Machine learning methods applied to the analysis of central exclusive production events in ALICE

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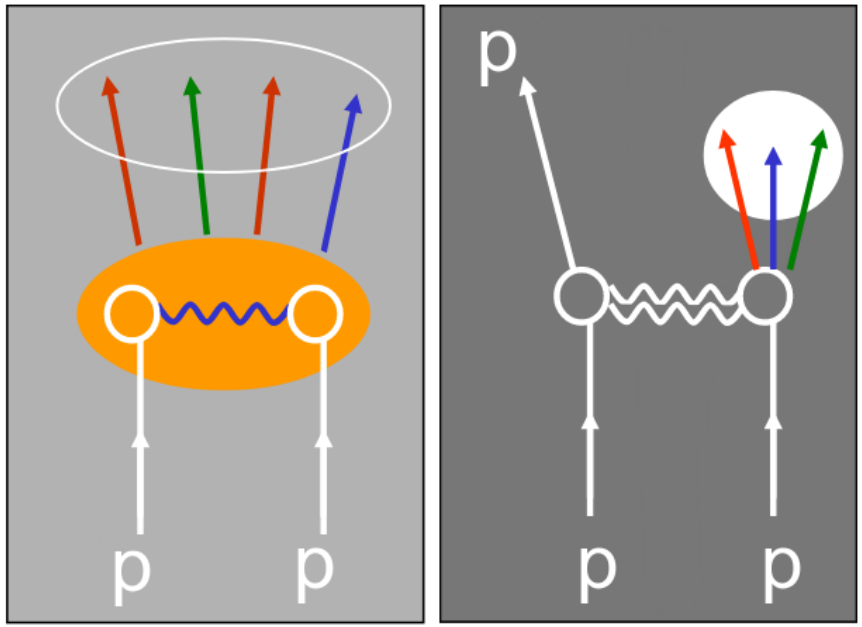
ÖAW ÖSTERREICHISCHE AKADEMIE DER WISSENSCHAFTEN

Outline

Diffractive events

Diffractive events are reactions where no quantum numbers are exchanged

Incident hadrons aquire color
$\rightarrow$ break apart



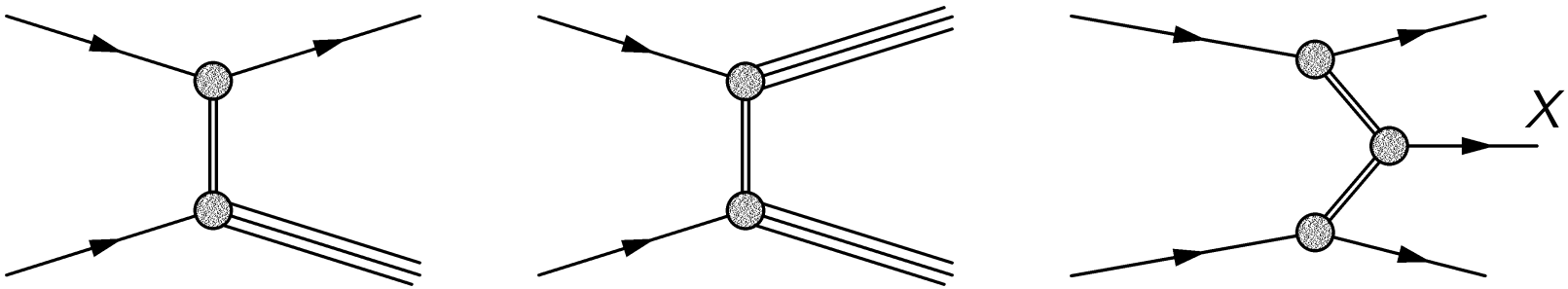
Colorless exchange with *vacuum* quantum numbers

η gap exponentially supressed

η gap not supressed

Diffractive processes

Different types of diffractive events are distinguished



Single diffractive | Double diffractive | CEP

Described by *Regge* theory

Regge theory - short overview

- Reactions characterized by a color neutral t -channel exchange carrying vacuum quantum numbers
- t-channel process governed by exchange of resonances sitting on *Regge trajectory* $\alpha(t) = \alpha + \alpha' t$
- Resonance of mass m sitting on the trajectory at $t = m^2$ has angular momentum of value $\alpha(m^2)$
- Trajectory makes contribution to total inelastic cross section $\sigma_{tot}(s) \propto s^{\alpha-1}$

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- Pomeron $\mathbb{P}$ represents special Regge trajectory & is a color singlet state of gluons & has vacuum quantum numbers
- Contribution to σ_{tot} grows with increasing energy
- Double Pomeron exchange = production mechanism to study glueballs in the mass region below 2 MeV
- Pomeron exchange leads to restriction of quantum numbers of X
  $\rightarrow J^{PC} = (\text{even})^{++}$

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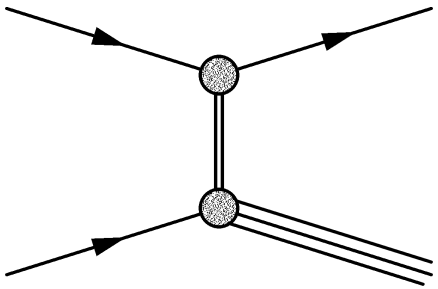
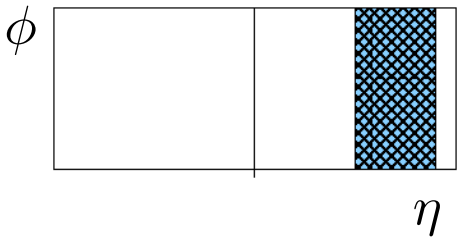
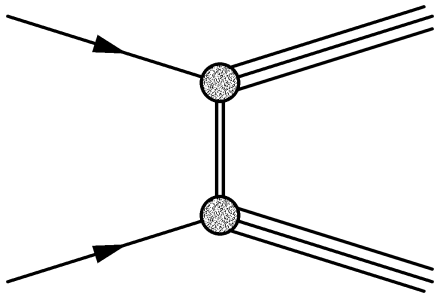
Event topology

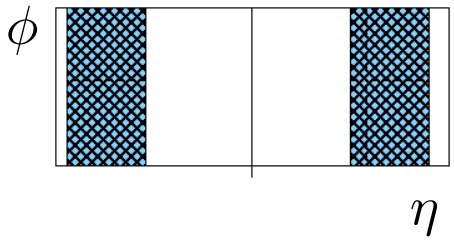
Single diffractive



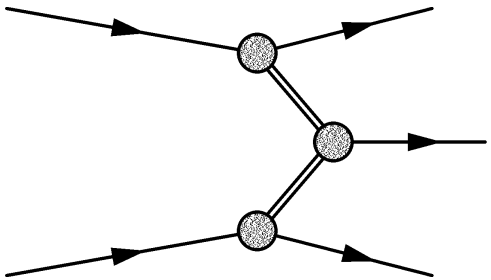


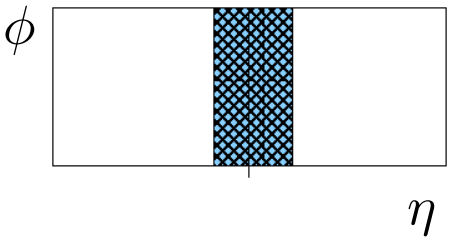
Double diffractive





CEP





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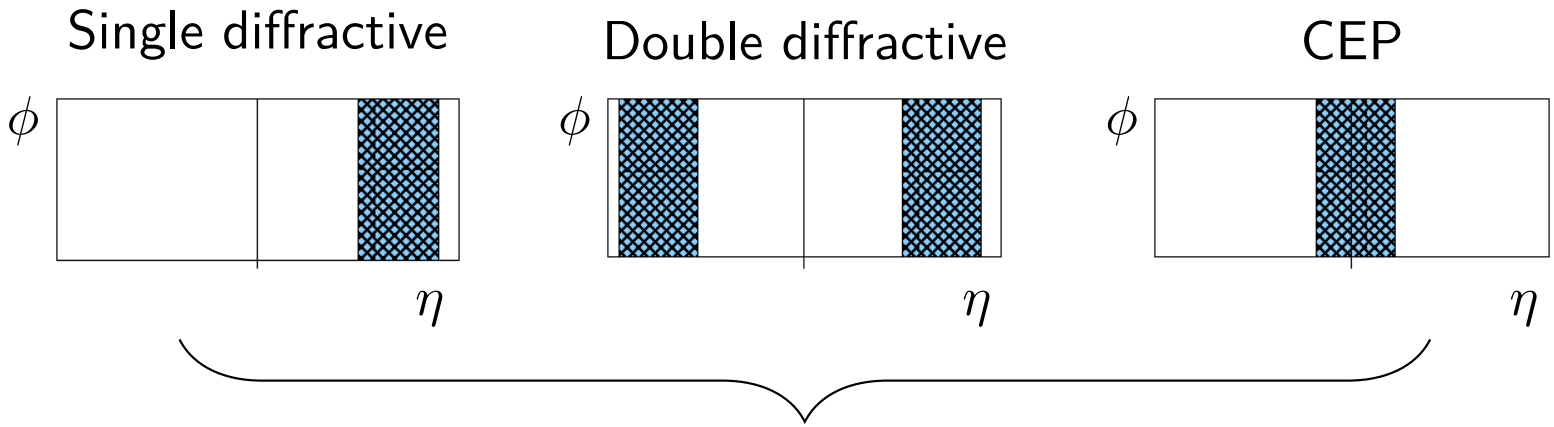
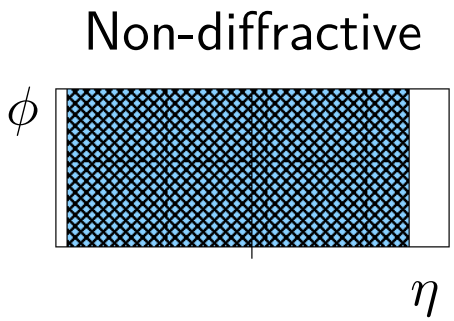
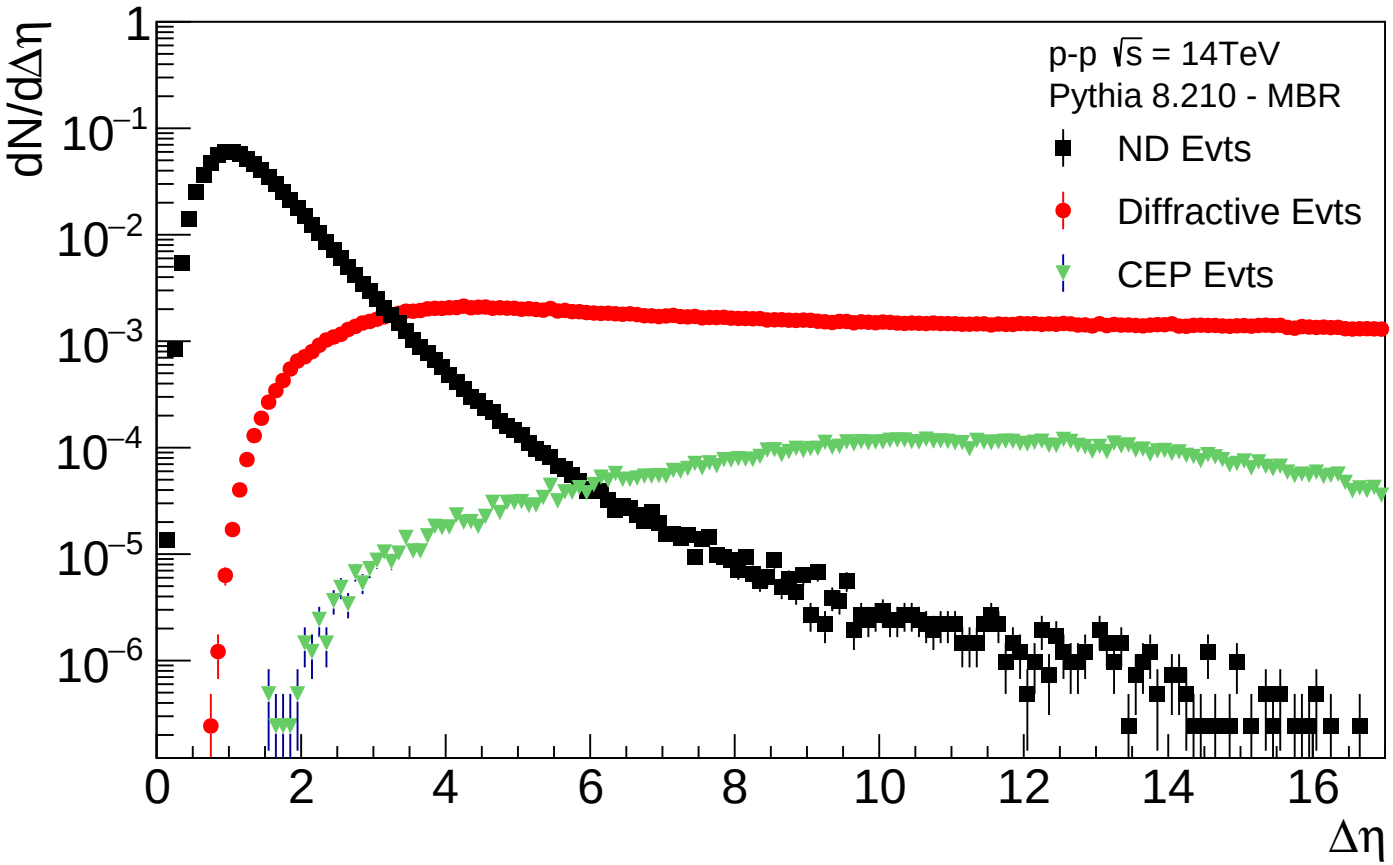




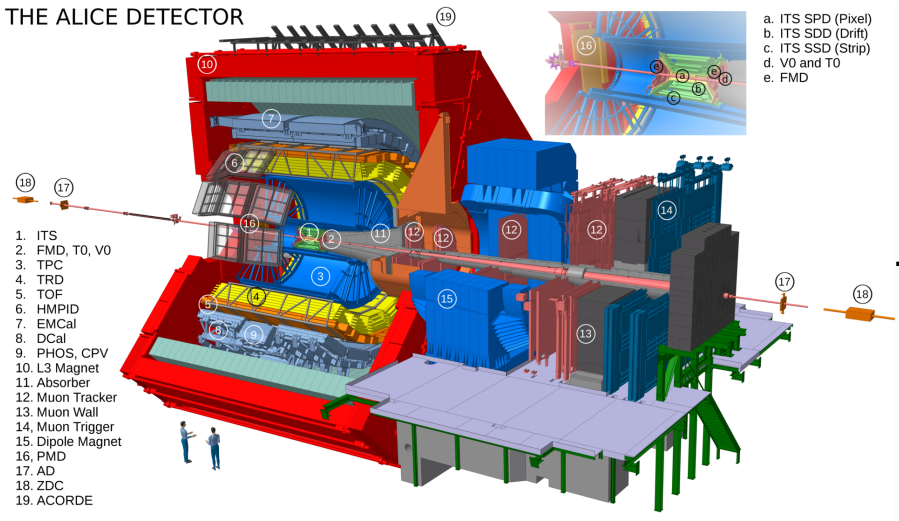
Event selection

Large rapidity gaps in *non-diffractive* events are exponentially supressed

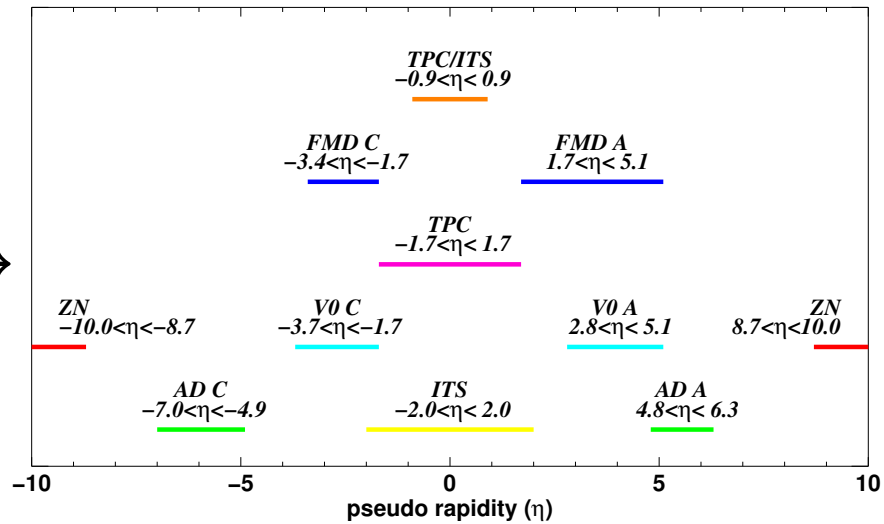


The ALICE detector system

ALICE detector



η coverage



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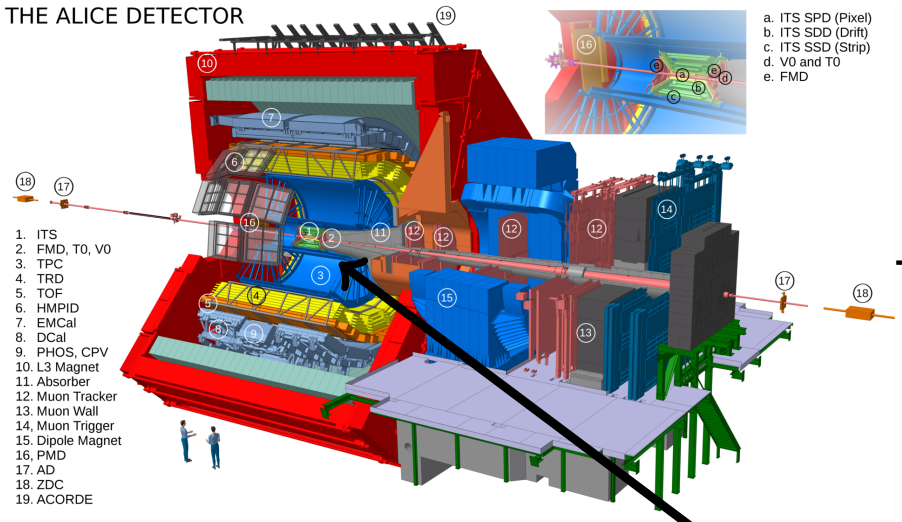

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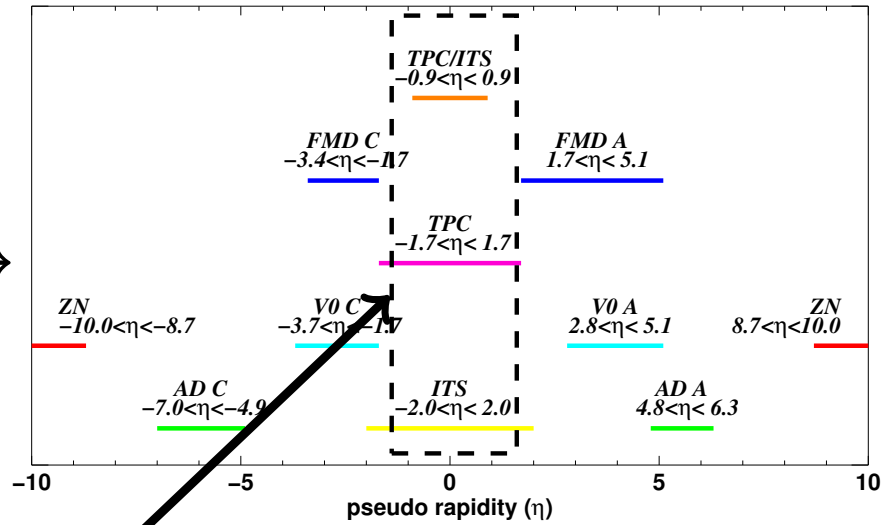

Central barrel $\rightarrow$ determine p^{μ}

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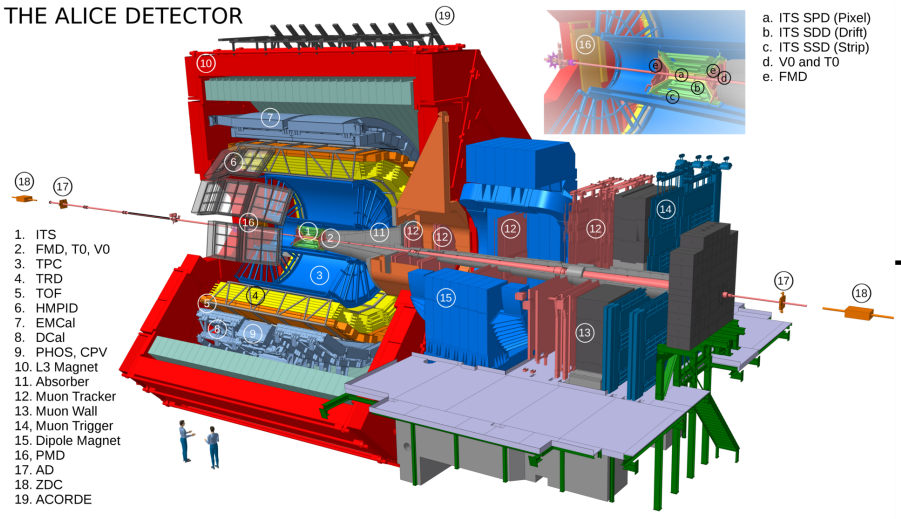

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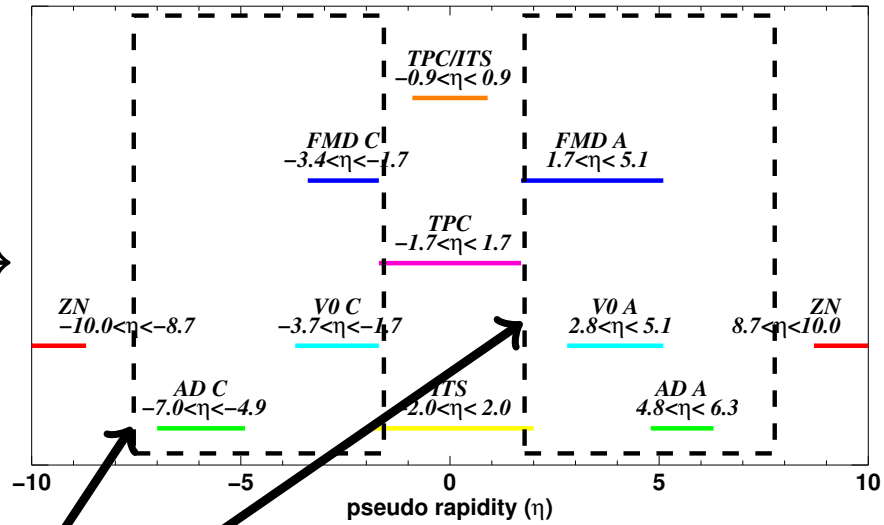


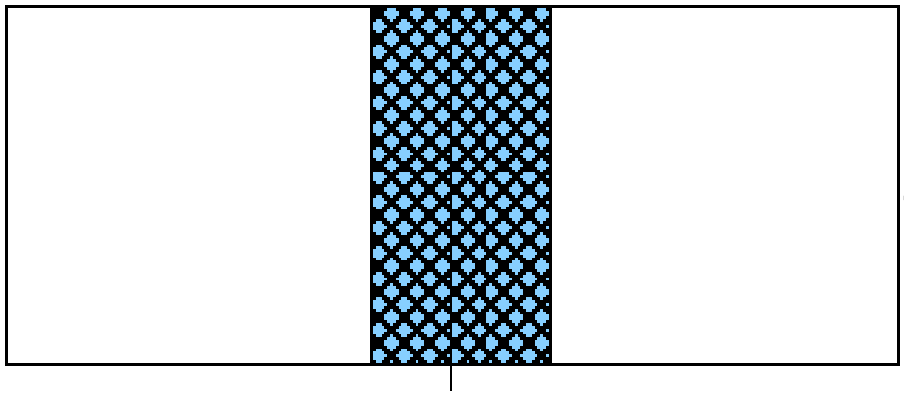
Small detectors for global event characterisation

Central exclusive production at ALICE

To study the CEP events a η gap condition is used

1. Signal in the central barrel
2. No activity in veto detectors

CEP event



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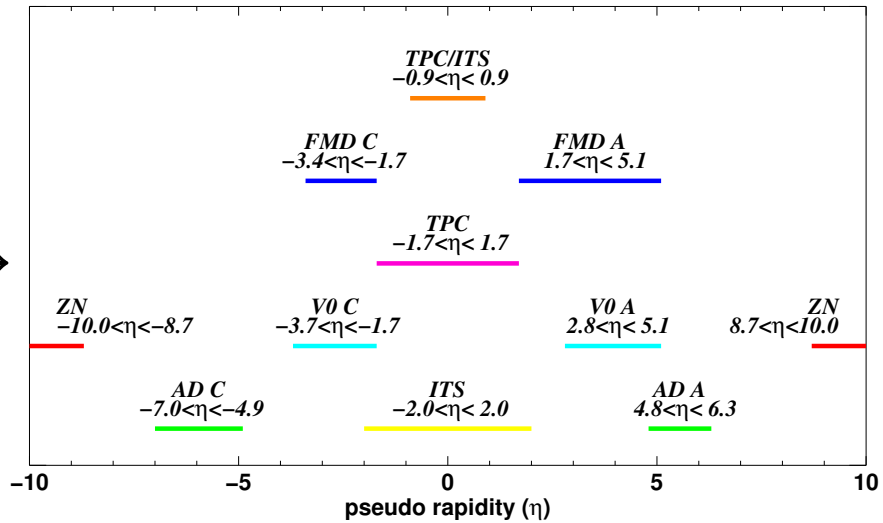

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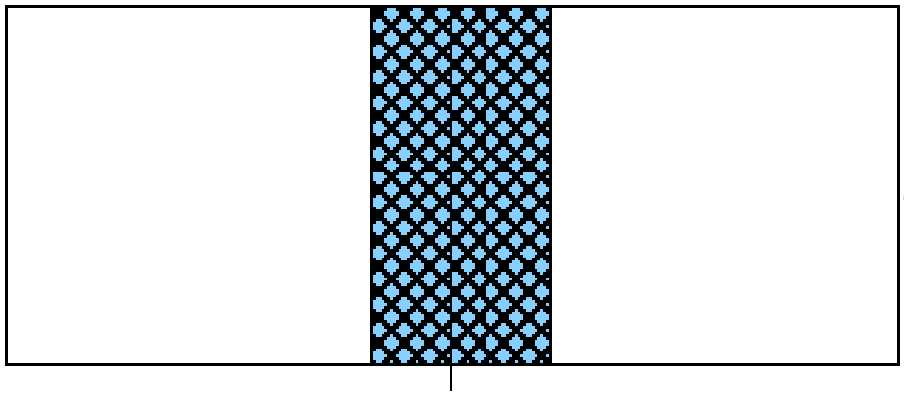

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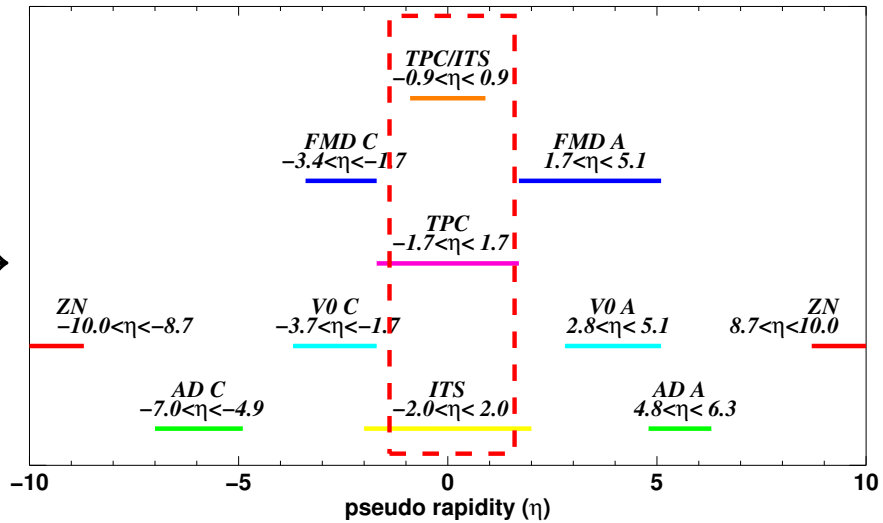

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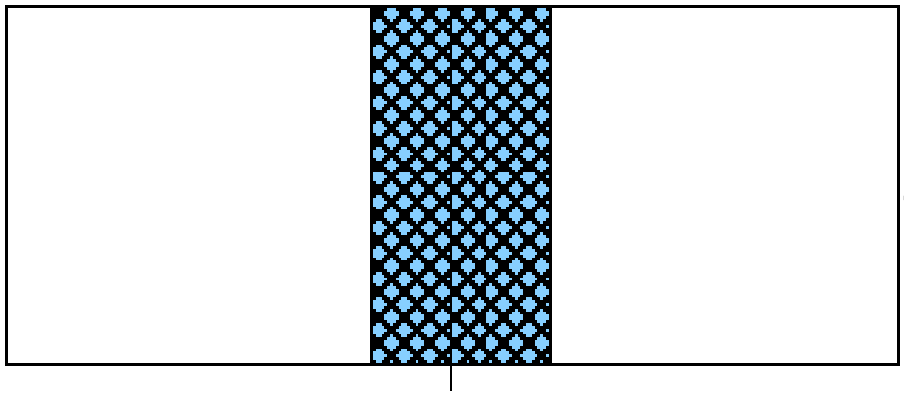

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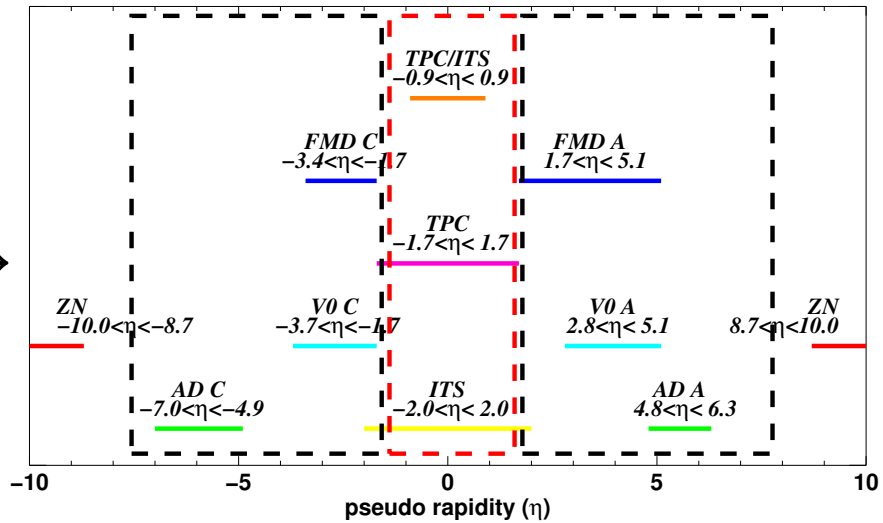
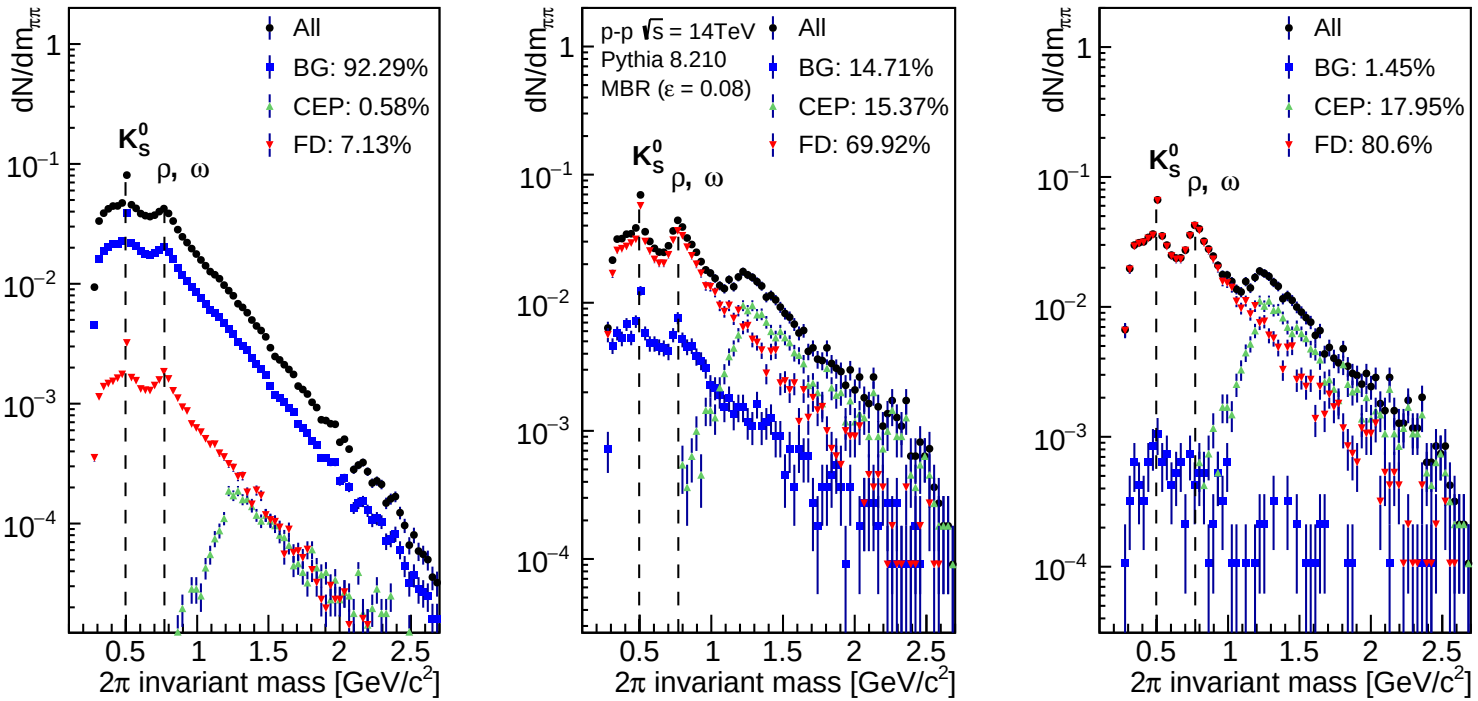


Invariant mass spectrum

Studying *Pythia-8* simulations yield

- Enforcing η gap cut reduces non-diffractive almost entirely
- Remaining background are partially recontructed CEP events - **feed down**



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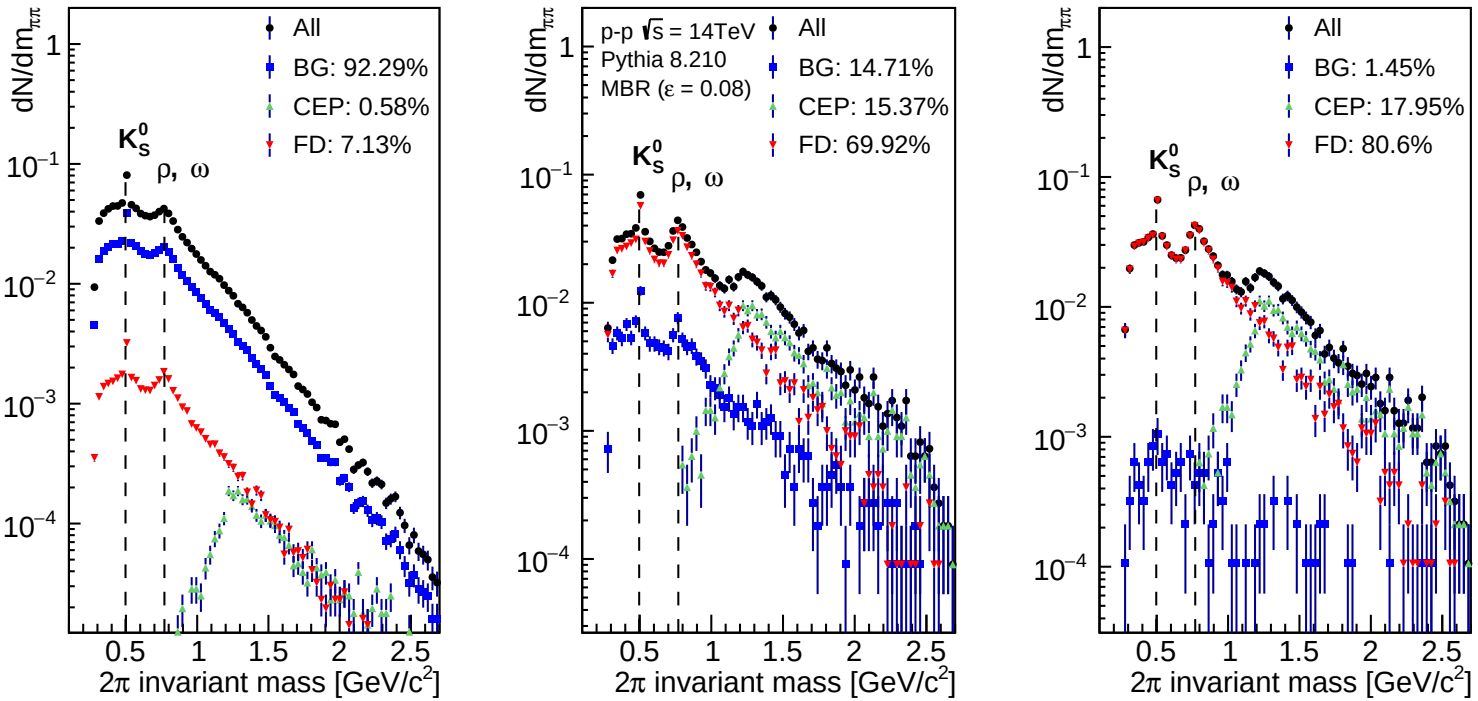

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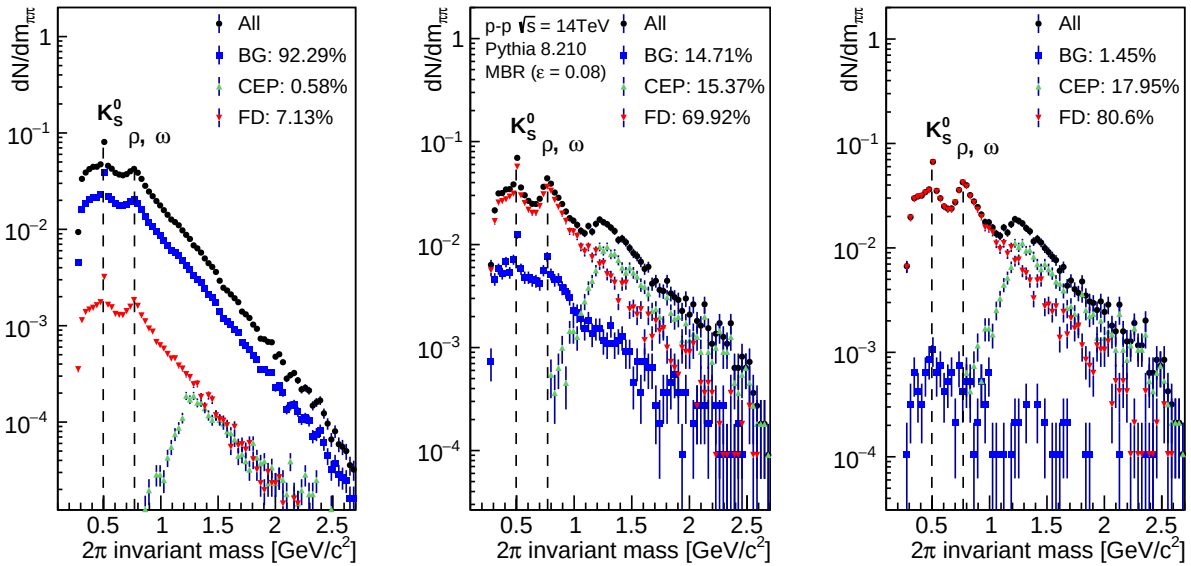

ML: an overview

In general ML represents a contrast to a *rule based systems*

Rule-based system

System that uses rules to make deductions or choices

- Domain-specific expert system
- Knowledge base: facts & rules (if $\rightarrow$ then statement)
- Rules manually specified (by expert) $\rightarrow$ expensive, incomplete

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- Alorithms that learn from *data* & make predictions on *data*
- Automatic methods $\rightarrow$ no human needed
- Human work required for defining problem & assessing the data

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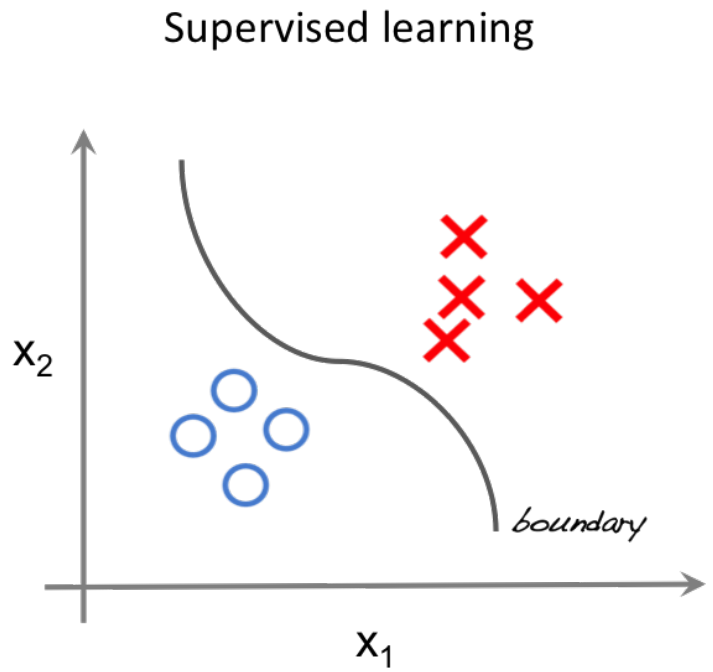
Types of ML

- Supervised
  - Classification
  - Regression
- Unsupervised



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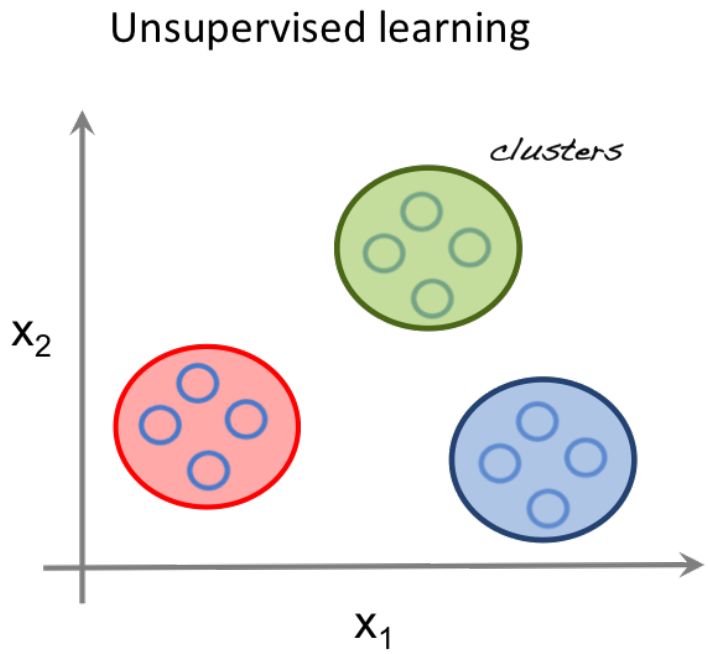
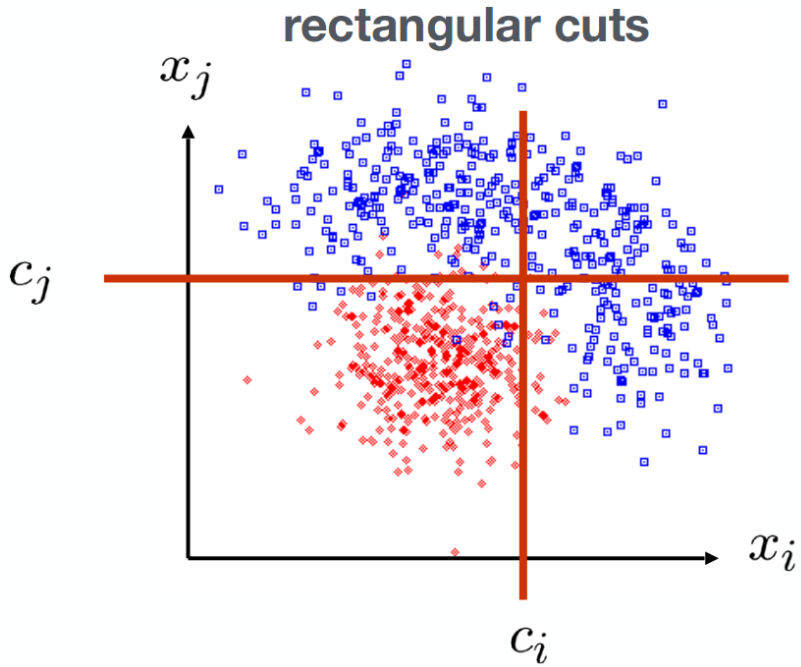


Rectangular cuts

Standard cut in one variable

- Cuts only in lower-dimensional subspaces
- Ignores possible dependencies between the input variables
- Signal might behave like BG in several observables
  $\rightarrow$ misclassification



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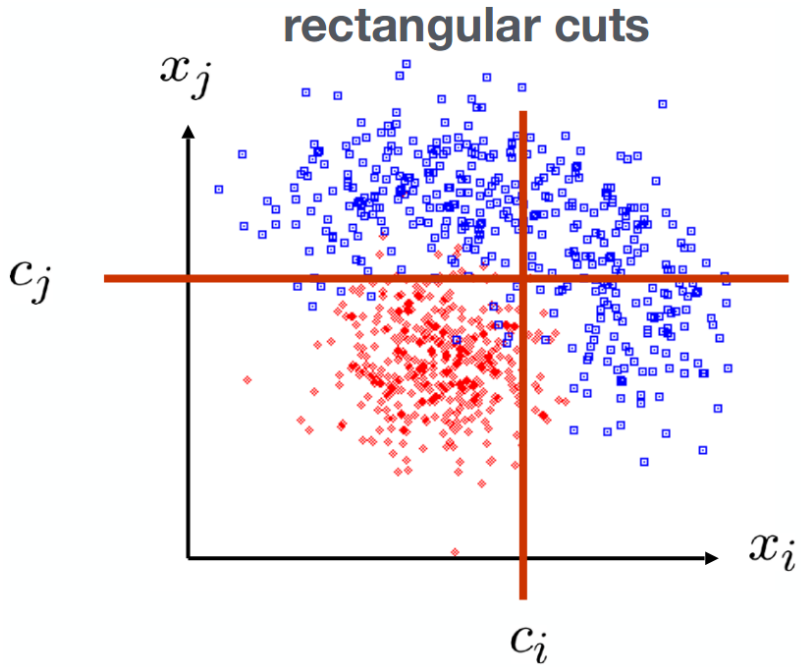

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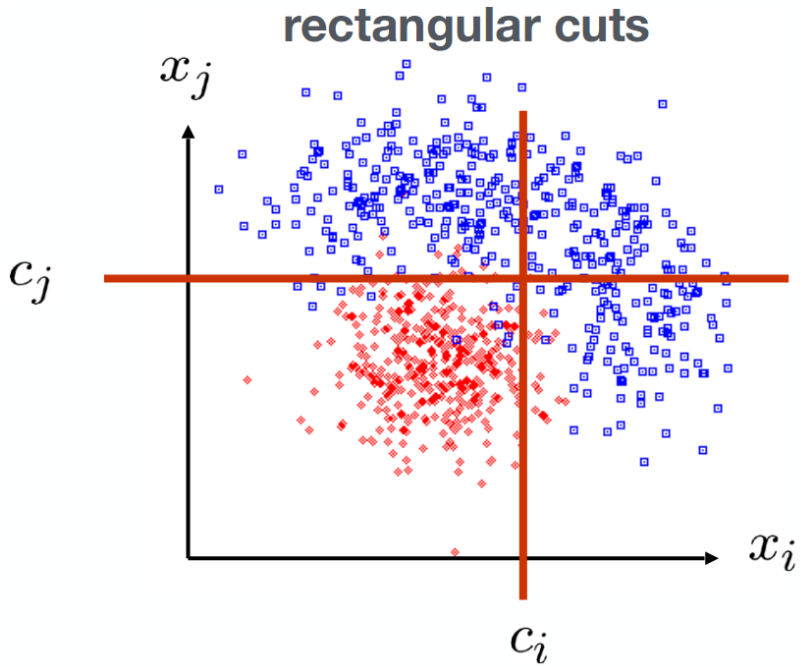
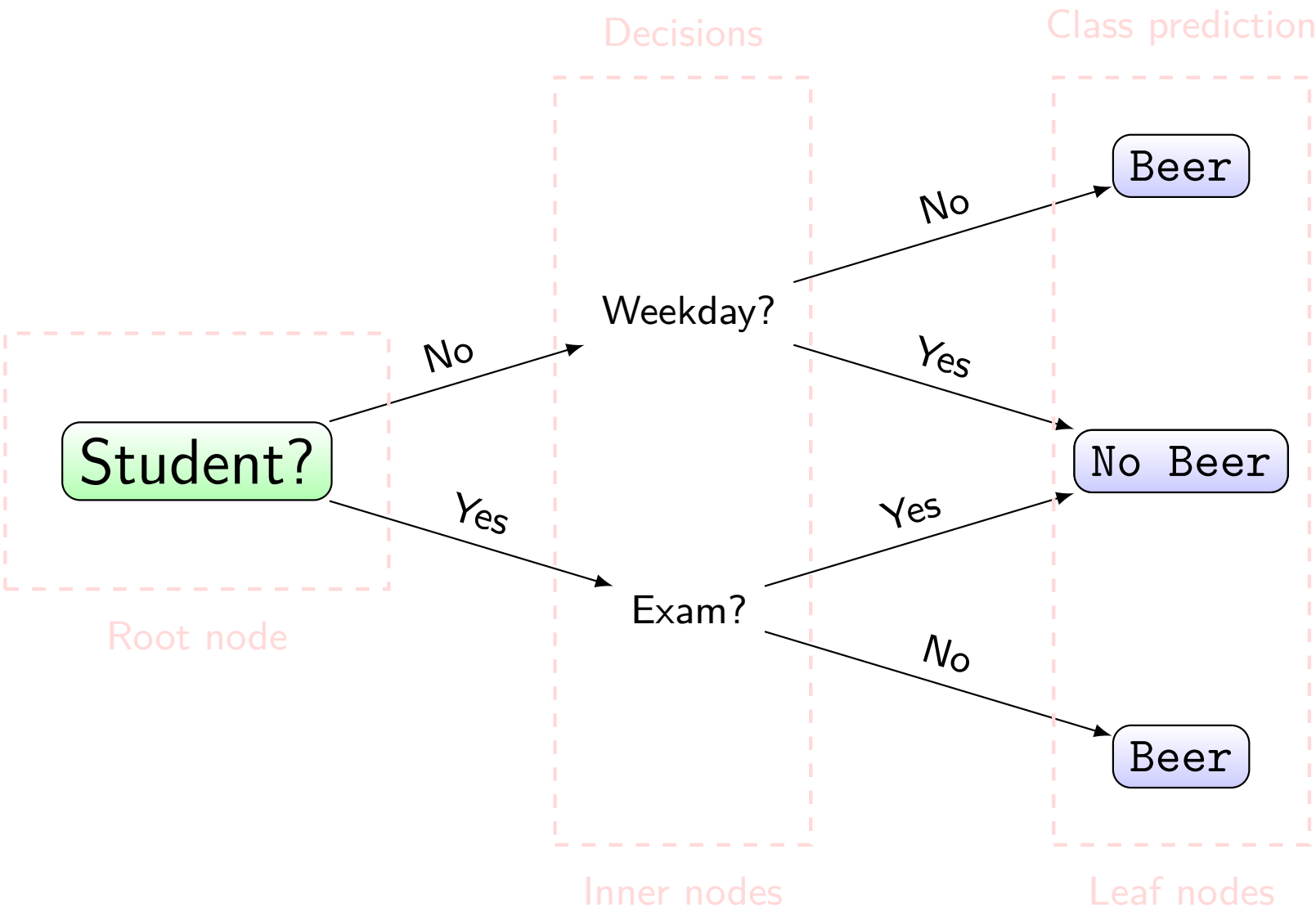


Rectangular cuts with *decision trees*

- Tree-like graph $\rightarrow$ flowchart
- Easy to understand
- Either be manually modelled by experts or learned from training data

Rectangular cuts with *decision trees*



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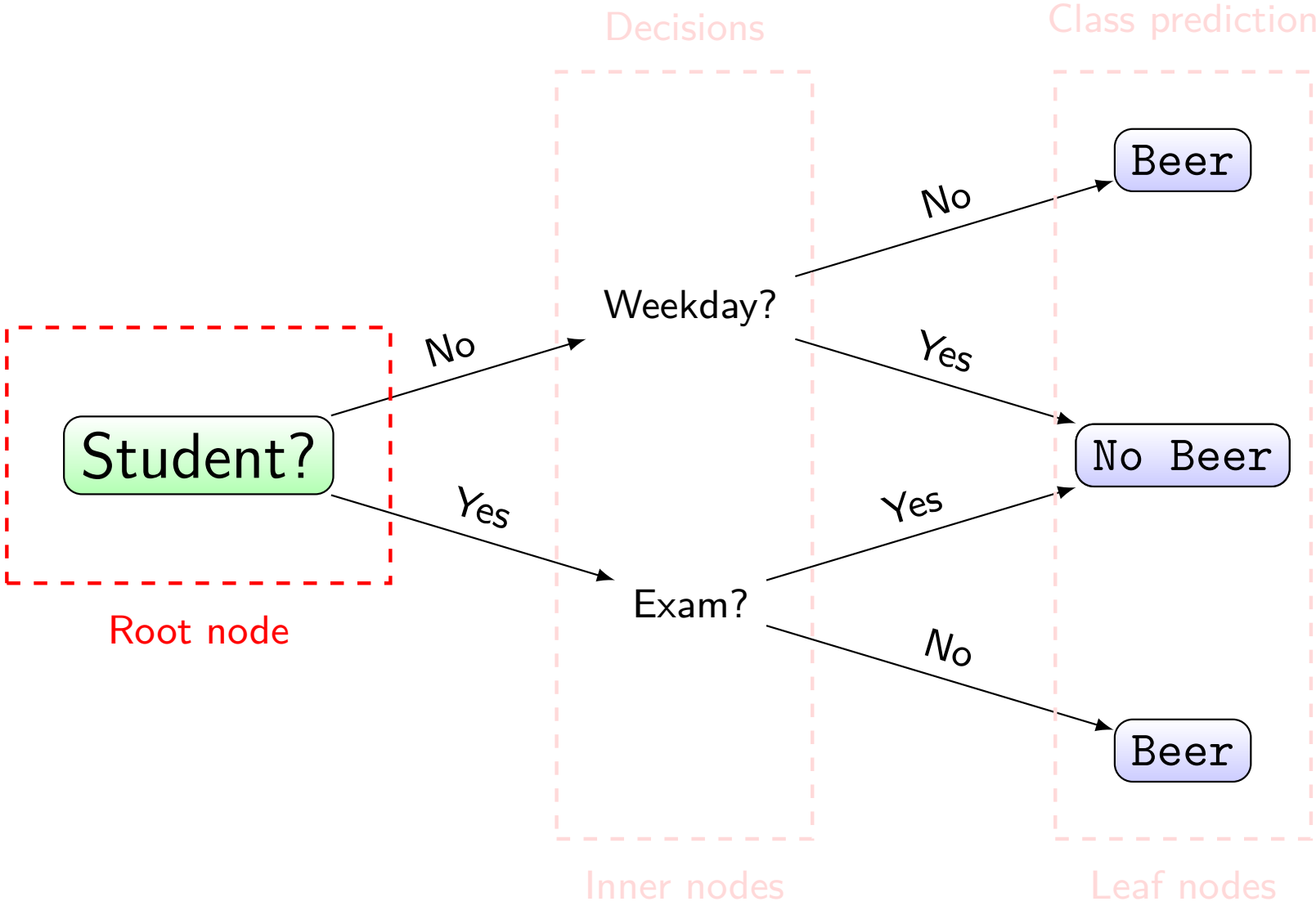

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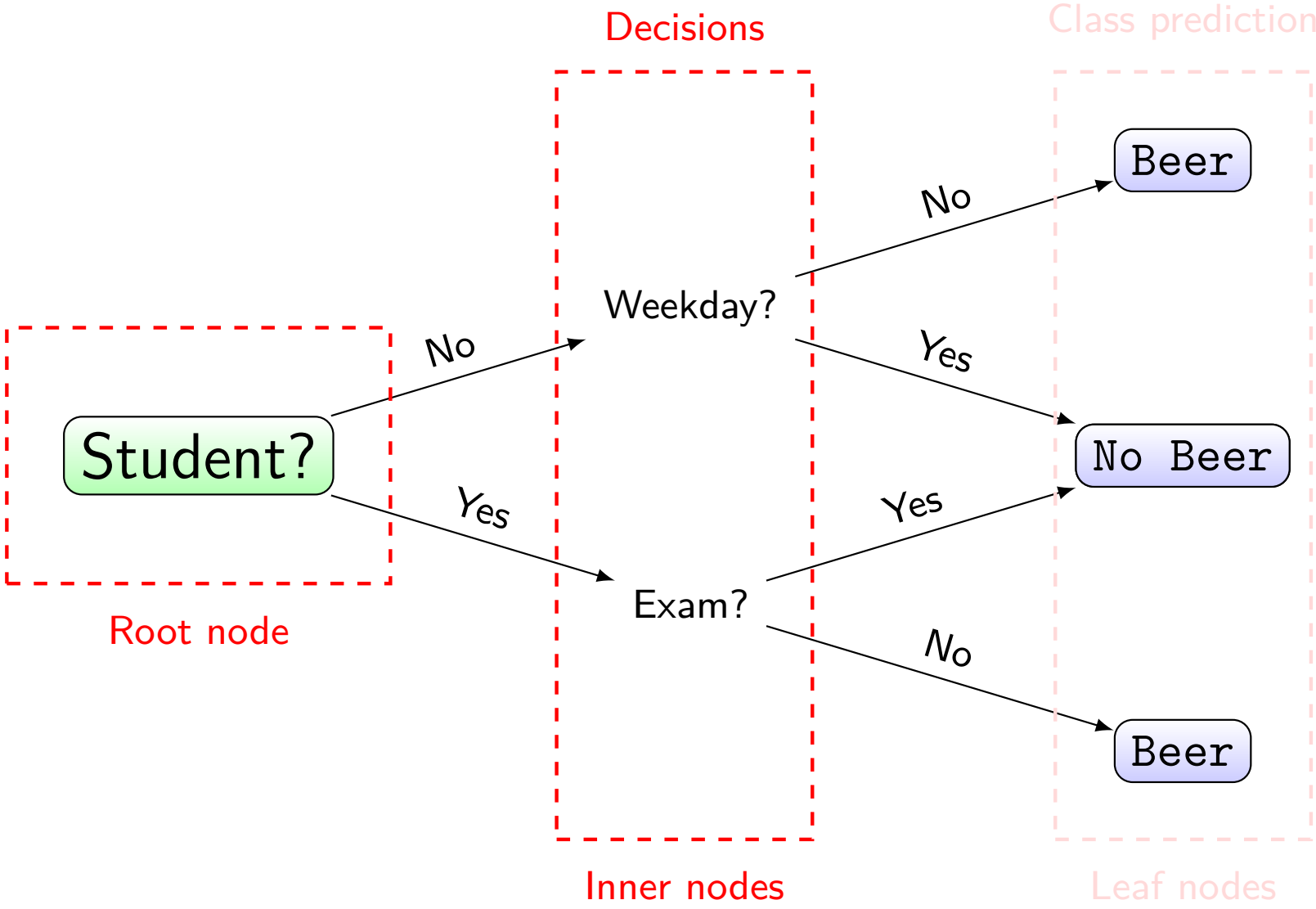

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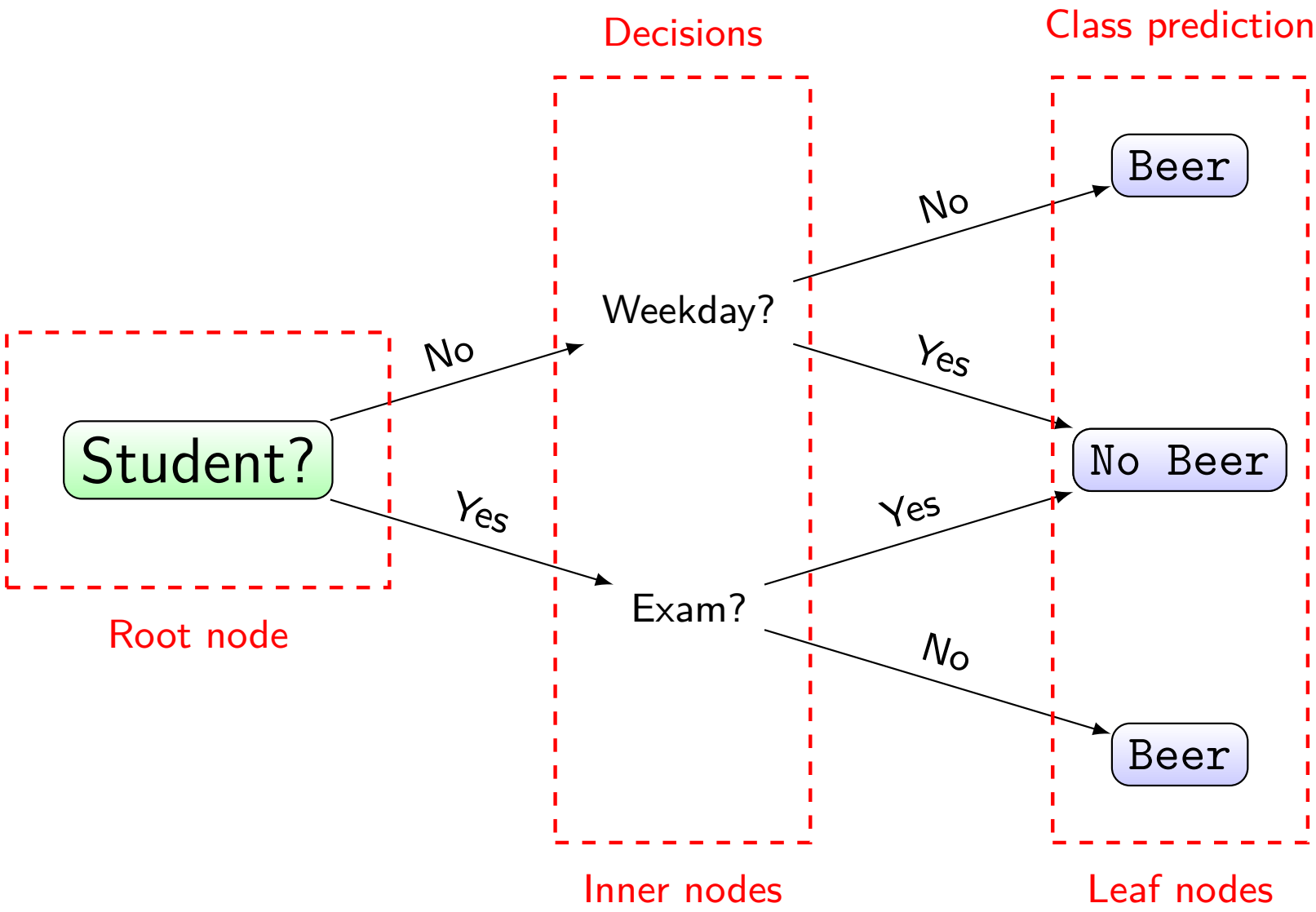


Decision tree learning

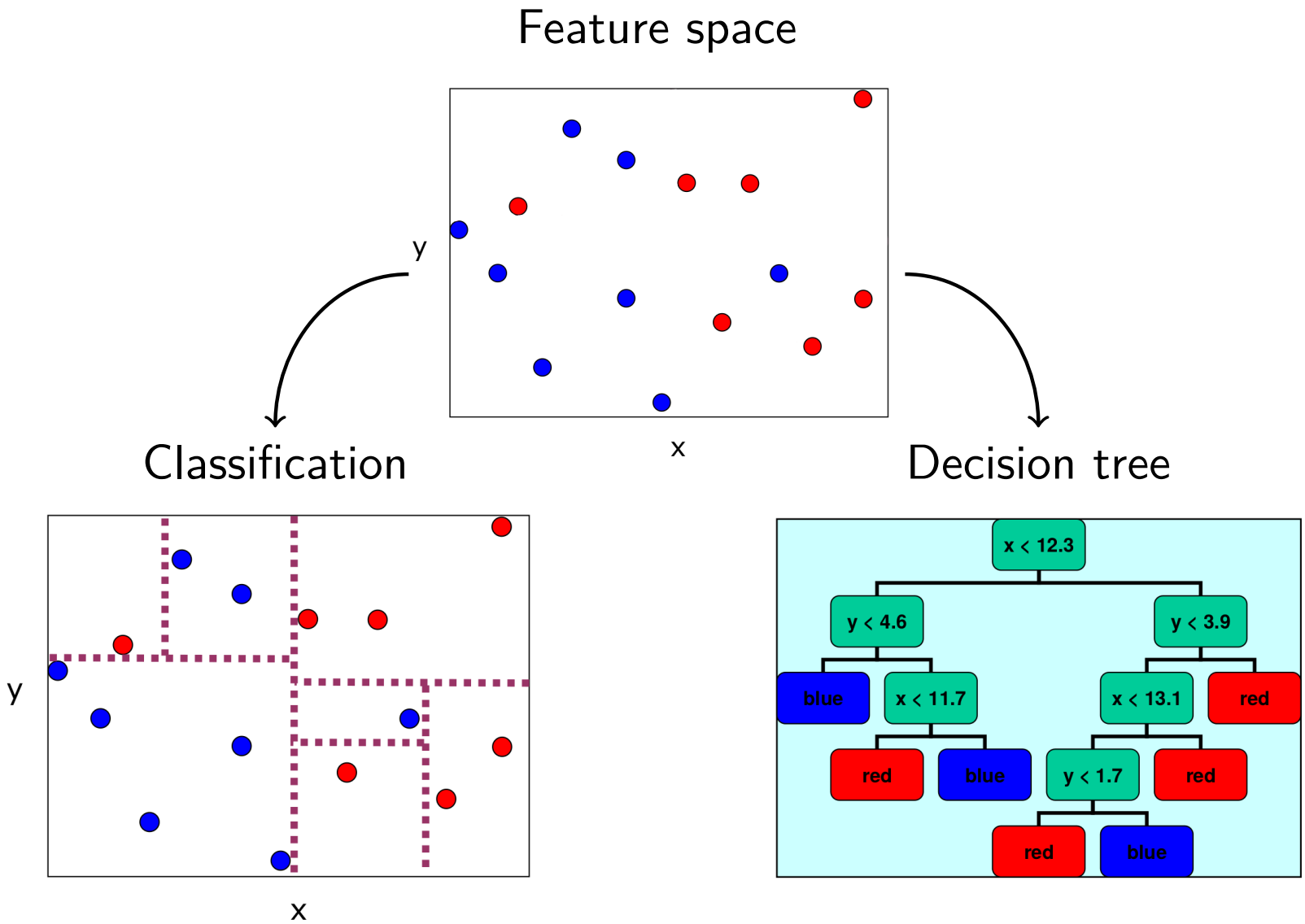
Training

Recursively split feature space into sub-spaces at each step

$\rightarrow$ Measures to evaluate split

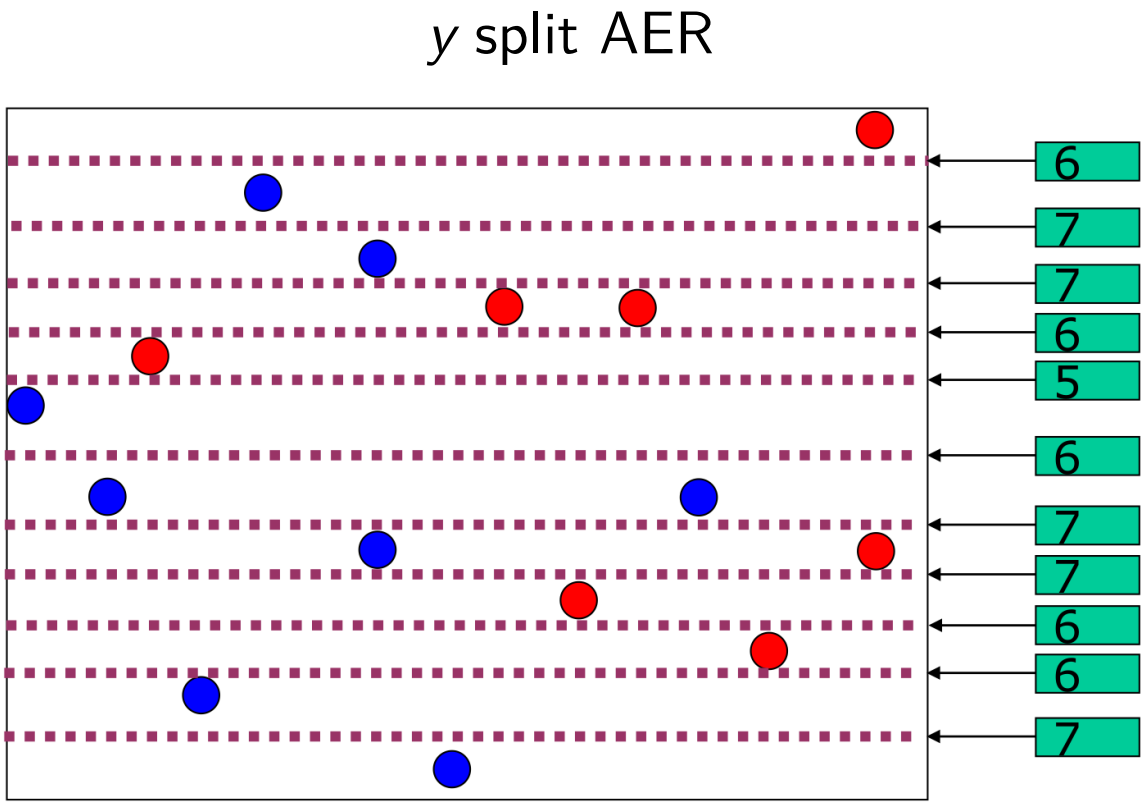
- Error rate
- Information gain
- Gini index

Decision tree learning



Decision tree learning

1) We compute a measure for *each possible split* in each feature
   $\rightarrow$ here **absolute error rate** (AER)



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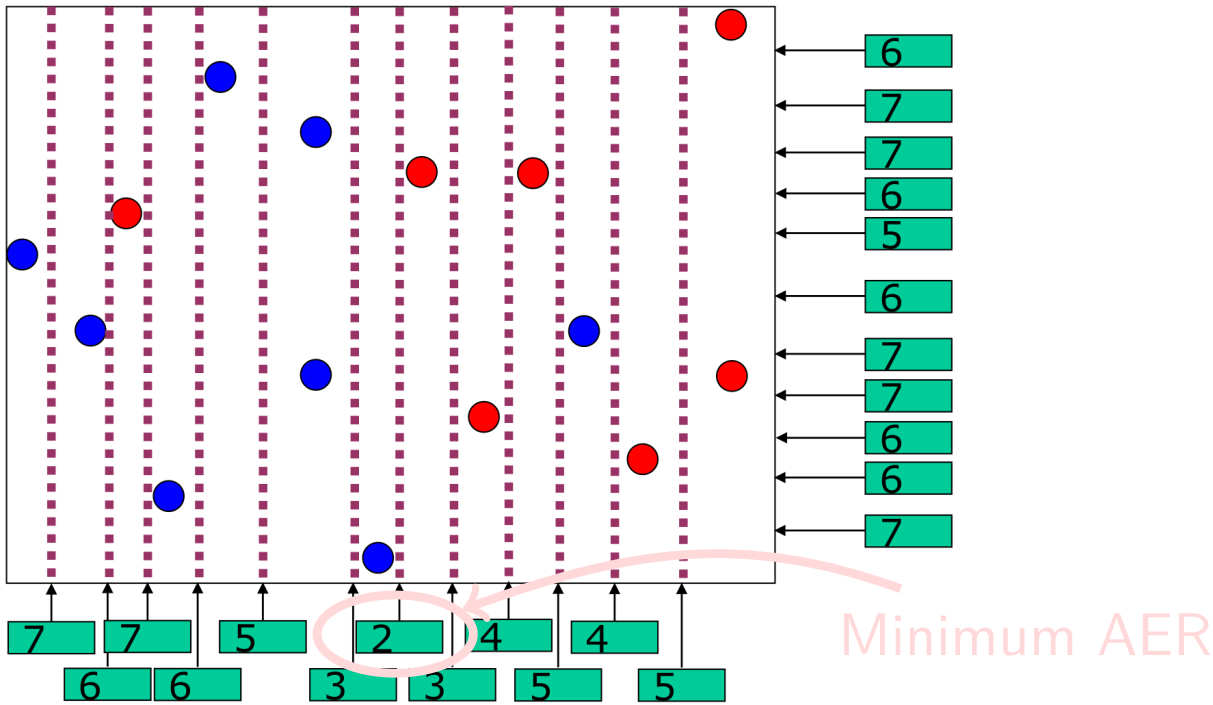
x-*y* split AER



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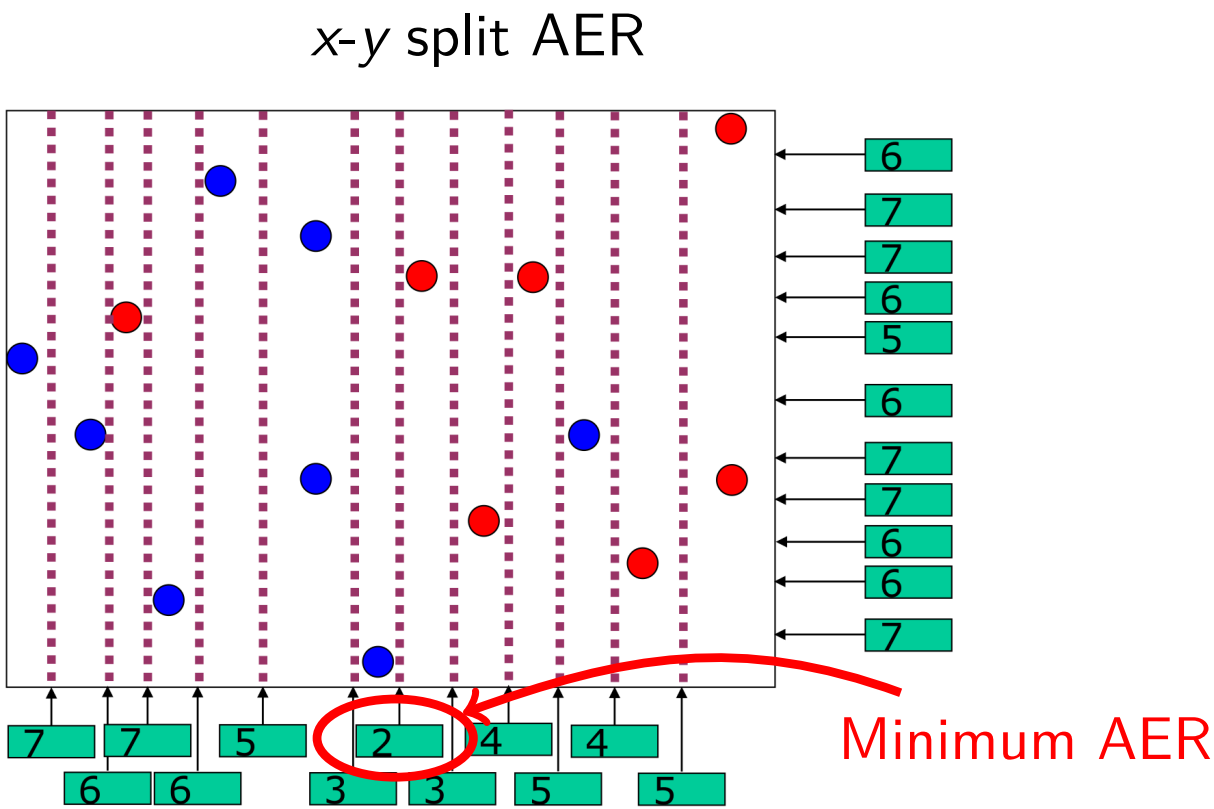

Decision tree learning

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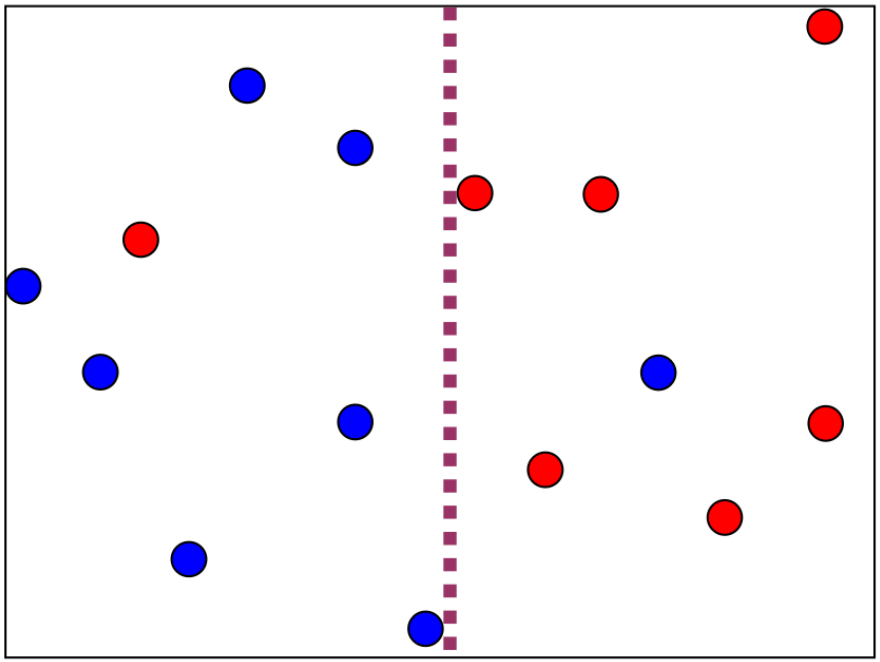

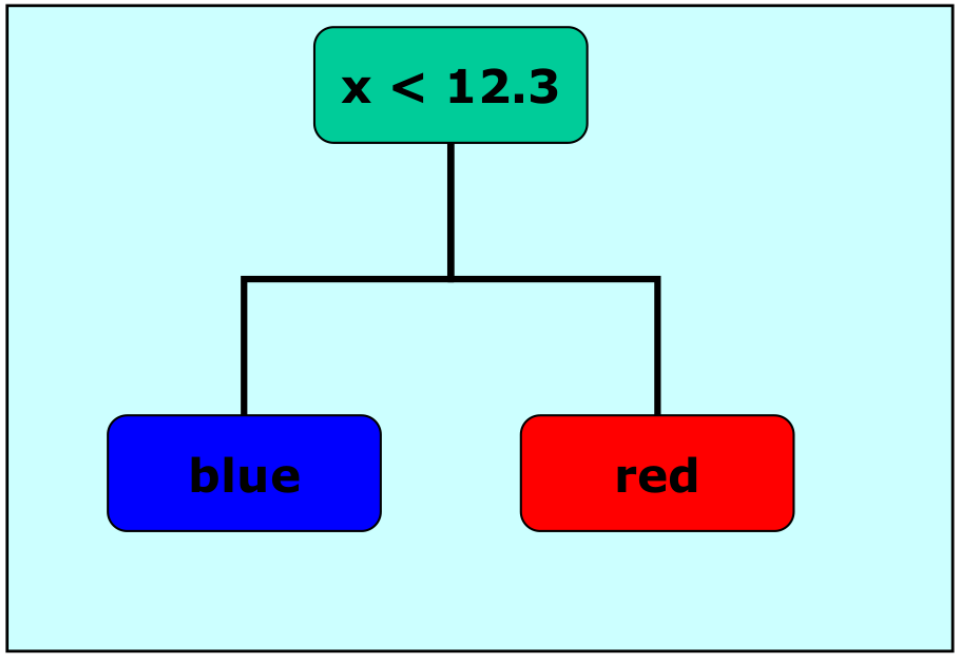

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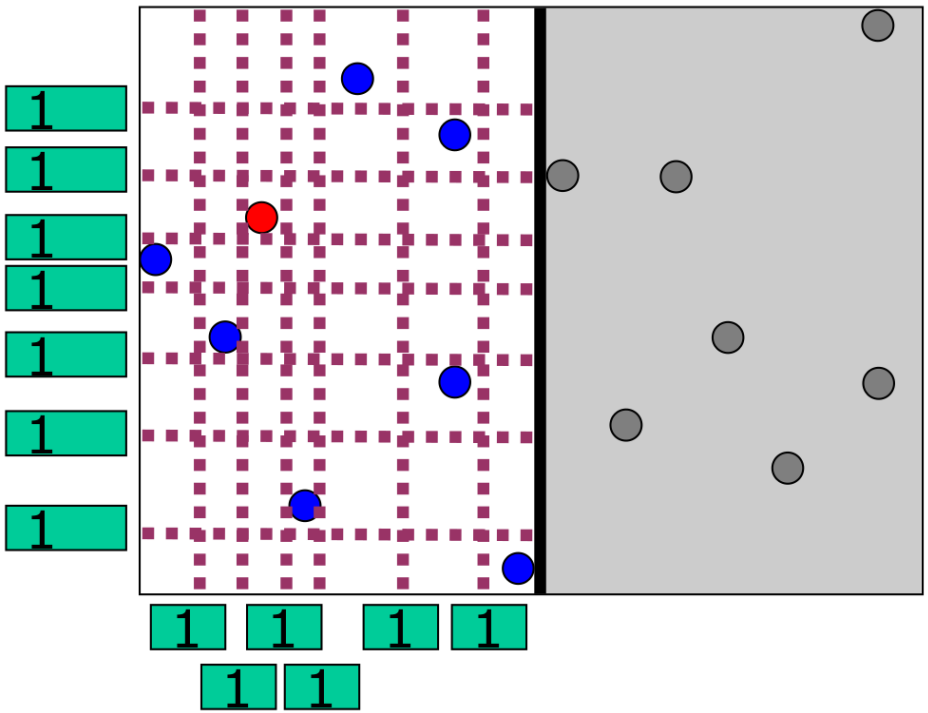

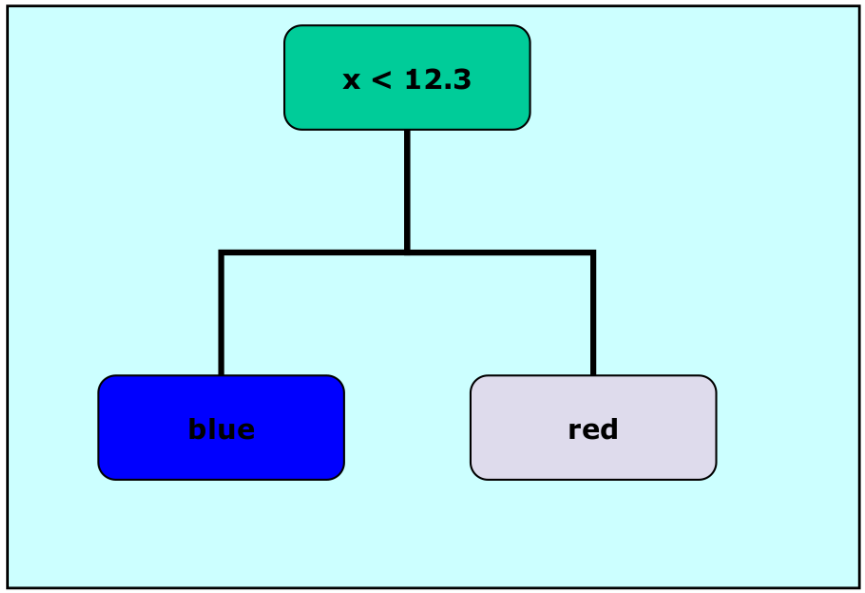

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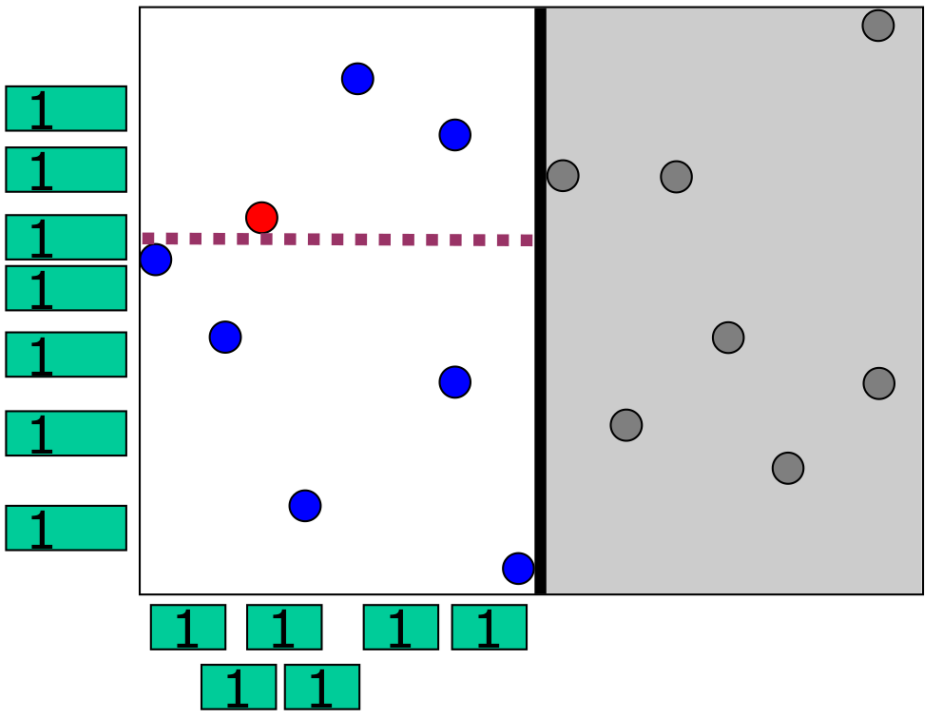

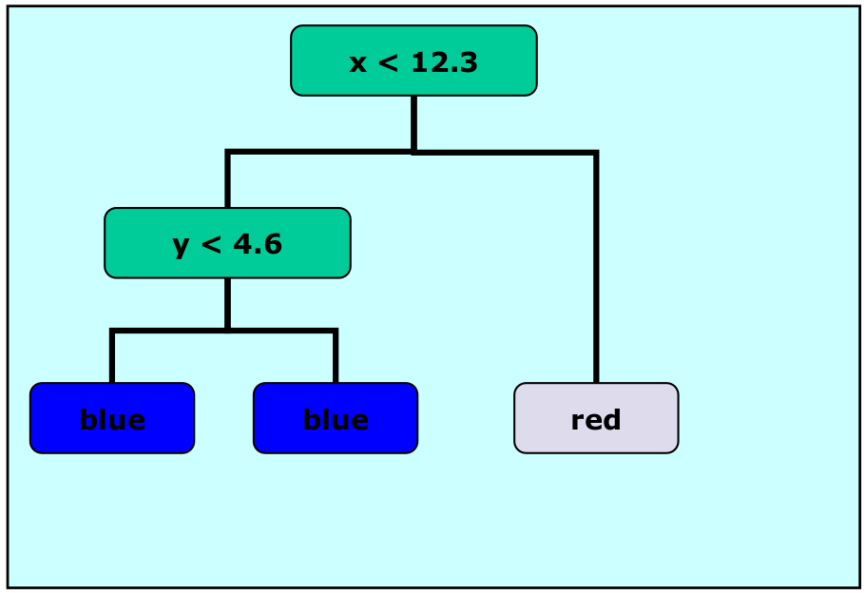

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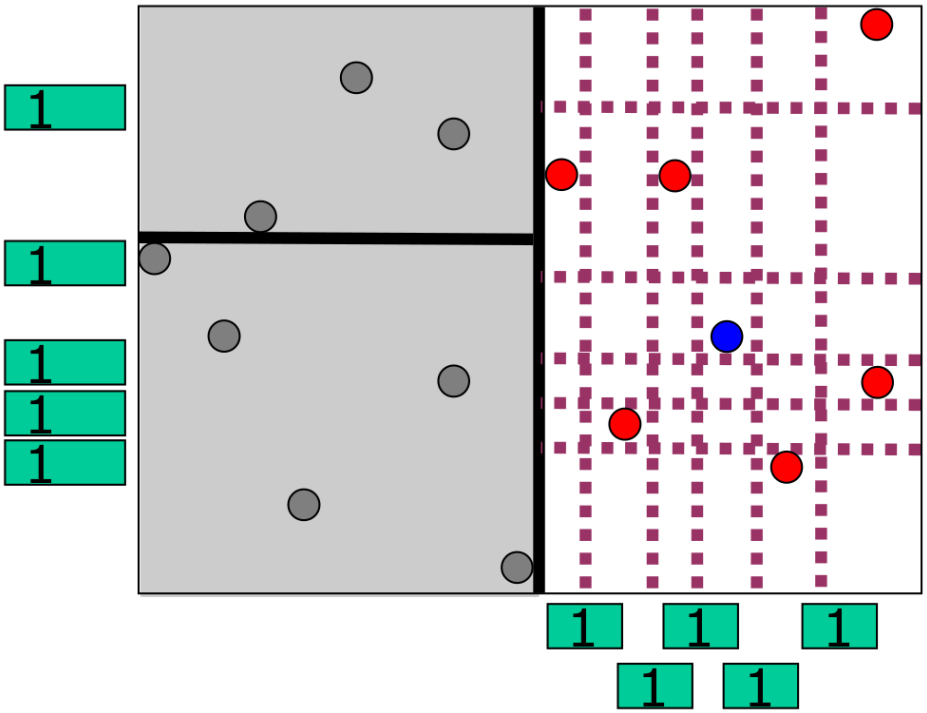

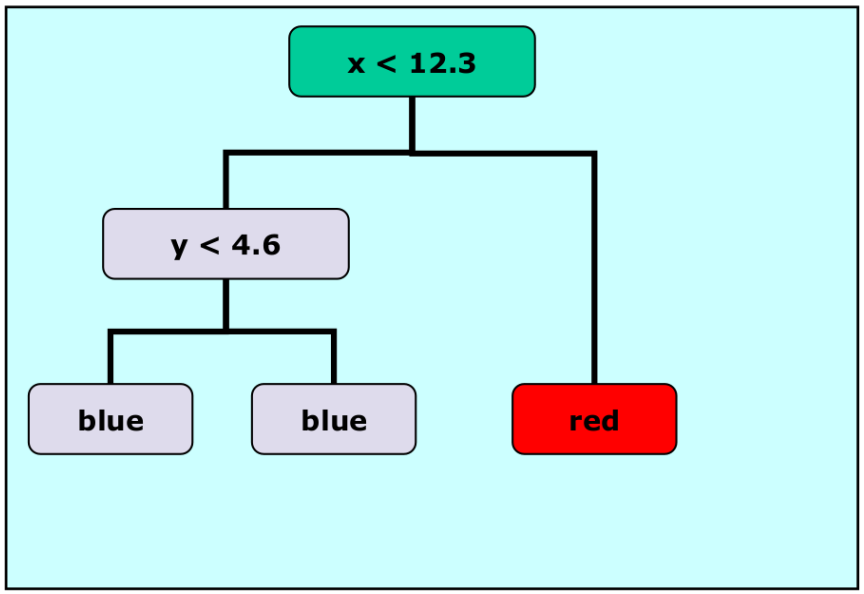

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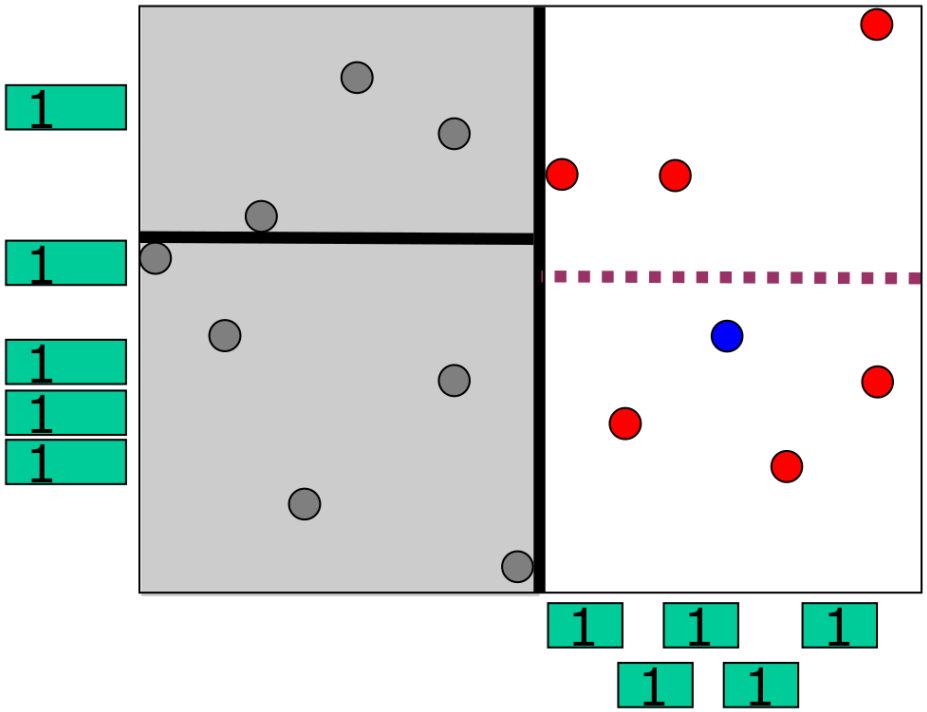

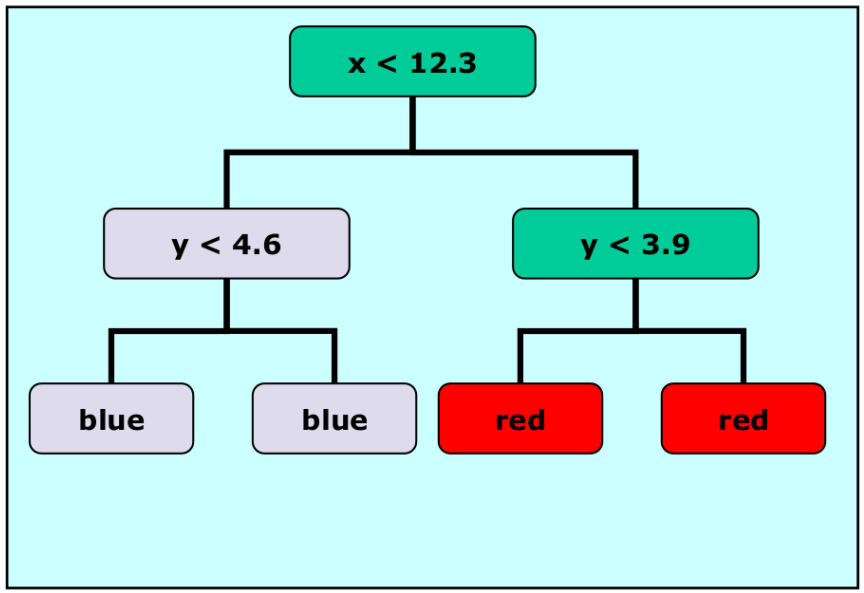

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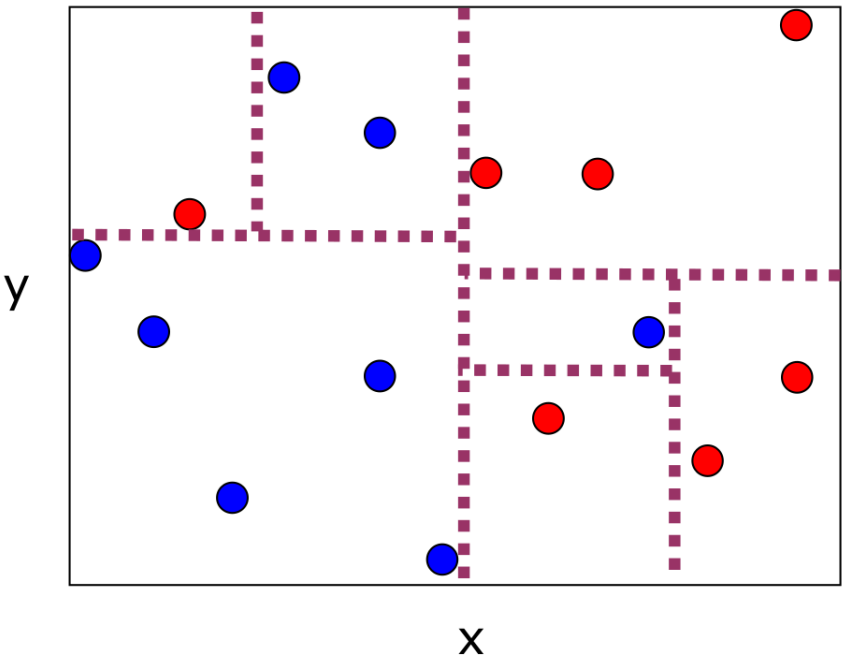
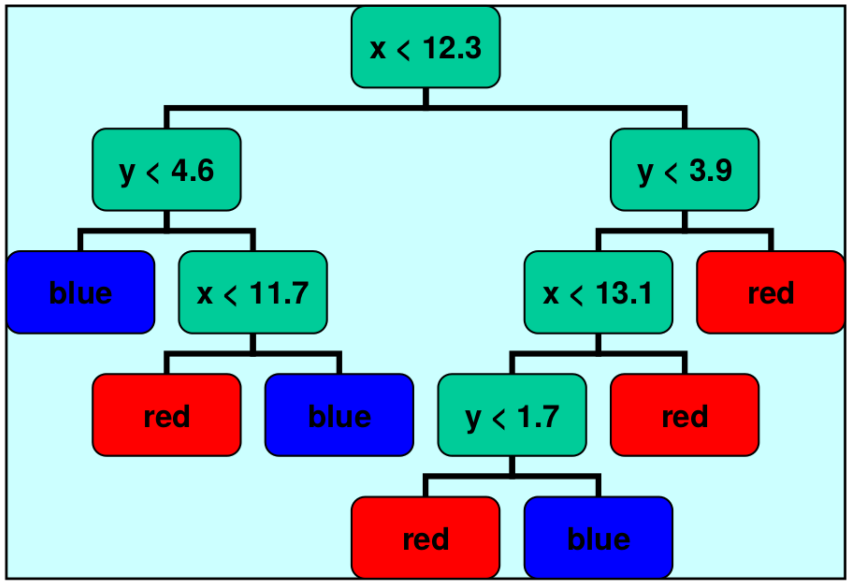
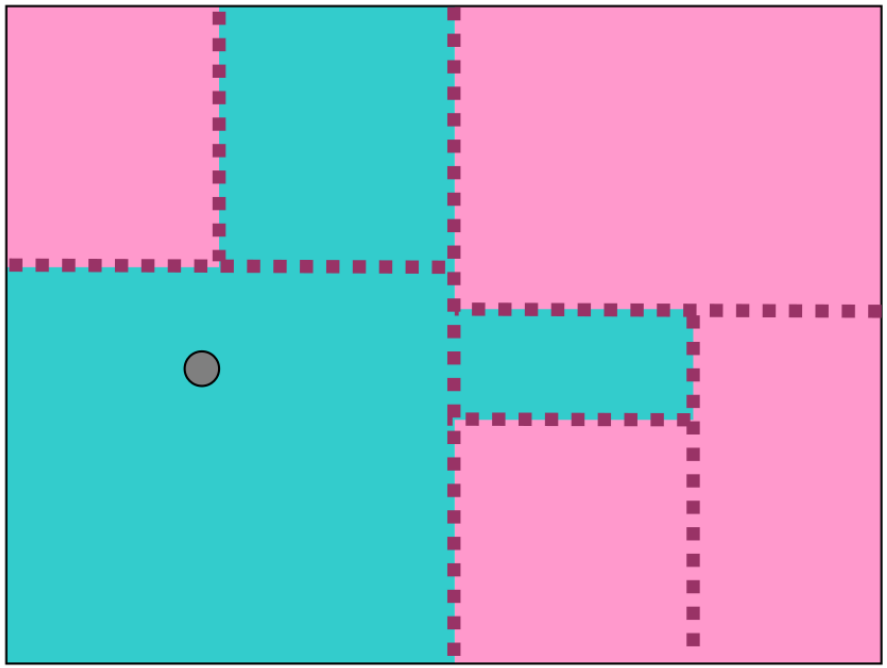
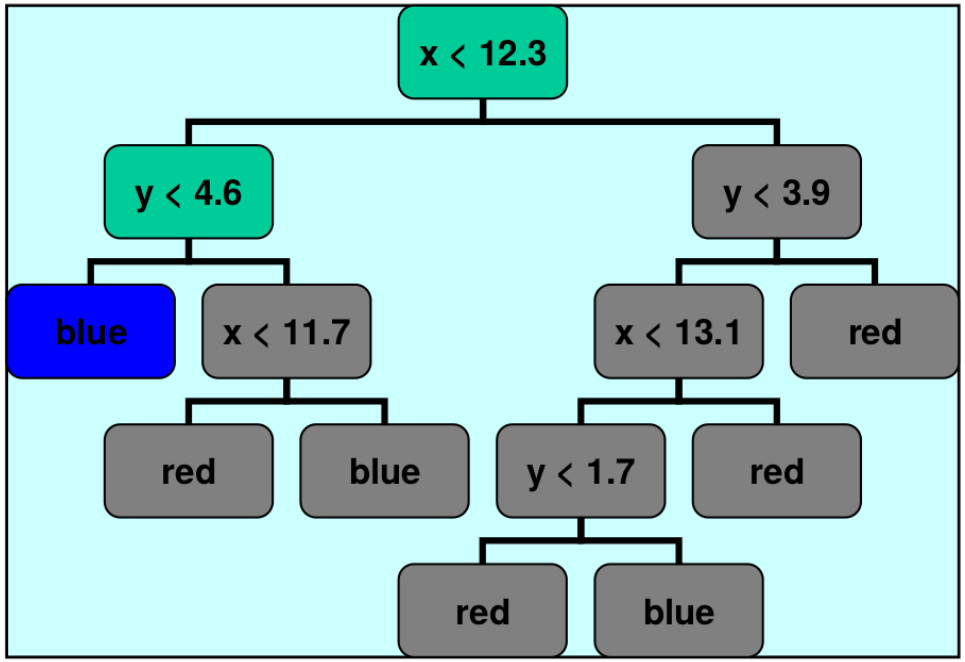




Decision tree classification

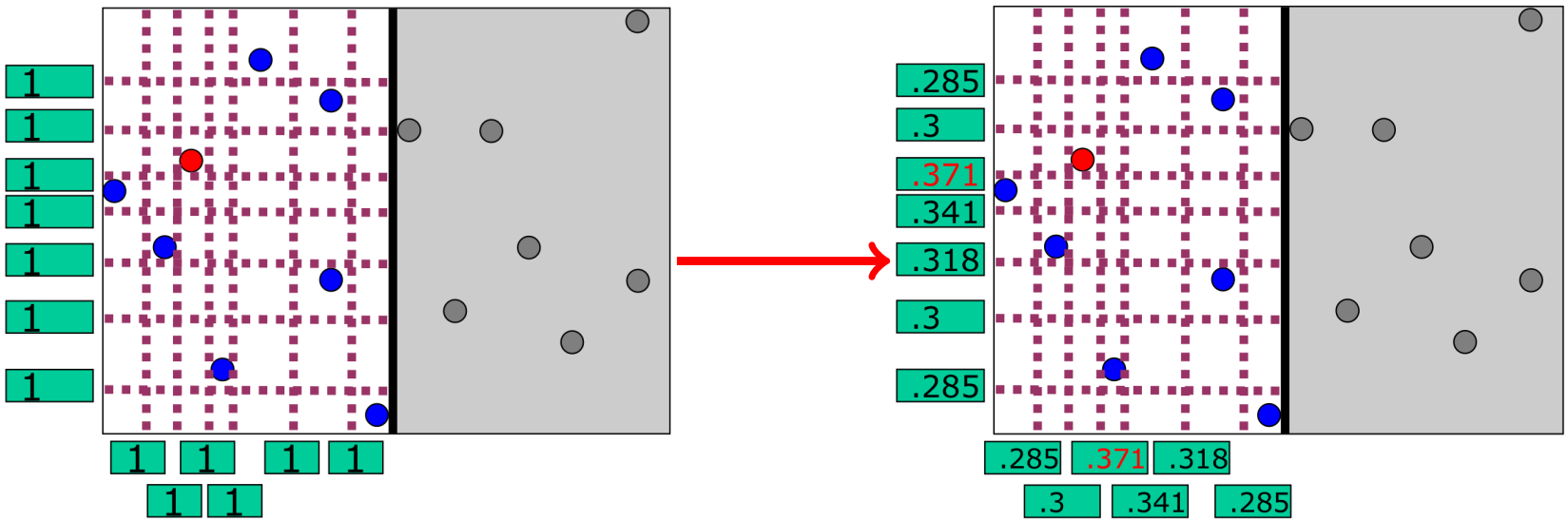
3) Classification





Decision tree improvements I

- Use more sophisticated split measures
  - *Information gain* $\leftrightarrow$ (im-)purity of splitted sub-sets
  - Gini index
- Pruning



Absolute error rate

Information gain

Decision tree improvements II

Random forest

- Ensemble of DTs
- For each tree use:
  - Random sub-sample (=*bootstrapping*)
  - Random number of the original features
  - → large number of rather shallow trees
- Classify data by majority voting of individual trees

Boosted DT

- Sequential ensemble of evolving DTs
- Assign weights to training samples → initially equal weights
- Adjust weights & give more importance to misclassified samples
- Subsequent predictors thus should focus on those

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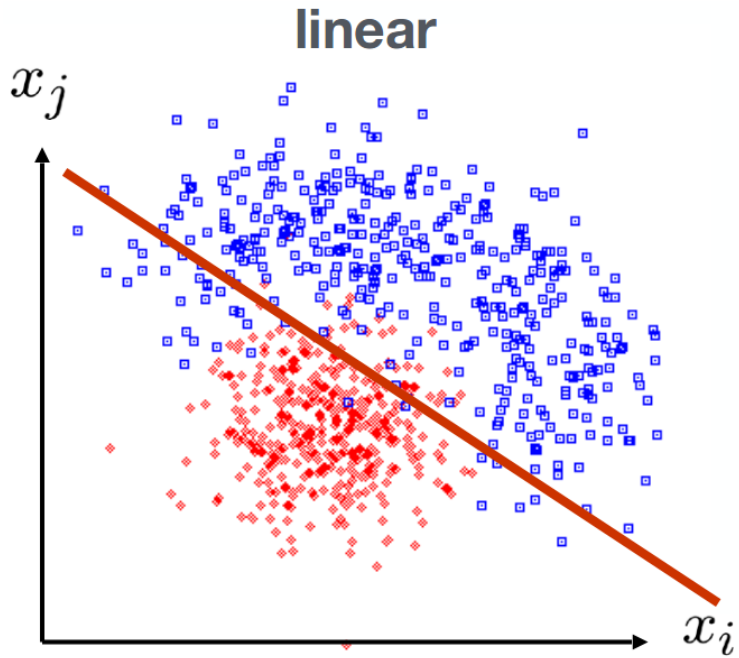
Linear cuts

More degrees of freedom than rectangular cut

- Simple white box methods
- Very fast classification
- Can become very powerful by using *kernel trick*



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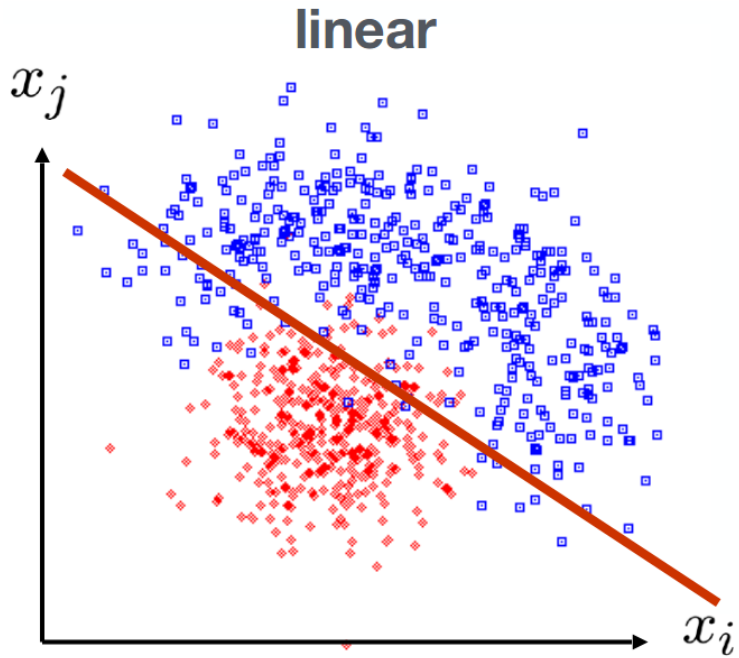

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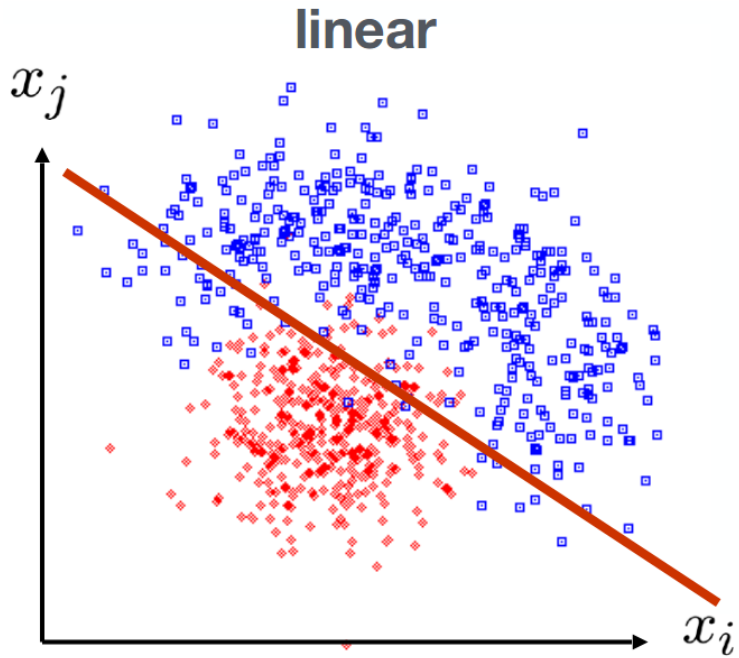

Linear models

Takes a *linear function* of its inputs $\boldsymbol{x} = (x_1, \ldots x_n)$ to base its decision on.

$$y : \mathbb{R}^n \to \mathbb{R} \mid \boldsymbol{x} \mapsto y = f(\boldsymbol{w} \cdot \boldsymbol{x}) = f(\sum_j w_j x_j)$$

$\boldsymbol{w} \ldots$ weight vector

Simplest case

$$y = f(x) = \Theta(x) = \begin{cases} 0 & x < 0 \quad \text{signal} \\ 1 & x \geq 0 \quad \text{background} \end{cases}$$

$\rightarrow$ Function can be approximated by **single layer perceptron**

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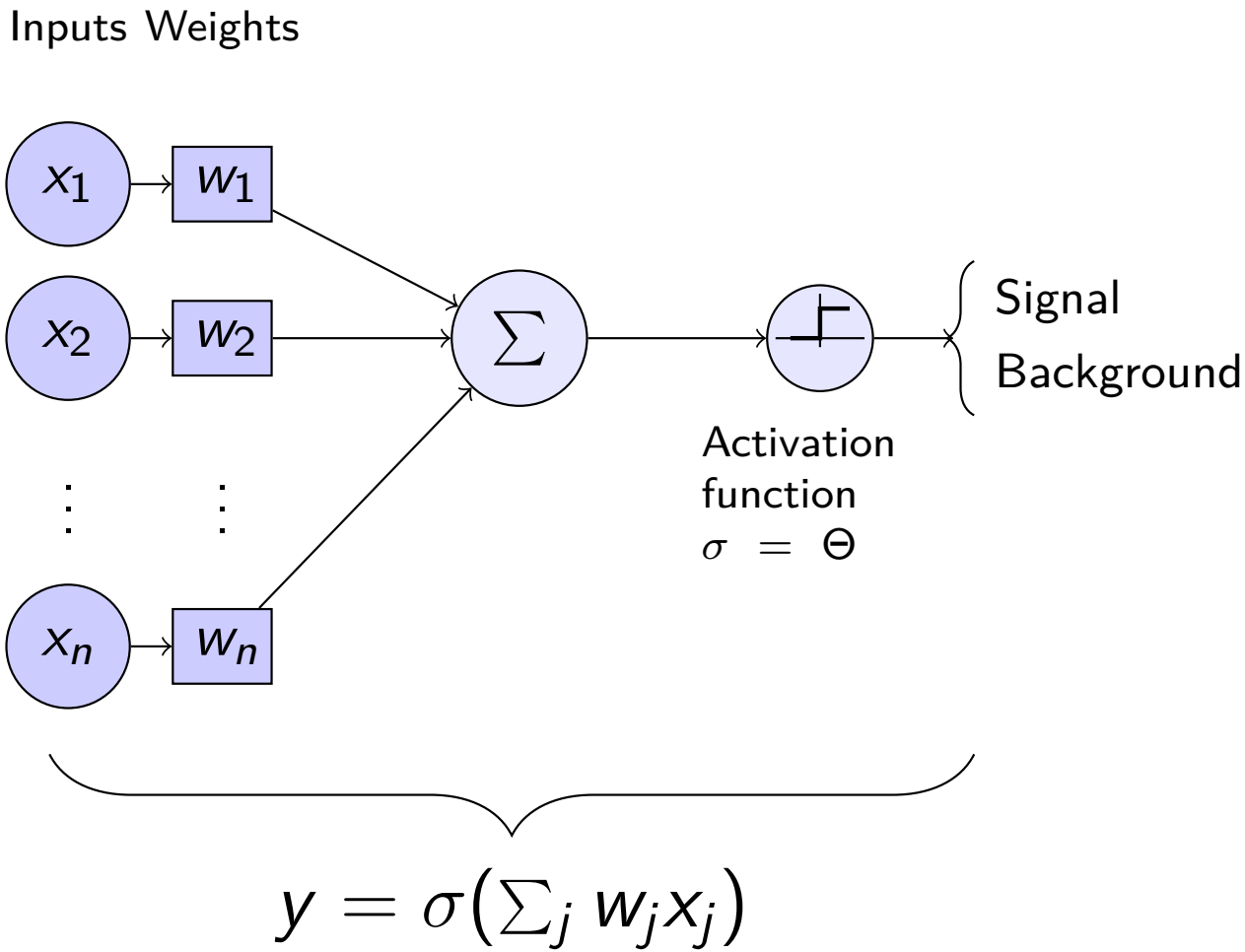
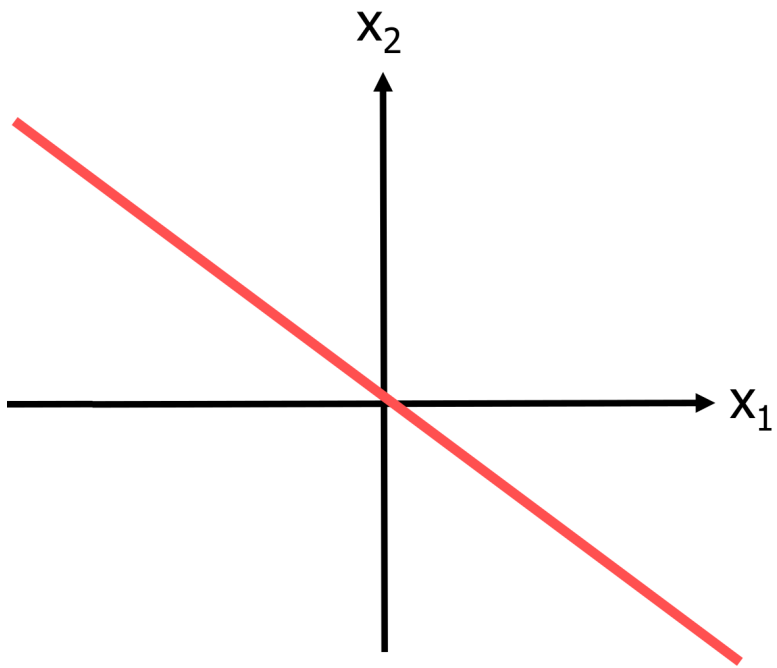
Single layer perceptron (SLP)



SLP training

Algorithm

1. Initialize weights $\boldsymbol{w}_{init}$
2. Repeat until $y = y_{target}$:
   1. Present training sample x
   2. Predict sample label $y = \Theta(x\boldsymbol{w}_{init})$ and compute error $\Delta = y_{target} - y$
   3. If $\Delta \neq 0 \rightarrow$ update weights $\boldsymbol{w}' = \boldsymbol{w} + \alpha\Delta\boldsymbol{x}$



$$y = w_1 x_1 + w_2 x_2$$

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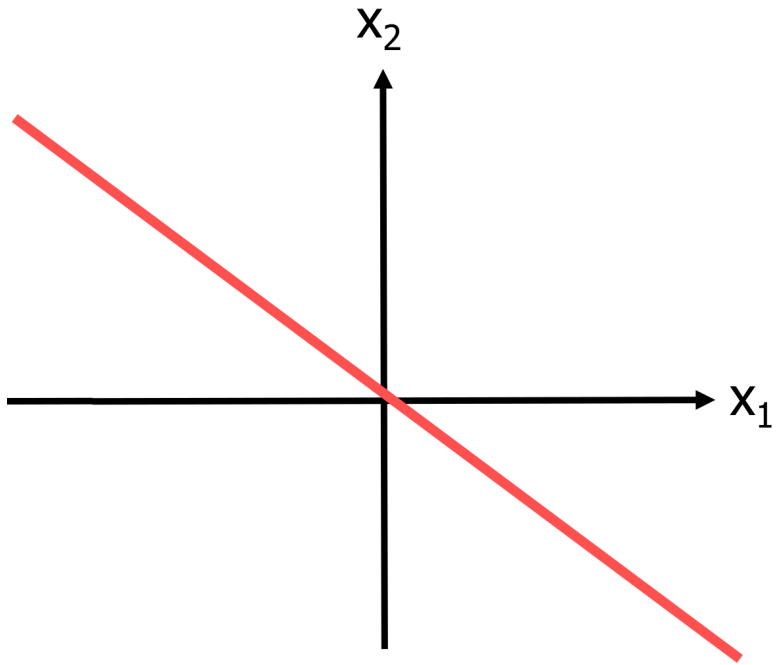

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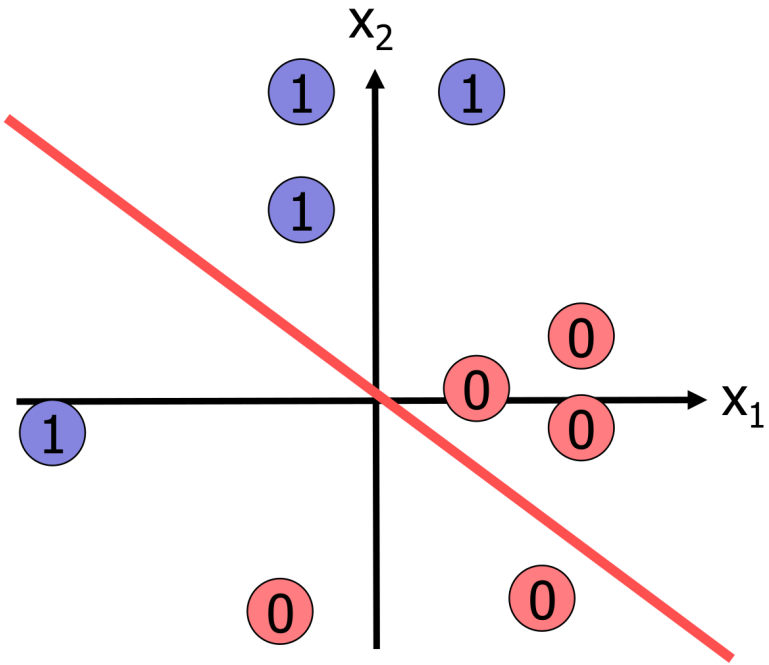

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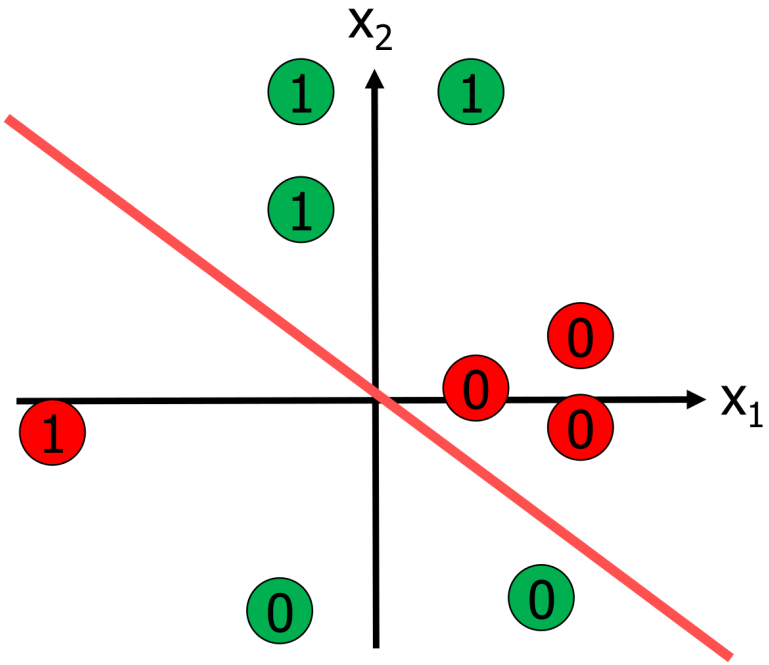

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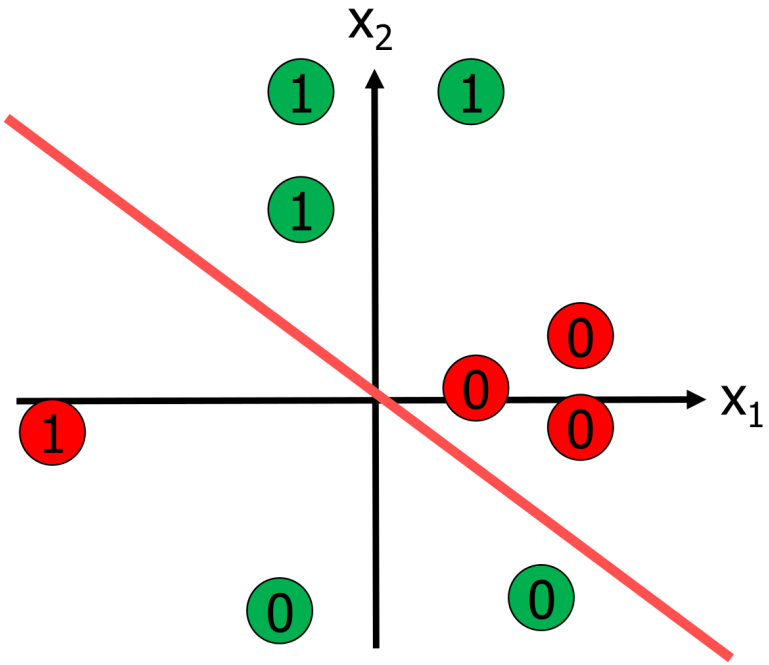

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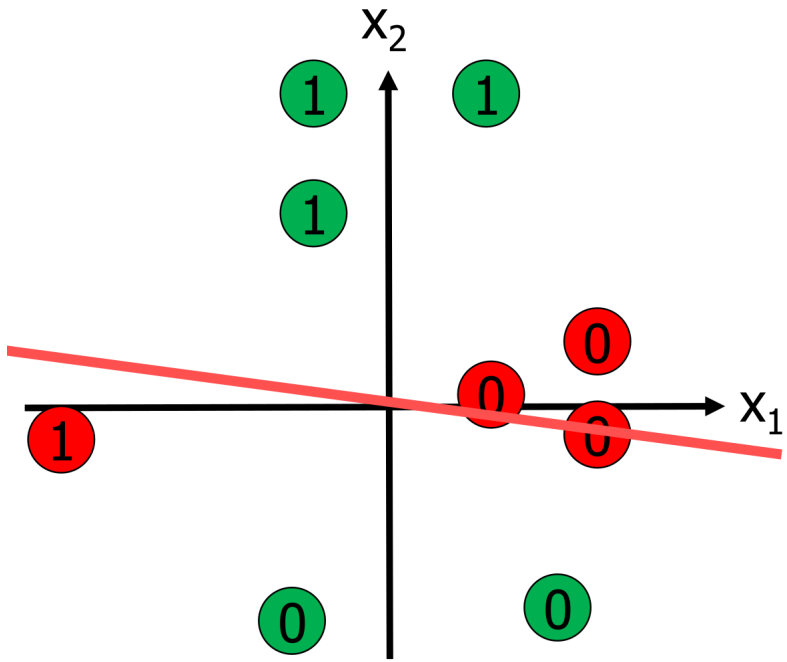

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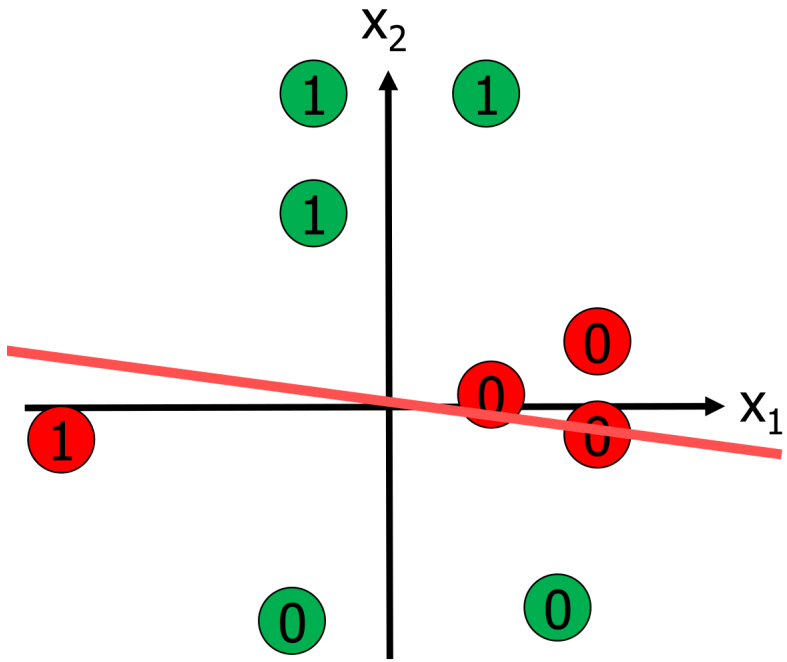

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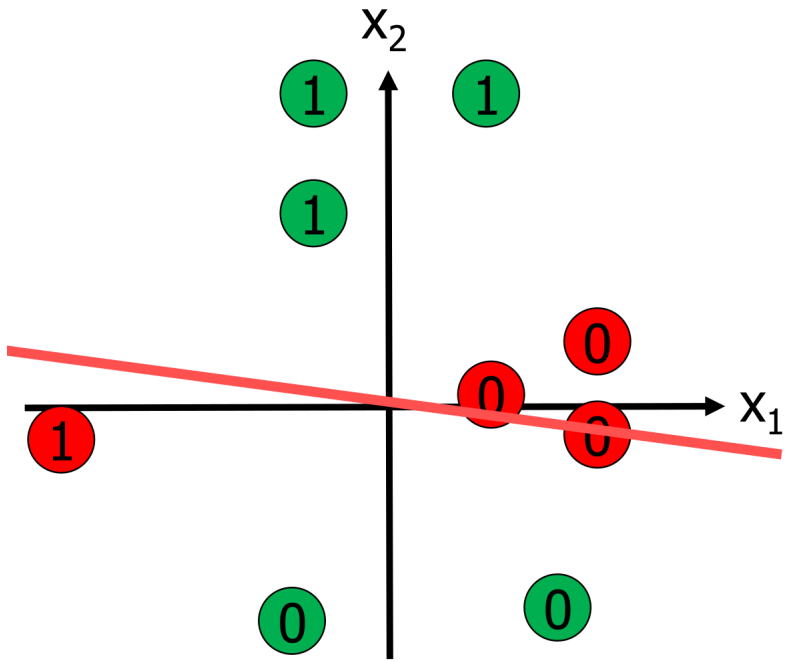

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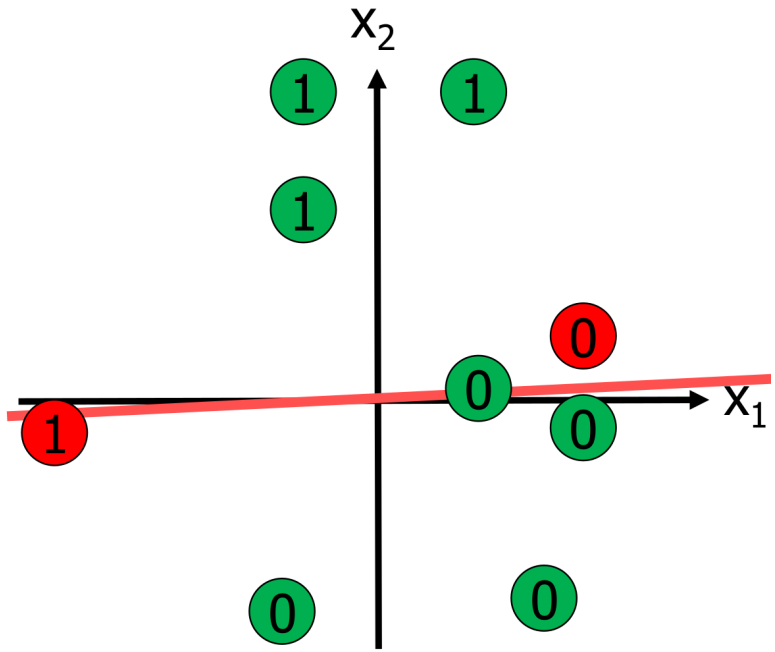

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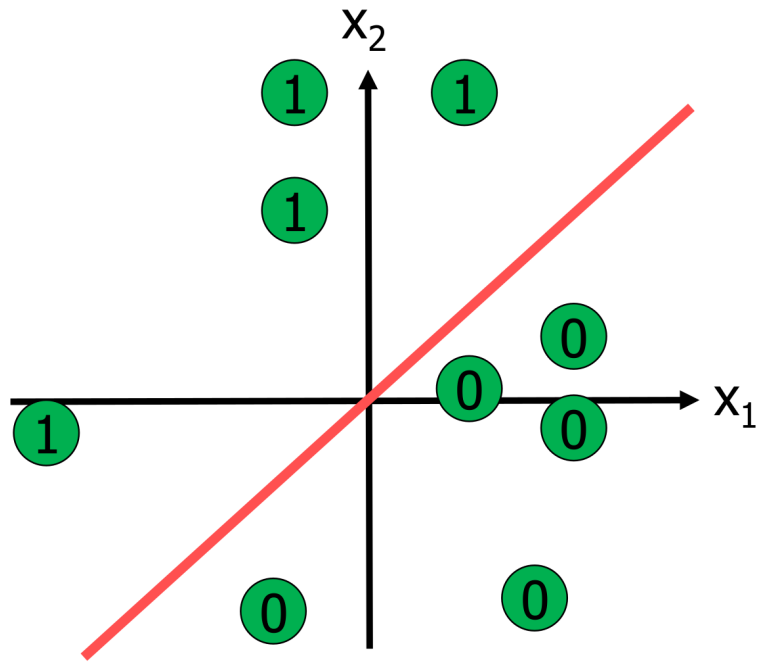
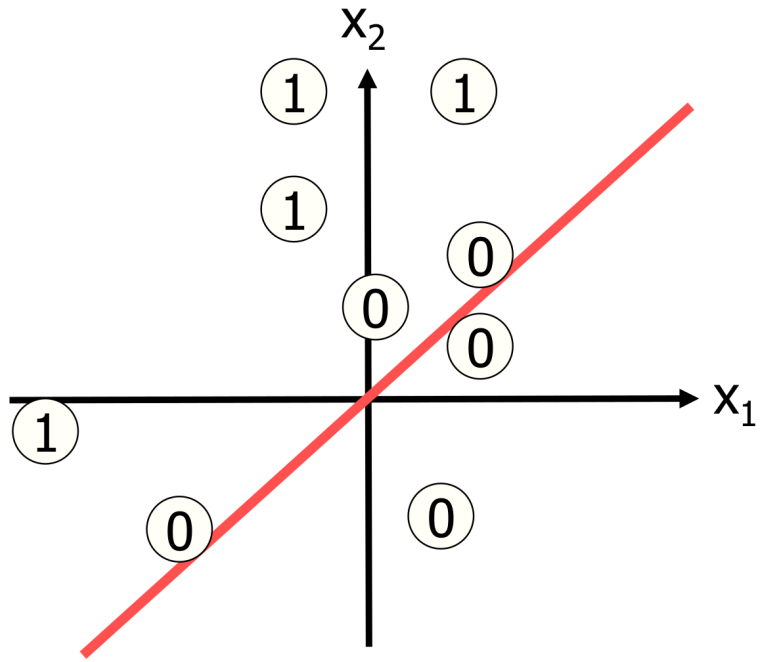


SLP bias term



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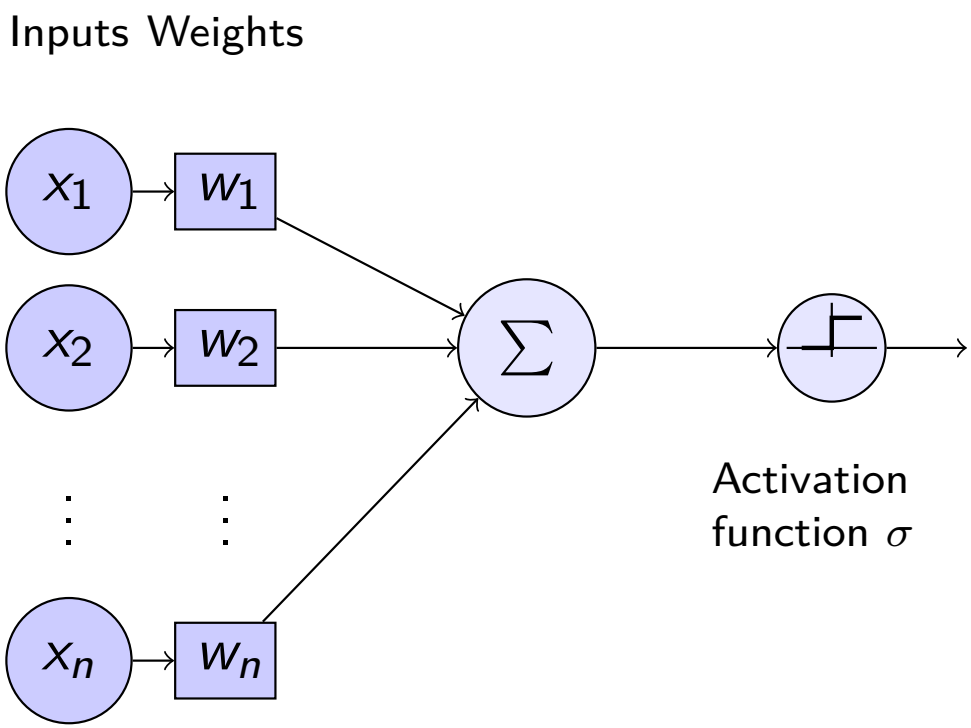
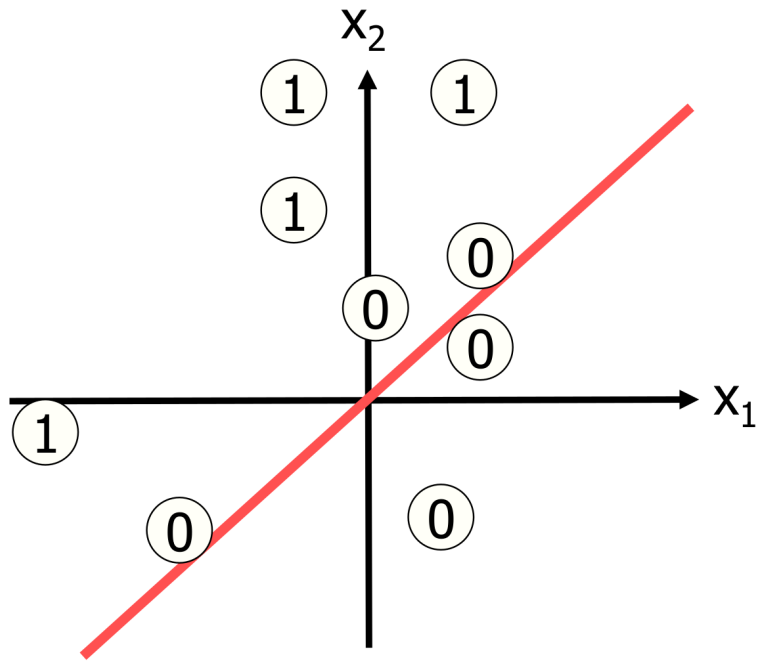
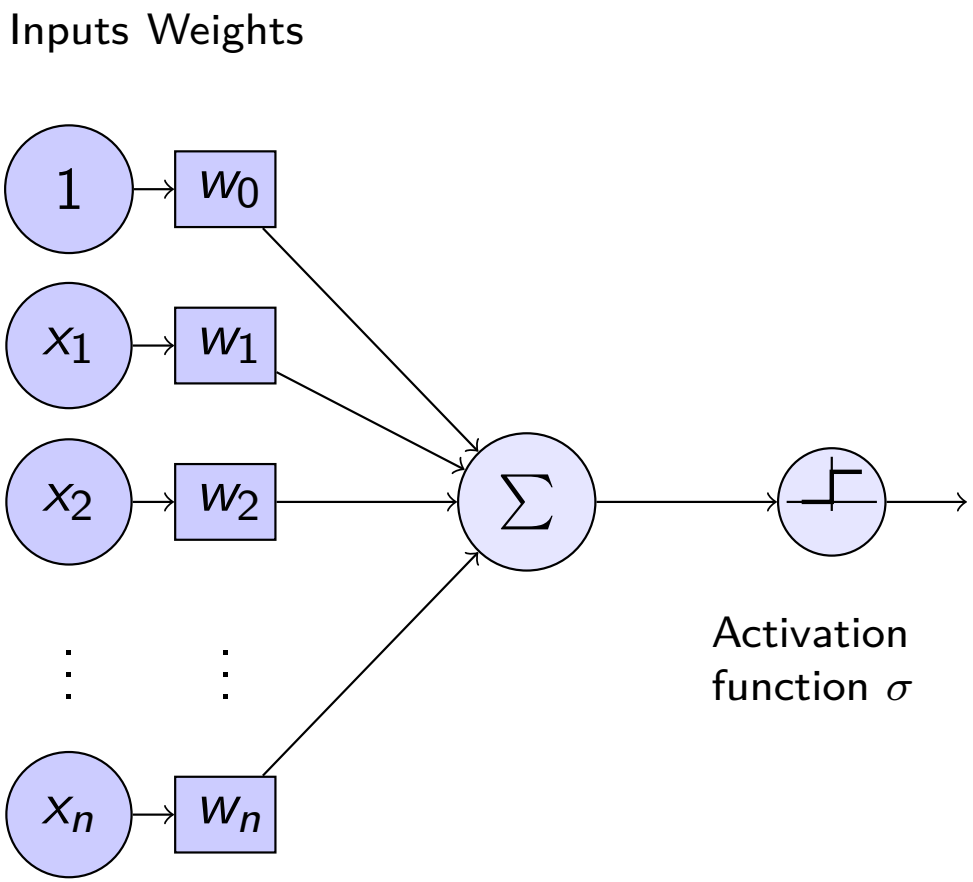
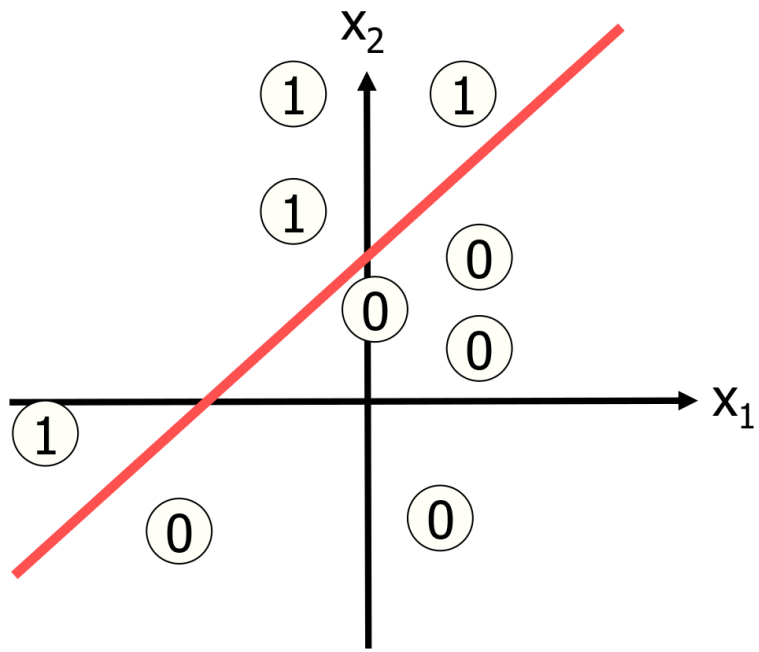




SLP bias term





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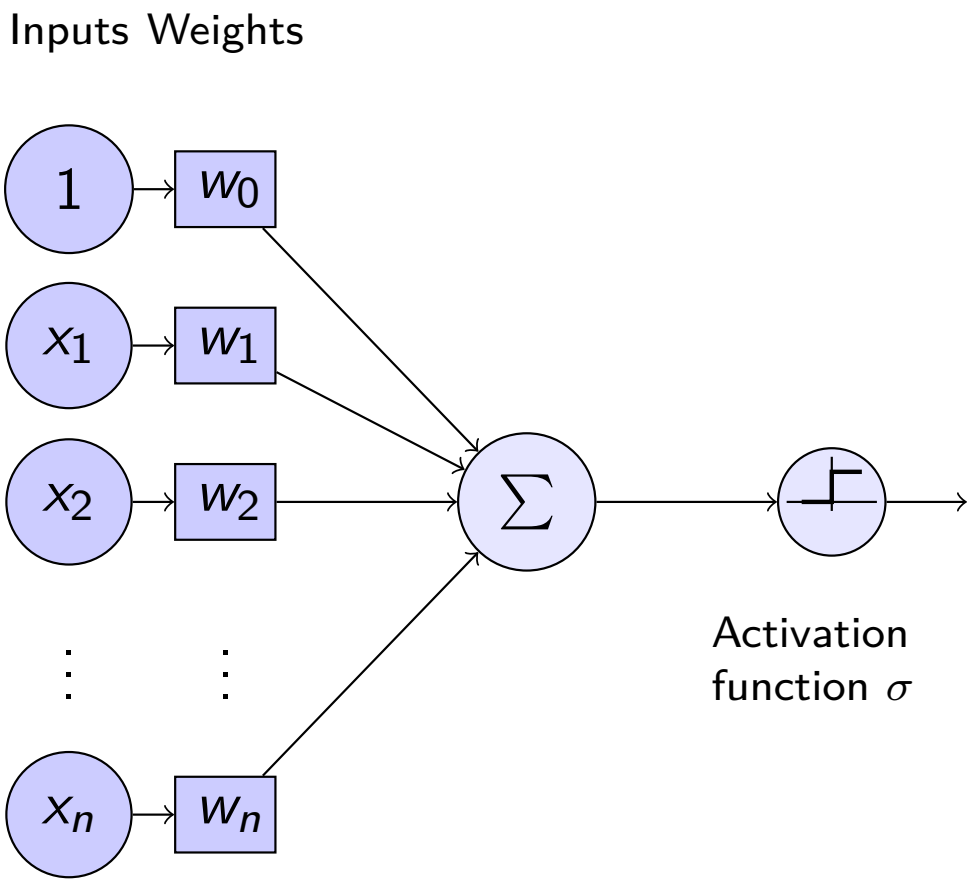

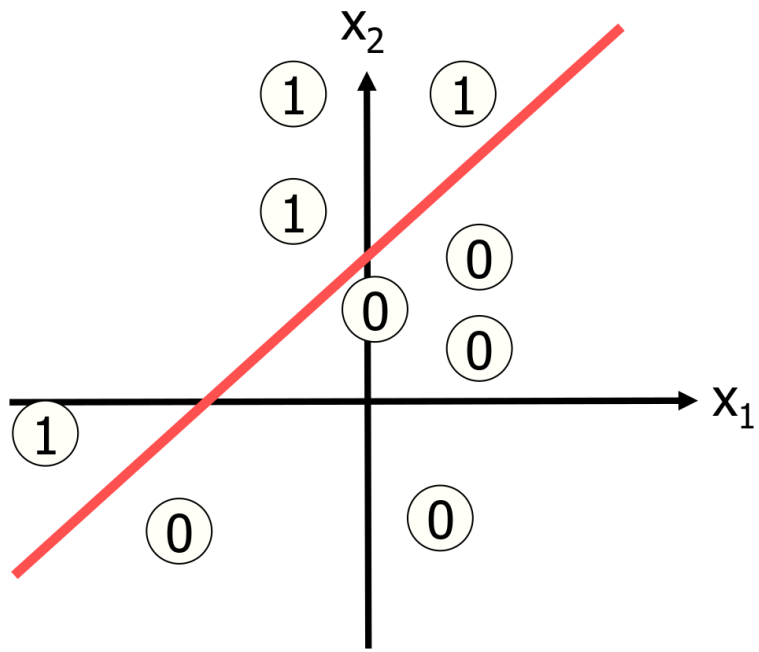

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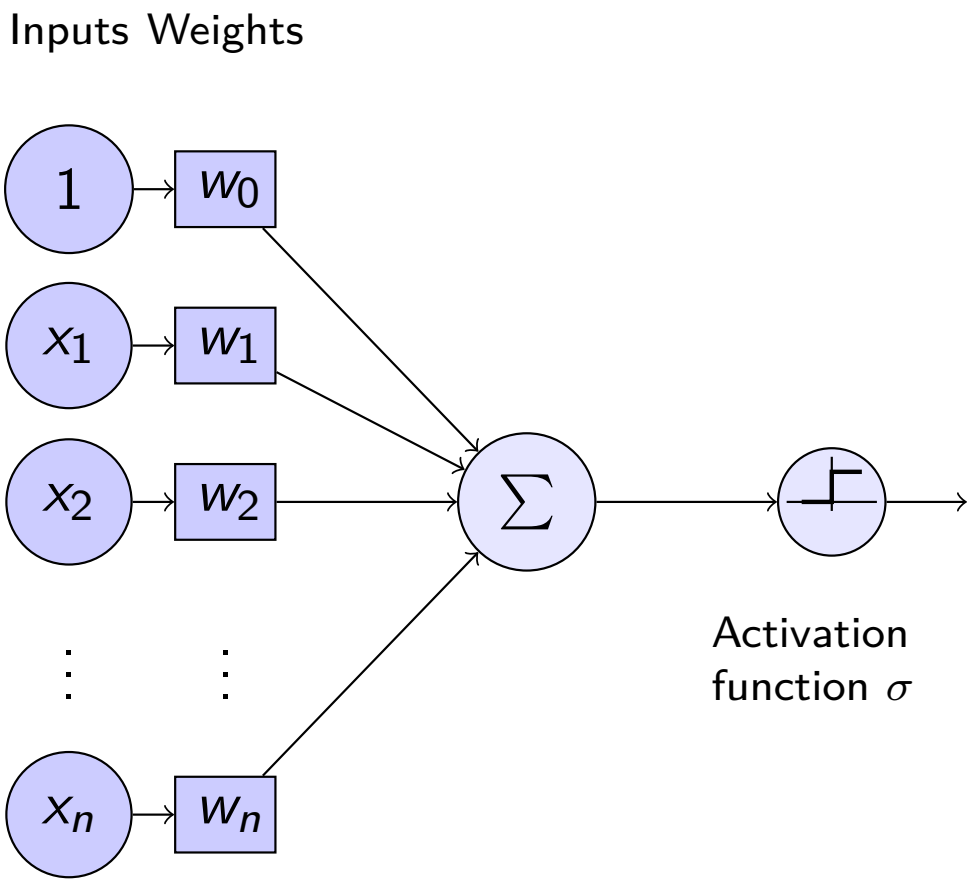
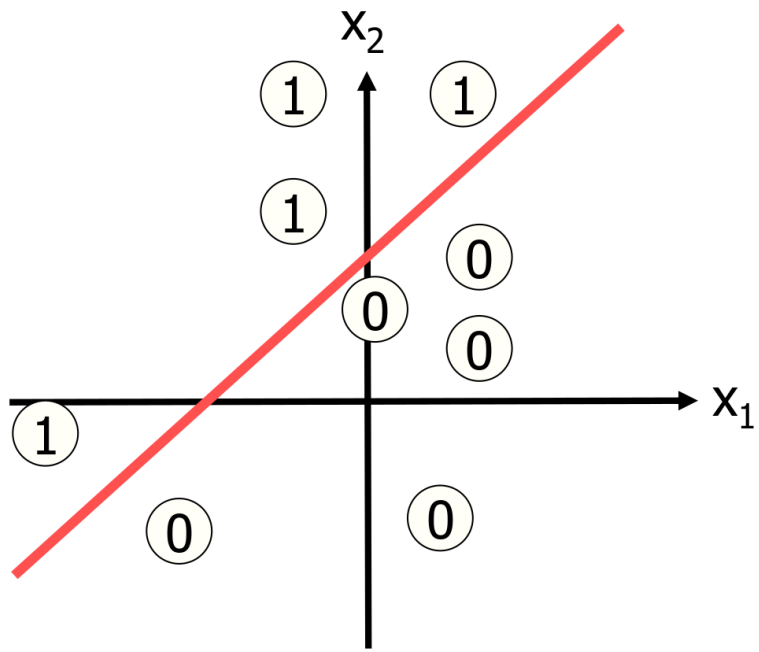
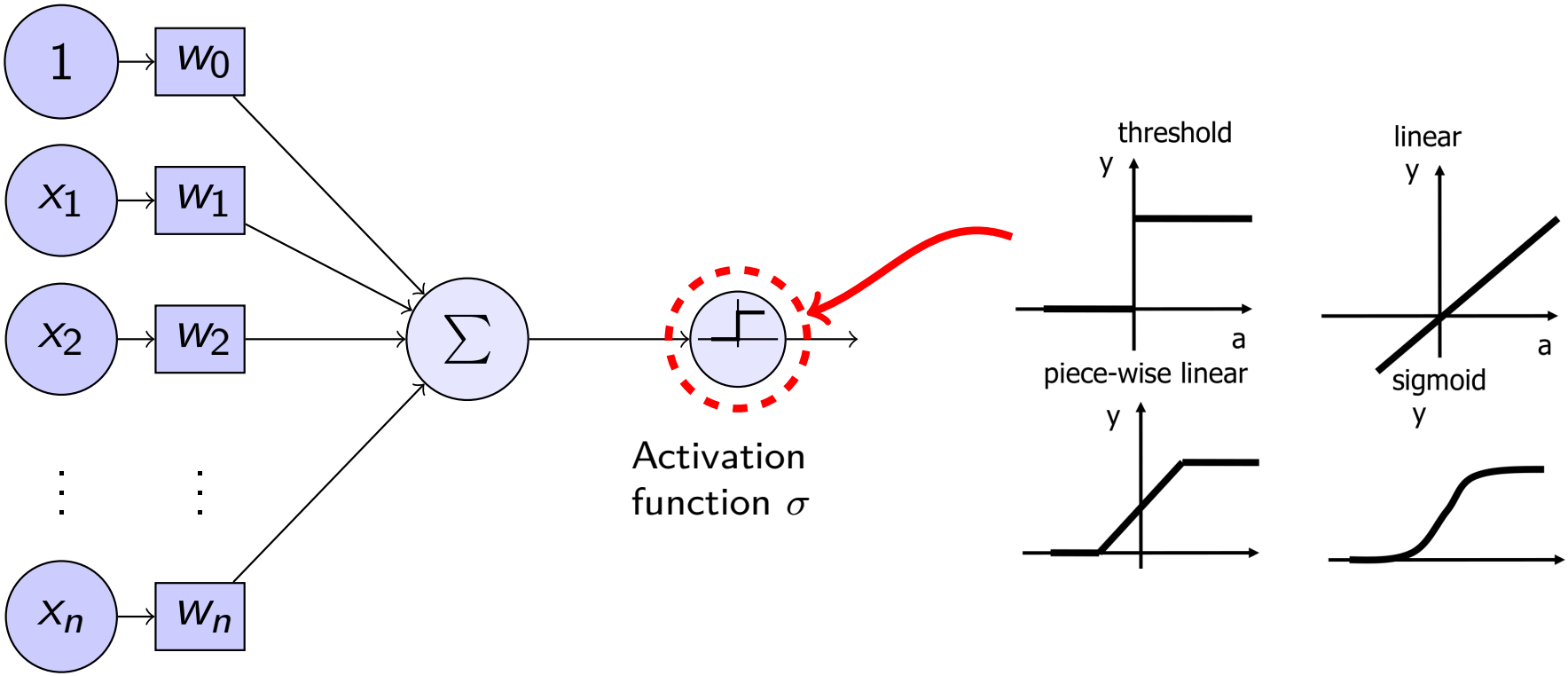




Bias weight w_0 learned just as the other weights

$$y = \sigma(w_0 + \sum_{j=1}^{n} w_j x_j)$$

SLP activation functions



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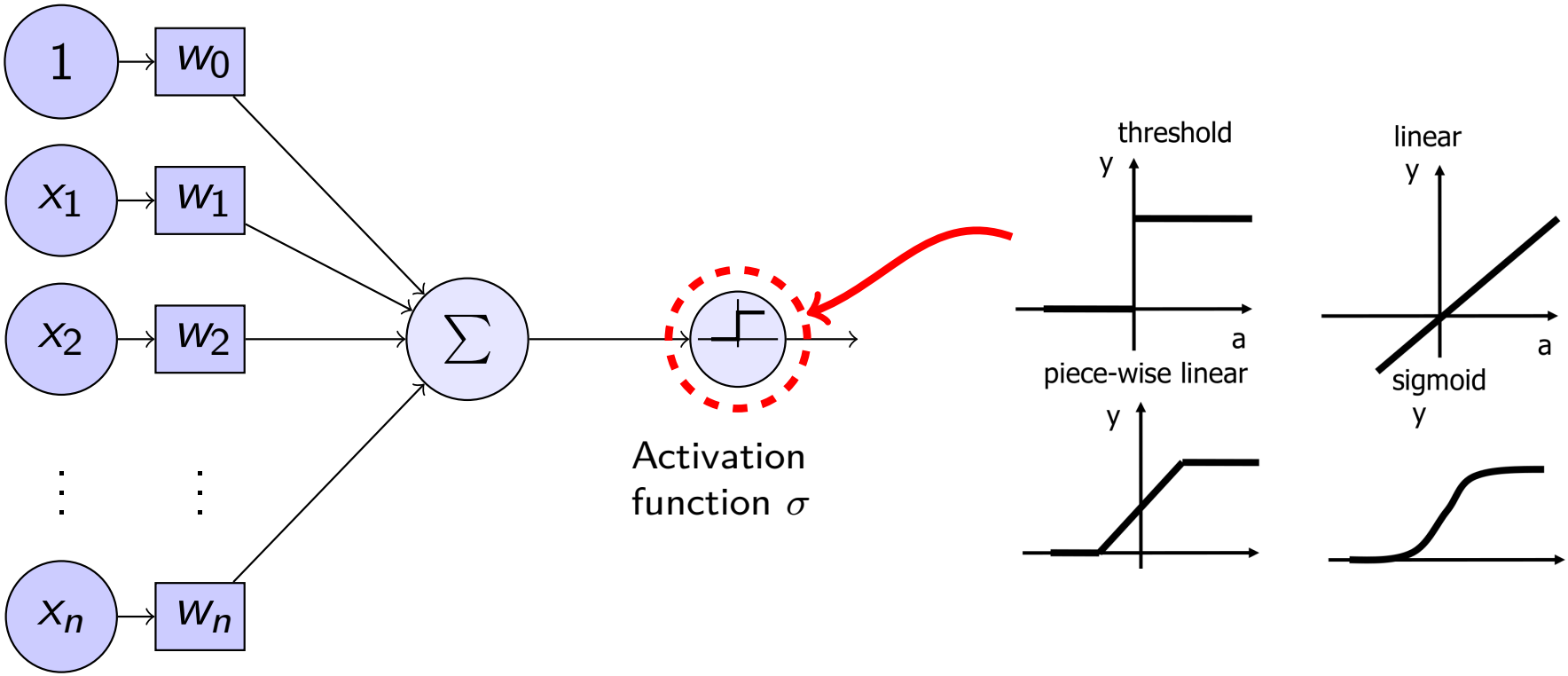
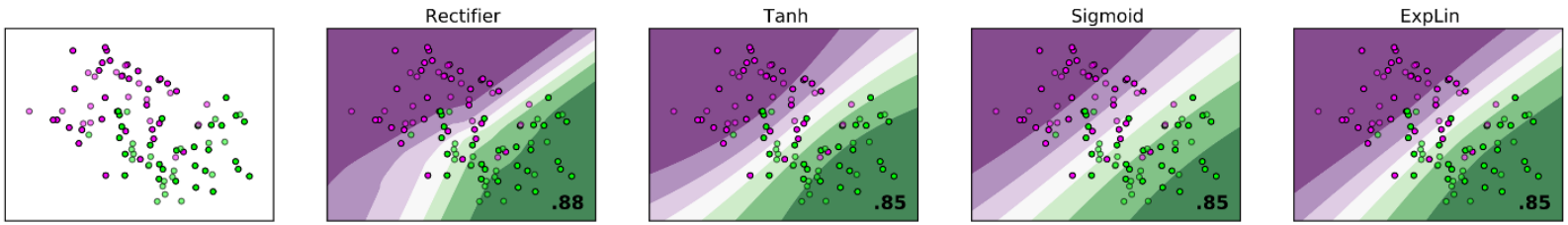
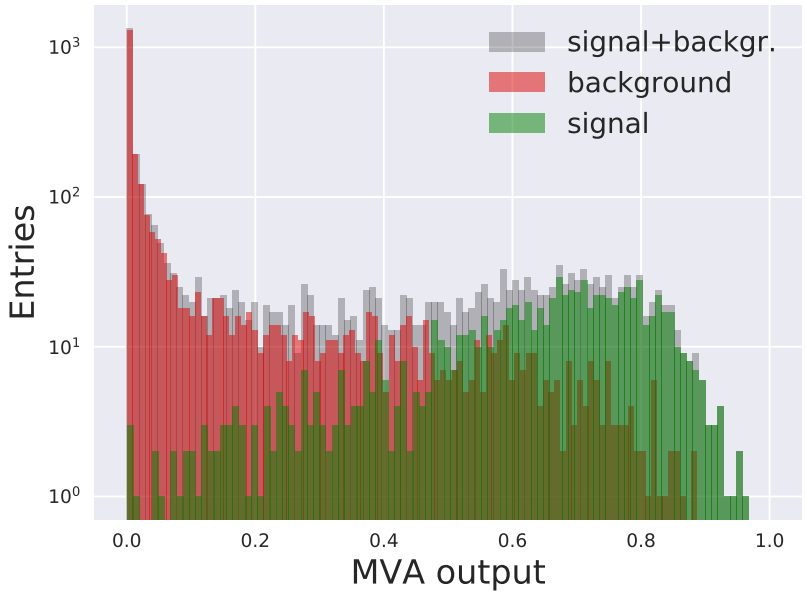


Often used: *sigmoid* $\rightarrow$ output $\in (0, 1)$

SLP improvement INon-linear activation functions output





Improving linear methods

Kernel trick

Map data to a higher dimensional space where linear hyperplane can again be found

Improving linear methods

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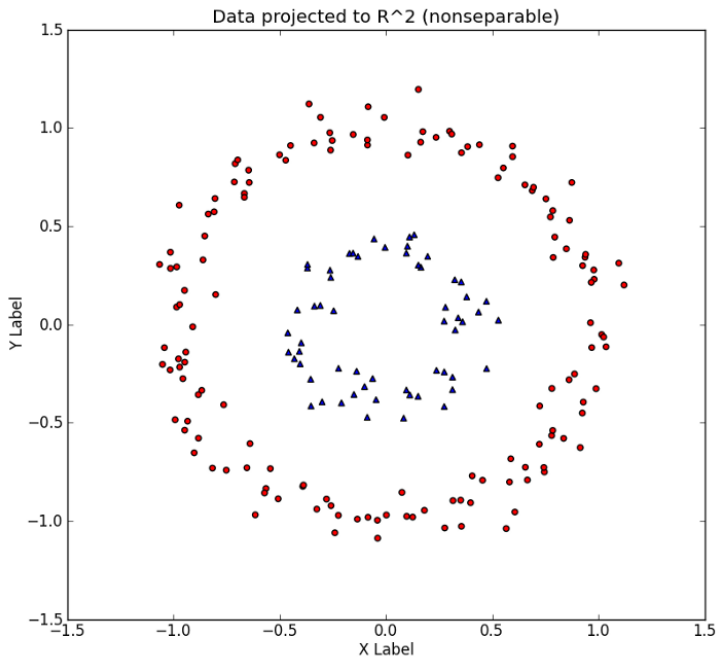
Map data to a higher dimensional space where linear hyperplane can again be found



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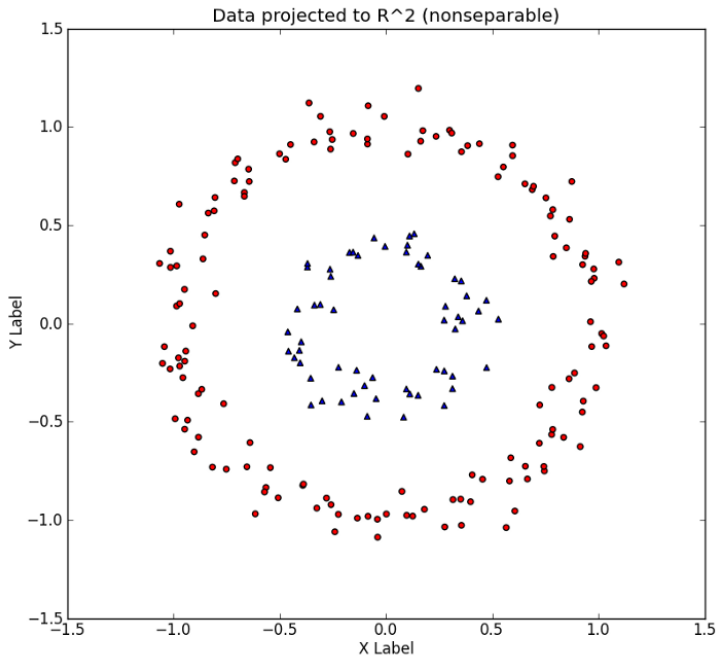
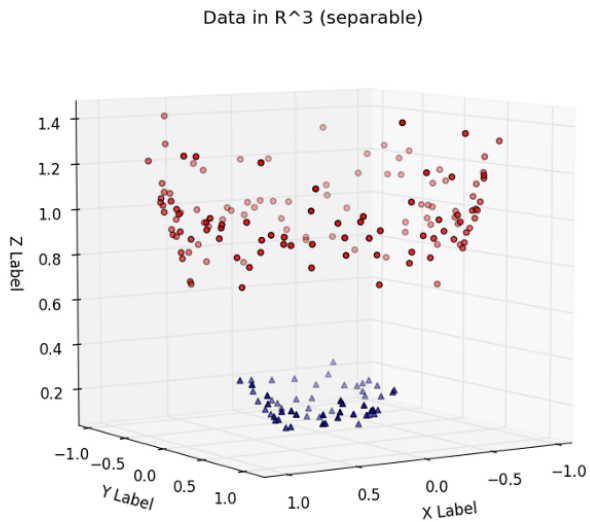




Non-linear models

Assumtion

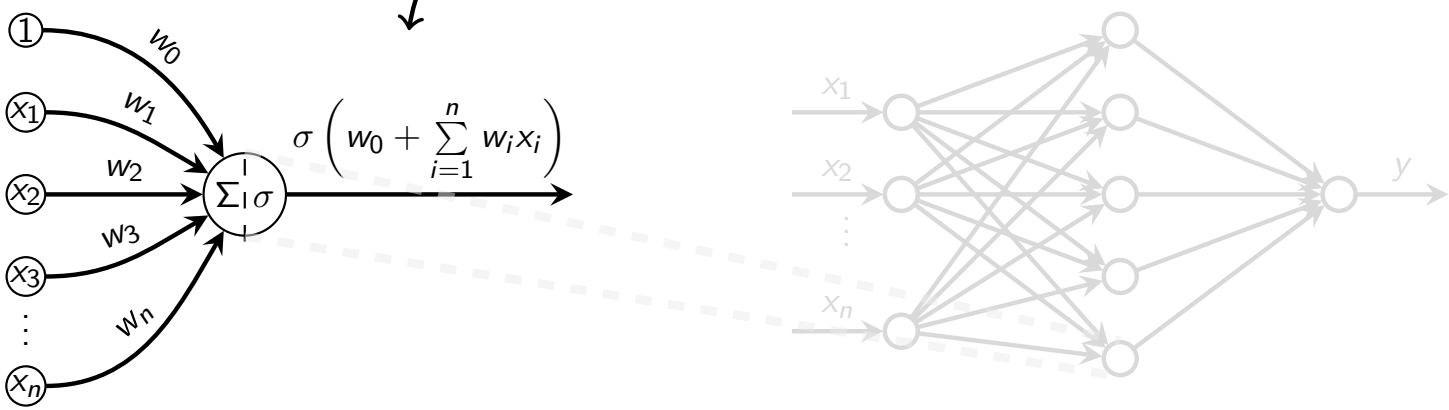
Take *kernel trick* idea: map inputs $\boldsymbol{x} = (x_1, \dots x_n)$ to higher dimensional space $\mathbb{R}^m$ with $m > n$ where linear seperation is possible:

$$y : \mathbb{R}^n \to \mathbb{R}^m \to \mathbb{R} = \sigma\left(w_0^2 + \sum_{i=1}^{m}\left[w_i^{(2)} + \sigma\left(w_{0,i}^{(1)} + \sum_{k=1}^{n} w_{k,i}^{(1)}\ x_k\right)\right]\right)$$
$$= \sigma\left[w_0^{(2)} + \boldsymbol{w}^{(2)} \cdot \sigma(\boldsymbol{w}_0^{(1)} + \boldsymbol{W}^{(1)} \cdot \boldsymbol{x})\right]$$

$\to$ *m single layer perceptrons*

Visualisaion

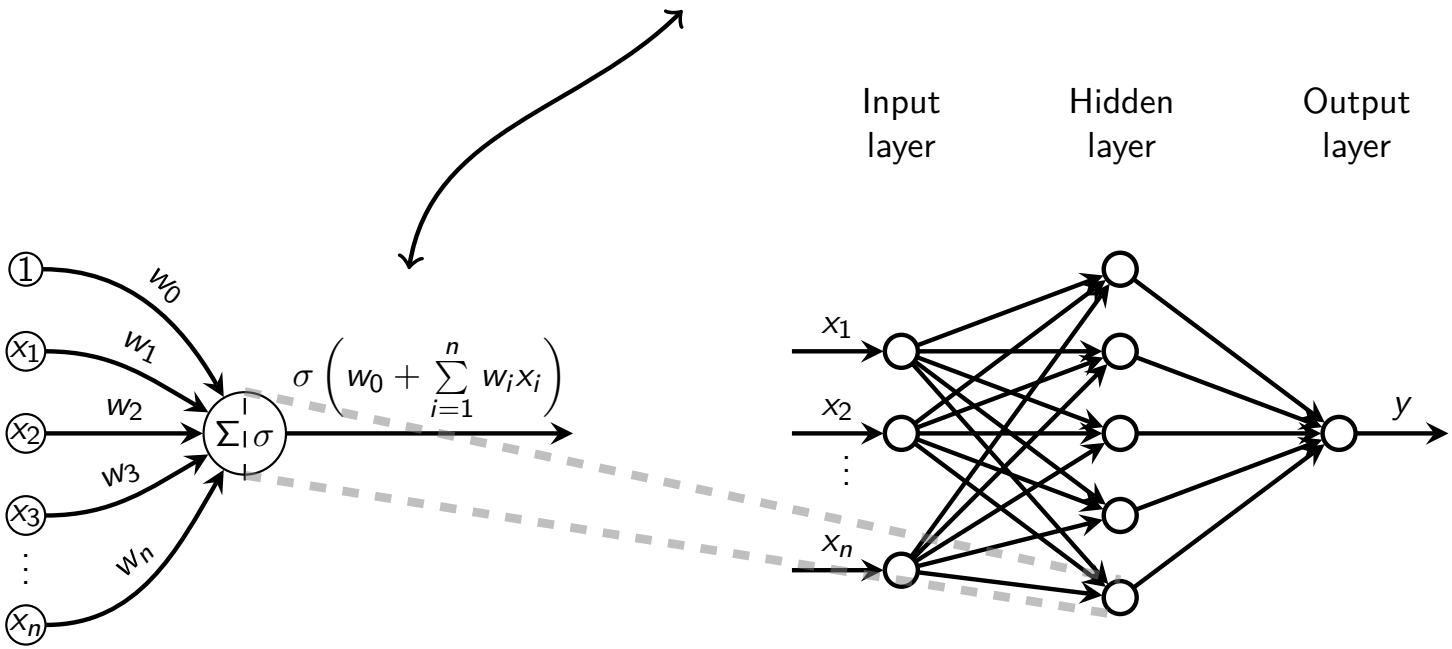
$$y = \sigma[w_0^{(2)} + \overbrace{\boldsymbol{w}^{(2)}}^{\mathbb{R}^m} \cdot \underbrace{\sigma(\overbrace{\boldsymbol{w}_0^{(1)}}^{\mathbb{R}^m} + \overbrace{\boldsymbol{W}^{(1)}}^{\mathbb{R}^{m\times n}} \cdot \boldsymbol{x})}_{\text{Output of hidden layer: } \mathbb{R}^m}]$$



$\rightarrow$ The hidden layer *learns* a representation so that the data is linearly separable

Visualisaion

$$y = \sigma[w_0^{(2)} + \overbrace{\boldsymbol{w}^{(2)}}^{\mathbb{R}^m} \cdot \underbrace{\sigma(\overbrace{\boldsymbol{w}_0^{(1)}}^{\mathbb{R}^m} + \overbrace{\boldsymbol{W}^{(1)}}^{\mathbb{R}^{m\times n}} \cdot \boldsymbol{x})}_{\text{Output of hidden layer: } \mathbb{R}^m}]$$



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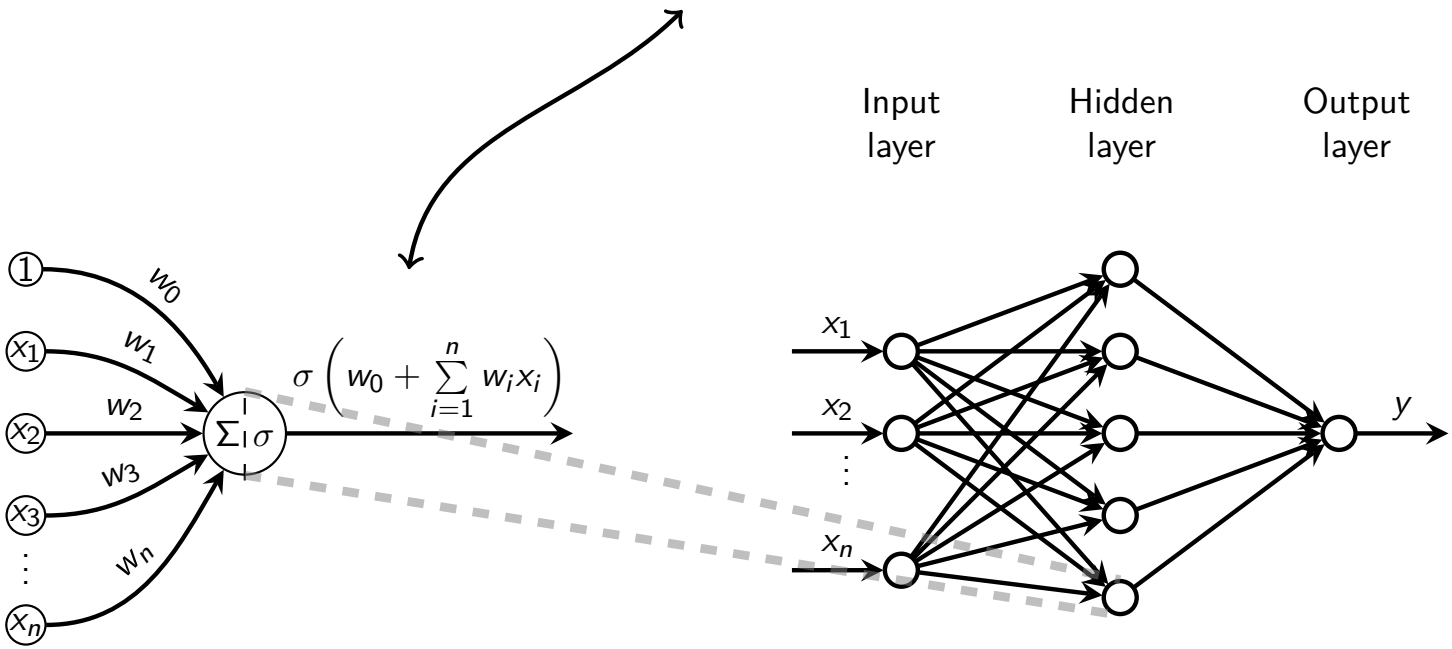

$\rightarrow$ The hidden layer *learns* a representation so that the data is linearly separable

Visualising the hidden layer

Effects of adding a hidden layer

Input vector $\boldsymbol{x}$ undergoes *linear transformation* by multiplication with weight matrix $\boldsymbol{W}$. The bias term $\boldsymbol{w}_0$ causes a *translation*.

$$y = \sigma[w_0^{(2)} + \boldsymbol{w}^{(2)} \cdot \underbrace{\sigma(\boldsymbol{w}_0^{(1)} + \boldsymbol{W}^{(1)} \cdot \boldsymbol{x})}_{\tilde{\boldsymbol{x}}}]$$

Visualising the hidden layer

Effects of adding a hidden layer

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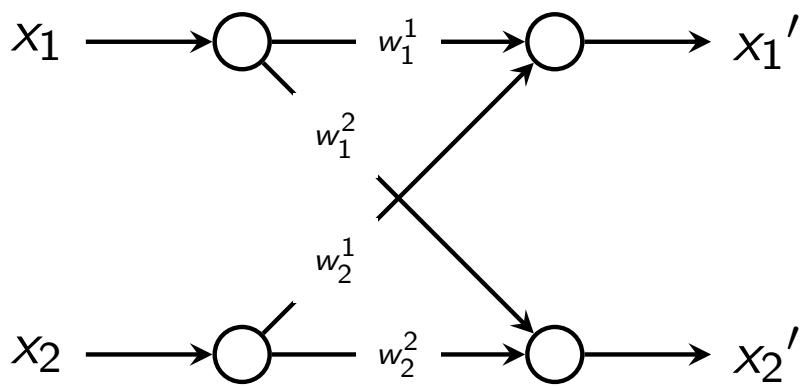
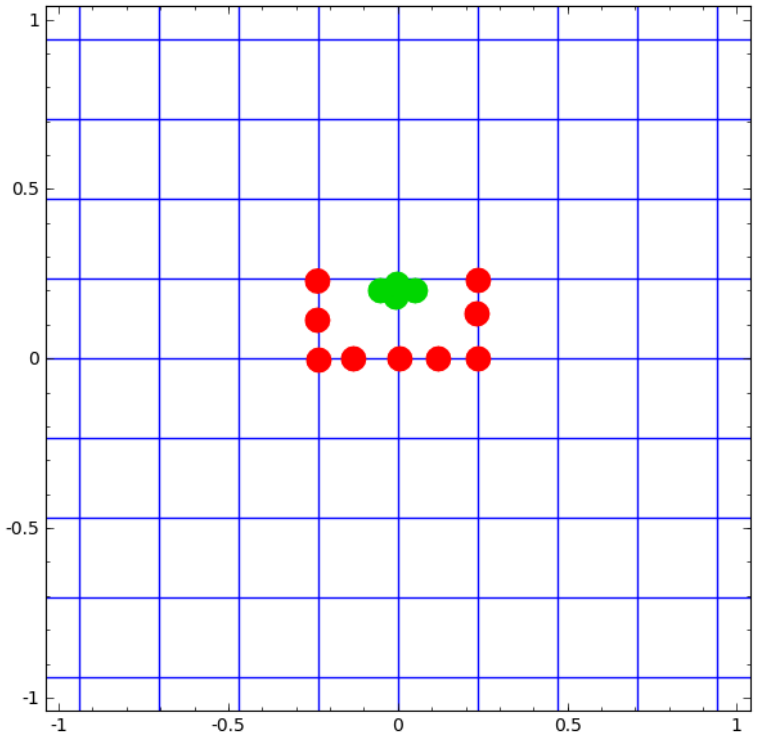
$$\tilde{\boldsymbol{x}} = \sigma(\boldsymbol{w}_0^{(1)} + \boldsymbol{W}^{(1)} \cdot \boldsymbol{x}) \quad \text{with } e.g. \ \boldsymbol{W} = \begin{pmatrix} w_1^1 & w_1^2 \\ w_2^1 & w_2^2 \end{pmatrix}$$



Visualising the hidden layer

1. Linear transformation: $\boldsymbol{W}\boldsymbol{x}$
2. Translation: $\boldsymbol{w}_0$
3. Non-linear activation: σ

$$\tilde{\boldsymbol{x}} = \boldsymbol{x}$$



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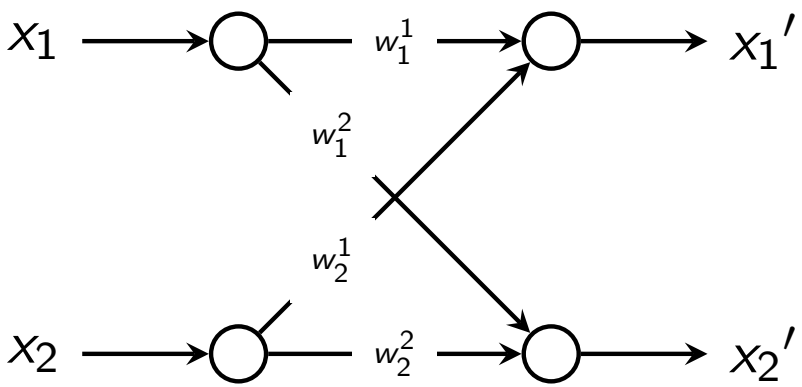
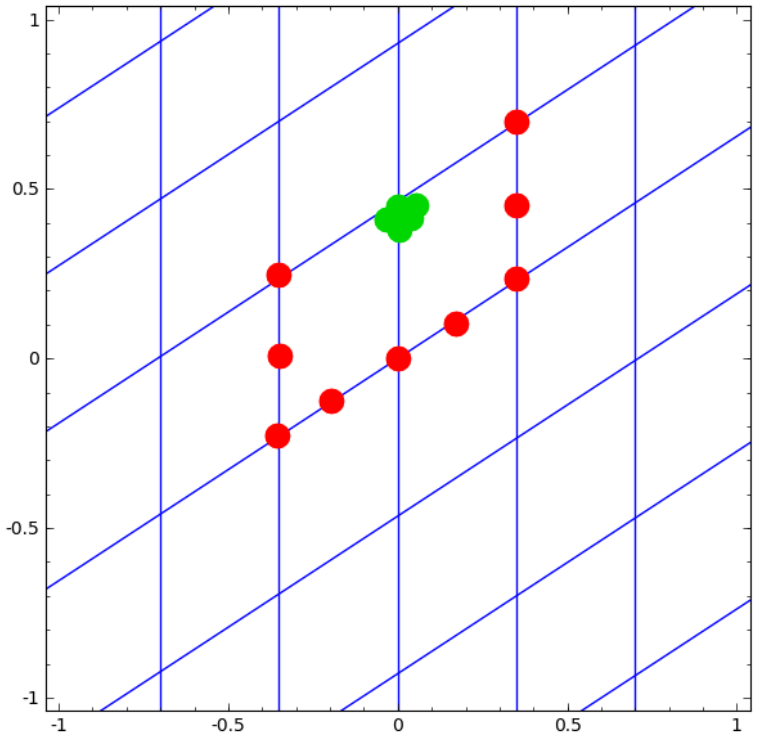
$$\tilde{\boldsymbol{x}} = (\boldsymbol{W}^{(1)} \cdot \boldsymbol{x})$$





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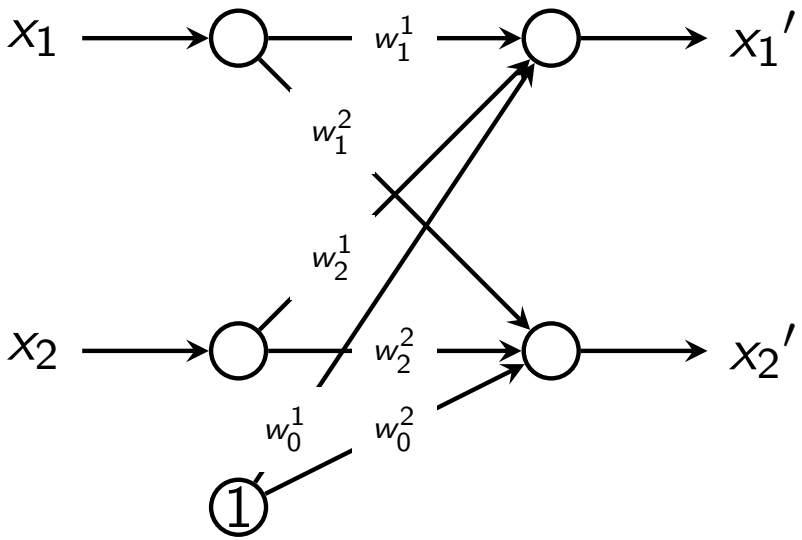

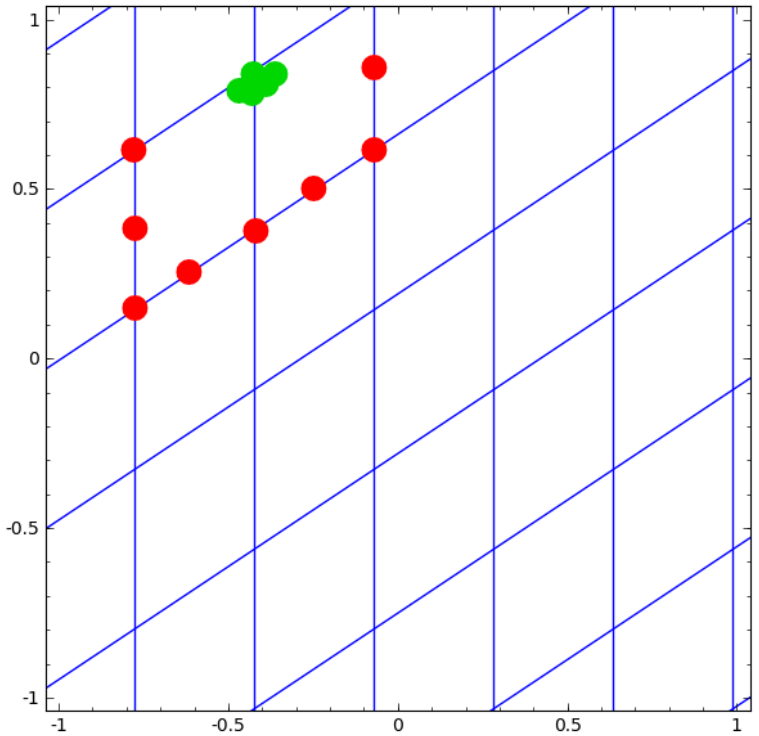

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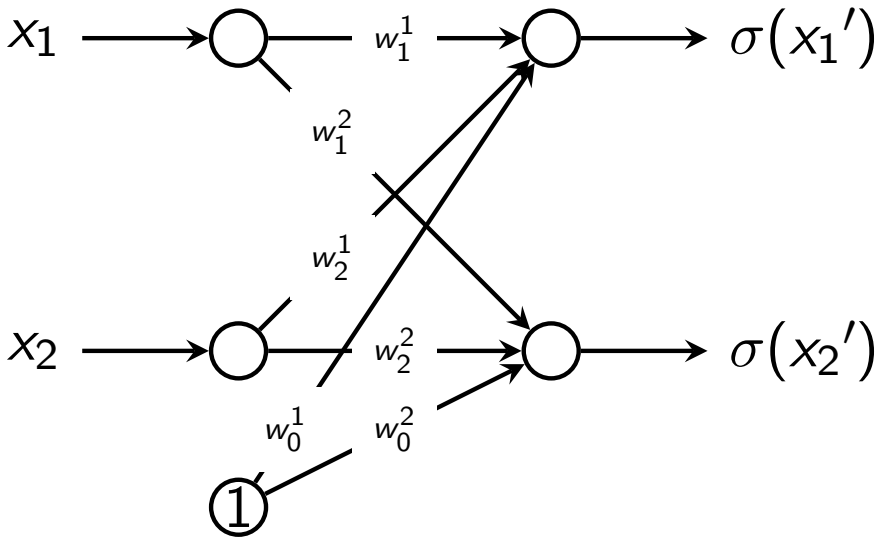

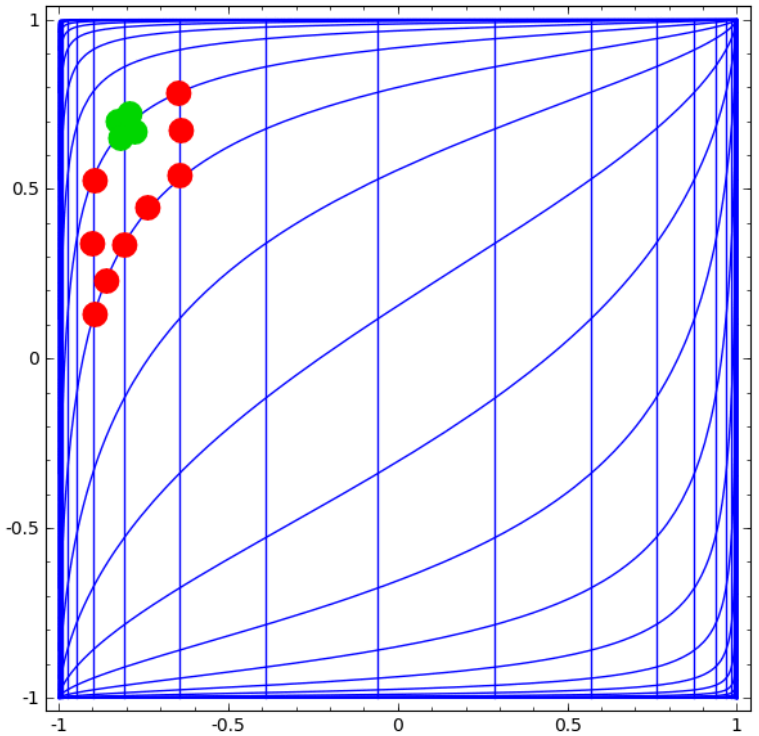

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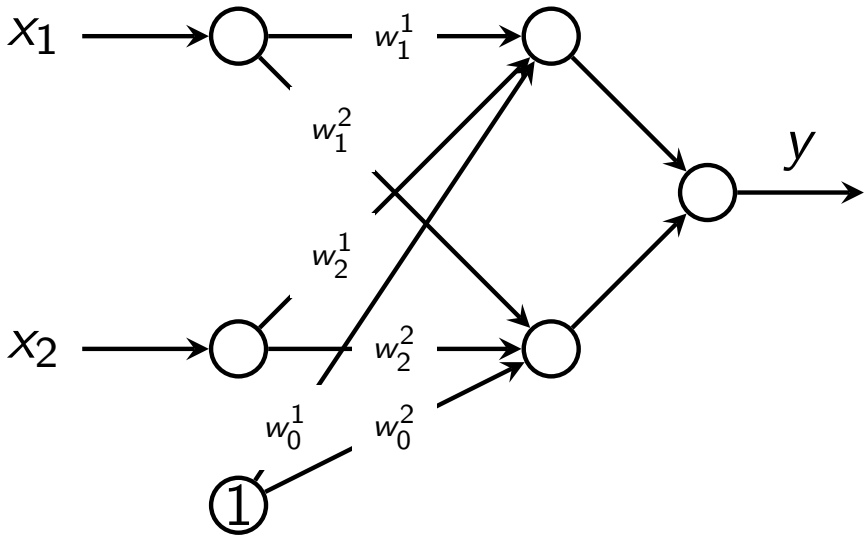

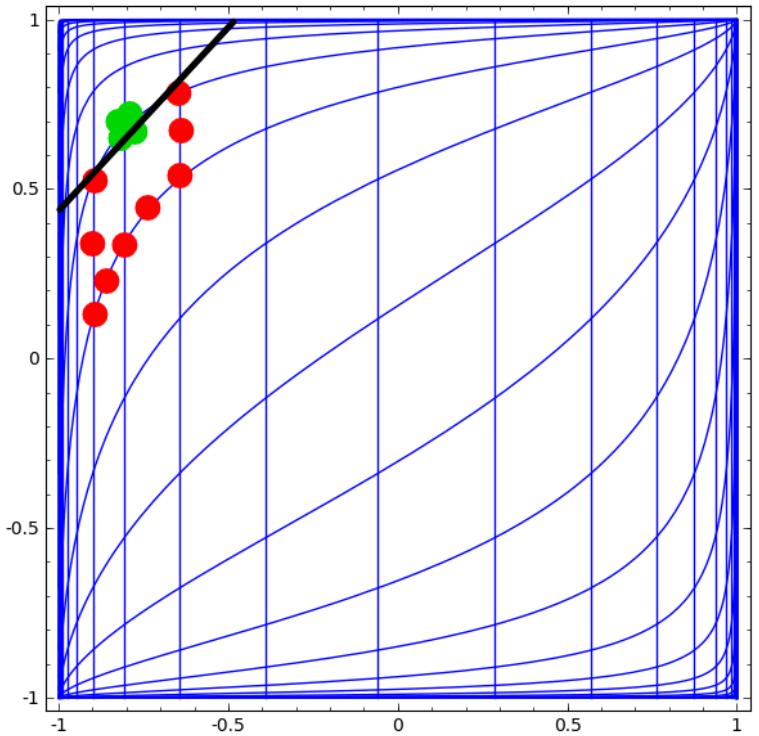

Update weights via backpropergation

Backpropergation

Adapt weights by going backwards in the network

- Initialize weigts
- Evaluate $y_{predict} = f(\boldsymbol{x})$ and calculate $\Delta = (y_{true} - y_{predict})$
- Update weights: Weight adaption often denoted via loss $L \propto \Delta$
  $\rightarrow$ minimize loss $\rightarrow$ find best fit

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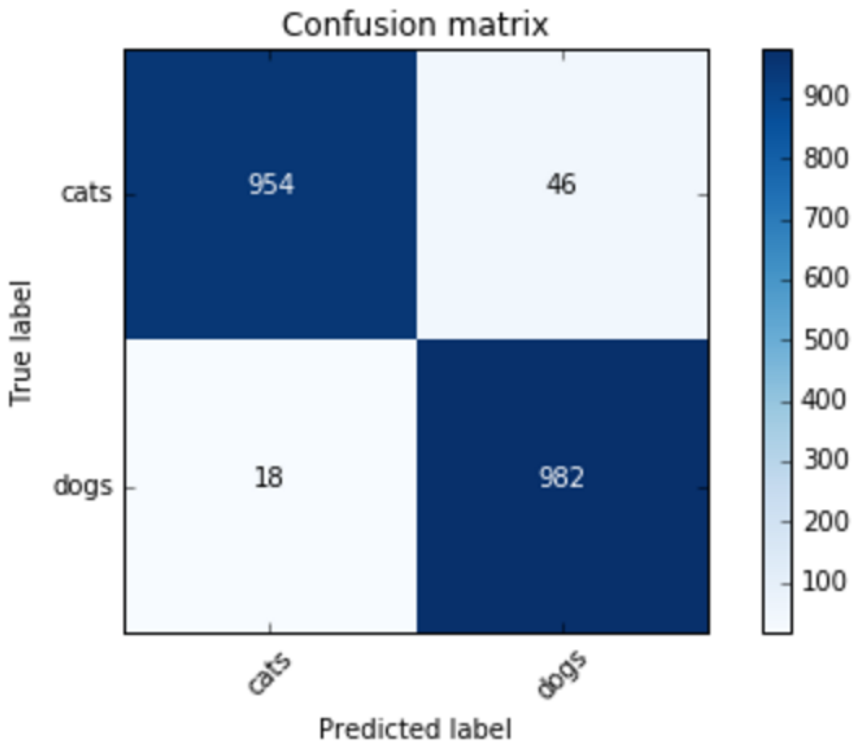
Quantify MVA output

Evaluate classifier performance

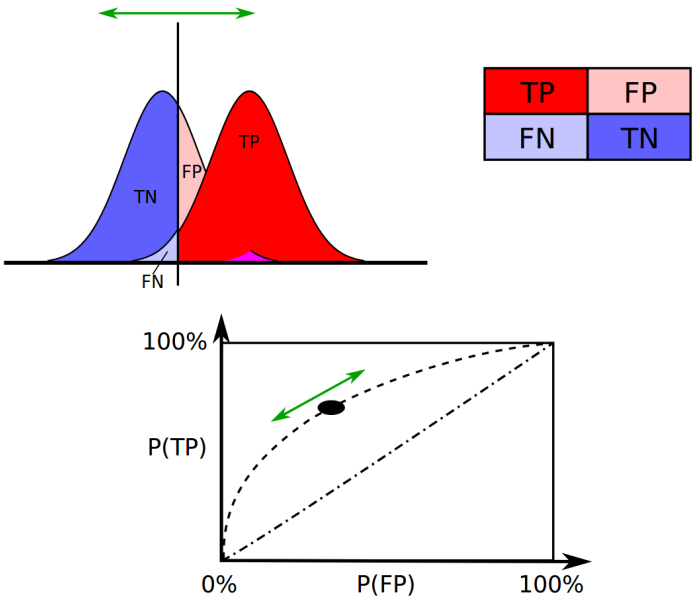
- Compare predicted class labels with the true ones → confusion matrix



Quantify MVA output

Evaluate classifier performance

- ROC curve: continuously scan y & plot background acceptance (FPR) vs. signal efficiency (TPR)



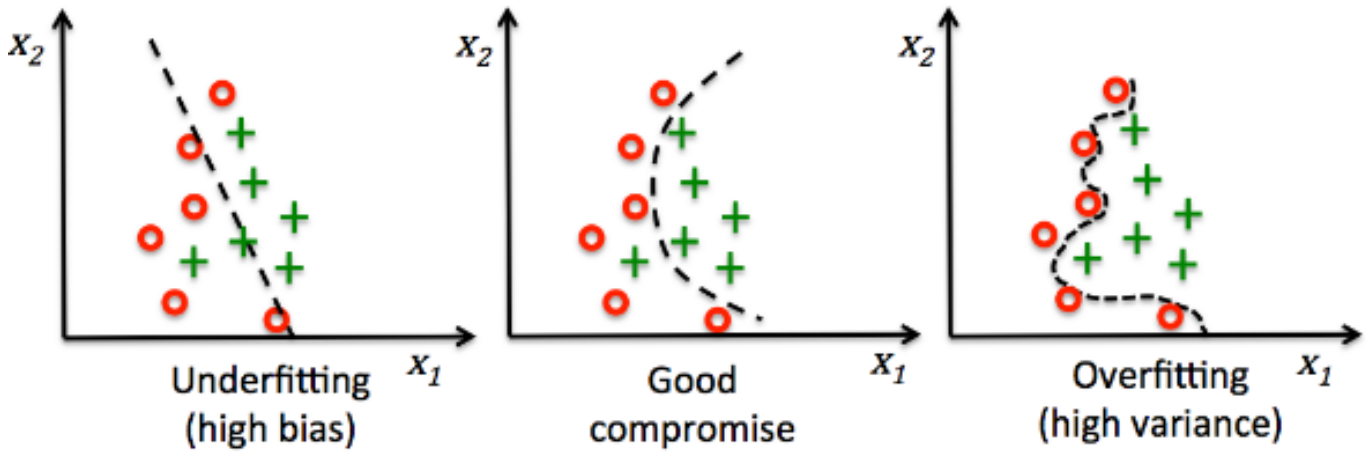
$$\text{FPR} = \text{FP}/(\text{FP}+\text{TN})$$

$$\text{TPR} = \text{TP}/\ (\text{TP} + \text{FN})$$

ROC-AUC: probability that classifier ranks randomly chosen positive sample higher than randomly chosen negative one

Bias-variance tradeof

- Small variance: Classifiers with low degrees of freedom are less prone to statistical fluctuations
  $\rightarrow$ different training samples result in similar classification boundaries
- However: if data contain features that a model with few degrees of freedom cannot describe, a bias is introduced



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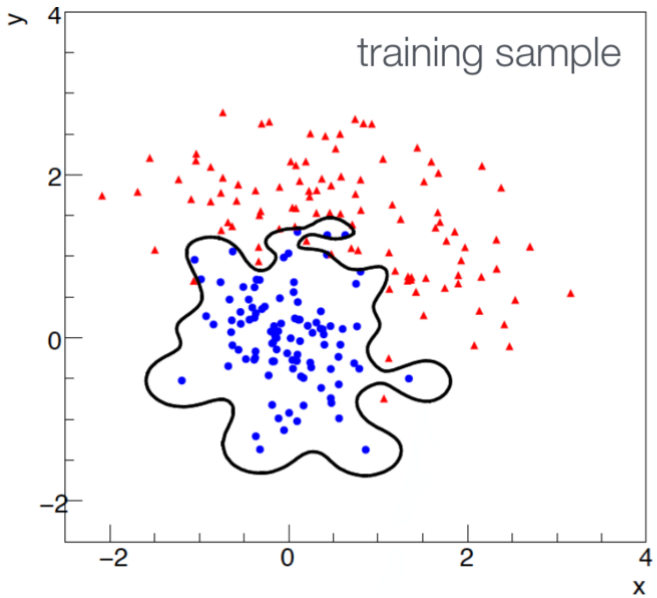
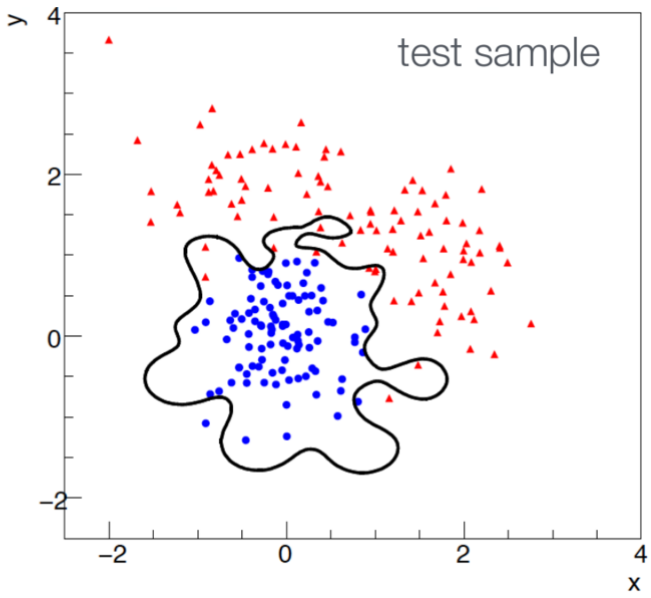
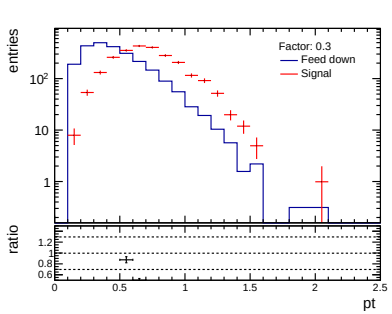
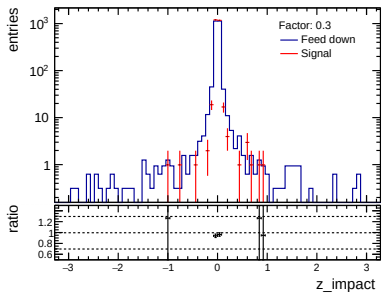
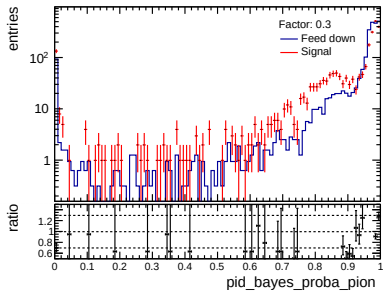




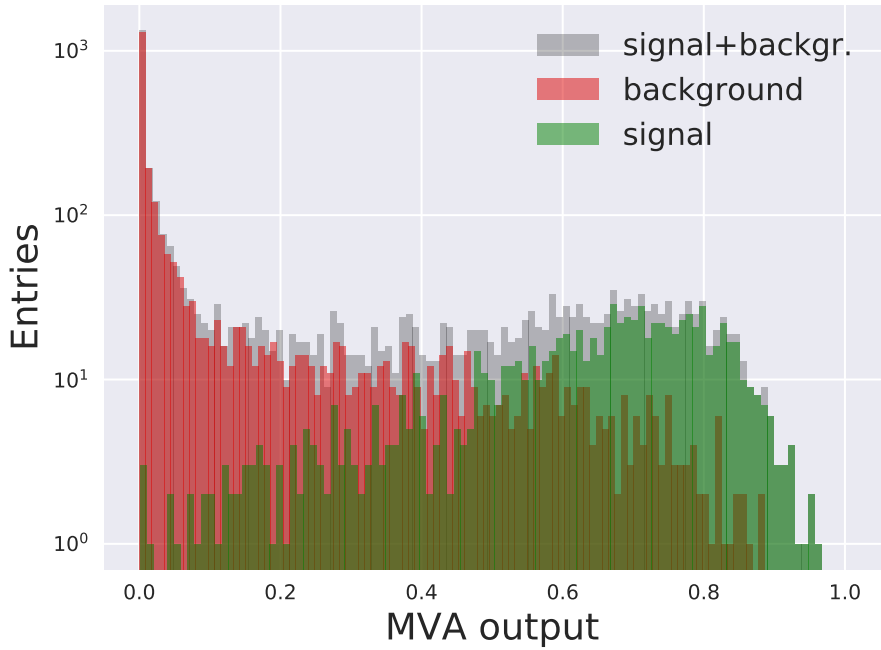
Results







$$\mathbb{R}^n \rightarrow \mathbb{R}$$



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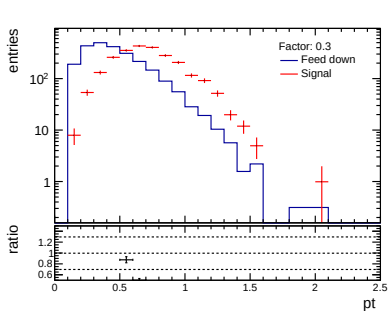
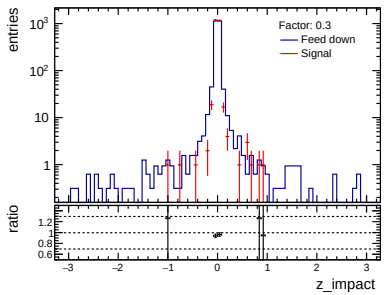
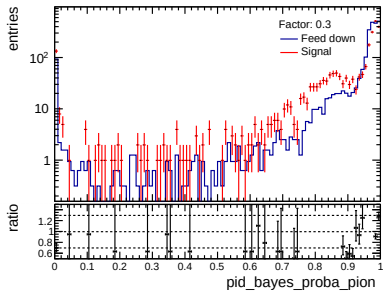
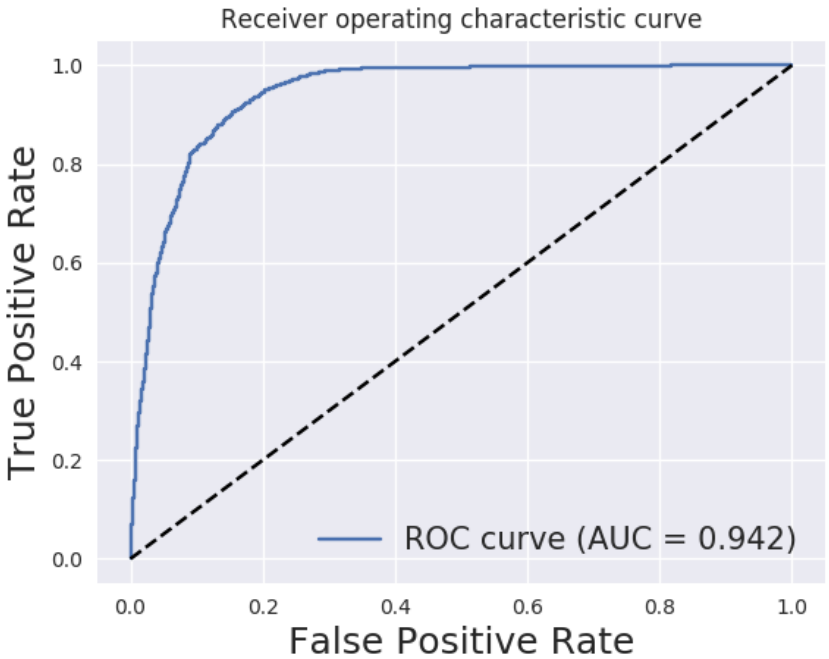




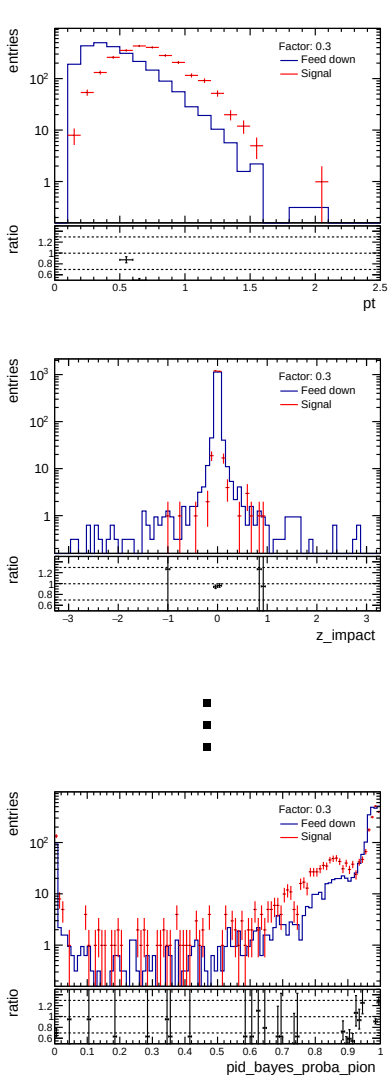


$$\mathbb{R}^n \rightarrow \mathbb{R}$$

ROC train

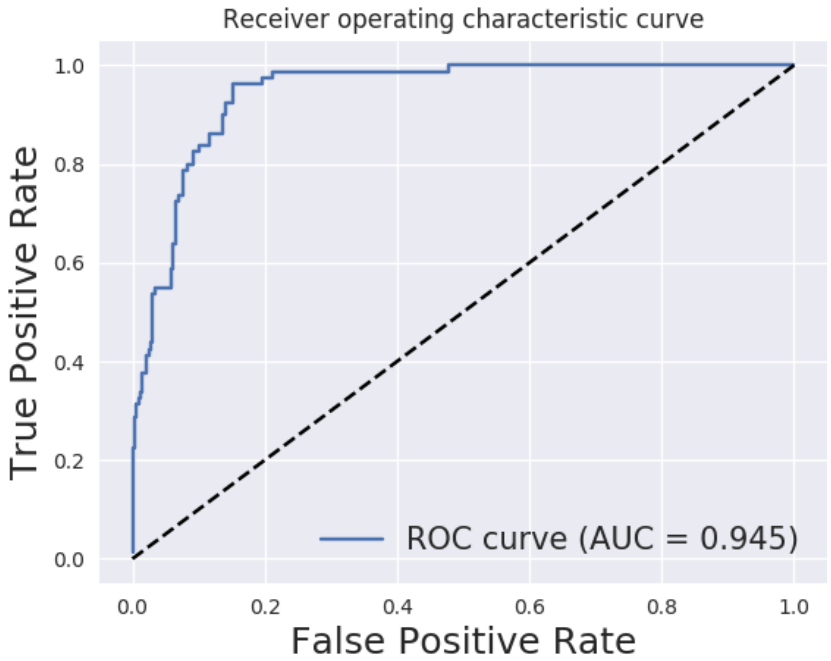


Results

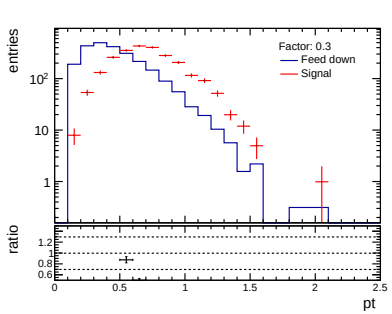


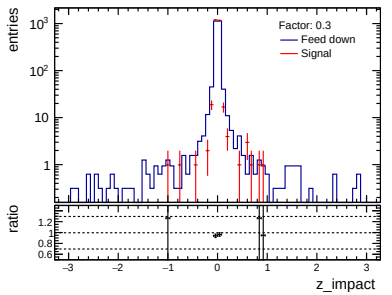
$\mathbb{R}^n \rightarrow \mathbb{R}$

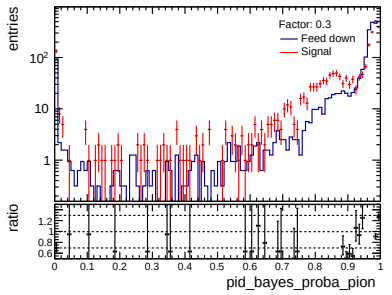
ROC test



Results

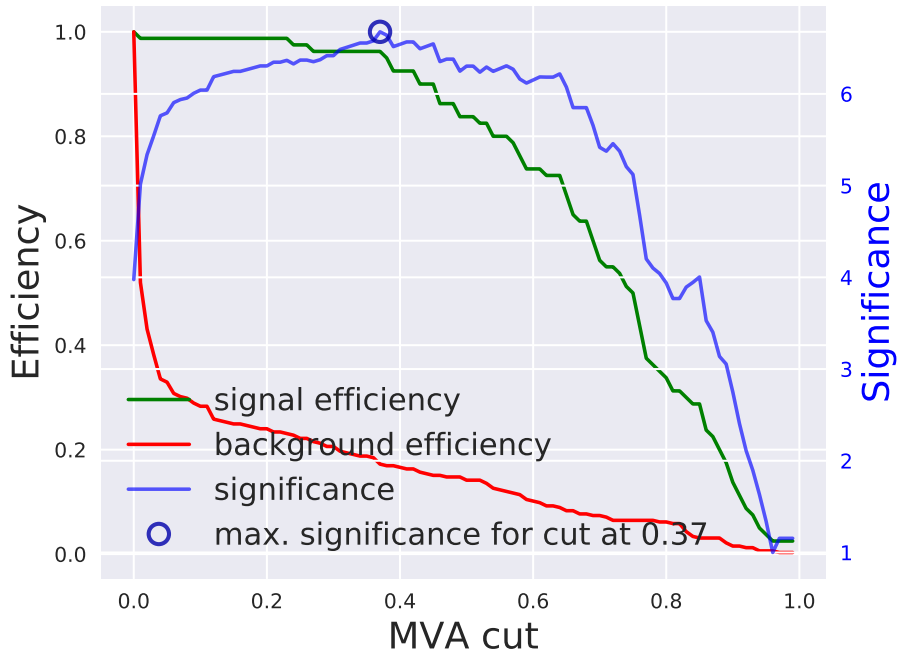




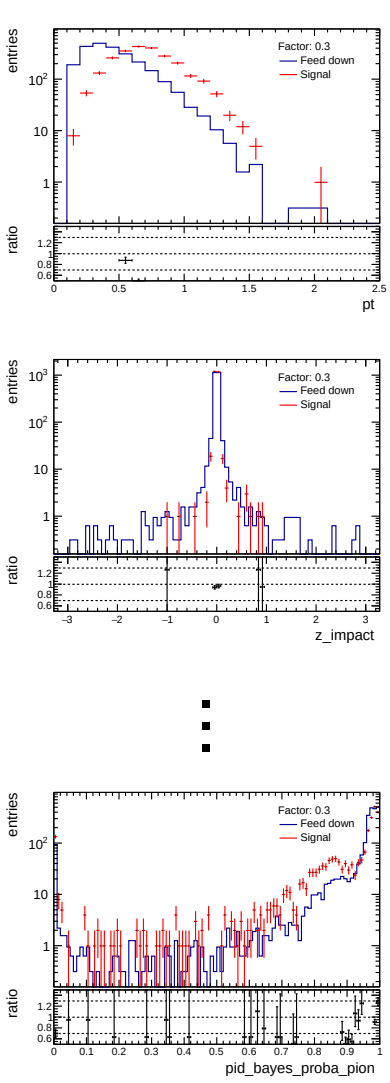


$$\mathbb{R}^n \to \mathbb{R}$$

Significance $S = N_{sig} / \sqrt{N_{sig} + N_{BG}}$

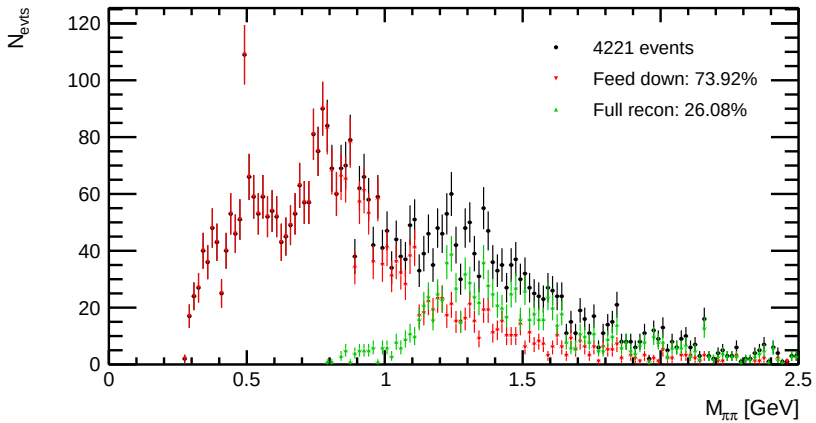


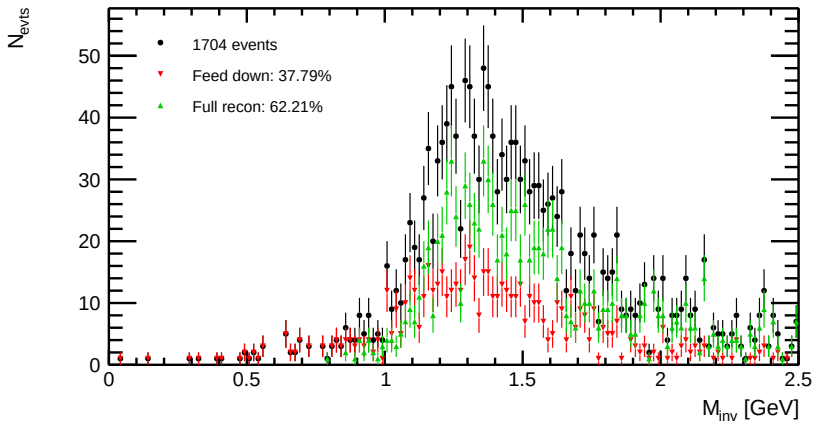
Results



$\mathbb{R}^n \rightarrow \mathbb{R}$

no MVA cut





with MVA cut