

# **Python for Data Science 2**

## **Lecture 10- Machine Learning**

**Amir Farbin**

# Test Statistic

- In your lab you are investigating different observables (aka features)  $\{\vec{x}_i\}$ 
  - Each has separation power between signal and background.
    - Some are better than others
    - We can refer to any of these observables as a **test statistic**
      - A statistical variable that we can use to perform a test (i.e. is it signal?).
      - Many were created after years of careful “feature engineering”.
  - Many are very correlated → Capturing similar information
  - But not 100% correlated → Capture unique information
  - Suggests combining selections on multiple observables might be good idea.
    - → Difficult to do... lose statistical power.
- Can we find a single observable that optimally combines all of the observable?
  - Single test statistic  $f(\{\vec{x}_i\}) \equiv t_i$

# Hypothesis Testing

- Neyman-Pearson lemma: best possible test statistic, given a set of observables is
- But it is rather difficult to obtain  $P$ .
  - Unless you know it analytically, you'll have to rely on Data with ground truth or Simulation (ground truth inputed)
    - → Build Probability Density Function (high dimensional histogram)
    - Curse of Dimensionality → very difficult to populate a high dimensional histogram.
  - Alternatives:
    - Feature Engineering - That's what was attempted with the observables you are using.
    - Machine Learning - Algorithm that learn an optimal test statistic for your task.

# AI vs ML vs DL

- ***Artificial Intelligence***: Any technique that mimics human behavior
  - Code, Logic, Symbolic systems, Knowledge Bases
- ***Machine Learning***: Any technique that learns from experience (aka Data)
  - Logistic regression (aka fits), Decision Trees, Clustering, Kernel Methods
  - ***Representation Learning***: Techniques that learn representations of data amenable to specific or general tasks
    - Shallow Auto-encoders
    - ***Neural Networks***: Biologically inspired ML
      - ***Deep Learning***: Multi-layered Neural Networks
        - MLP, DNN, CNN, RNN, ...

# Supervised ML

- **Tasks:** Classification, Classification with missing inputs, Regression, Transcription, Machine Translation, Structured Output
- “Traditional” Techniques:
  - Linear/Logistic Regression
  - Support Vector Machines
  - Decision Trees

# Un-supervised ML

- **Tasks:** Clustering, Anomaly Detection, Imputation of Missing Values, Synthesis & Sampling, Denoising, Density Estimation
- “Traditional” Techniques:
  - Principle Component Analysis
  - k-means Clustering

# Ingredients of ML

- **Problem Formulation.** Specify:
  - **Data Set:** Inputs/Outputs
  - **ML technique:**  $F(\text{Input} \mid \text{Parameters}) = \text{Output}$
  - **Target: Cost (aka loss) function**
    - *Supervised:* Compare  $F$  vs Ground Truth Output
    - *Unsupervised:* e.g. Cluster like inputs
    - *Semi-supervised:*  $F(\text{Input}) = \text{Input}$
  - **Training: Optimization**
    - Choose how to find best parameters

# Machine Learning

# Basic Formulation

- **AI Algorithm:**  $\text{Input} \longrightarrow \text{AI Algorithm} \longrightarrow \text{Output}$ 
  - $X \longrightarrow F(\theta) \longrightarrow y: y = F(X|\theta)$ 
    - $X$ : observable inputs
    - $\theta$ : Model parameters (most likely learned)
    - $y$ : observable outputs
- **Typical HEP ML task:** Isolate signal in real data  $\{x_d\}_i$ 
  - **Formulate problem:**  $X = x_d, y = 0$  or  $1$  if  $c = \text{background or signal}$
  - **Obtain training data:** generate simulated labeled Dataset  $\{x_d, c\}_i$ 
    - **Separate dataset:** into *Train*, *Test*, and possibly *Validation* subsets
  - **Choose:** Pick an ML algorithm  $F$
  - **Train:** Use labeled Dataset  $\{x_d, c\}_i$  to obtain  $\theta$
  - **Test:** Estimate  $P(F(X|\theta)|c_j)$  using Test sample
  - **Optimize:** Select  $F(X|\theta) > \text{cut}$  to optimize sensitivity for a hypothesis test
    - $P(F(X|\theta)| \text{signal}) / P(F(X|\theta)| \text{background})$
  - **Validate:** Obtain signal / background efficiency using Validation sample
  - **Apply:** to data  $\{x_d\}_i$

# ML Models (Linear)

- Linear Models:  $F(\vec{x}) = \mathbf{W}\vec{x} + \vec{b}$

- Solve equation  $\vec{y} = \mathbf{W}\vec{x} + \vec{b}$

- for “weights” w in matrix W and biases b

- by minimizing  $\frac{1}{N} \sum_i^N (F(\vec{x}_i | \mathbf{W}, \vec{b}) - \vec{y}_i)^2$

- Note

- W is d by m matrix

- x is d component vector

- y is m component vector

- Simple example: b = 0, W is 1 by d

- $\Rightarrow$  Analytic solution

$$W = (X^T X)^{-1} X^T Y$$

$$X = \begin{pmatrix} \vec{x}_1 \\ \vec{x}_2 \\ \vdots \\ \vec{x}_N \end{pmatrix} \quad Y = \begin{pmatrix} \vec{y}_1 \\ \vec{y}_2 \\ \vdots \\ \vec{y}_N \end{pmatrix}$$

# ML Models (LDA)

- Linear Discriminant Analysis (Fisher Discriminant)
  - Assume 2 classes: 0 and 1
    - Means  $\mu_0, \mu_1$  and covariance matrices  $\Sigma_0, \Sigma_1$
  - Model:  $\vec{y} = \mathbf{W}\vec{x}$ 
    - Again W is 1 by d, b=0
    - Maximize: 
$$S = \frac{(\mathbf{W} \cdot \vec{\mu}_0 - \mathbf{W} \cdot \vec{\mu}_1)^2}{\mathbf{W}^T \Sigma_0 \mathbf{W} - \mathbf{W}^T \Sigma_1 \mathbf{W}}$$
      - Maximal separation between means
      - Smallest possible variance
    - Analytic Solution:  $\mathbf{W} = (\Sigma_0 + \Sigma_1)^{-1} (\vec{\mu}_0 - \vec{\mu}_1)$

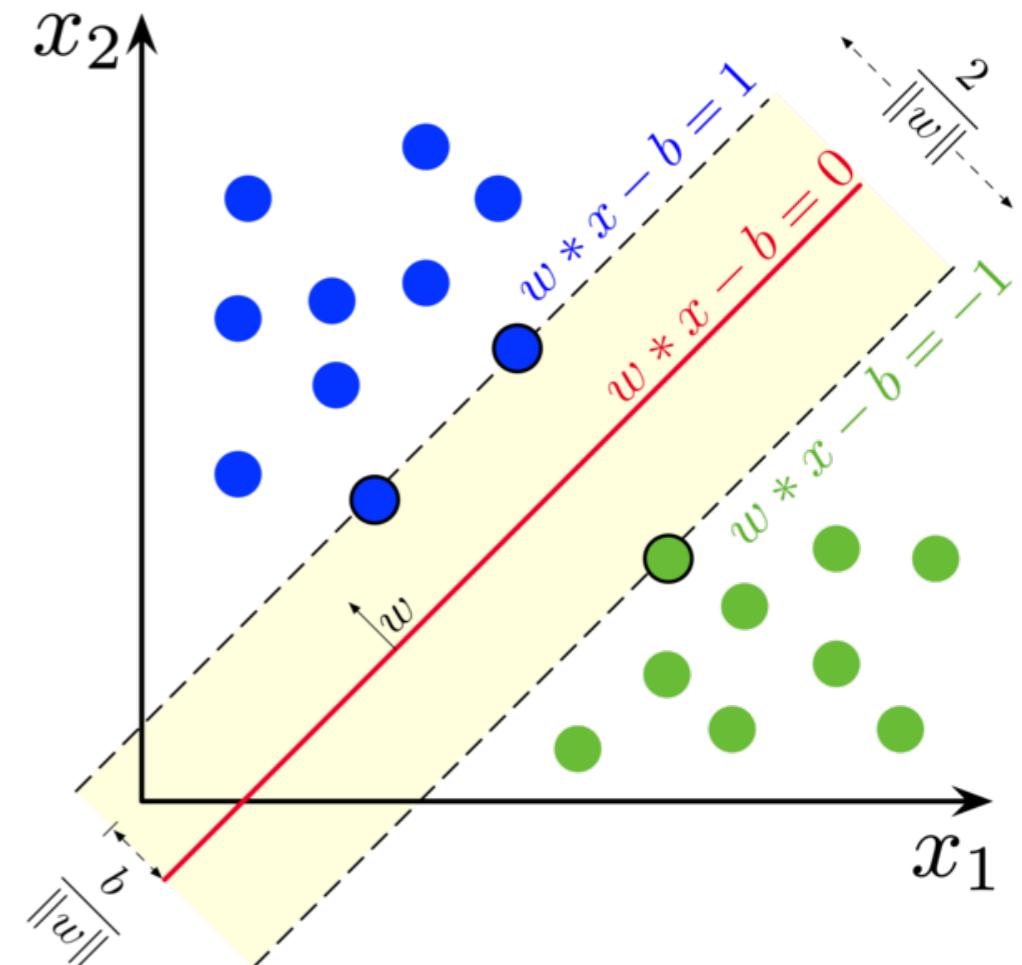
# ML Models (Linear SVM)

- Support Vector Machines:

- Same setup...  $\vec{y} = \vec{W} \cdot \vec{x} + \vec{b}$
- Note that this is an equation for a hyperplane —> formulate problem as finding the hyperplane that optimally separates two classes.
- Maximize boundary between two classes  $\Rightarrow$  plane depends on points closest to the plane / most difficult to separate... the *Support Vectors*.
- Solving this problems is equivalent to solving a dual problem of solving for  $a_i$

$$f(\vec{x}) = \left( \sum_i^N a_i y_i \vec{x}_i \right) \cdot \vec{x} + \vec{b}$$

- Where  $y_i = \{+1, -1\}$  depending on class.
- $a_i \geq 0$ .
- Dot product measures similarity.
  - $\rightarrow$  Sign of output dependent on sign of the most similar example in training set.
  - Support vectors still most important for defining boundary

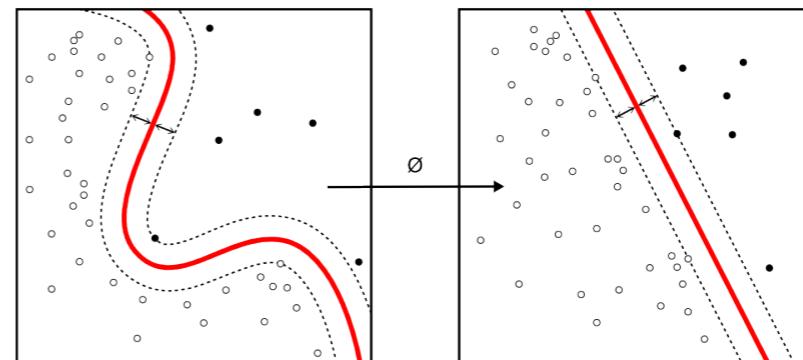


# ML Models (Kernel SVM)

- If boundary not linear  $\Rightarrow$  Kernel Trick:

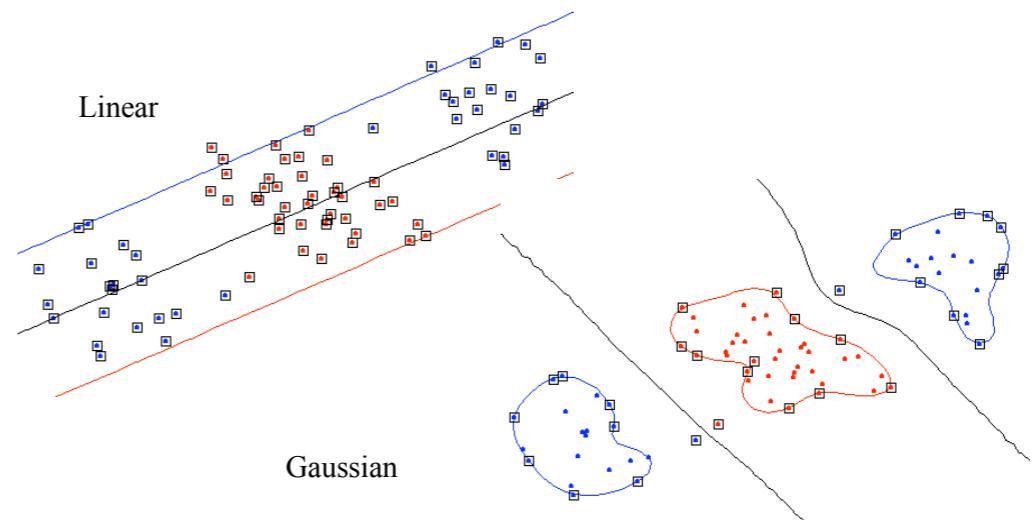
- Replace dot product:  $f(\vec{x}) = \sum_i^N a_i y_i k(\vec{x}_i, \vec{x}) + \vec{b}$      $k(\vec{x}_i, \vec{x}) = \phi(\vec{x}_i) \cdot \phi(\vec{x})$

- Example: if  $x$  is in radial coordinates, then kernel gets back proper dot product.

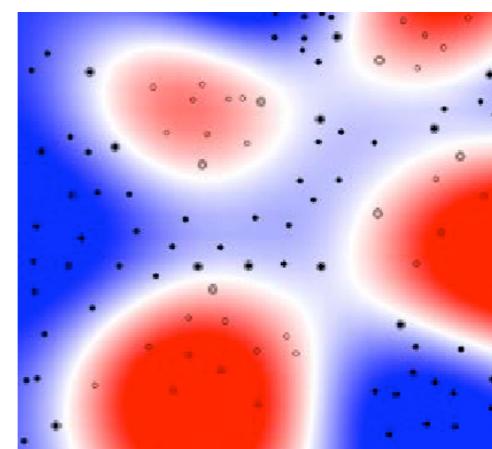


- Example: Gaussian Kernels

- Euclidian Distance in the exponential
- If close to an example in training data  $\Rightarrow$  large value
- Equivalent to template matching



Radial Basis Functions

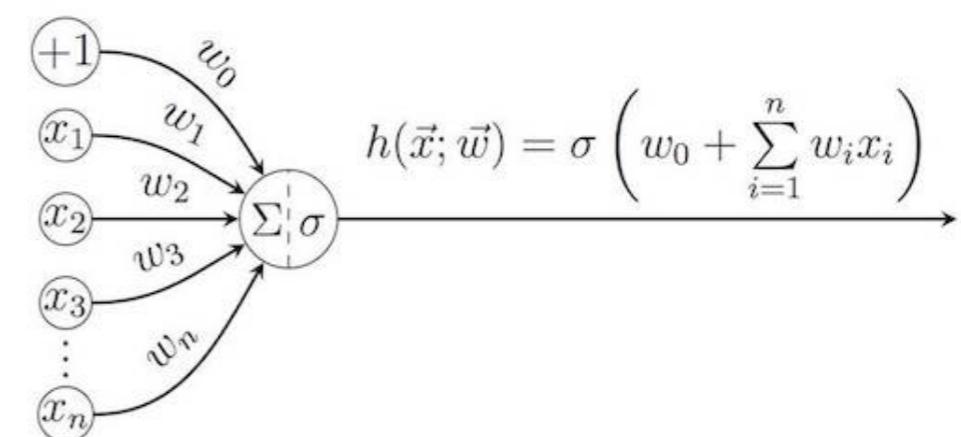
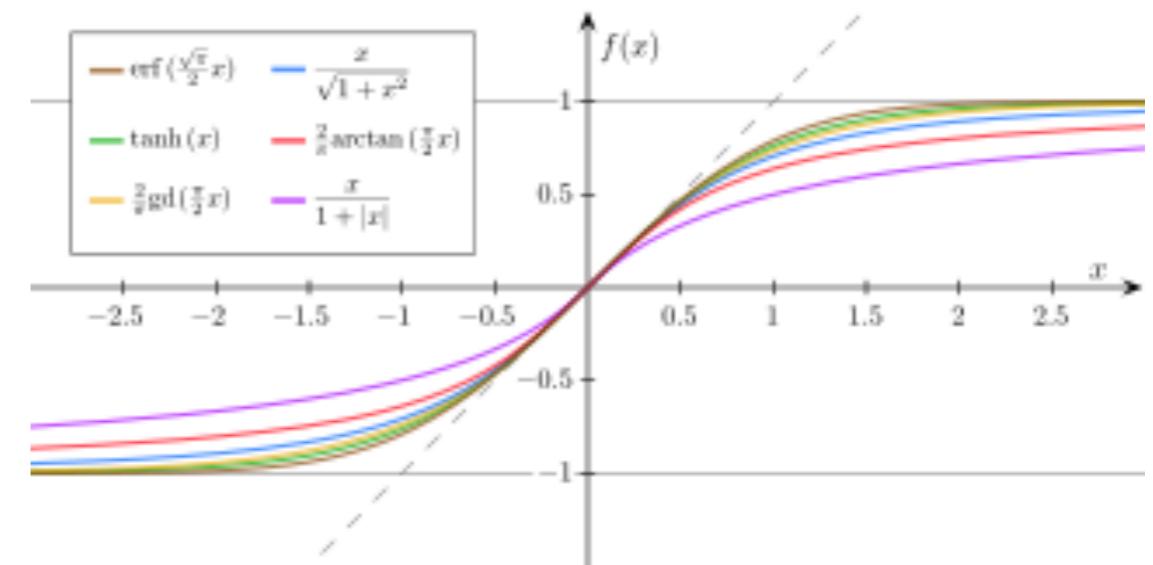


# Features

- $X \rightarrow \phi(X) \rightarrow$  Linear Model
- $\phi$  are features or representation derived from  $X$
- $\phi$  is:
  - Generic, e.g. polynomials  $\rightarrow$  e.g. SVM
  - Manually constructed  $\rightarrow$  Feature Engineering
  - Learned  $\rightarrow$  Feature Learning

# Artificial Neural Network

- A simple one layer NN
  - $F(\mathbf{X} | \mathbf{a} = \mathbf{W}, \mathbf{b}) = f(\mathbf{W} \mathbf{X} + \mathbf{b})$
  - $\mathbf{W}, \mathbf{b}$  = “weights”, “biases”
  - $f(x)$  = “activation function”
    - Must be non-linear.
  - Universal Computation Theorem.



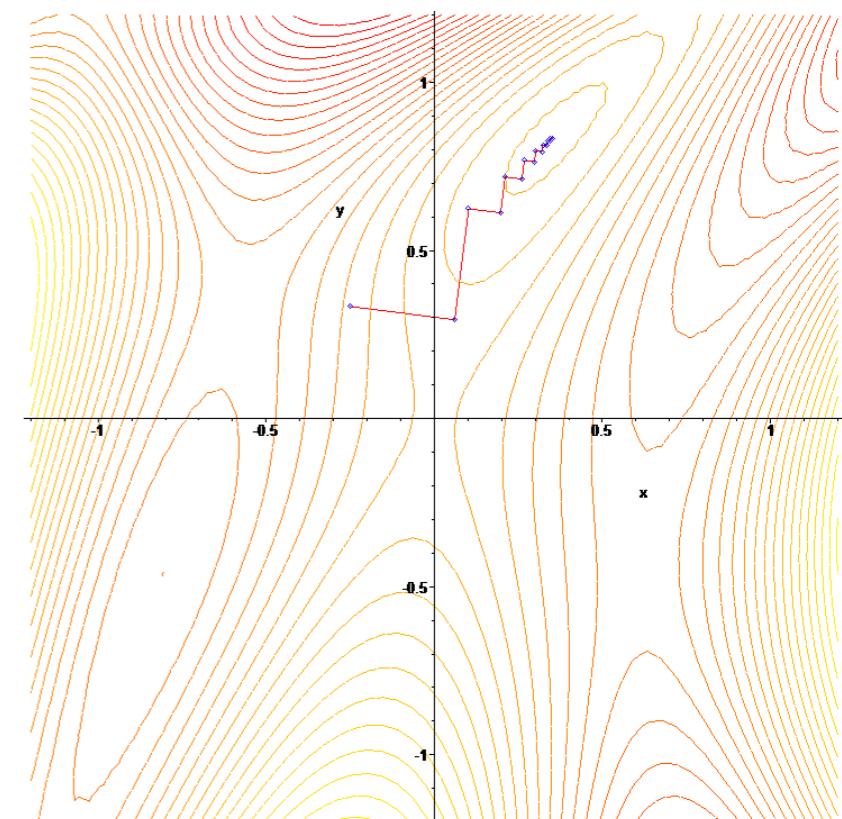
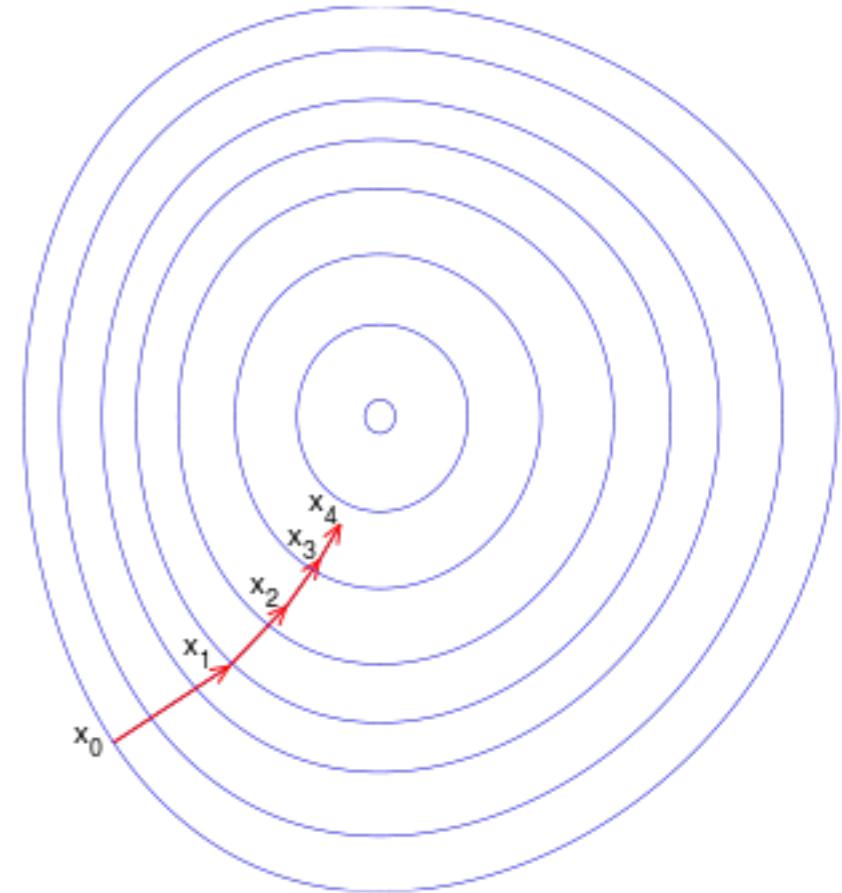
# Training == Optimization

- Training = Minimizing cost function w.r.t. parameters  $\vec{\alpha}$

$$C[F(\vec{X}_{train}|\vec{\alpha}), \vec{Y}_{train}] \equiv C(\vec{\alpha})$$

- Gradient Decent (Newton's Method):
  - Gradient points to direction of maximal change.
  - Iterate ( $\epsilon$  sets the step size == *Learning Rate*)

$$\vec{\alpha}_{i+1} = \vec{\alpha}_i - \epsilon \nabla C(\vec{\alpha})$$

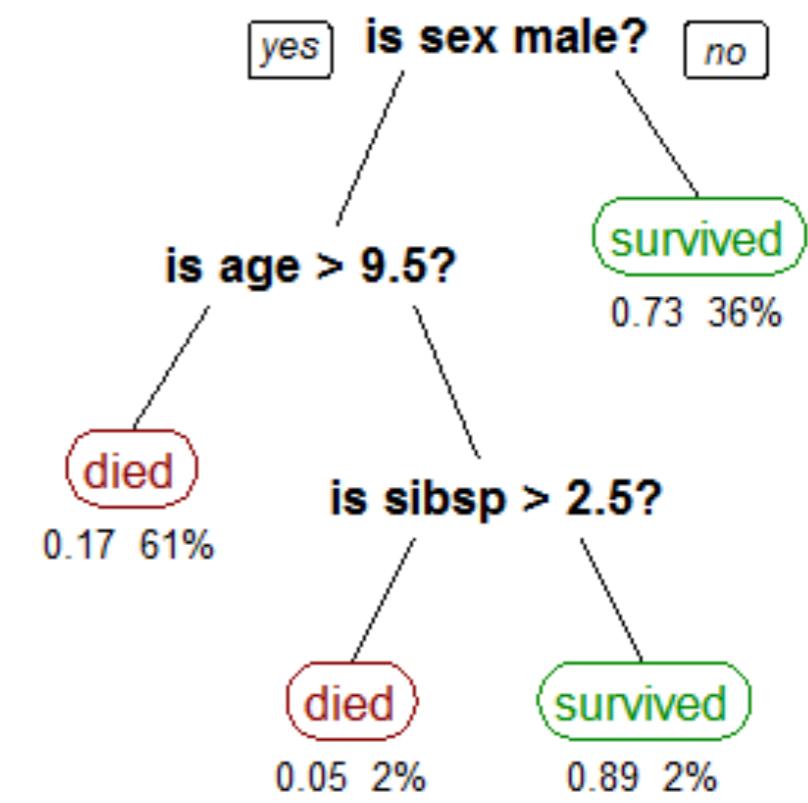


# Bayesian vs Frequentist

- ***Supervised Learning:***
  - Data:  $(X, Y)$
  - True:  $f^*(X) = Y$
  - Learn:  $f(X|\theta) \sim f^*$
- ***Frequentist:***
  - $(X, Y)$  random.
  - Ideal  $\theta$  exists.
  - Estimate  $\theta$ .
- ***Bayesian:***
  - $(X, Y)$  fixed.
  - $\theta$  is random.
  - Learn  $p(\theta)$
- ***Bayesian Learning:***
  - For example:  $\theta$  is Gaussian distributed  $\Rightarrow$  learn  $\mu, \sigma$
  - Allows you to propagate uncertainties  $\Rightarrow$  estimate uncertainty on output  $Y$

# Decision Trees

- Doesn't fit the  $F(\mathbf{X} | \mathbf{W}, \mathbf{b})$  formulation.
- Powerful technique
  - Random Forest
  - Boosting
- Covered by Daniele
- Up to recently, in HEP, Boost Decision Trees (BDTs) on well constructed/chosen features



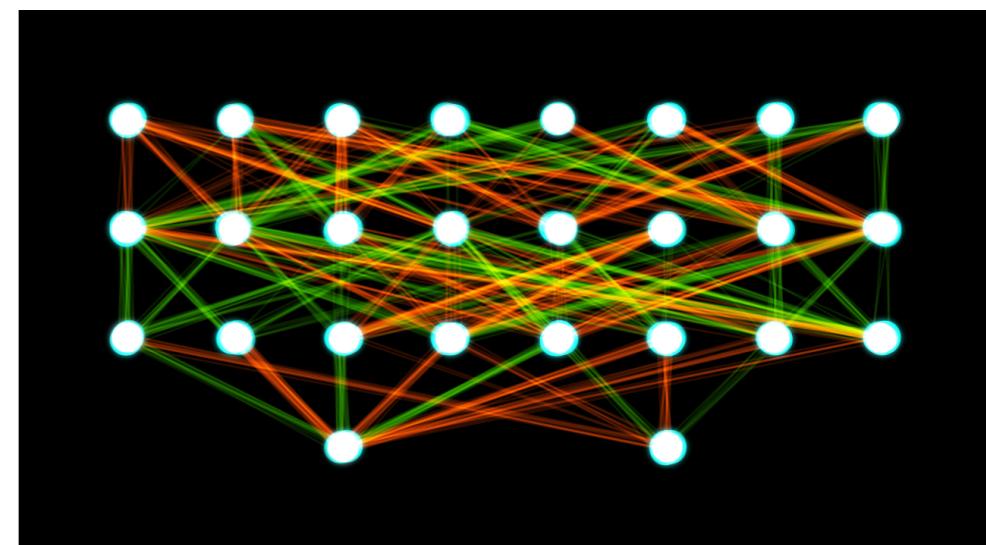
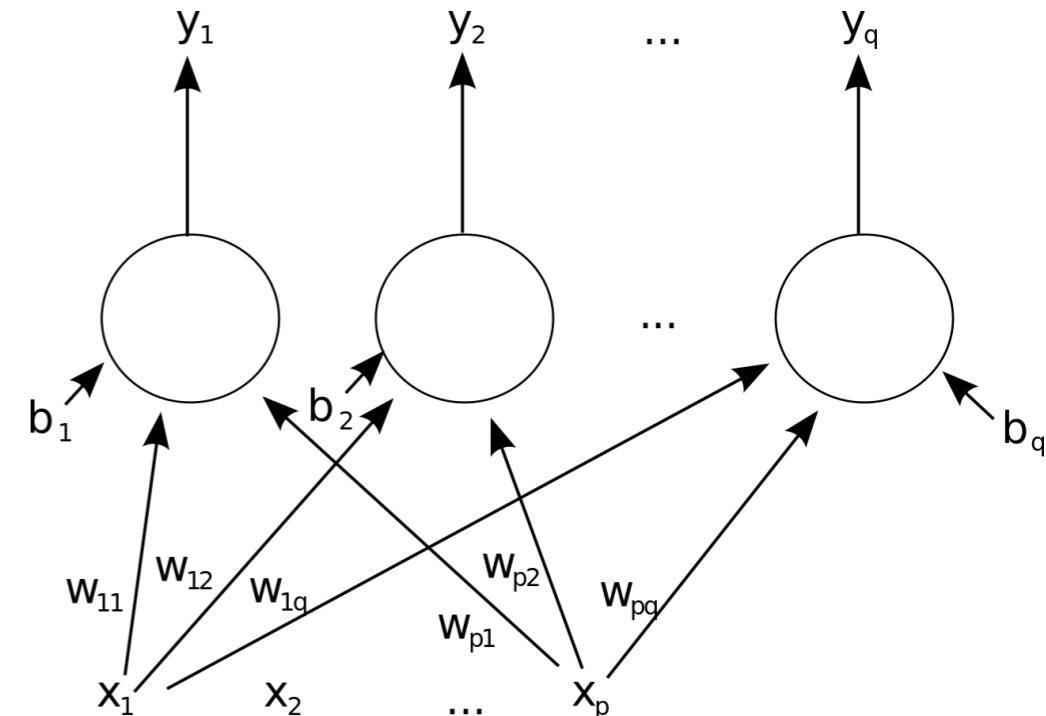
**Titanic Survivors**

- have been the best performing techniques, and
- become the standard to beat,

# Deep Learning

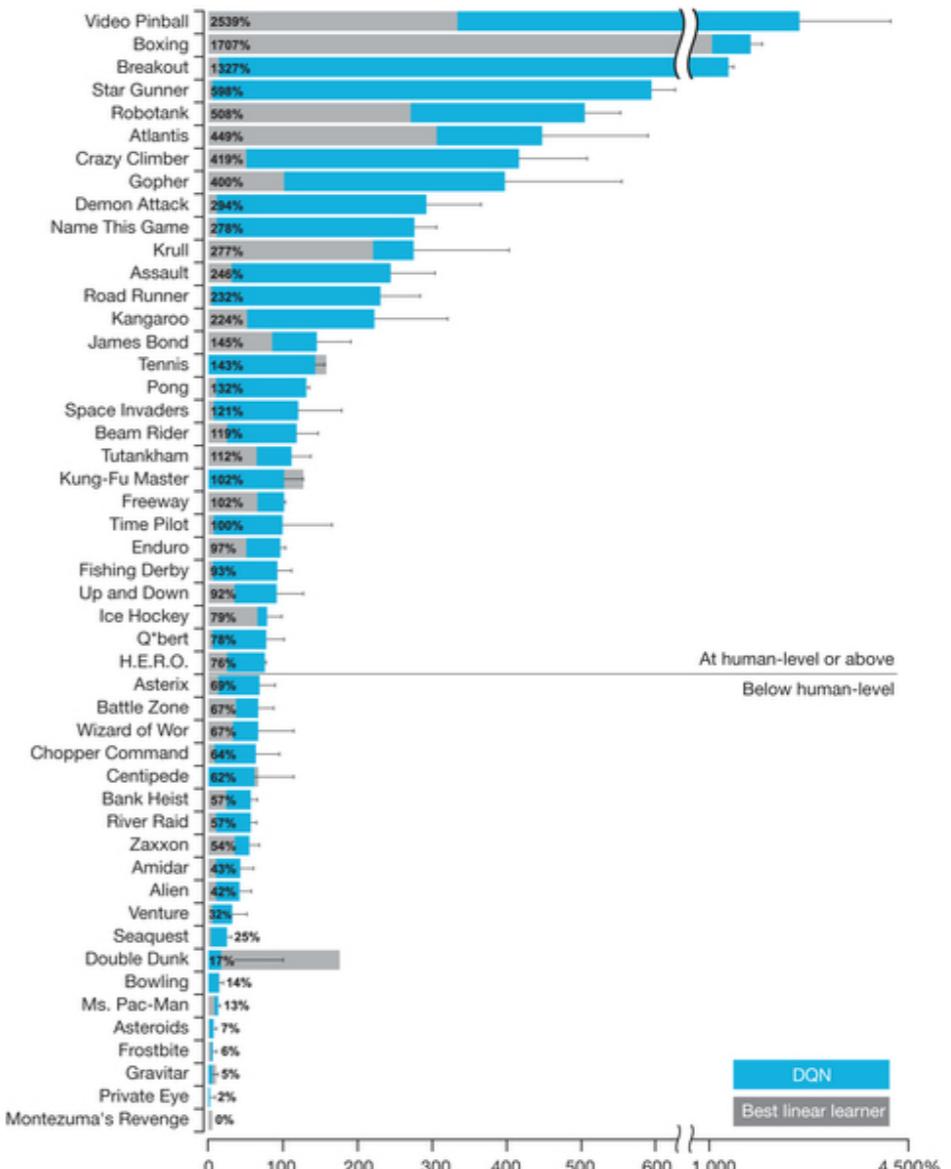
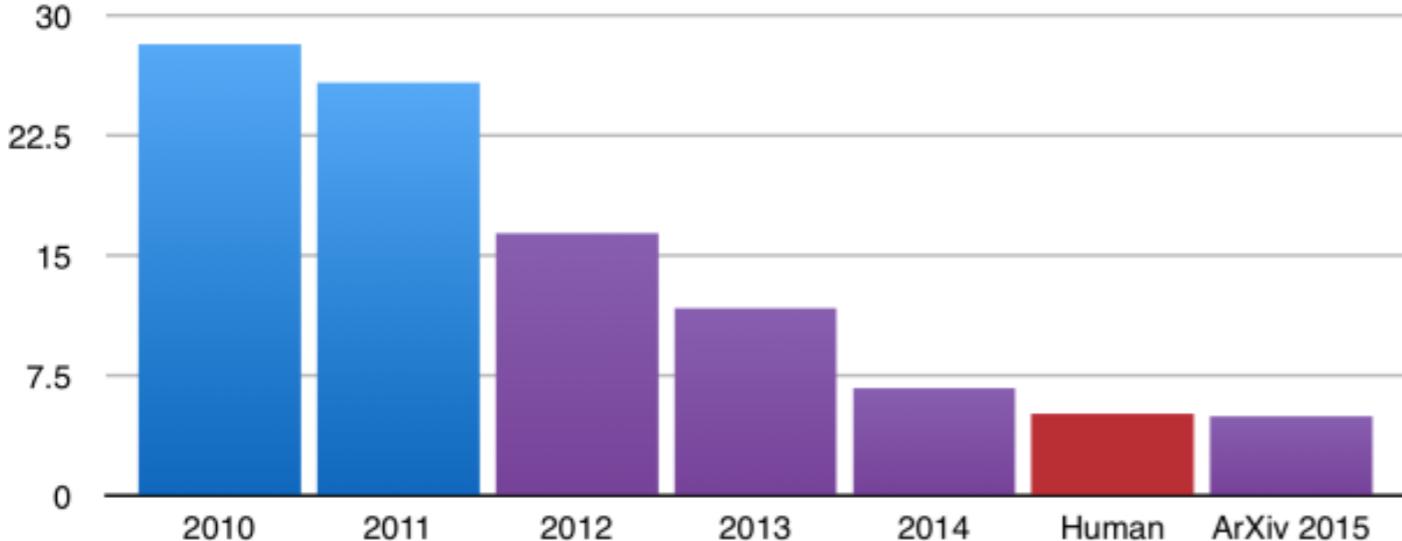
# Artificial Neural Networks

- **Biologically inspired computation**, (first attempts in 1943)
  - **Probabilistic Inference**: e.g. signal vs background
  - **Universal Computation Theorem** (1989)
- Multi-layer (**Deep**) Neutral Networks:
  - Not a new idea (1965), just impractical to train. **Vanishing Gradient problem** (1991)
  - Solutions:
    - New techniques: e.g. better activation or layer-wise training
    - **More training**: big training datasets and lots of computation ... **big data and GPUs**
  - **Deep Learning Renaissance**. First DNN in HEP (2014).
  - **Amazing Feats**: Audio/Image/Video recognition, captioning, and generation. Text (sentiment) analysis. Language Translation. Video game playing agents.
  - **Rich field**: Variety of architectures, techniques, and applications.

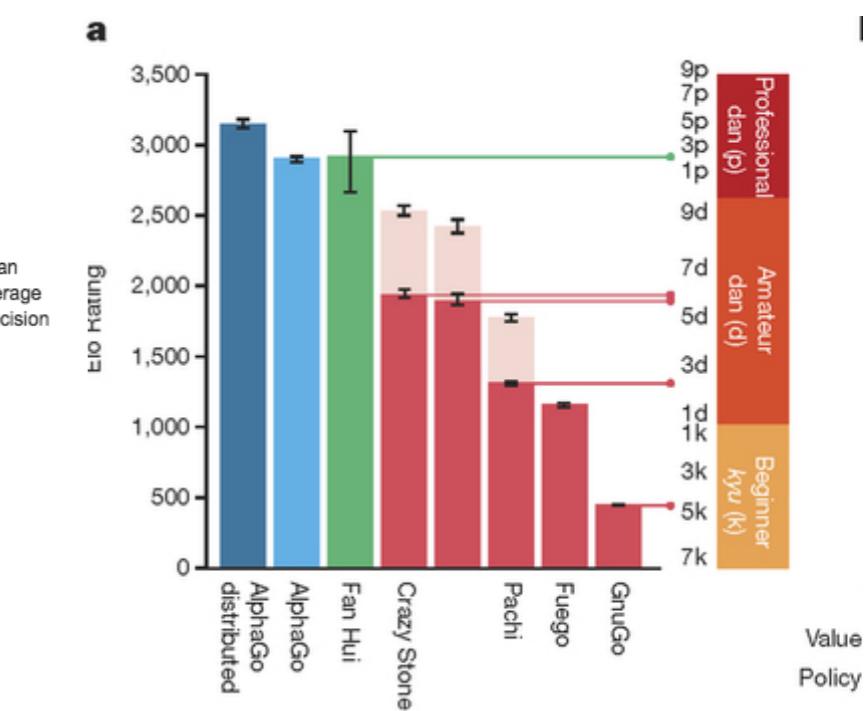
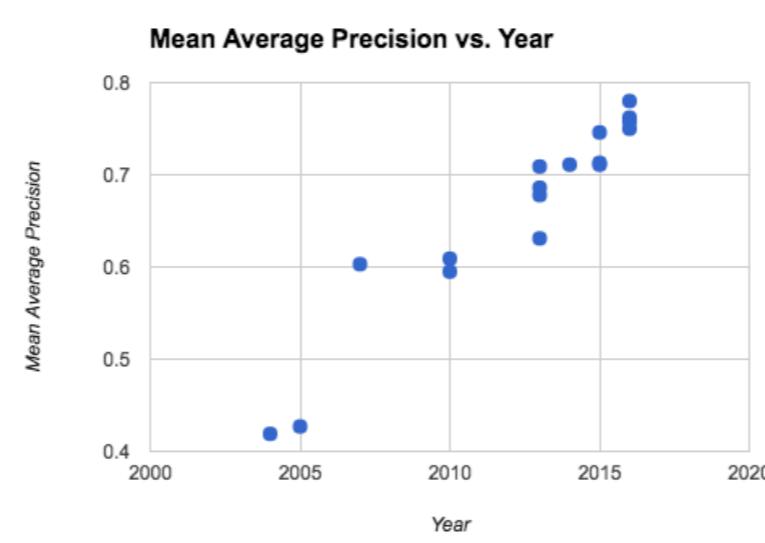
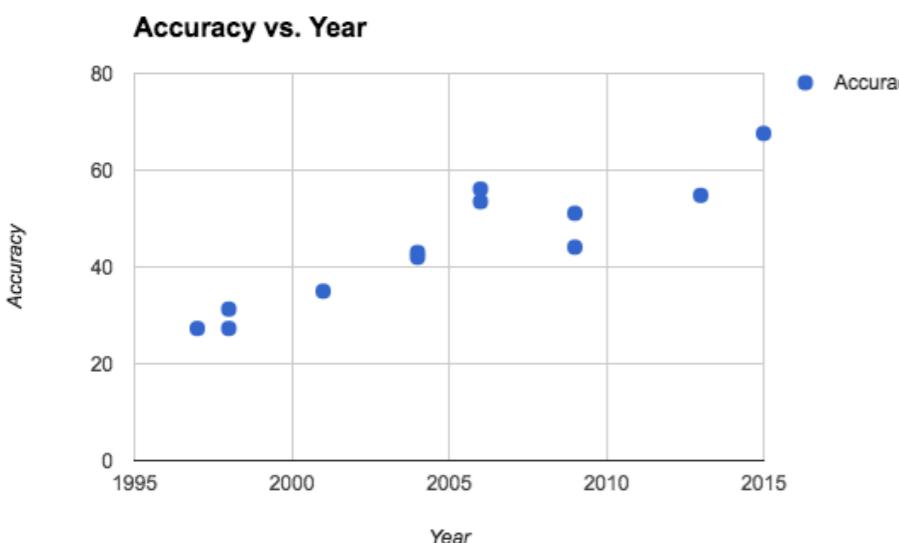
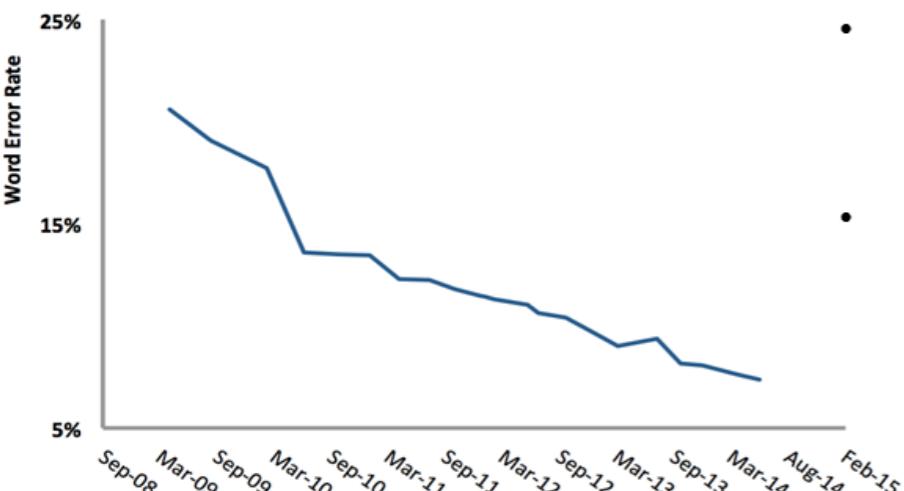


Images from Wikipedia

# ILSVRC top-5 error on ImageNet

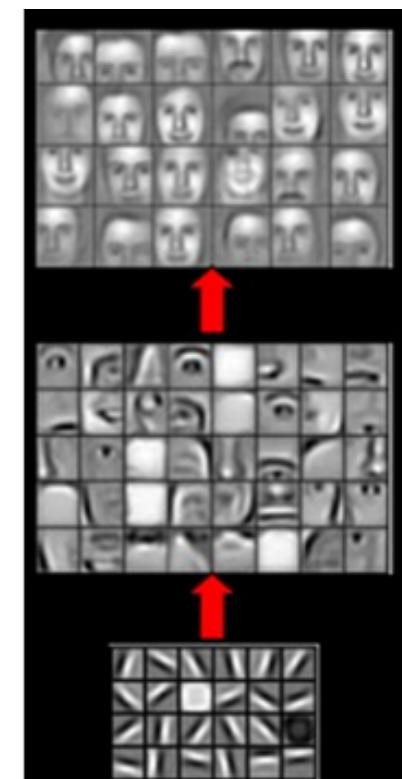
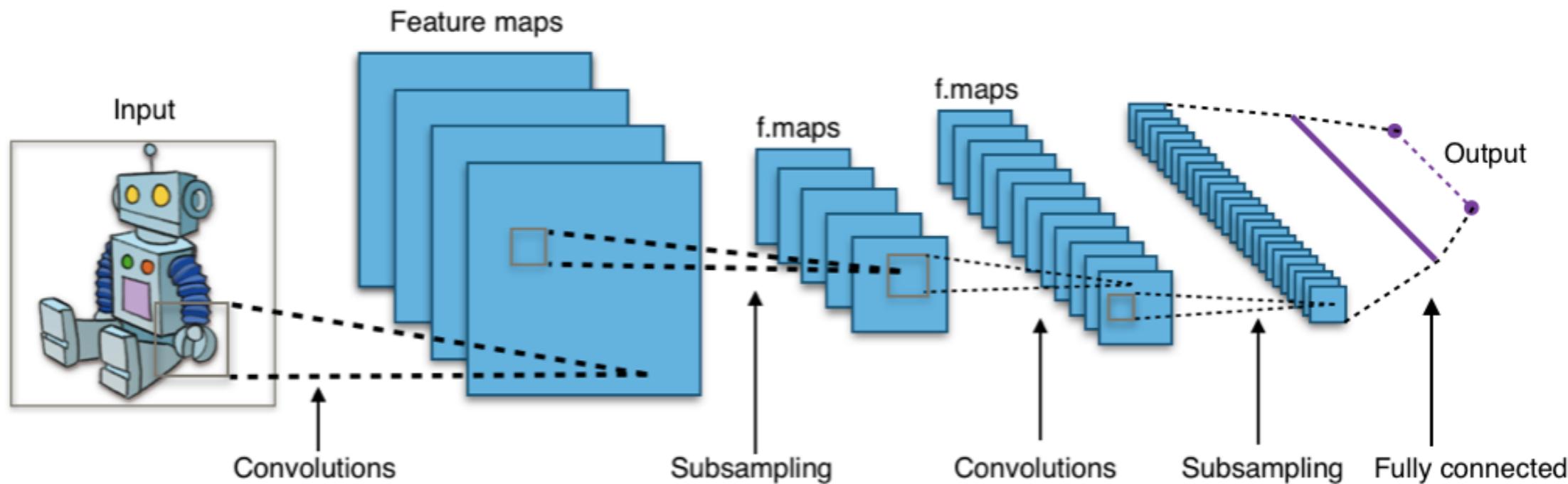


- Continuous server ASR word error rate (WER) reduction ~18% / year: combination of algorithms, data, and computing
- Deep learning (DNNs) is driving recent performance improvements in ASR and meaning extraction

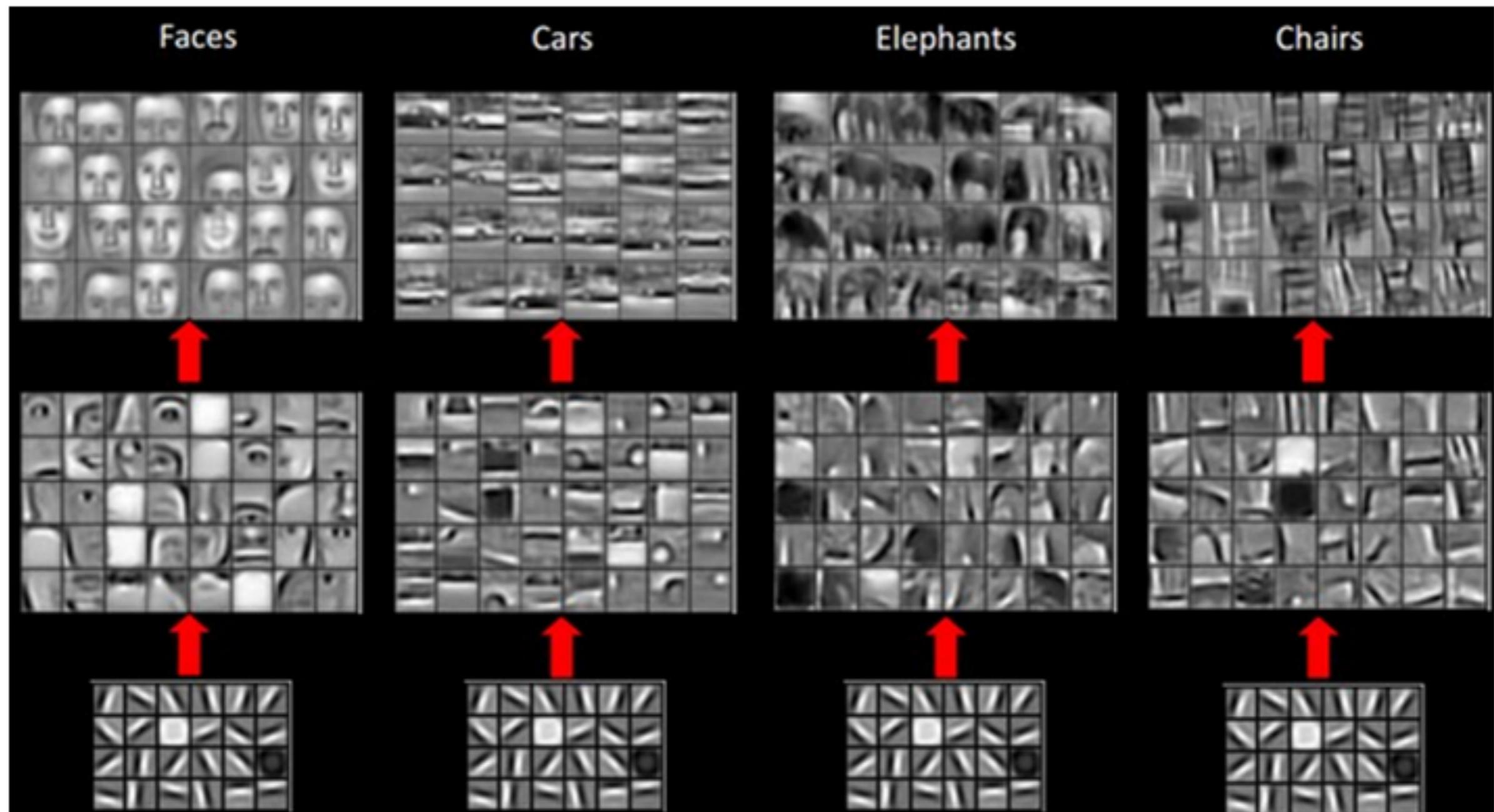


# Feature Learning

- **Feature Engineering:** e.g. Event Reconstruction ~ Feature Extraction, Pattern Recognition, Fitting, ...
- Deep Neural Networks can **Learn Features** from **raw data**.
- Example: **Convolutional Neural Networks** - Inspired by visual cortex
  - **Input:** Raw data... for example 1D = Audio, 2D = Images, 3D = Video
  - **Convolutions** ~ learned feature detectors
  - **Feature Maps**
  - **Pooling** - dimension reduction / invariance
  - **Stack:** Deeper layers recognize higher level concepts.

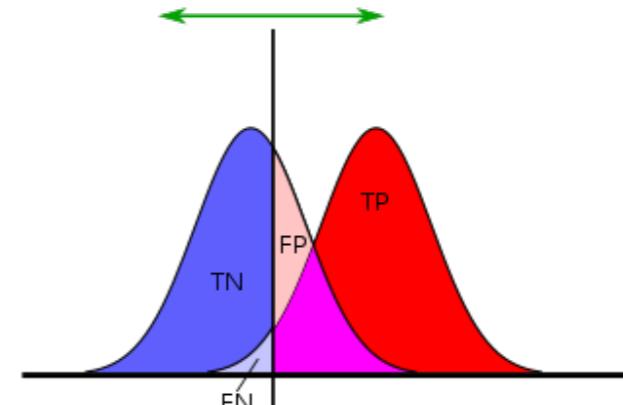
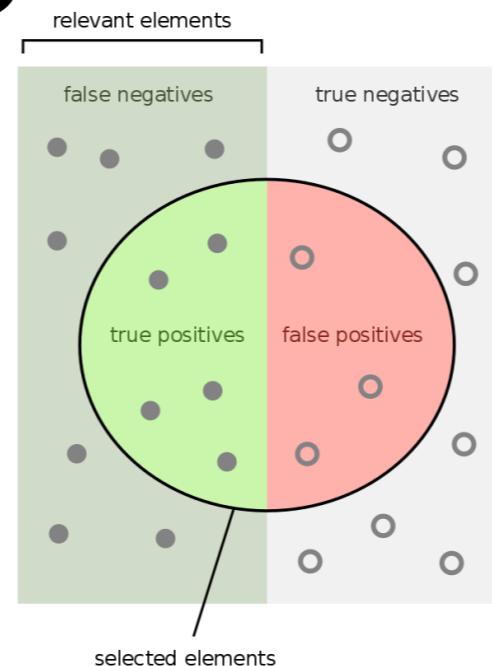


# Deep Neutral Networks

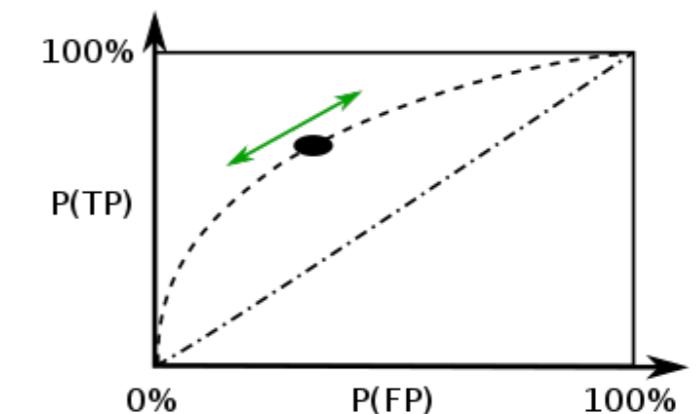


# Assessing Performance

- **True Positive Rate (TPR):** Efficiency
- **False Positive Rate (FPR):** Background efficiency, 1/Background Rejection
- **Receiver Operator Curve (ROC):** TPR vs FPR
- **Area Under Curve (AUC):** Area under ROC



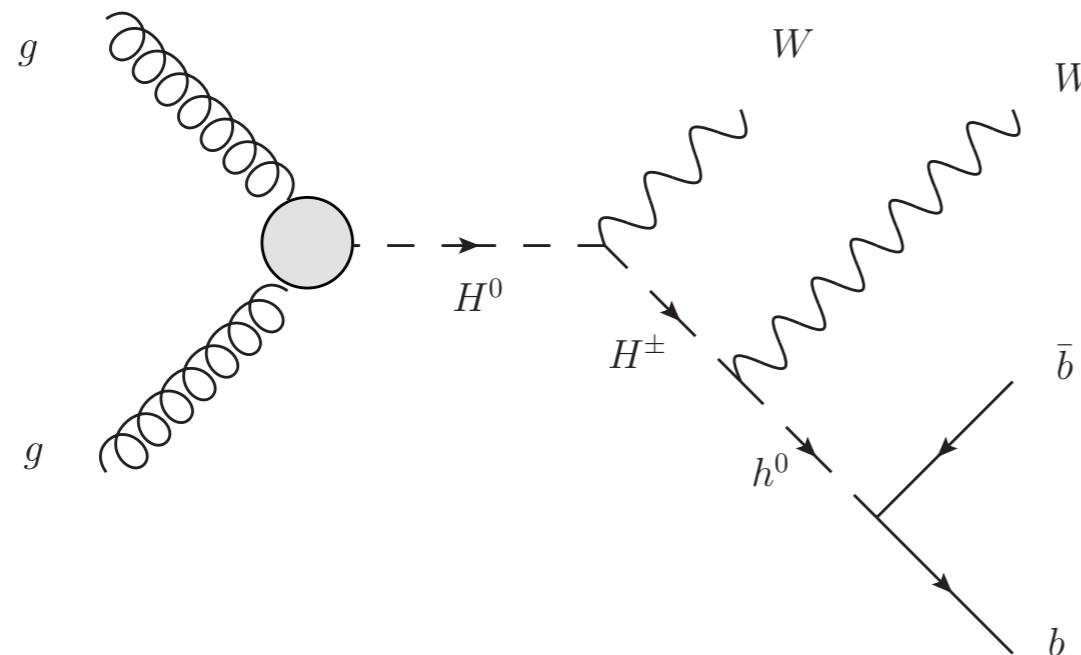
TP	FP
FN	TN



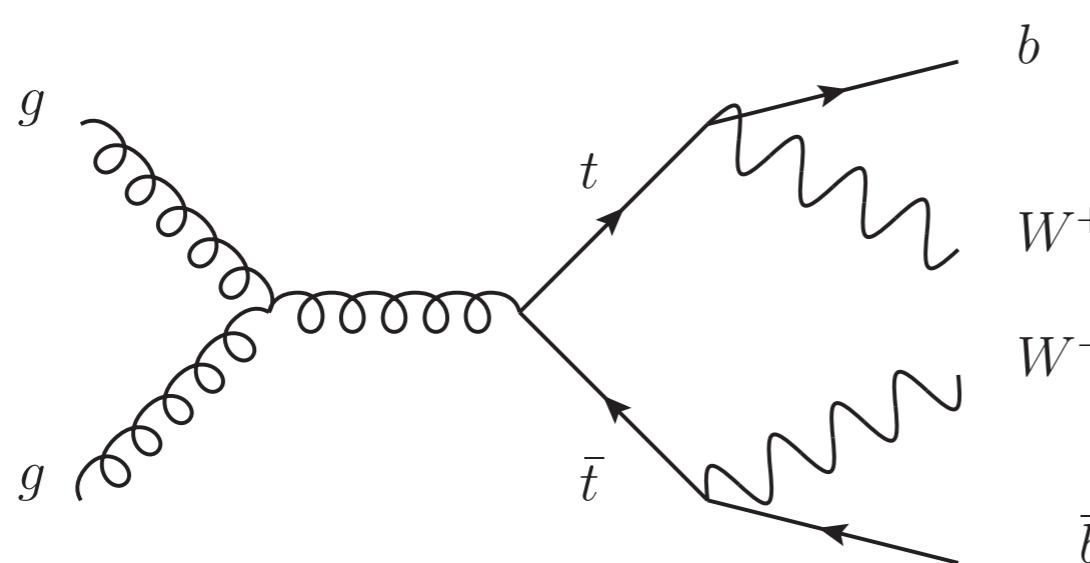
		True condition		Prevalence = $\frac{\sum \text{Condition positive}}{\sum \text{Total population}}$	Accuracy (ACC) = $\frac{\sum \text{True positive} + \sum \text{True negative}}{\sum \text{Total population}}$
		Condition positive	Condition negative		
Predicted condition	Predicted condition positive	True positive	False positive, Type I error	Positive predictive value (PPV), Precision = $\frac{\sum \text{True positive}}{\sum \text{Predicted condition positive}}$	False discovery rate (FDR) = $\frac{\sum \text{False positive}}{\sum \text{Predicted condition positive}}$
	Predicted condition negative	False negative, Type II error	True negative	False omission rate (FOR) = $\frac{\sum \text{False negative}}{\sum \text{Predicted condition negative}}$	Negative predictive value (NPV) = $\frac{\sum \text{True negative}}{\sum \text{Predicted condition negative}}$
		True positive rate (TPR), Recall, Sensitivity, probability of detection, Power = $\frac{\sum \text{True positive}}{\sum \text{Condition positive}}$	False positive rate (FPR), Fall-out, probability of false alarm = $\frac{\sum \text{False positive}}{\sum \text{Condition negative}}$	Positive likelihood ratio (LR+) = $\frac{\text{TPR}}{\text{FPR}}$	Diagnostic odds ratio (DOR) = $\frac{\text{LR+}}{\text{LR-}}$
		False negative rate (FNR), Miss rate = $\frac{\sum \text{False negative}}{\sum \text{Condition positive}}$	Specificity (SPC), Selectivity, True negative rate (TNR) = $\frac{\sum \text{True negative}}{\sum \text{Condition negative}}$	Negative likelihood ratio (LR-) = $\frac{\text{FNR}}{\text{TNR}}$	
					$F_1 \text{ score} = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$

# DEEP LEARNING IN HEP

Baldi, Sadowski, Whiteson  
arxiv:1402.4735

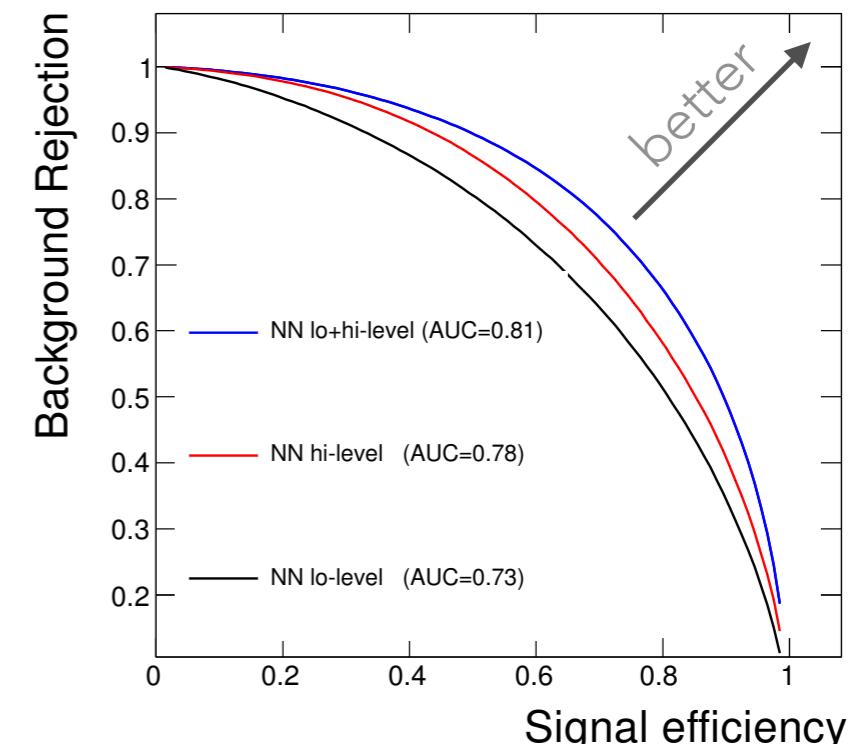


(a)

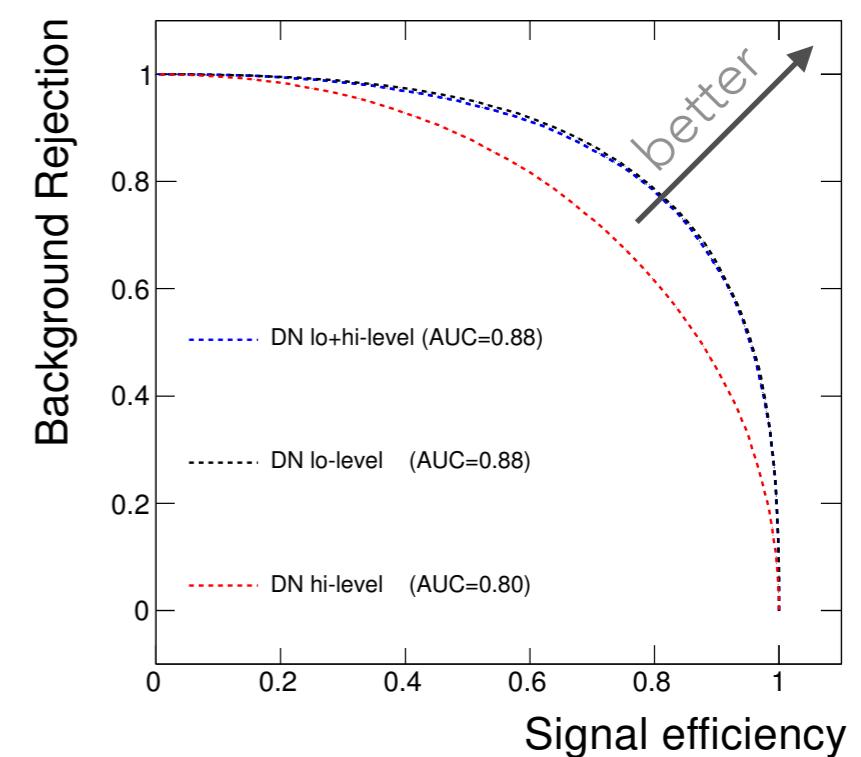


(b)

Slide from Kyle Cranmer



(a)



# Data Representation

- Data are stored in “tensors”.
  - Basically an N- Dimensional Array with a “shape”
    - `shape = ()`: Scalar
    - `shape = (N,)`: Vector
    - `shape = (N,M)`: Matrix
    - `shape = (N1, N2, N3, ..., NR)`: Rank R Tensor
  - Inputs: **X**
    - Can be arbitrary shape. Typically first dimension is the example index (usually an “event” or collision in HEP)
    - Example: Let’s say your examples are students, and your data is their age, sex, years at University, undergrad/grad, and department
      - `X = [ [ 20, 0, 2, 0, 4] , # 20 year old, 0=male, 2=junior, 0=undergrad, 4=computer science`
      - `[ 25, 1, 2, 1, 3] , # 25 year old, 1=female, 2=3rd year, 0=grad, 4=physics`
      - `[ 23, 0, 0, 1, 3] ] # 25 year old, 1=make, 2=1st year, 0=grad, 4=physics`
    - `X[0] = [20, 0, 2, 0, 4]`: the first students data.
    - `X[0][3] = 1`. This is a graduate student
  - Outputs : **Y**
    - Can be arbitrary shape. Typically first dimension is the example index (usually an “event” or collision in HEP)
    - Example: `Y = 0/1`, student does not / does know python

# Machine Learning Problem Formulation

- Split *Datasets*:
  - $(\mathbf{X}_{\text{train}}, \mathbf{Y}_{\text{train}})$  = training dataset
  - $(\mathbf{X}_{\text{test}}, \mathbf{Y}_{\text{test}})$  = test dataset
  - $(\mathbf{X})$  = unlabeled data
- Set *Goal*:
  - *Inference* algorithm/function  $F(\mathbf{X} | \mathbf{a}) = \mathbf{Y}_{\text{predict}}$ .
    - $F$  can be a heuristic. e.g. if (computer science student) then (student knows python).
    - $F$  can be anything
  - $\mathbf{a}$  are parameters of the function, for Neural Networks, these are weights.
  - Note that in a simple classification problem,  $\mathbf{Y}_{\text{train}}$  can be 0 or 1 for any example. But  $\mathbf{Y}_{\text{predict}}$  will usually be between 0 and 1.
- *Training*: (for Neural Networks)
  - Optimize (usually a minimization) a *cost function*  $F(\mathbf{X} | \mathbf{a}) = C(F(\mathbf{X}_{\text{train}} | \mathbf{a}), \mathbf{Y}_{\text{train}})$  w.r.t.  $\mathbf{a}$
  - For example,  $C = [F(\mathbf{X} | \mathbf{a}) - \mathbf{Y}_{\text{train}}]^2$
  - $\mathbf{a}_{\text{trained}}$ = result of training
- Validation:
  - Compute cost function on test data  $C(F(\mathbf{X}_{\text{test}} | \mathbf{a}_{\text{trained}}), \mathbf{Y}_{\text{test}})$
  - Other metrics. For example:
    - Select  $\mathbf{Y}_{\text{test}}=1$  and see how often  $F(\mathbf{X}_{\text{test}} | \mathbf{a}_{\text{trained}}) > 0.5$
- Inference:
  - $\mathbf{Y}_{\text{predict}} = F(\mathbf{X} | \mathbf{a}_{\text{trained}})$