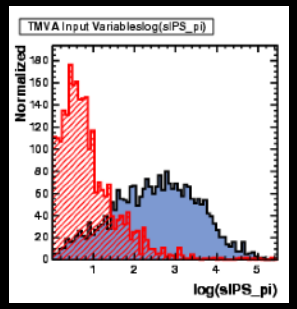
Regression

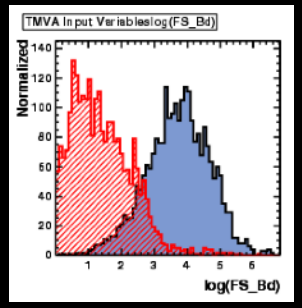


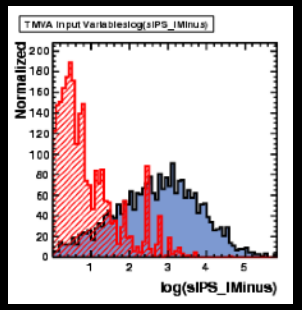


- Easy cases: Fit of known functional form f(**x**) to data point
- General: Build approximation of f(x) - model
  - piecewise approximation
  - superposition of basis functions

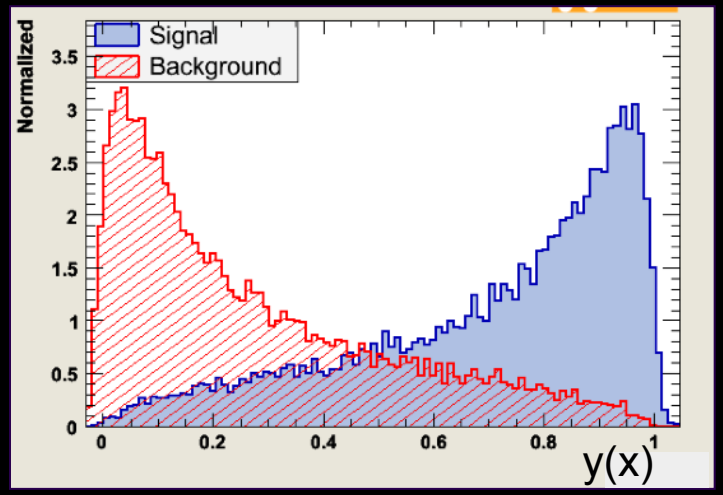
Object classification





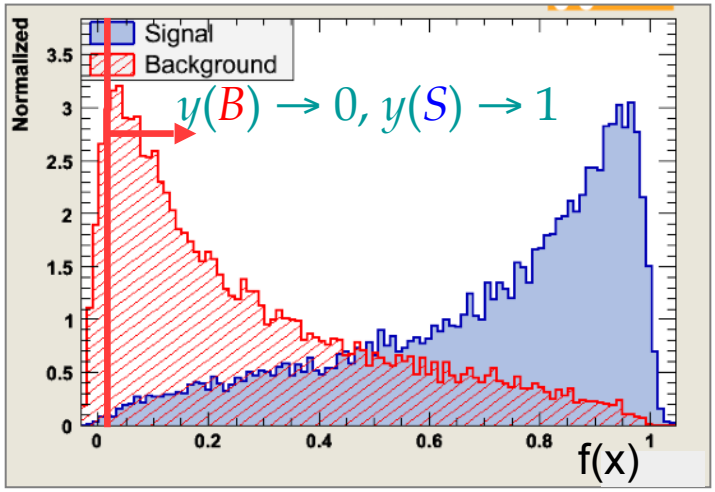


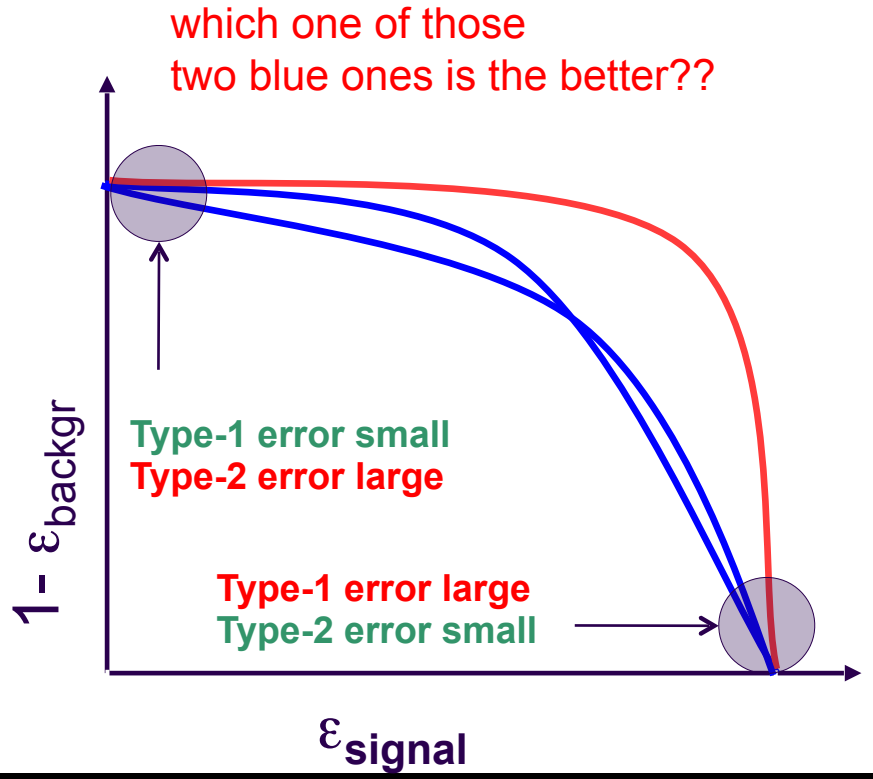
- Suppose each object has D features, $x_1 \ldots x_D$
- Goal is to label objects as **signal** or **background**
- Define function f(**x**) to label objects as **signal-like** or **background-like**
- Use supervised ML to determine best f(**x**)
- f(**x**) summarizes information from D features



Receiver Operating Characteristic (ROC) curve

Signal /Background discrimination





- Type 1 error: wrongly accept background event (reduces “Purity”)
- Type 2 error: wrongly reject signal event (reduces “Efficiency”)

Change “cut” in f(x): Move decision boundary hypersurface in feature space

Classification →find mapping function f(**x**)

- Need “training sample” where we know what is class “signal” or class “background”
  - each training object: (**x**,t) where t = signal or t=background
- Use training sample to find mapping function f(x)
  - make cut in y = f(x) to define **working point**
  - **working point** defines boundary in feature space
- How do we obtain training sample?
  - Detector simulations using software
  - Data-driven methods using data events with known outcome
- Often split sample into training and test samples

Why is this difficult?

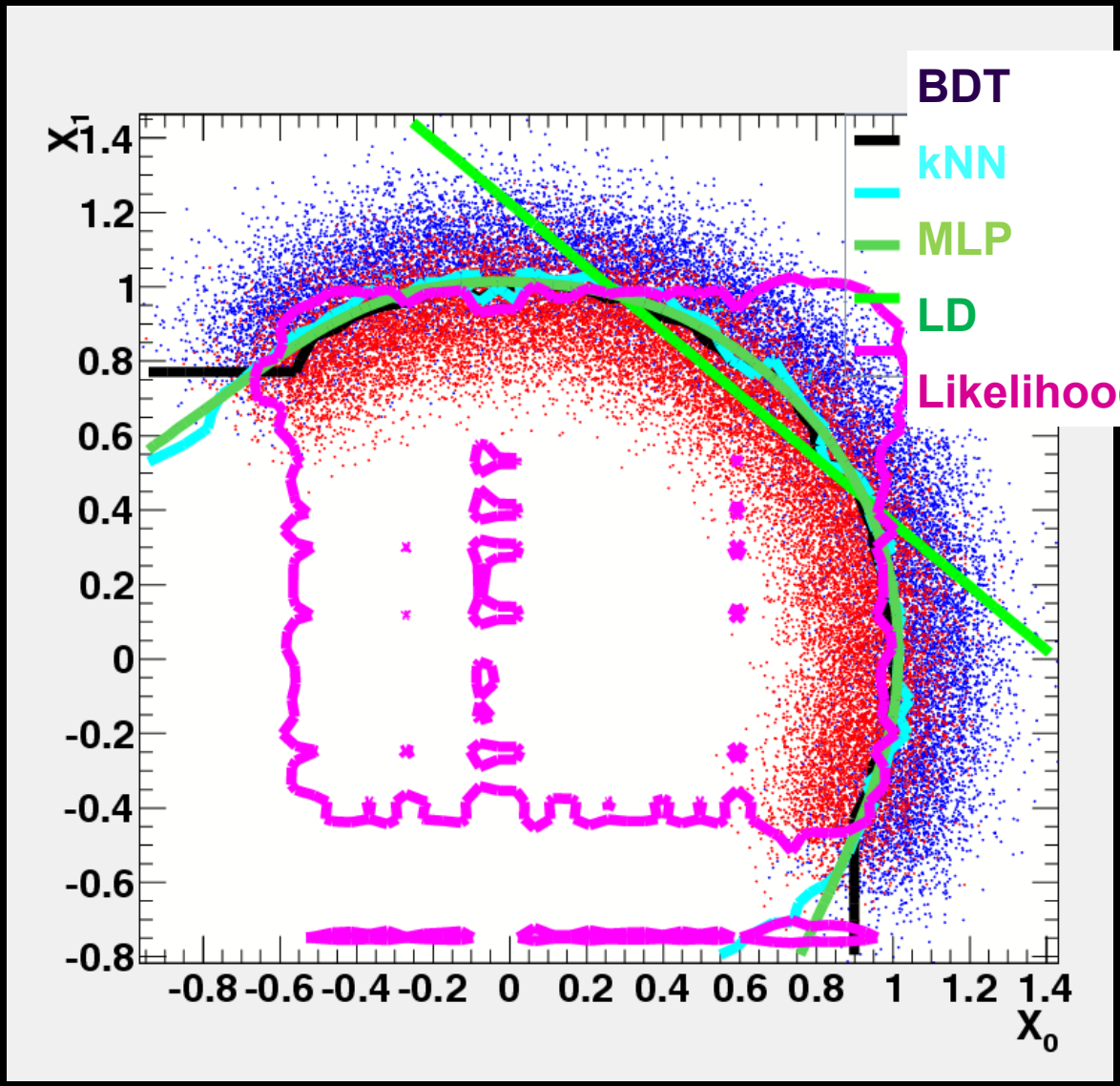
- Curse of dimensionality:
  - Most interesting cases have D > 1-2
  - For D = 4, 10% selection fills 56% in each dimension ($0.1 = 56^4$)
  - need many training events to fill D dimensional space

- Overfitting:
  - Complexity of model (e.g., nodes in decision tree) grows exponentially with number of variables; if there are not enough training events, model will “learn” to fit random fluctuations in training sample perfectly

How to train your classifier: loss function

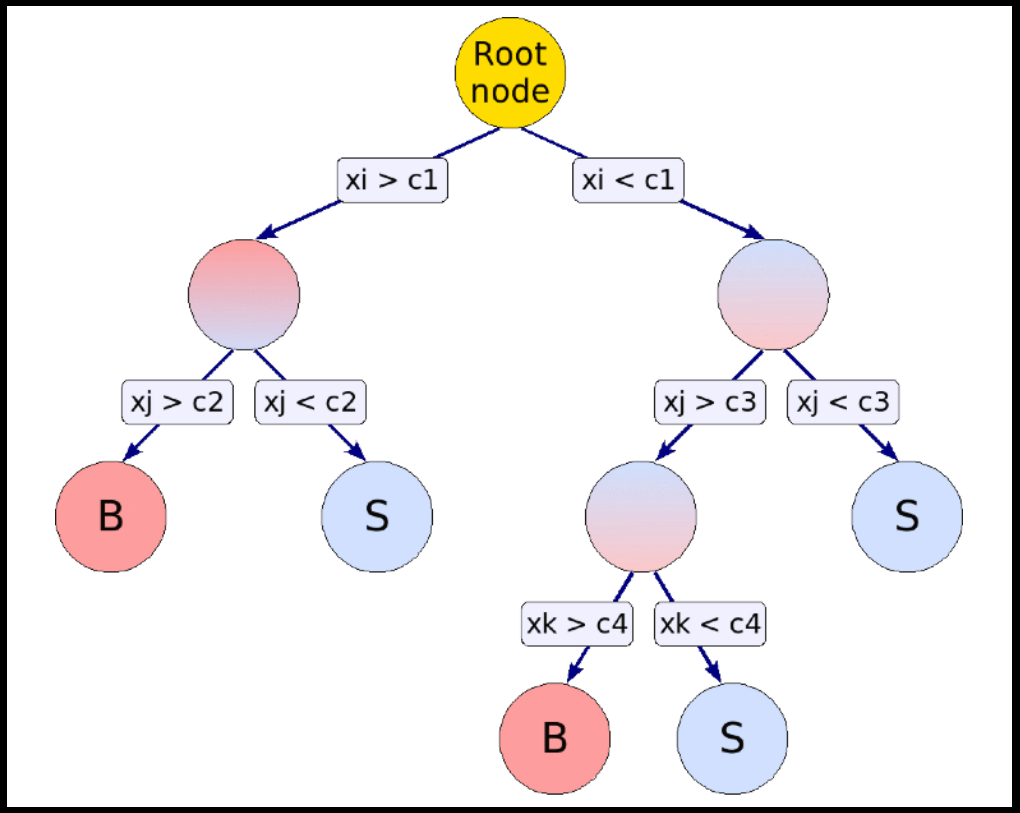
- To optimize decision boundary, need to tell ML algorithm which solutions are better or worse: Loss function
  - Sometimes called *error function*
  - Remember the χ^2 when fitting? similar
- Example loss function:
  - Sum over all events, +1 if background event classified as signal and +0 if background event classified correctly
- Model building $\rightarrow$ change parameters to minimize the loss function

Example of decision boundaries



Boosted Decision Trees

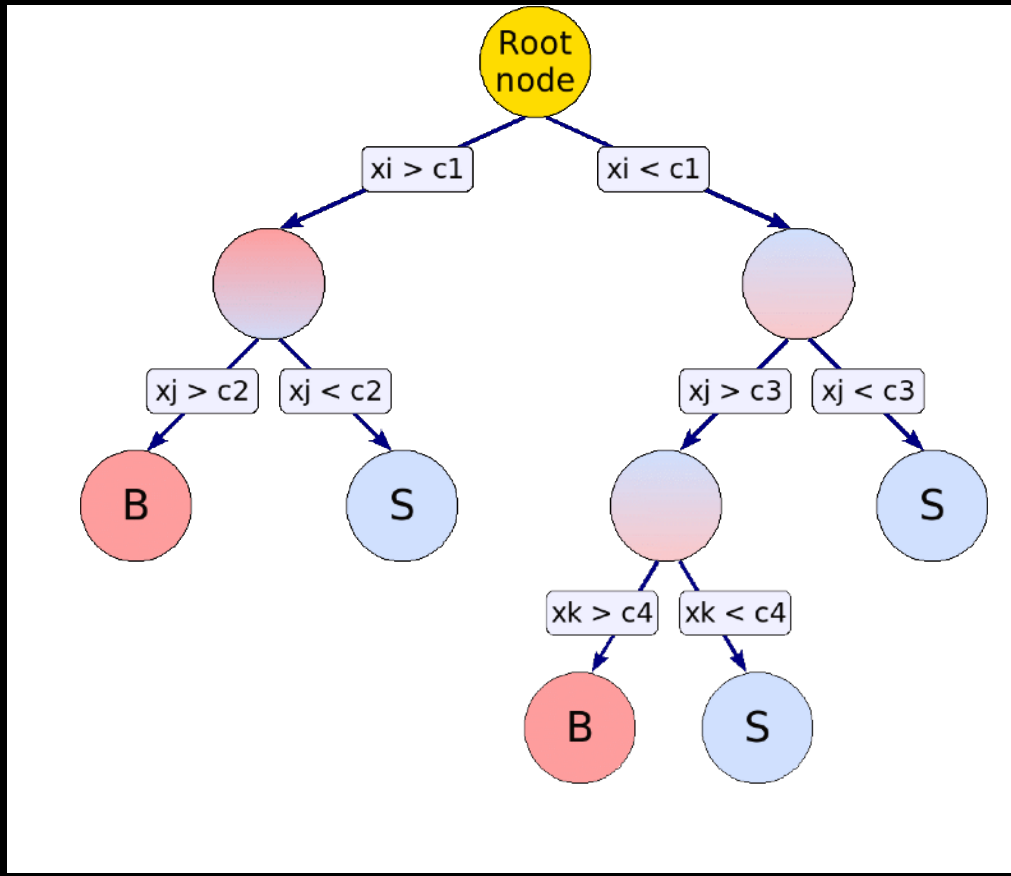
Decision Trees



- Sequential application of cuts
- Each cut on different variable
- Final cut in each branch splits data into signal and background

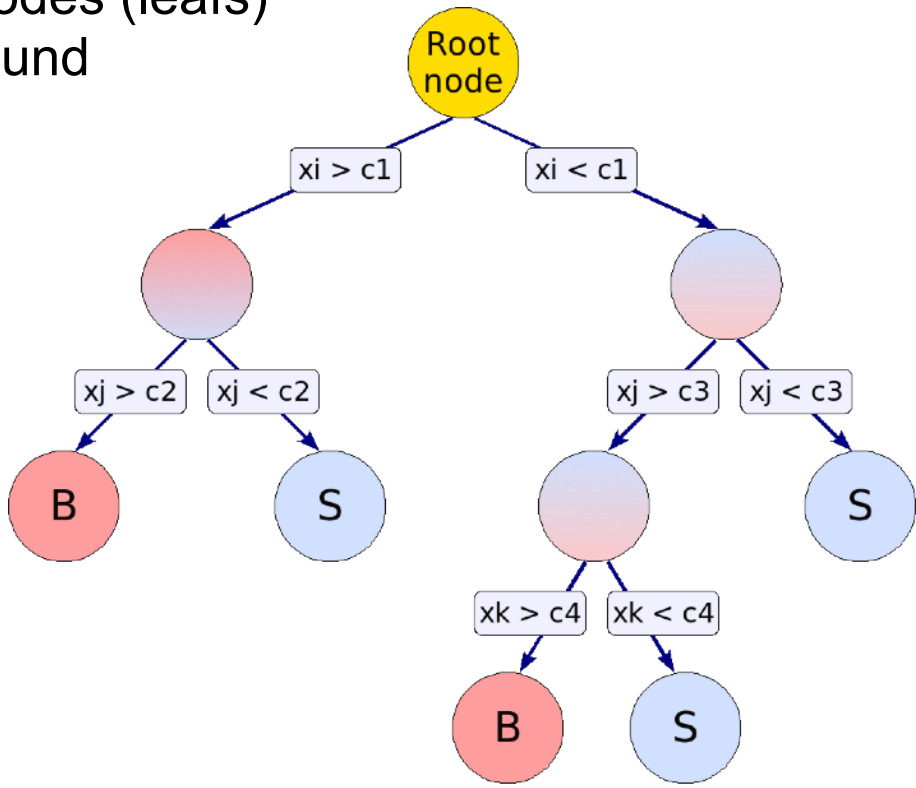
Growing a Decision Tree

- start with training sample at root node
- split training sample at node into two, using a cut in variable that gives best separation gain
- continue splitting until:
  - minimal #events per node
  - maximum number of nodes
  - maximum depth specified



Boosted Decision Trees

- Decision Tree: Sequential application of cuts splits the data into nodes, where the final nodes (leafs) classify an event as signal or background

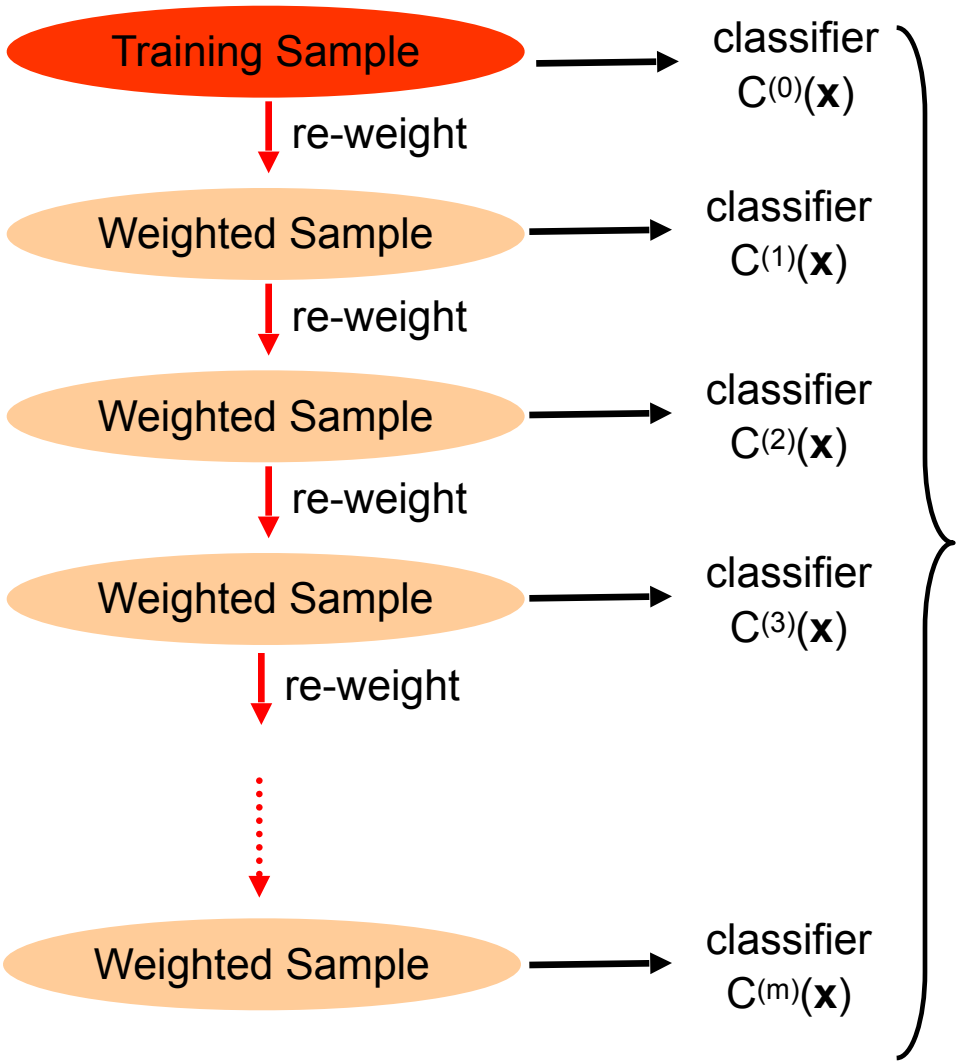


- Each branch → one standard "cut" sequence
  - easy to interpret, visualize
  - independent of monotonous variable transformations, immune against outliers
  - weak variables are ignored (and don't (much) deteriorate performance)
- Disadvantage → sensitive to statistical fluctuations in training data

- Boosted Decision Trees (1996): combine a whole forest of Decision Trees, derived from the same sample, e.g. using different event weights.
  - overcomes stability problem
  - increases performance

→ became popular in HEP since MiniBooNE, B.Roe et.a., NIM 543(2005)

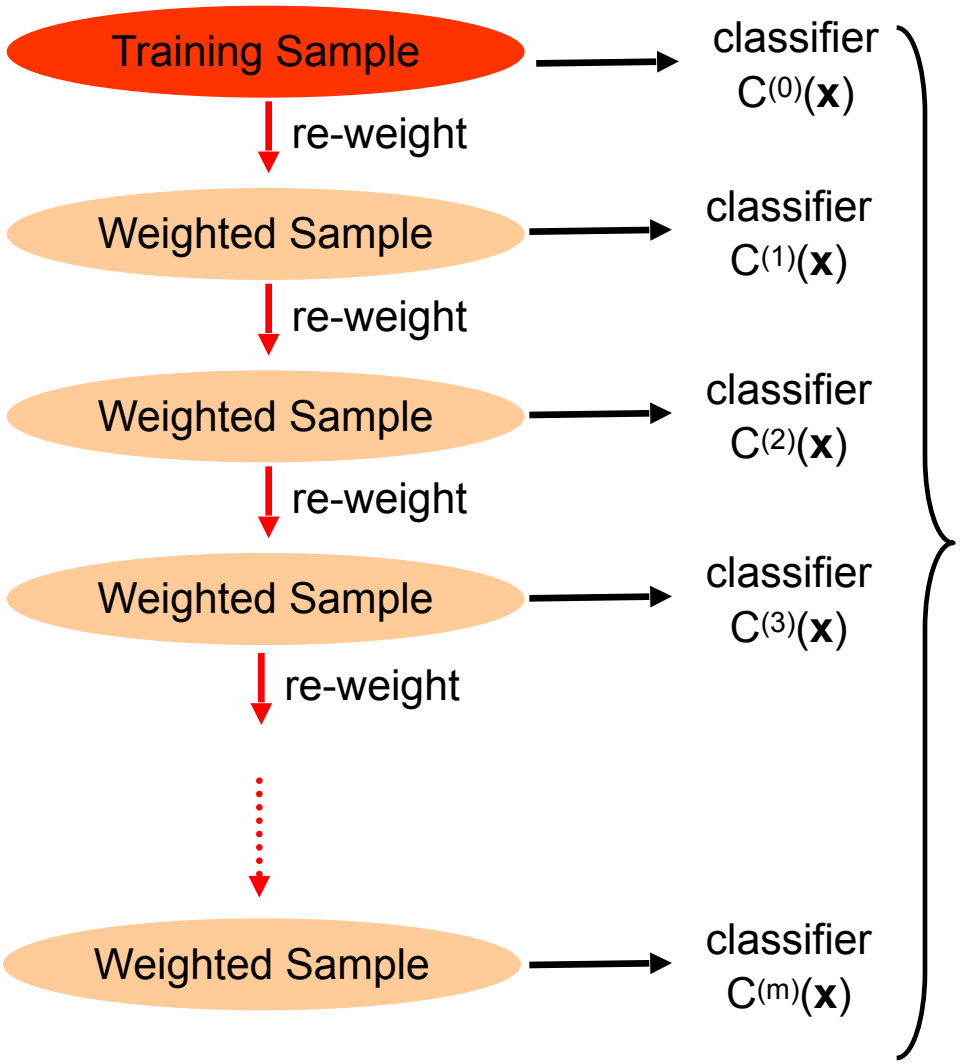
Boosting



- Boosted Decision Trees:
- combine many decision trees, derived from the same sample
  - overcomes overfitting problem
  - increases performance

$$y(x) = \sum_{i}^{N_{Classifier}} w_i C^{(i)}(x)$$

Adaptive Boosting (AdaBoost)



- AdaBoost re-weights events misclassified by previous classifier by:

$$\frac{1-f_{err}}{f_{err}} \quad \text{with :}$$

$$f_{err} = \frac{\text{misclassified events}}{\text{all events}}$$

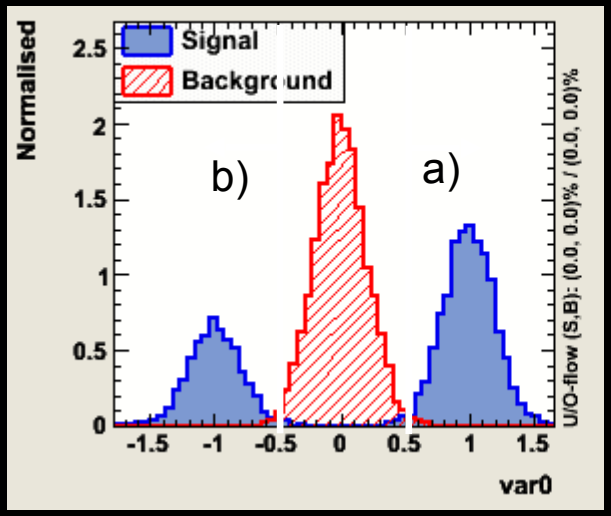
- AdaBoost weights the classifiers also using the error rate of the individual classifier according to:

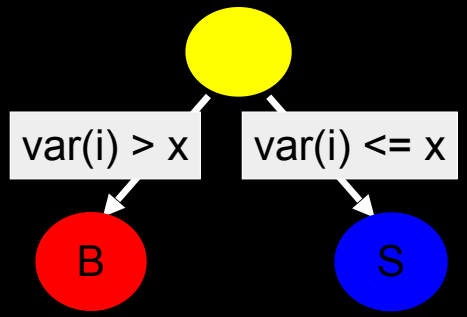
$$y(x) = \sum_{i}^{N_{Classifier}} \log\left(\frac{1-f_{err}^{(i)}}{f_{err}^{(i)}}\right) C^{(i)}(x)$$

AdaBoost: A simple demonstration

Example:

- Data file with three “bumps”
- Weak classifier (i.e. one single simple “cut” ↔ decision tree stumps)





a) Var0 > 0.5 → ε_{sig}=66% ε_{bkg} ≈ 0% misclassified events in total 16.5%

or

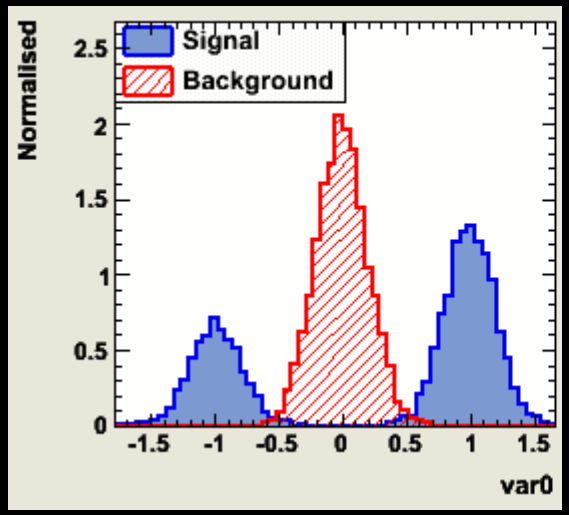
b) Var0 < -0.5 → ε_{sig}=33% ε_{bkg} ≈ 0% misclassified events in total 33%

the training of a single decision tree stump will find “cut a)”

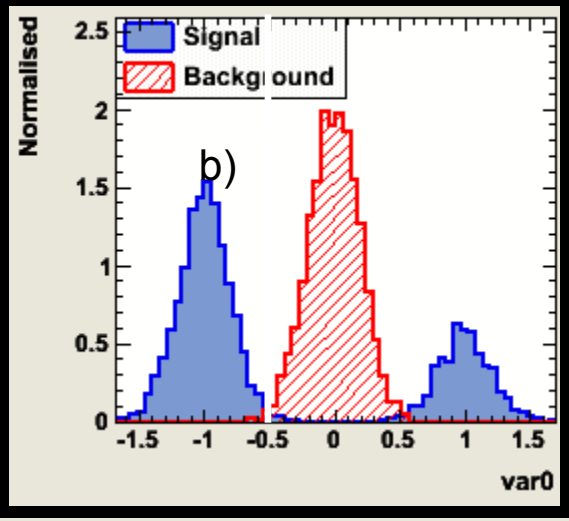
AdaBoost: A simple demonstration

➔ before building the next “tree”: weight wrong classified training events by (1-err/err)) ≈ 5

➔ the next “tree” sees essentially the following data sample:

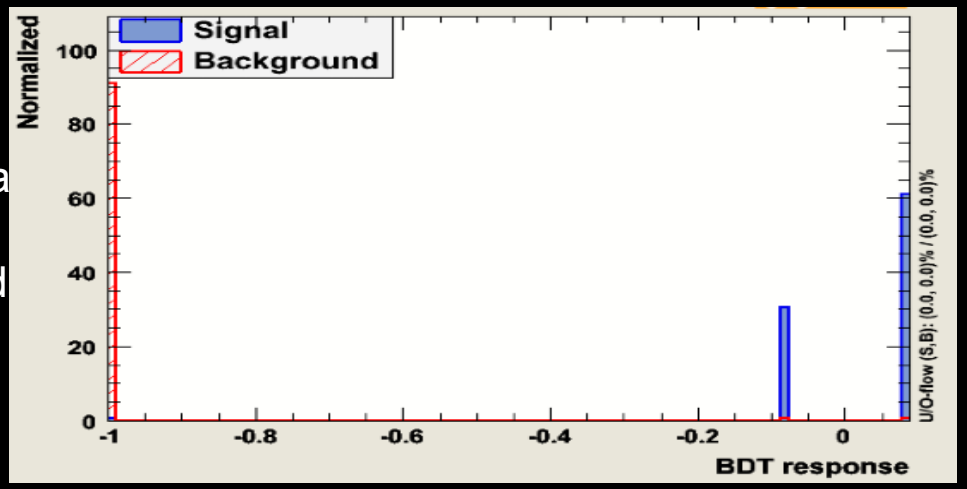


re-weight

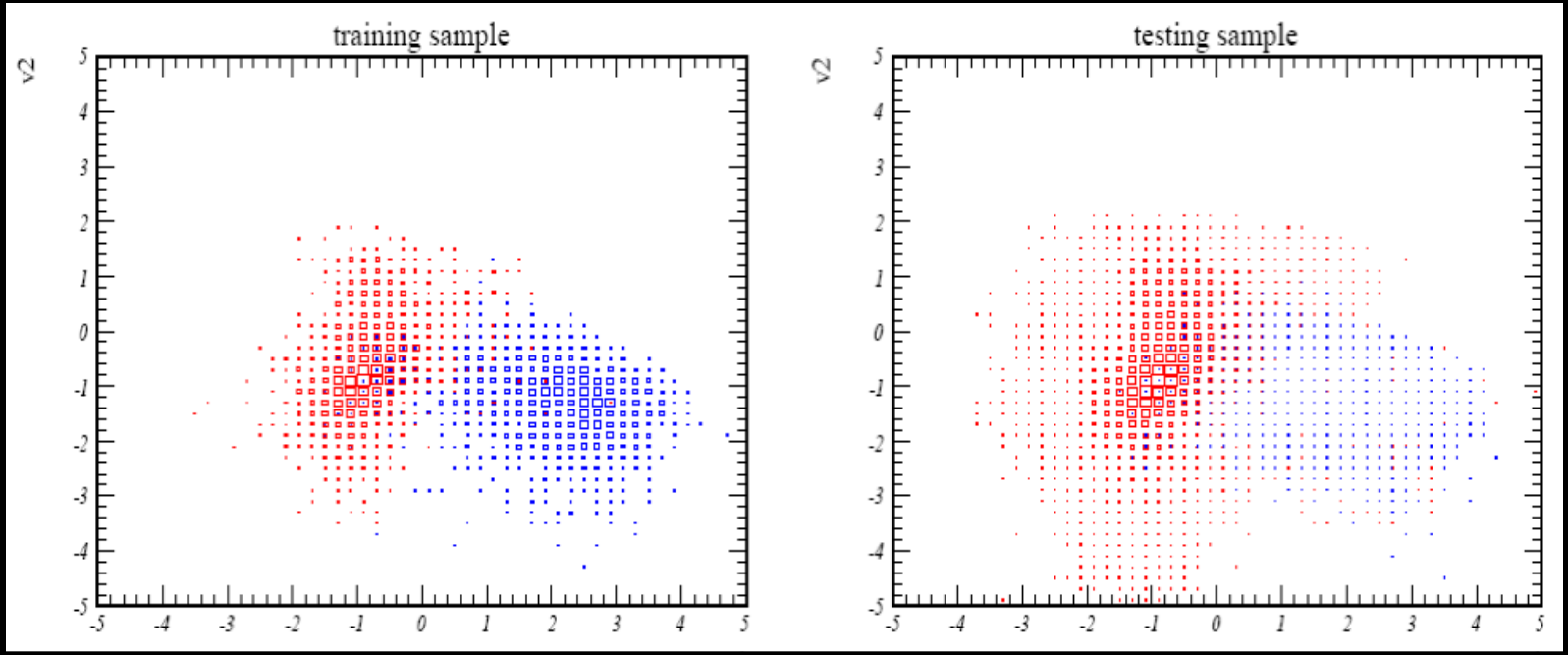


.. and hence will chose: “cut b)”: Var0 < -0.5

The combined classifier: Tree1 + Tree2
the (weighted) average of the response to a test event from both trees is able to separate signal from background as good as one would expect from the most powerful classifier



Training and test sample



- training and test sample do not have to be identical
- Can train on different ratios of signal and background events

General Advice for (MVA) Analyses

There is no magic in MVA-Methods:

- you typically still need to make careful tuning and do some “hard work”
- no “artificial intelligence” … just “fitting decision boundaries” in a given model

The most important thing at the start is finding good observables

- good separation power between S and B
- little correlations amongst each other
- no correlation with the parameters you try to measure in your signal sample!

Think also about possible combination of variables

- this may allow you to eliminate correlations
  - rem.: you are MUCH more intelligent than your computer

Apply pure preselection cuts and let the MVA only do the difficult part.

“Sharp features should be avoided” → numerical problems, loss of information when binning is applied

- simple variable transformations (i.e. log(variable)) can often smooth out these areas and allow signal and background differences to appear in a clearer way

Treat regions in the detector that have different features “independent”

- can introduce correlations where otherwise the variables would be uncorrelated!

Artificial Neural Networks

Artificial Neural Networks

Human brain

- Neuron switching time ~.001 second
- Number of neurons ~10^{10}
- Connections per neuron ~$10^{4\text{-}5}$
- Scene recognition time ~.1 second
- Requires a lot of training
- Lots of parallel computation!

Artificial neural networks (ANNs):

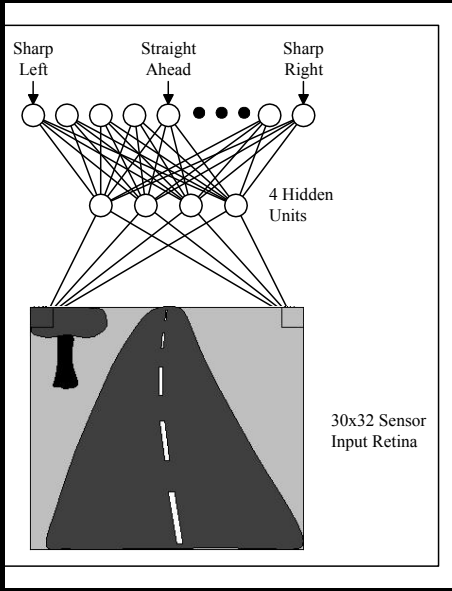
- Many neuron-like threshold switching units

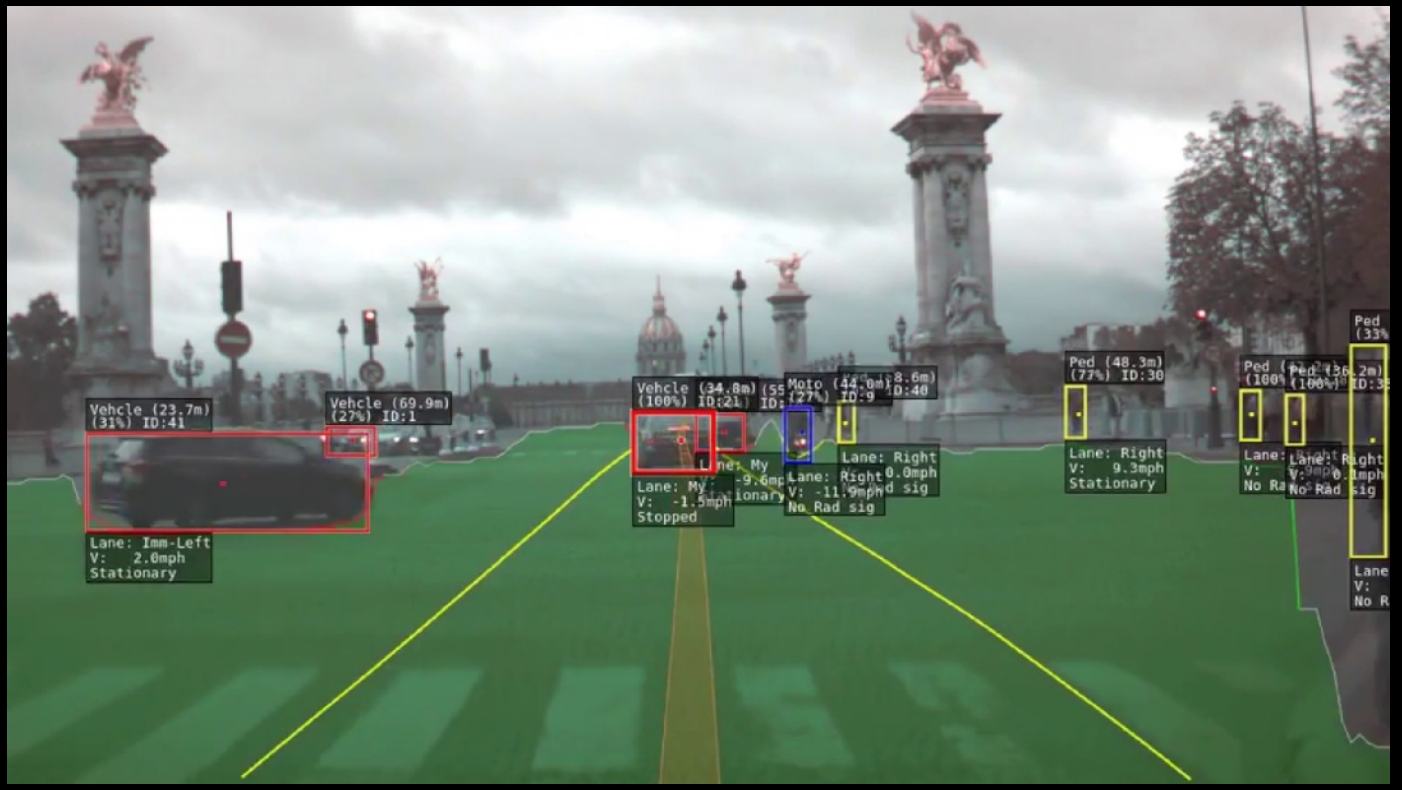
When to Consider Neural Networks

- Input is high-dimensional discrete or real-valued (e.g., combining information from different measurements or detectors)
- Output is discrete or real valued
- Output is a vector of values
- Possibly noisy data
- Form of target function is unknown
- Human readability of result is *unimportant*

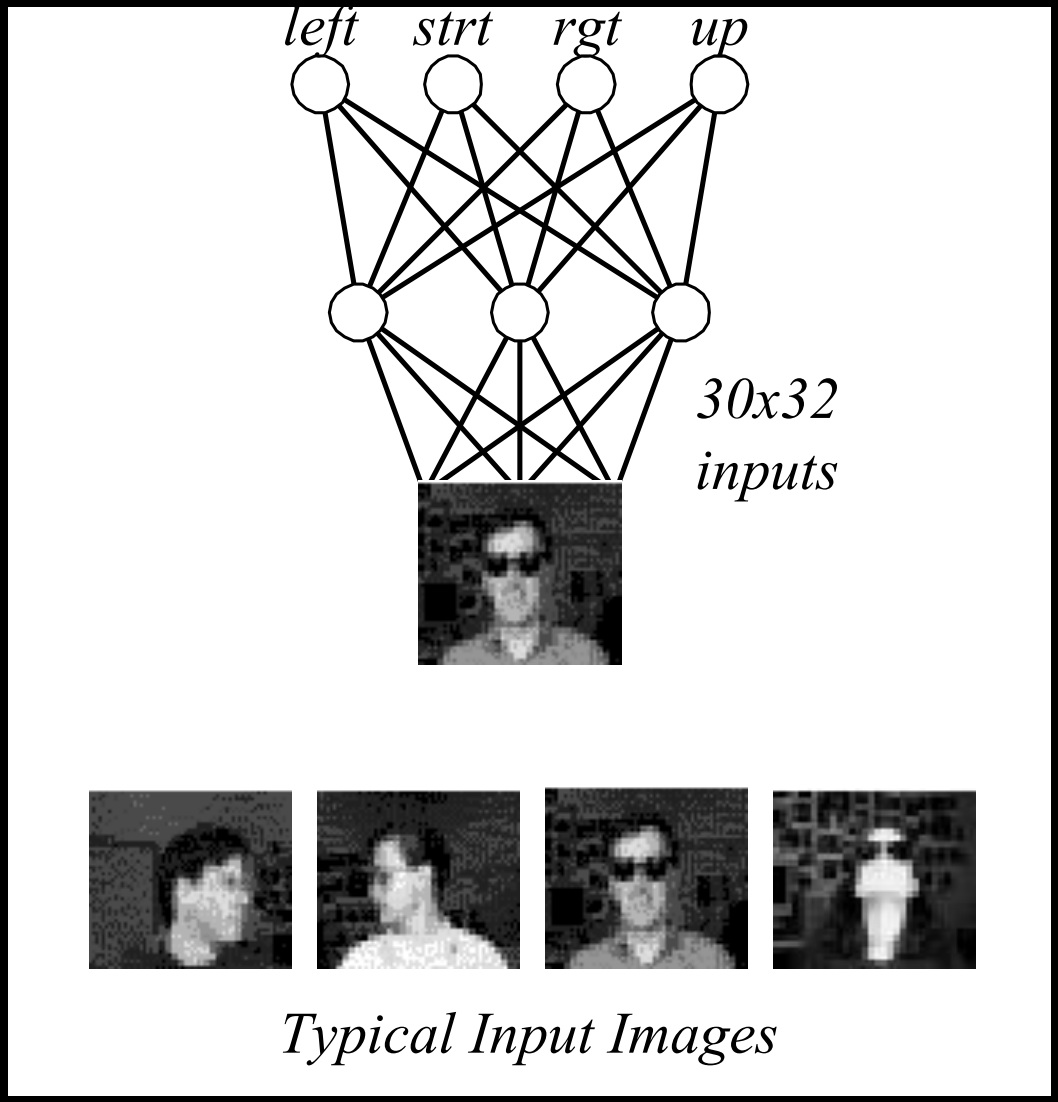
Examples:

ANN drives through Paris



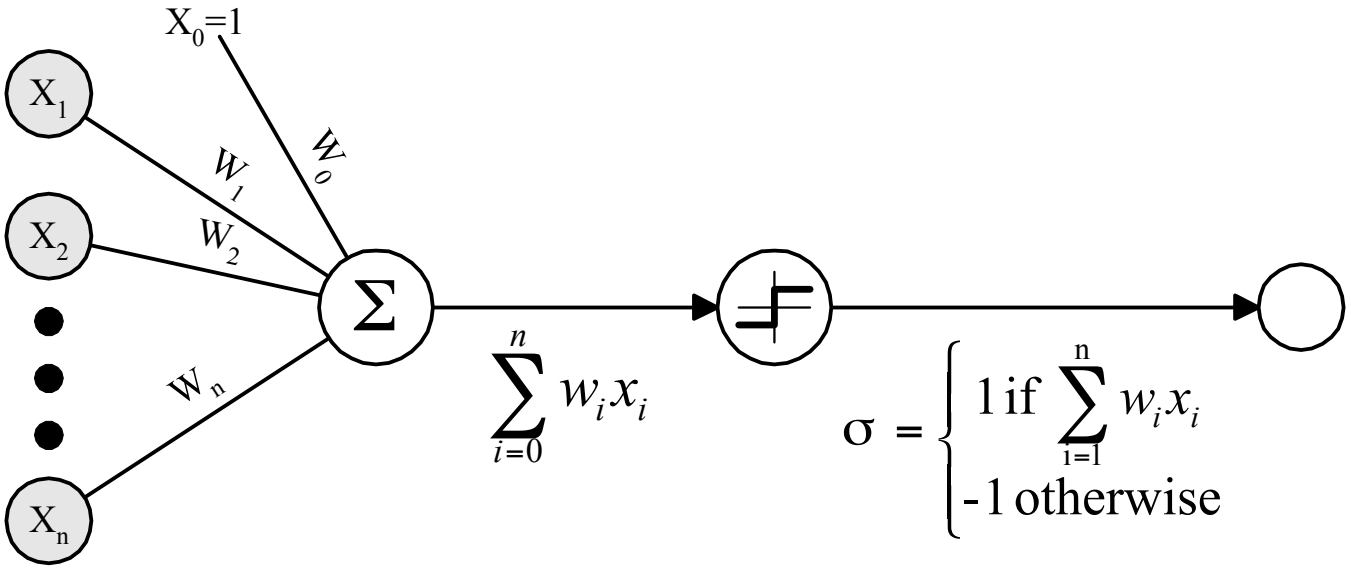


ANN recognizes faces



Typical Input Images

Basic unit: Perceptron

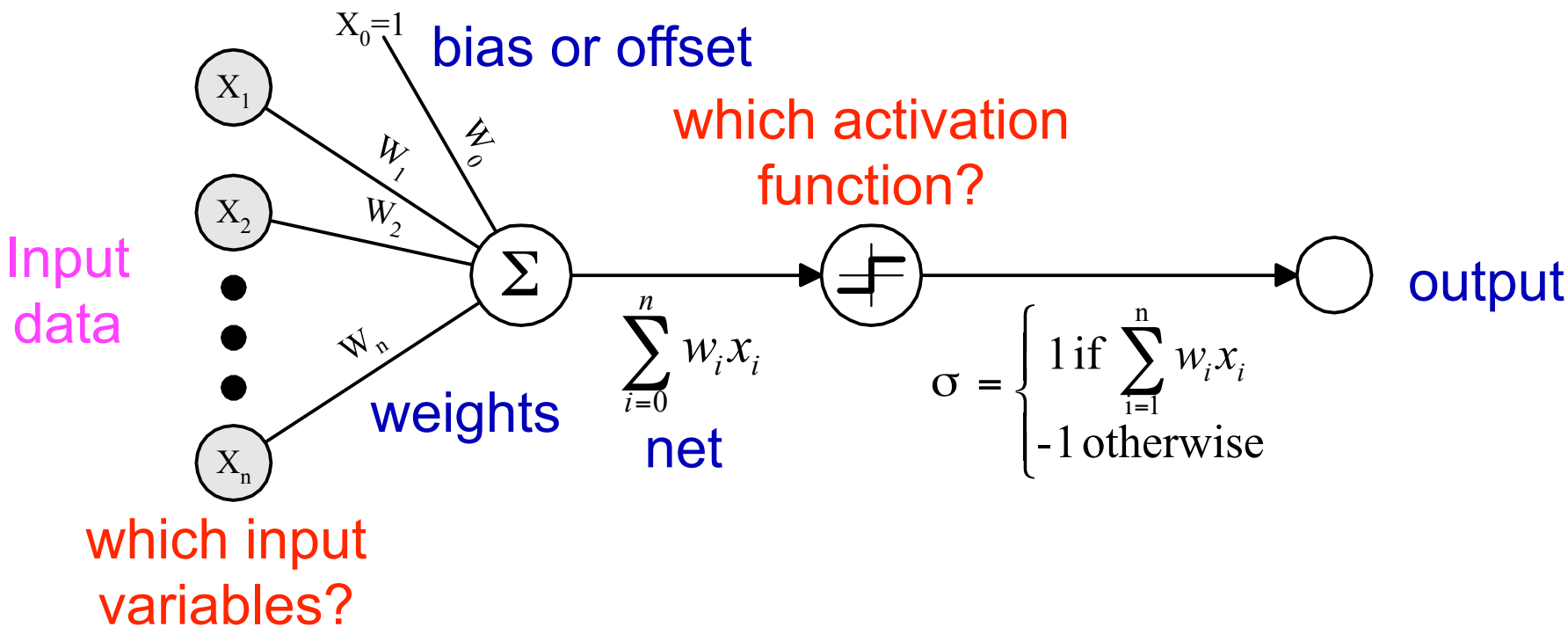


$$o(x_1,\ldots,x_n) = \begin{cases} 1 \text{ if } w_0 + w_1 x_1 + \ldots + w_n x_n > 0 \\ -1 \text{ otherwise} \end{cases}$$

Sometimes we will use simpler vector notation :

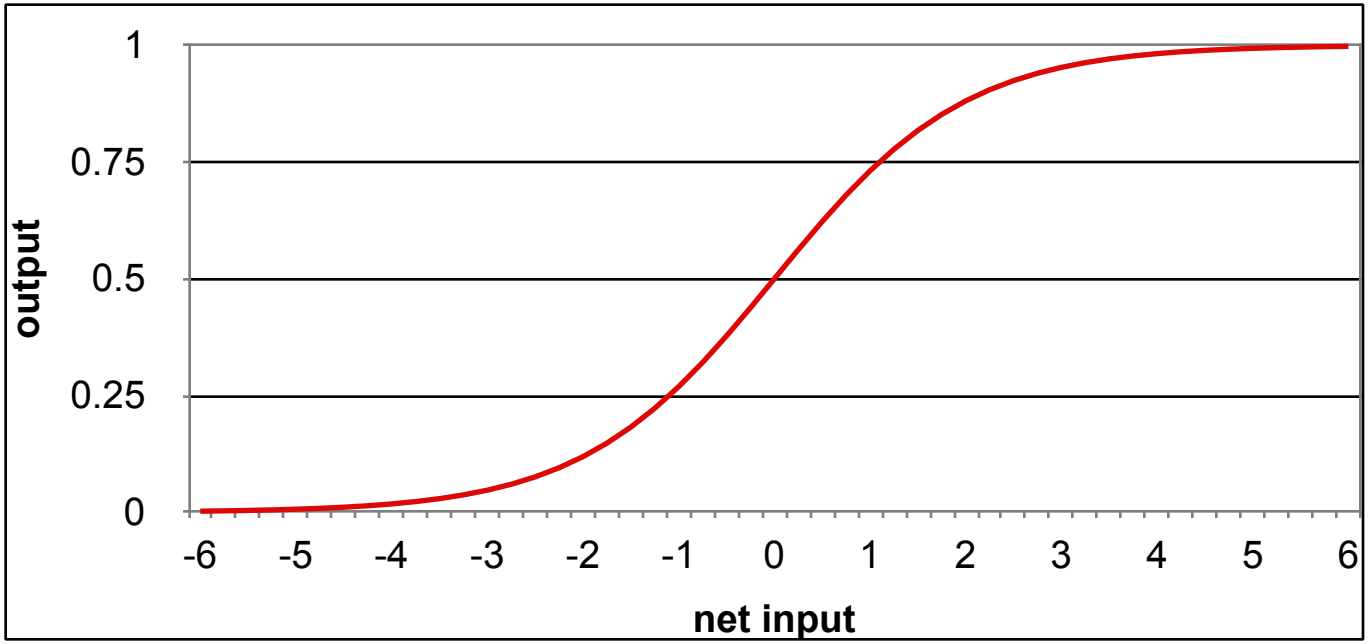
$$o(\vec{x}) = \begin{cases} 1 \text{ if } \vec{w} \cdot \vec{x} > 0 \\ -1 \text{ otherwise} \end{cases}$$

Basic unit: Perceptron



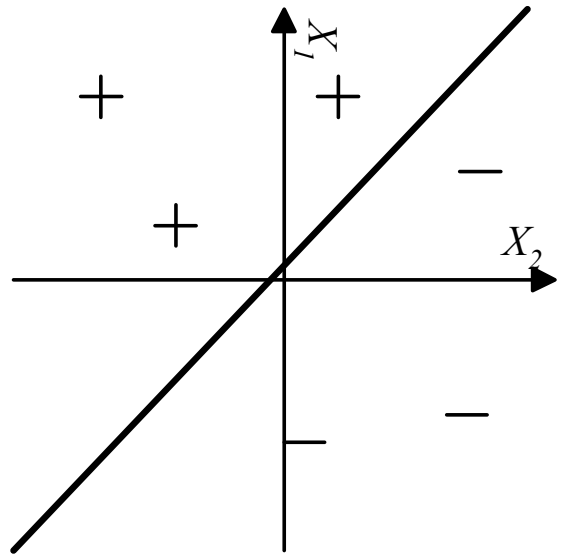
The Sigmoid Function

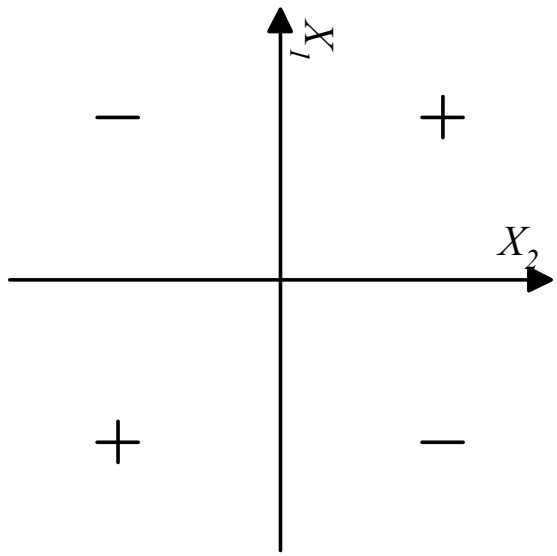
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



- "rounded" step function
- Unlike step function, can take derivative → helpful for learning

Perceptron decision boundaries





Represents some useful functions

- What weights represent $g(x_1,x_2) = AND(x_1,x_2)$?

But some functions not representable

- e.g., not linearly separable
- therefore, we will want networks of perceptrons

How to train your Perceptron

$$w_i \leftarrow w_i + \Delta w_i$$

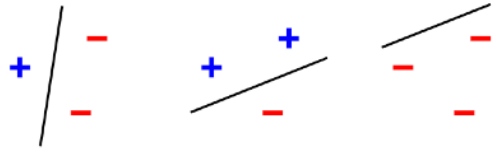
where

$$\Delta w_i = \eta\,(t - o)x_i$$

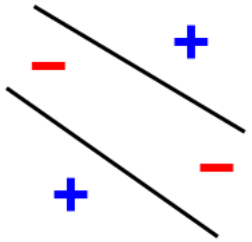
- $t = c(\vec{x})$ is target value
- o is perceptron output
- η is small constant (e.g., .1) called learning rate

Can prove it will converge

- If training data is linearly separable
- and η is sufficiently small



linearly separable



not l.s.

Again: Loss function

Now we just need to fix the parameters (weights) → Minimize Loss function E(**w**):

$$E(\mathbf{w}) = \sum_{i}^{events} \left(y_i^{train} - y(x_i) \right)^2$$

i.e. like usual χ^2 in fitting

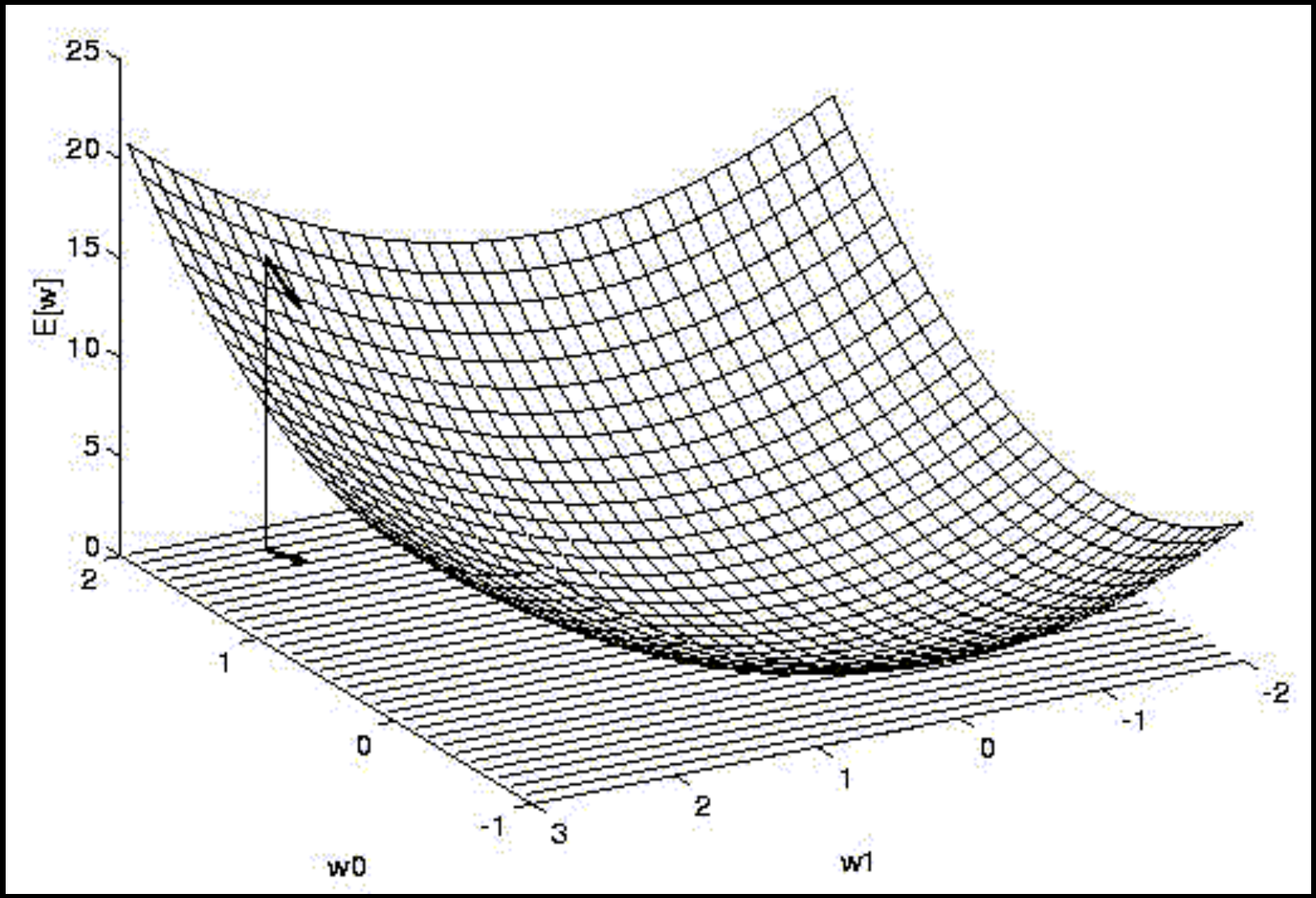
true

predicted

How to find weights w that minimize loss function?

- One global fit will usually not work
  - noisy data → many local minima
- Solution: Gradient descent optimization

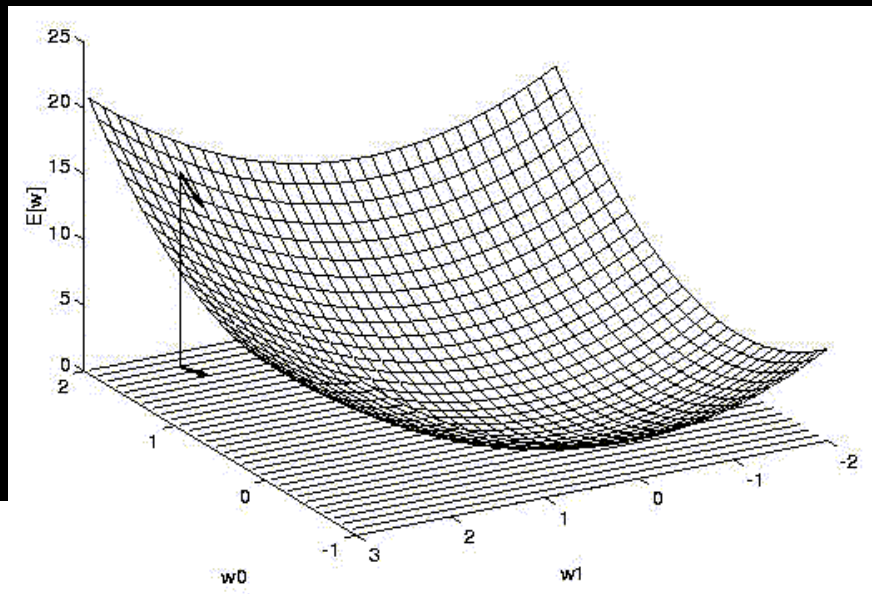
Gradient Descent



Make steps in the direction of the steepest slope of E(**w**)

Gradient Descent

Finding the optimal vector of weights **w**



Gradient $\nabla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \ldots, \frac{\partial E}{\partial w_n} \right]$ Slope of E(w) surface

Training rule: $\Delta w_i = -\eta \nabla E[\vec{w}]$ small step η down slope ∇E

i.e., $\Delta w_i = -\eta \frac{\partial E}{\partial w_i}$

Gradient Descent Training

GRADIENT – DESCENT(*training _ examples*, η)

Each training examples is a pair of the form $< \vec{x}, t >$ *, where* $\vec{x}$ *is the vector of input values and t is the t* arg *et output value.* η *is the learning rate (e.g.,* .05 *).*

- Initialize each w_i to some small random value
- Until the termination condition is met, do
  - Initialize each Δw_i to zero.
  - For each $< \vec{x}, t >$ in *training _ examples*, do
    - Input the instance $\vec{x}$ and compute output o
    - For each linear unit weight w_i, do

$$\Delta w_i \leftarrow \Delta w_i + \eta\,(t - o)x_i$$

  - For each linear unit weight w, do

$$w_i \leftarrow w_i + \Delta w_i$$

→ Obtain set of weights for which output is closest to target, as measured by Loss Function

Gradient Descent

Differentiate using chain rule

$$\frac{\partial E}{\partial w_i} = \frac{\partial}{\partial w_i}\frac{1}{2}\sum_d (t_d - o_d)^2$$

$$= \frac{1}{2}\sum_d \frac{\partial}{\partial w_i}(t_d - o_d)^2$$

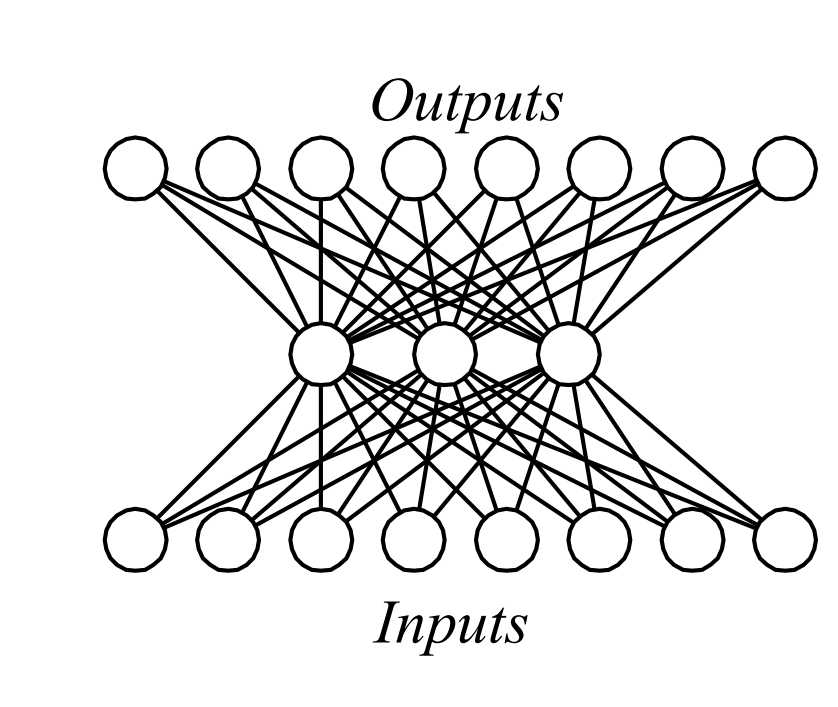
$$= \frac{1}{2}\sum_d 2(t_d - o_d)\frac{\partial}{\partial w_i}(t_d - o_d)$$

$$= \sum_d (t_d - o_d)\frac{\partial}{\partial w_i}(t_d - \vec{w}\cdot\vec{x}_d)$$

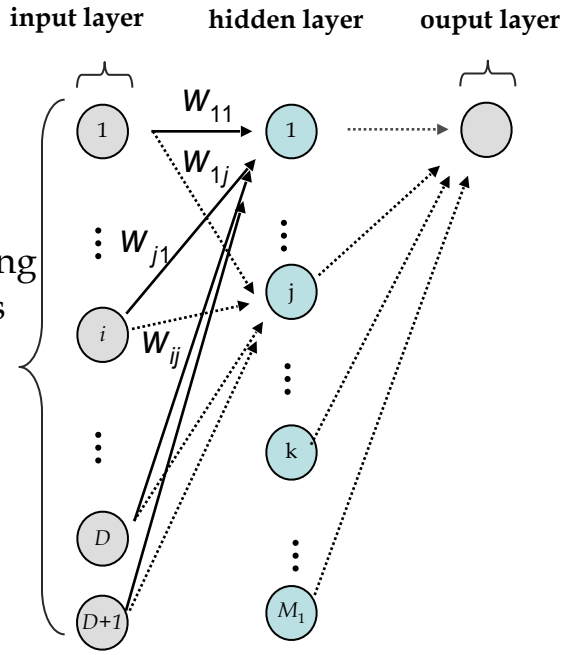
$$\frac{\partial E}{\partial w_i} = \sum_d (t_d - o_d)(-x_{i,d})$$

Networks of perceptrons

- Linear units correspond to *hyperplanes* as decision boundary
- How to approximate arbitrary hyper surfaces?
- → Multi-layer perceptron (MLP)



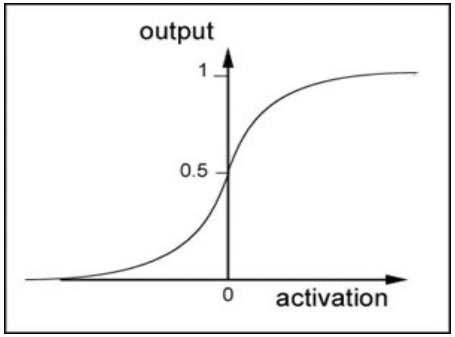
Multilayer Perceptron - MLP



D discriminating input variables as input + 1 bias

output:

$$y(x)=\sum_{i}^{M} w_{0i} A\left(w_{i0} + \sum_{j=1}^{D} w_{ij} \cdot x_j \right)$$



"Activation" function e.g. sigmoid:

$$A(x) = \left(1 + e^{-x}\right)^{-1}$$

or tanh
or …

- Nodes in hidden layer have "activation functions" whose arguments are linear combinations of input variables → non-linear response to the input
- The output is a linear combination of the output of the activation functions at the internal nodes
- Input to the layers from preceding nodes only → feed forward network (no backward loops)
- It is straightforward to extend this to additional layers

Backpropagation

- How to change weights for hidden layers?
- Can’t take derivative of E wrt hidden layer weights directly
- Use same idea (gradient descent), but recursively
- Start with output layer, calculate update to weights from hidden layer
- Then update hidden layer weights
  - continue if multiple hidden layers
  - repeat until satisfied with network performance

Backpropagation

Initialize all weights to small random numbers. Until satisfied, do

- For each training example, do

  1. Input the training example and compute the outputs
  2. For each output unit k

$$\delta_k \leftarrow o_k(1-o_k)(t_k - o_k)$$

  3. For each hidden unit h

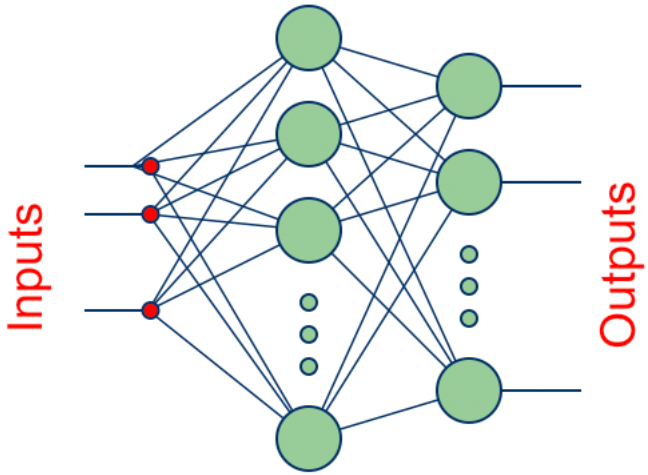
$$\delta \leftarrow o_h(1-o_h)\sum_{k \in outputs} w_{h,k}\delta_k$$

  4. Update each network weight $w_{i,j}$

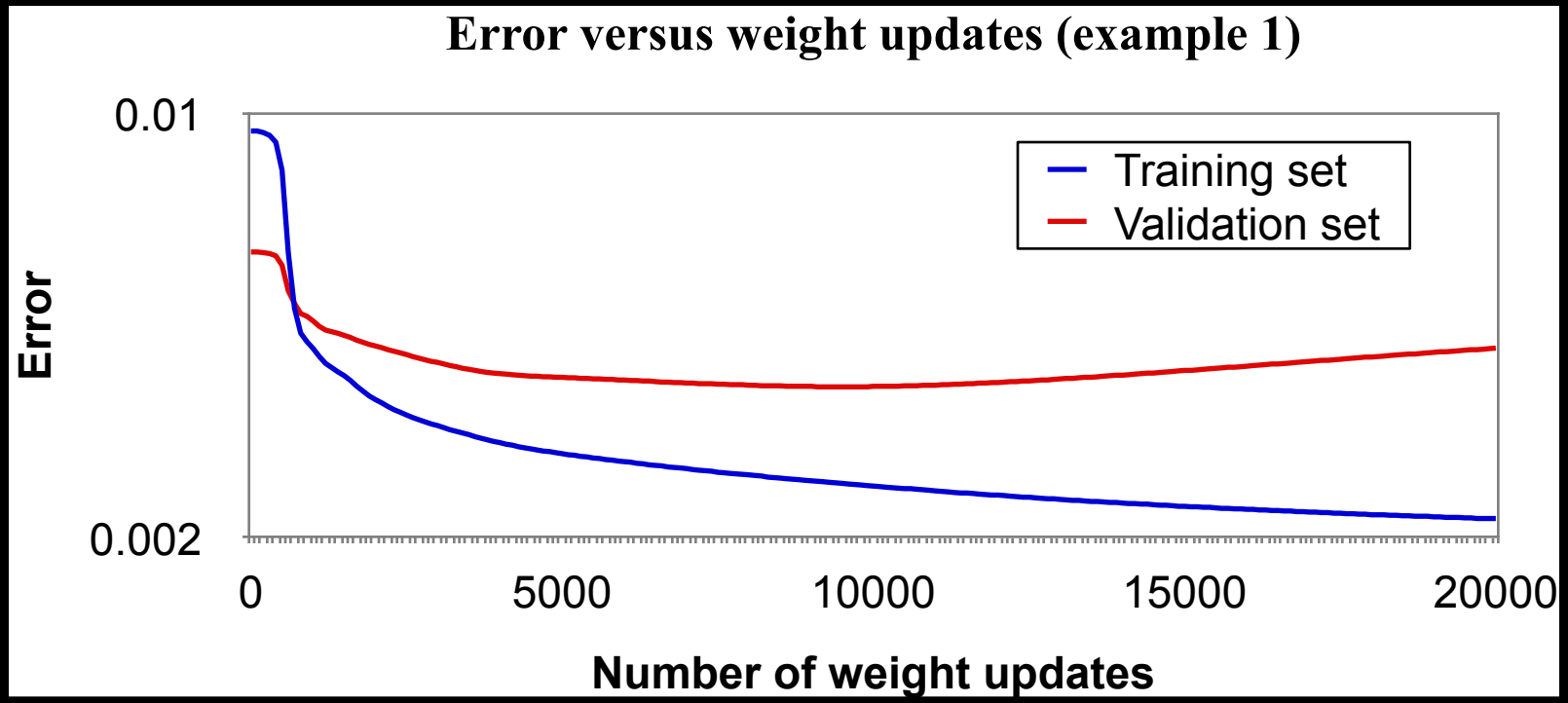
$$w_{i,j} \leftarrow w_{i,j} + \Delta w_{i,j}$$

where

$$\Delta w_{i,j} = \eta\, \delta_j x_{i,j}$$



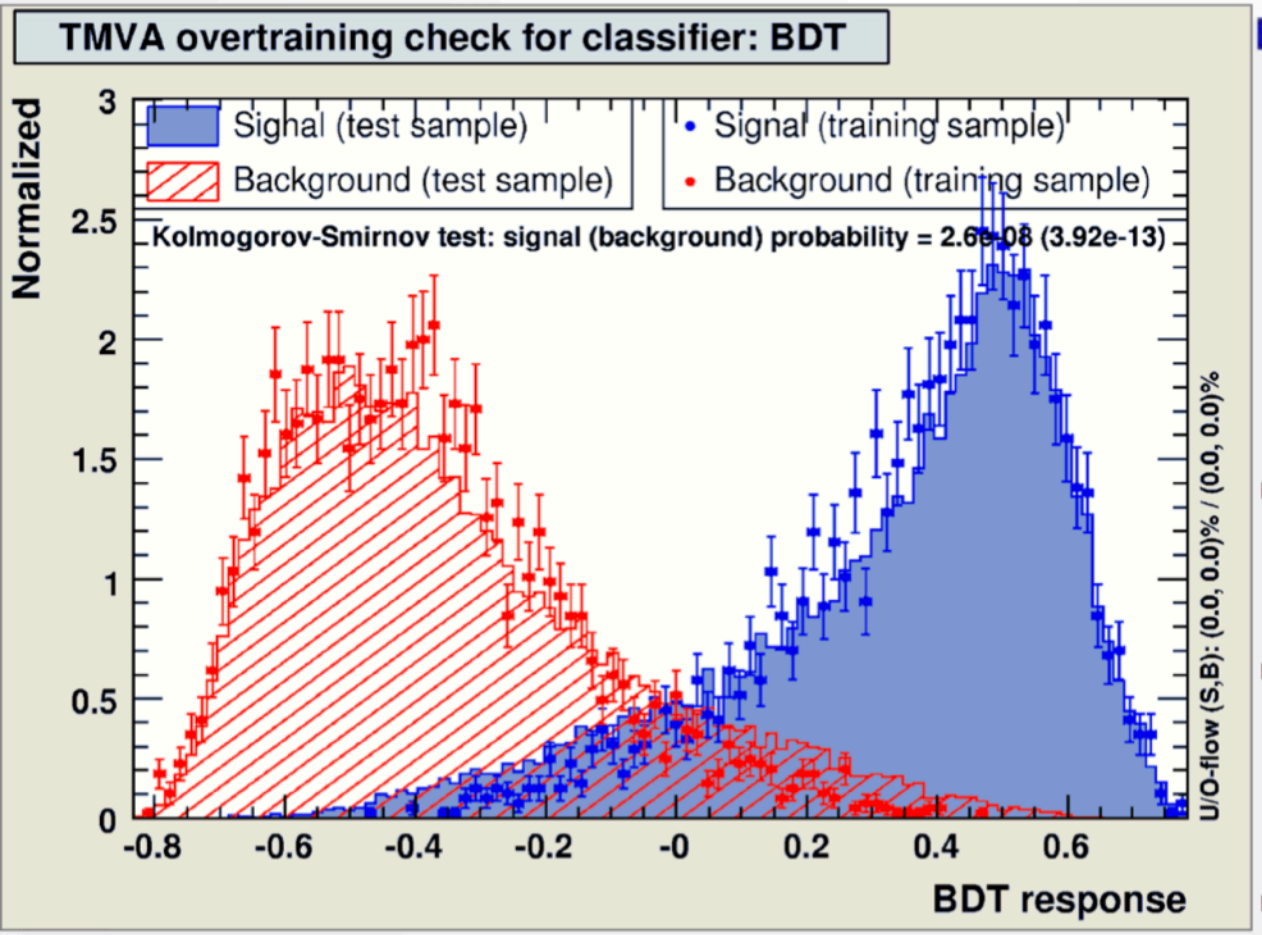
Convergence/Overfitting in ANNs



Train on ***Training set***, check results
on independent ***Validation set*** *(or Test set)*

Overtraining MVAs

- Check for overtraining: classifier output for test *and* training samples



- Remark on **overtraining**
  - Occurs when classifier training has too few degrees of freedom because the classifier has too many adjustable parameters for too few training events
  - Sensitivity to overtraining depends on classifier: *e.g.*, Fisher weak, BDT strong
  - Compare performance between training and test sample to detect overtraining
  - Actively counteract overtraining: *e.g.*, smooth likelihood PDFs, prune decision trees

Gradient Descent (simplified example)

To understand, consider simple *linear unit*, where

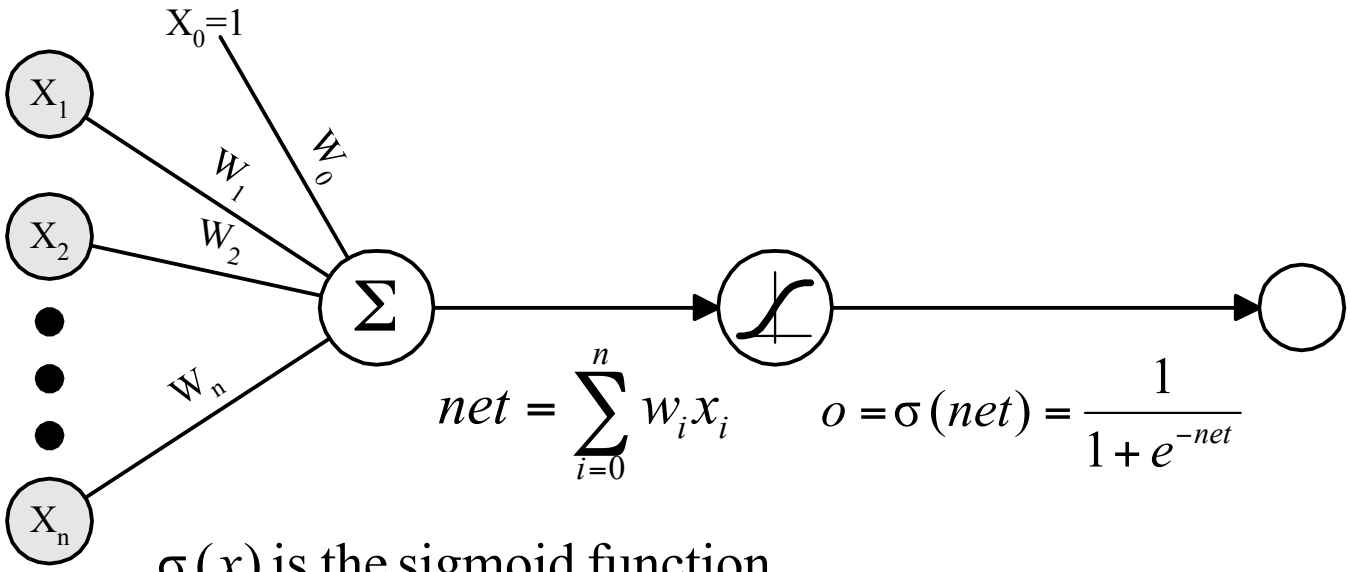
$$o = w_0 + w_1 x_1 + \ldots + w_n x_n$$

Idea : learn w_i's that minimize the squared error

$$E[\vec{w}] \equiv \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$$

Where D is the set of training examples

Sigmoid Unit



$$net = \sum_{i=0}^{n} w_i x_i \qquad o = \sigma(net) = \frac{1}{1 + e^{-net}}$$

$\sigma(x)$ is the sigmoid function

$$\frac{1}{1 + e^{-x}}$$

Nice property : $\frac{d\sigma(x)}{dx} = \sigma(x)(1 - \sigma(x))$

We can derive gradient descent rules to train

- One sigmoid unit
- *Multilayer networks* of sigmoid units → *Backpropagation*

Error Gradient for a Sigmoid Unit

$$\frac{\partial E}{\partial w_i} = \frac{\partial}{\partial w_i}\frac{1}{2}\sum_{d\in D}(t_d - o_d)^2$$

$$= \frac{1}{2}\sum_d \frac{\partial}{\partial w_i}(t_d - o_d)^2$$

$$= \frac{1}{2}\sum_d 2(t_d - o_d)\frac{\partial}{\partial w_i}(t_d - o_d)$$

$$= \sum_d (t_d - o_d)\left(-\frac{\partial o_d}{\partial w_i}\right)$$

$$= -\sum_d (t_d - o_d)\frac{\partial o_d}{\partial net_d}\frac{\partial net_d}{\partial w_i}$$

But we know :

$$\frac{\partial o_d}{\partial net_d} = \frac{\partial \sigma\,(net_d)}{\partial net_d} = o_d(1 - o_d)$$

$$\frac{\partial net_d}{\partial w_i} = \frac{\partial(\vec{w}\cdot\vec{x}_d)}{\partial w_i} = x_{i,d}$$

So :

$$\frac{\partial E}{\partial w_i} = -\sum_{d\in D}(t_d - o_d)o_d(1 - o_d)x_{i,d}$$

Incremental (Stochastic) Gradient

Batch mode Gradient Descent:
Do until satisfied:

1. Compute the gradient $\nabla E_D[\vec{w}]$
2. $\vec{w} \leftarrow \vec{w} - \eta \nabla E_D[\vec{w}]$

$$E_D[\vec{w}] \equiv \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$$

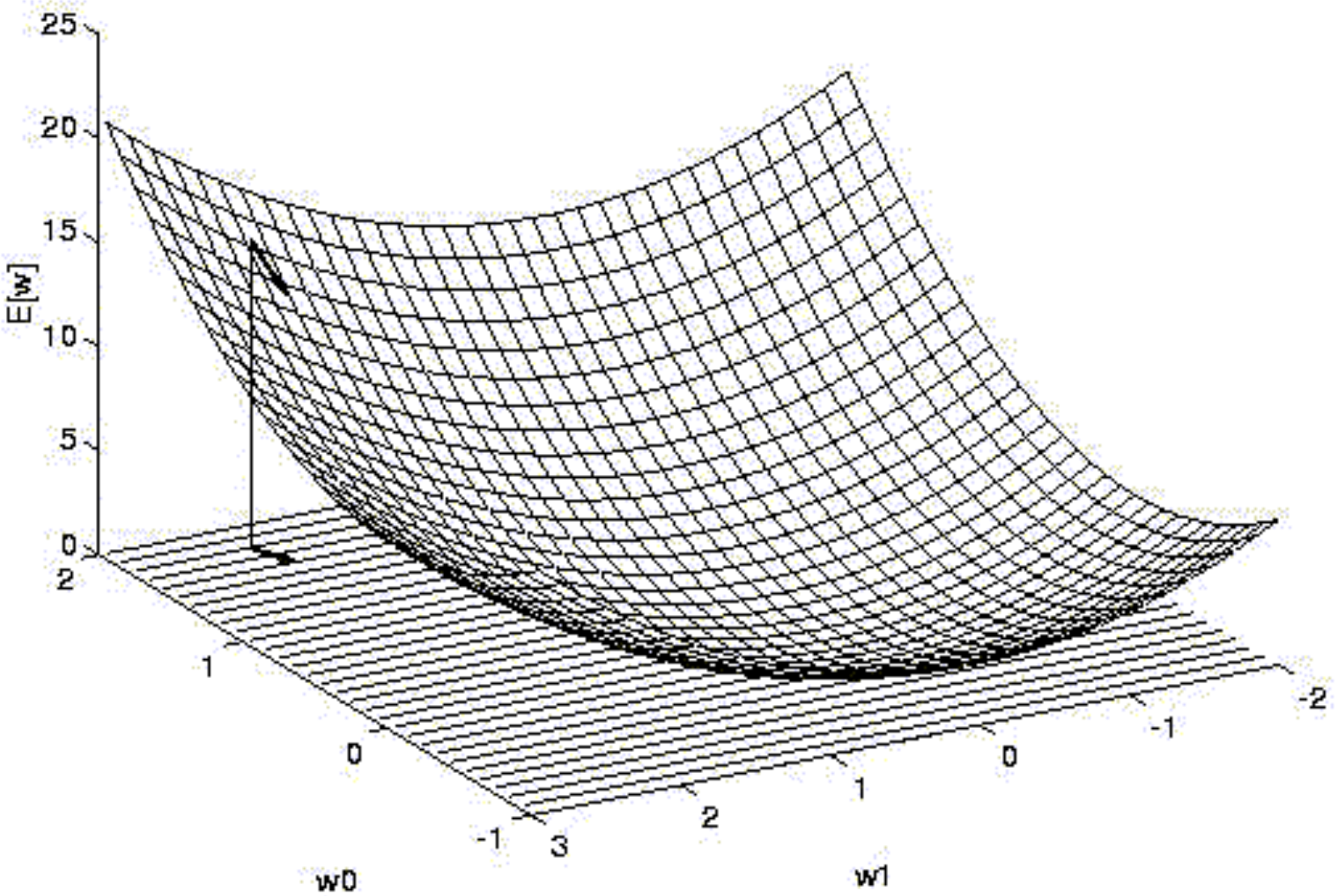
Incremental mode Gradient Descent:
Do until satisfied:
- For each training example *d* in *D*

1. Compute the gradient $\nabla E_d[\vec{w}]$
2. $\vec{w} \leftarrow \vec{w} - \eta \nabla E_d[\vec{w}]$

$$E_d[\vec{w}] \equiv \frac{1}{2} (t_d - o_d)^2$$

Incremental Gradient Descent can approximate *Batch Gradient Descent* arbitrarily closely if η made small enough

Example loss function vs (w_0,w_1)



Training: find **w**= (w_0,w_1) such that E(**w**) minimal