Python for Data Science 2

Lecture 19- Machine Learning

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Test Statistic

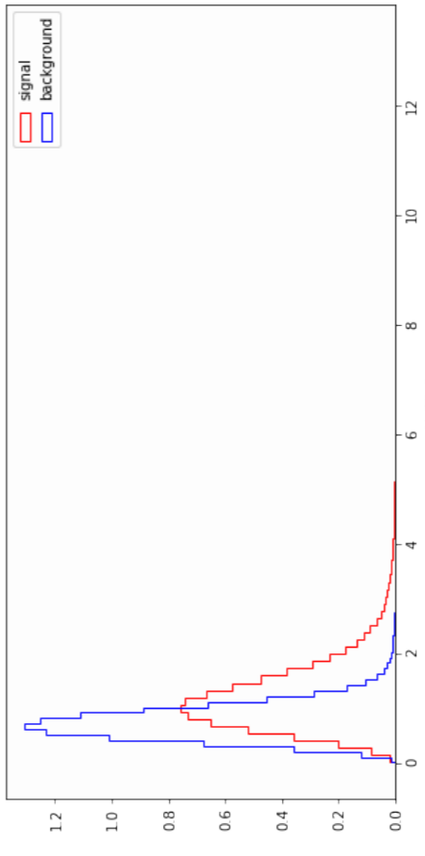
- In your lab you are investigating different observables (aka features) $\{\vec{x_i}\}$
  - Each has separation power between signal and background.
    - Some are better than others
    - We can refer to any of these observables as a ***test statistic***
      - A statistical variable that we can use 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 $f(\{\vec{x_i}\}) \equiv t_i$

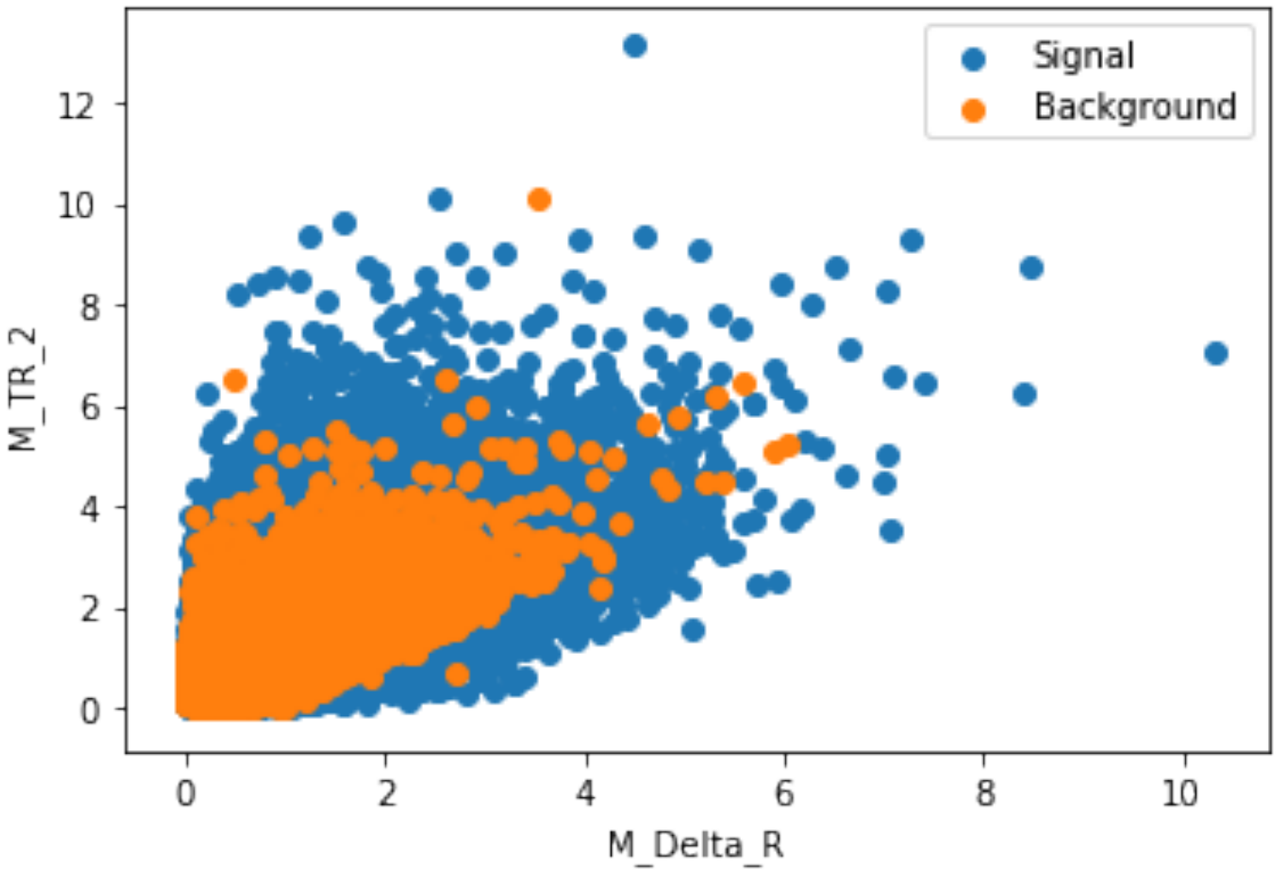
Hypothesis Testing

- Neyman-Pearson lemma: best possible best statistic, given a set of observables is

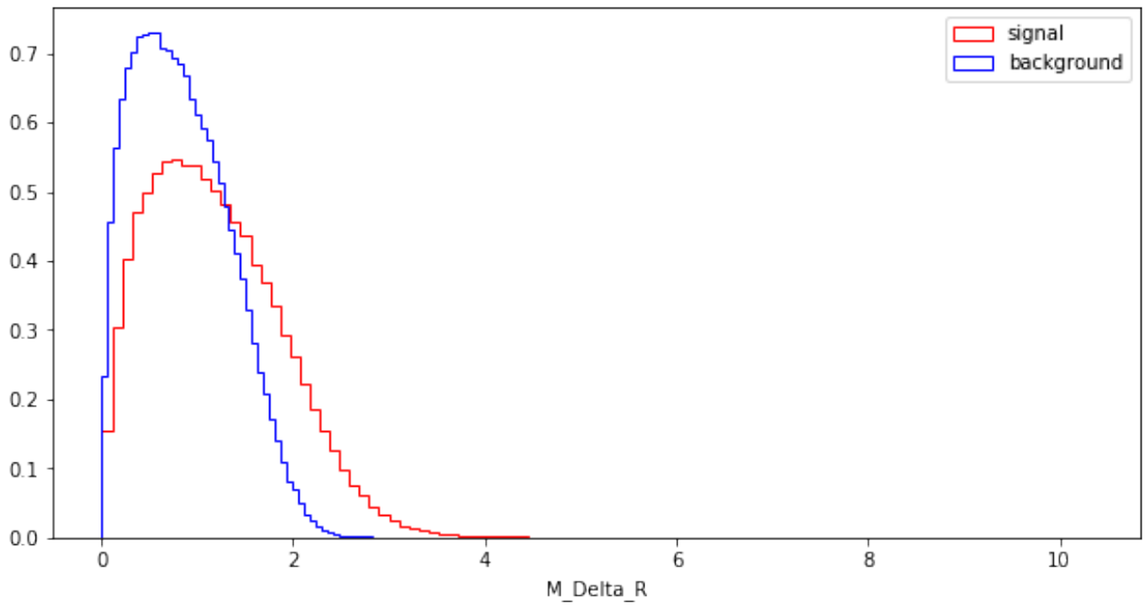
$$t_i = \frac{P(\{\vec{x_i}\}|H_1)}{P(\{\vec{x_i}\}|H_0)} > t_c$$

- But it is rather difficult to obtain *P.*
  - Unless you know it analytically, you'll have to rely on or 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.





	signal	background
M_TR_2>2.	0.114	0.006
M_Delta_R>2.	0.133	0.014
Product	0.015	0.000084
Combined	0.051	0.002



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 (Input | Parameters) = Output
  - ***Target: Cost (aka loss) function***
    - *Supervised*: Compare F vs Ground Truth Output
    - *Unsupervised*: e.g. Cluster like inputs
    - *Semi-supervised*: F(Input) = Input
- ***Training: Optimization***
  - Choose how to find best parameters

Machine Learning

Basic Formulation

- ***AI Algorithm***: *Input* ⟶ AI Algorithm ⟶ *Output*
  - $X \longrightarrow F(\theta) \longrightarrow y$: $y = F(X|\theta)$
    - X: observable inputs
    - θ: 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 = 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 θ
- ***Test***: Estimate $P(F(X|\theta)|c_j)$ using Test sample
- ***Optimize***: Select F(X|θ) > cut to optimize sensitivity for a hypothesis test
  - $P(F(X|\theta)|$ *signal* $) / P(F(X|\theta)|$ *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 $\frac{1}{N}\sum_{i}^{N}\left(F(\vec{x}|\mathbf{W},\vec{b}) - \vec{y}\right)^2$
  - 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
  - $\Longrightarrow$ Analytic solution

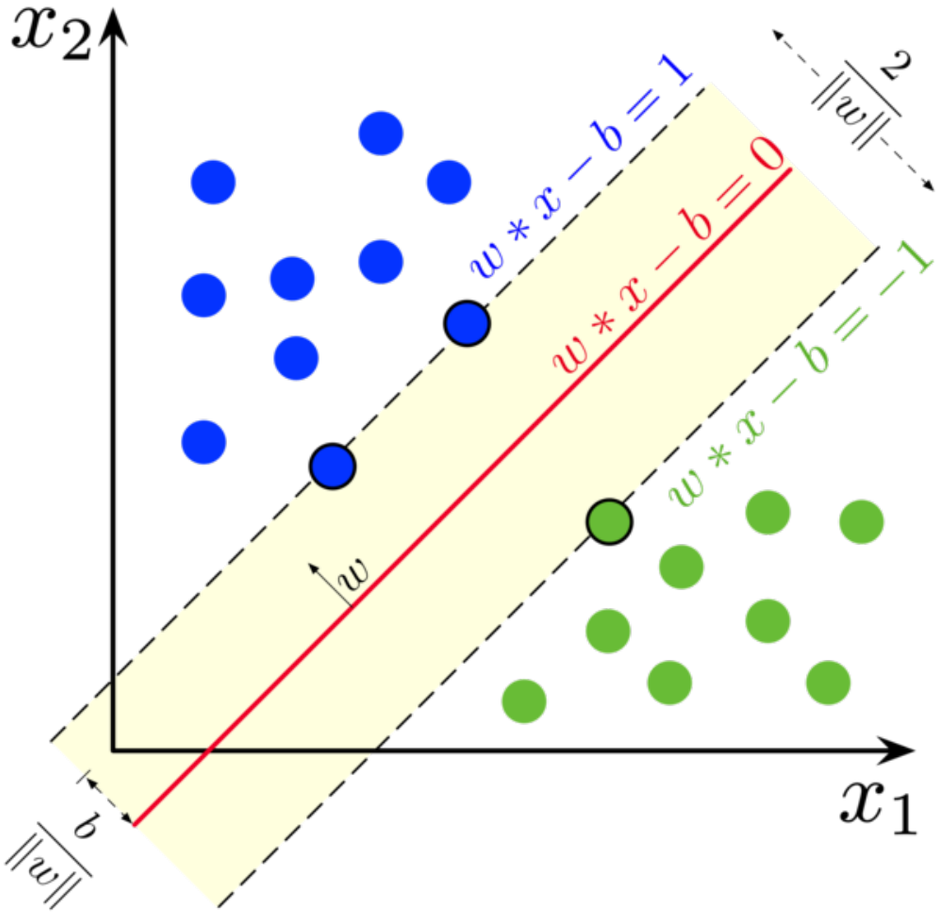
$$W = (X^T X)^{-1} X^T Y \qquad X = \begin{pmatrix} \vec{x}_1 \\ \vec{x}_2 \\ \dots \\ \vec{x}_N \end{pmatrix} \quad Y = \begin{pmatrix} \vec{y}_1 \\ \vec{y}_2 \\ \dots \\ \vec{y}_N \end{pmatrix}$$

ML Models (LDA)

- Linear Discriminant Analysis (Fisher Discriminant)
  - Assume 2 classes: 0 and 1
    - Means μ_0, μ_1 and covariance matrices Σ_0, Σ_1
  - Model: $\vec{y} = \mathbf{W}\vec{x}$
    - Again W is 1 by d, b=0
  - Maximize: $S = \frac{(\mathbf{W} \cdot \vec{\mu}_0 - \mathbf{W} \cdot \vec{\mu}_1)^2}{\mathbf{W}^T \boldsymbol{\Sigma}_0 \mathbf{W} - \mathbf{W}^T \boldsymbol{\Sigma}_1 \mathbf{W}}$
    - Maximal separation between means
    - Smallest possible variance
- Analytic Solution: $\mathbf{W} = (\boldsymbol{\Sigma}_0 + \boldsymbol{\Sigma_1})^{-1} (\vec{\mu_0} - \vec{\mu_1})$

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 ⟹ plane depends on points closest to the plane / most difficult to separate… the *Support Vectors*.



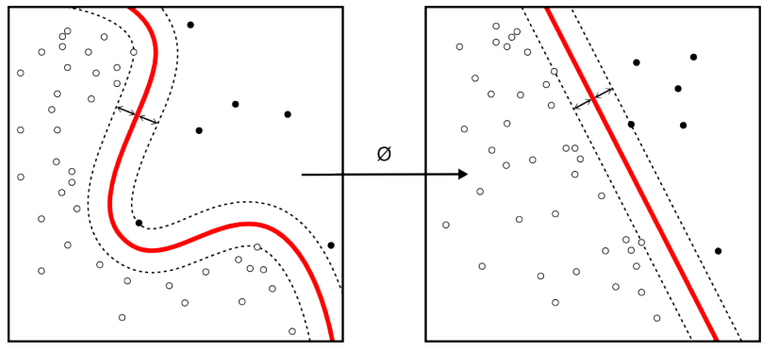
- Solving this problems is equivalent to solving a dual problem of solving for a_i

$$f(\vec{x}) = (\sum_{i}^{N} a_i y_i \vec{x}_i) \cdot \vec{x} + \vec{b}$$

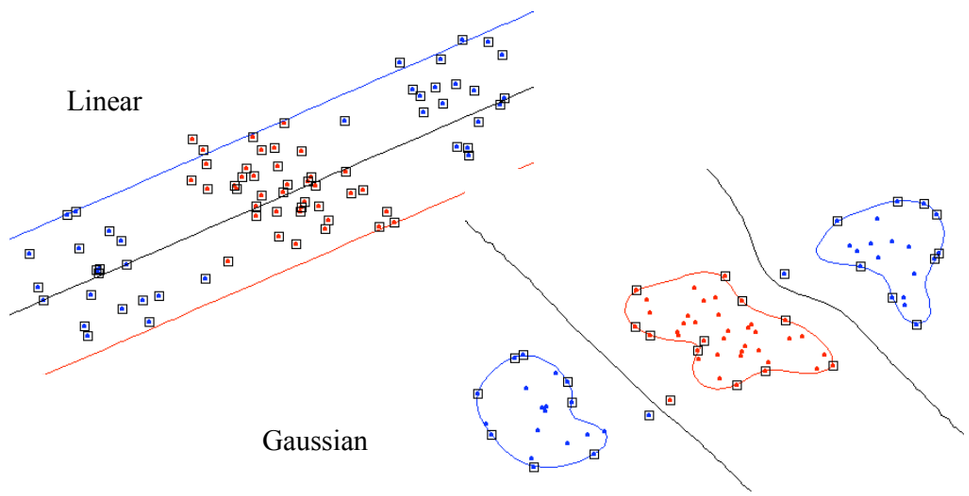
  - Where y_i={+1,-1} depending on class.
  - $a_i \geq 0$.
- Dot product measures similarity.
  - ⟶ Sign of output dependent on sign of the most similar example in training set.
  - Support vectors still most important for defining boundary

ML Models (Kernel SVM)

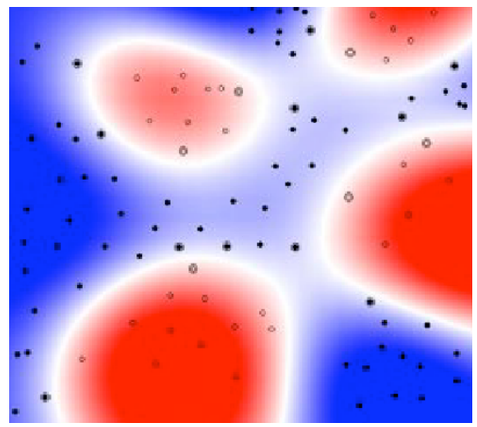
- If boundary not linear $\Longrightarrow$ Kernel Trick:
  - Replace dot product: $f(\vec{x}) = \sum_i^N a_i y_i k(\vec{x}_i, \vec{x}) + \vec{b} \qquad k(\vec{x}_i, \vec{x}) = \phi(\vec{x_i}) \cdot \phi(\vec{x})$
- Example: if *x* is in radial coordinates, then kernel gets back proper dot product.



- Example: Gaussian Kernels
  - Euclidian Distance in the exponential
  - If close to an example in training data $\Longrightarrow$ large value
  - Equivalent to template matching



Radial Basis Functions



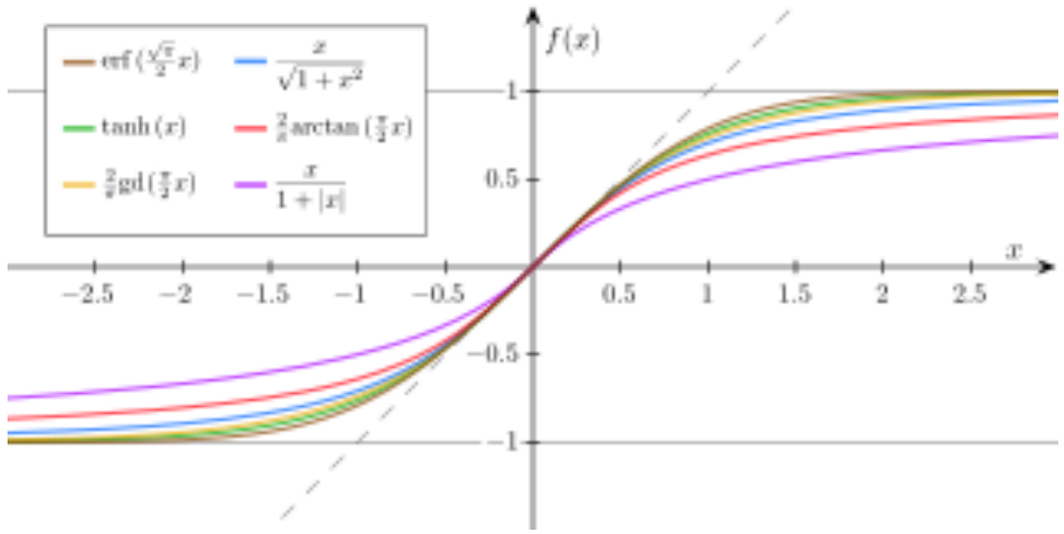
Examples from: http://web.mit.edu/6.034/wwwbob/svm-notes-long-08.pdf

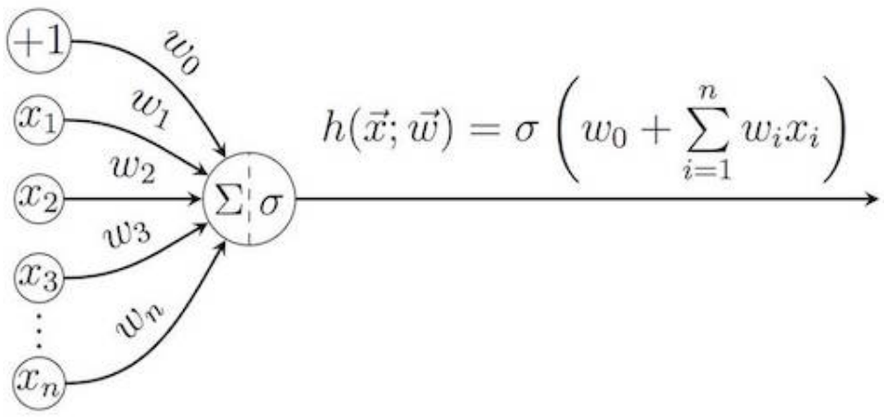
Features

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

Artificial Neural Network

- A simple one layer NN
  - F(**X** | **α**= **W**,**b**) = f (**W X** + **b**)
    - **W, b** = “weights”, “biases”
    - f(x)= “activation function”
      - Must be non-linear.





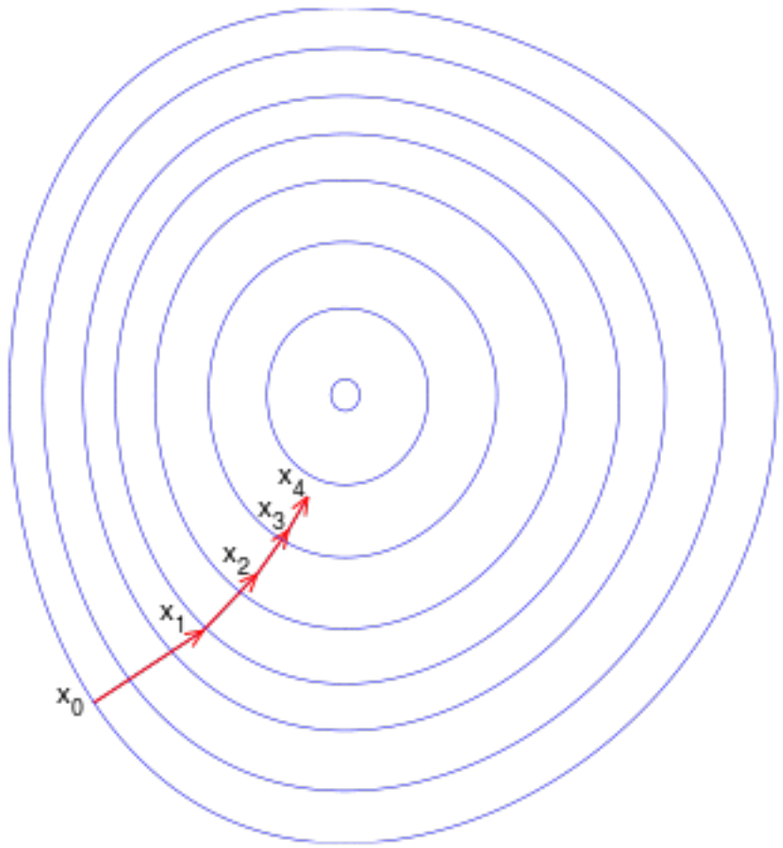
- Universal Computation Theorem.

Training == Optimization

- Training = Minimizing cost function w.r.t. parameters **α**

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

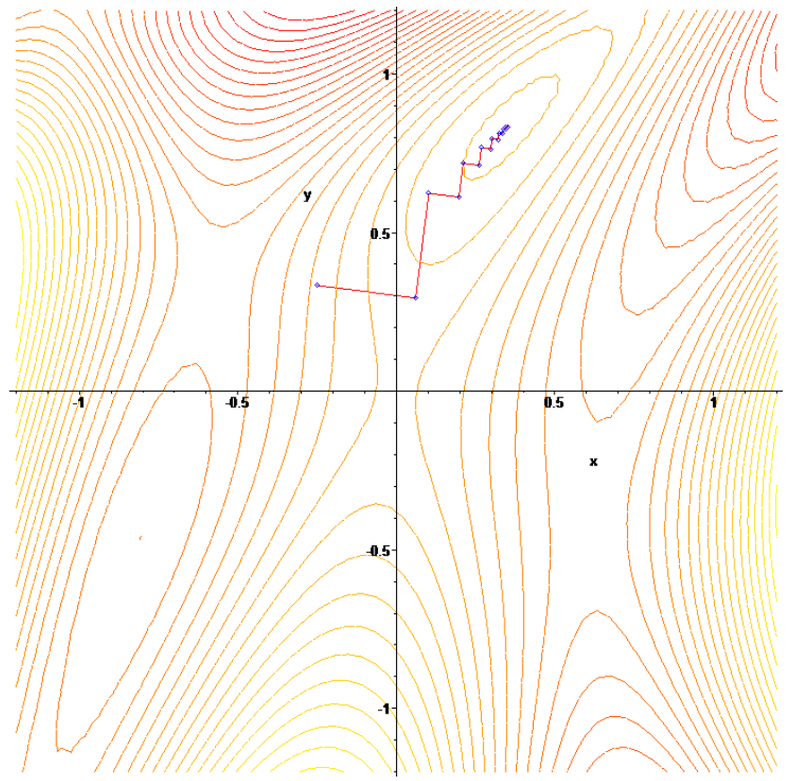
- Gradient Decent (Newton's Method):



- Gradient points to direction of maximal change.

- Iterate (ε sets the step size == *Learning Rate*)

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



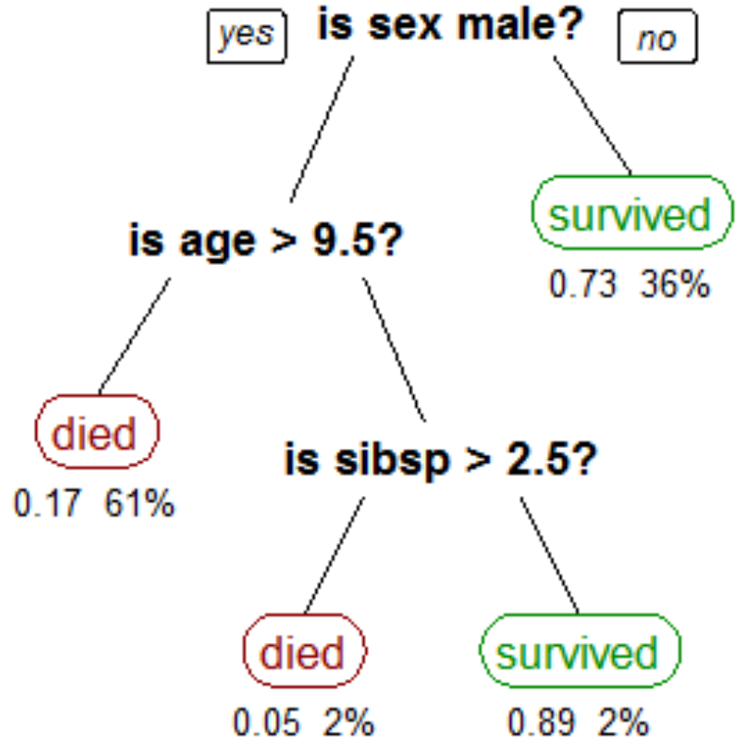
Bayesian vs Frequentist

- ***Supervised Learning:***
  - Data: (X , Y)
  - True: $f^*(X) = Y$
  - Learn: $f(X|\theta) \sim f^*$
- ***Frequentist***:
  - (X, Y) random.
  - Ideal θ exists.
  - Estimate θ.
- ***Bayesian***:
  - (X, Y) fixed.
  - θ is random.
  - Learn $p(\theta)$

- ***Bayesian Learning:***
  - For example: θ is Gaussian distributed $\Longrightarrow$ learn μ, σ
  - Allows you to propagate uncertainties $\Longrightarrow$ estimate uncertainty on output Y

Decision Trees

- Doesn’t fit the F(**X** | **W**,**b**) formulation.
- Powerful technique
  - Random Forest
  - Boosting
- Up to recently, in HEP, Boost Decision Trees (BDTs) on well constructed/chosen features
  - have been the best performing techniques, and
  - become the standard to beat,

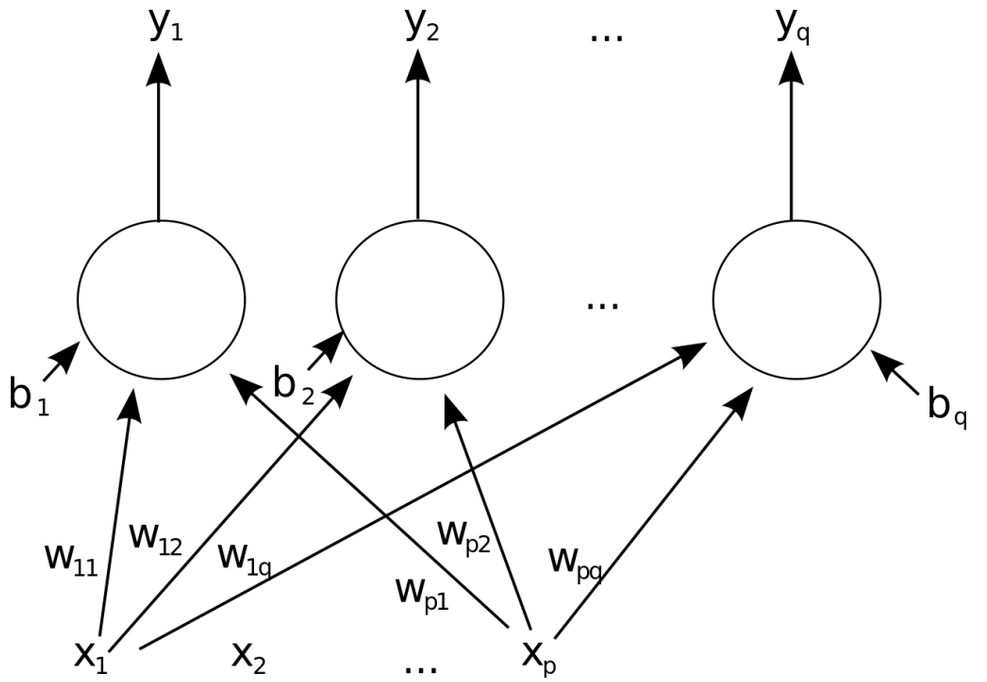


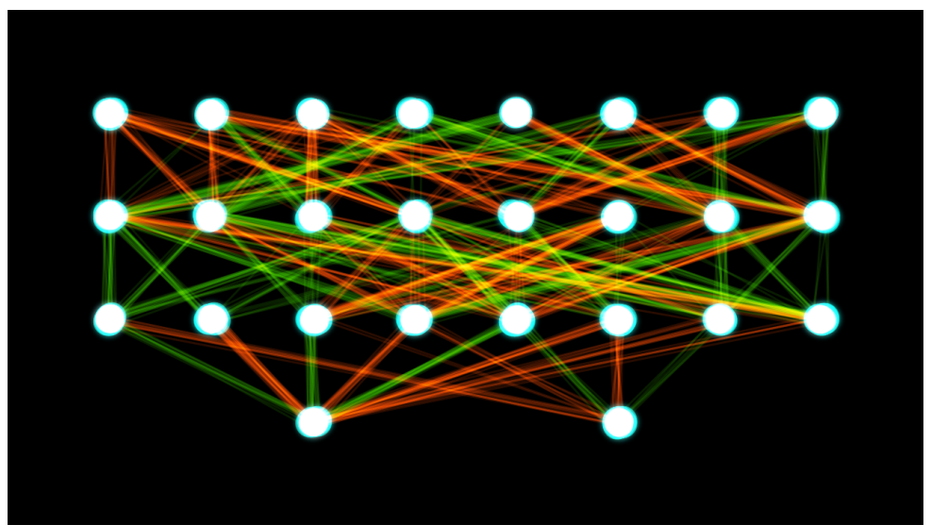
Titanic Survivors

Deep Learning

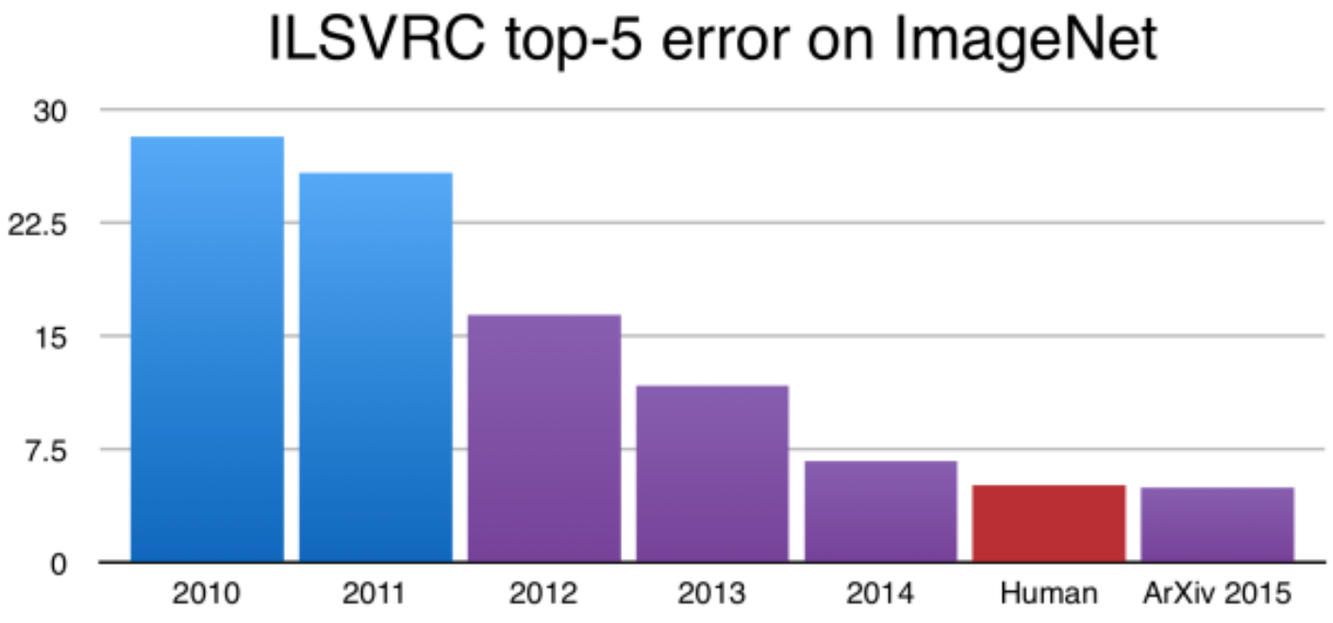
Artificial Neural Networks

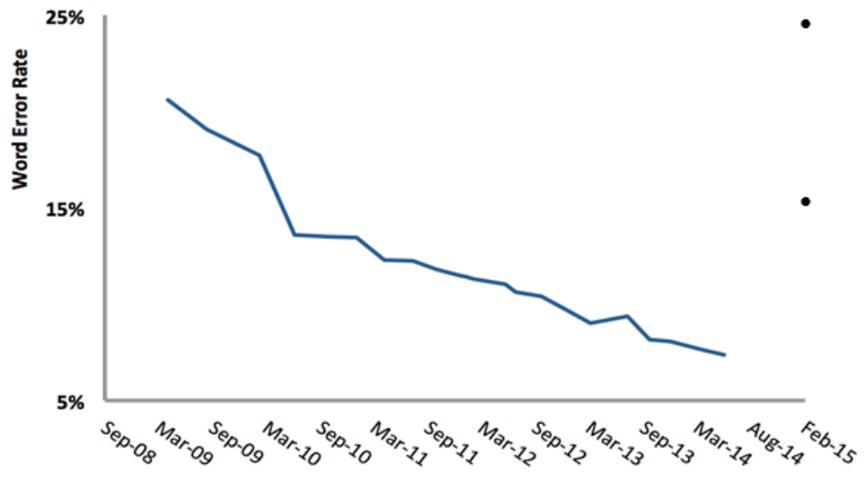
- ***Biologically inspired computation***, (first attempts in 1943)
  - ***Probabilistic Inference***: e.g. signal vs background
  - ***Universal Computation Theorem*** (1989)
- Multi-layer (***Deep***) Neutral Networks:
  - Not a new idea (1965), just impractical to train. ***Vanishing Gradient problem*** (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.



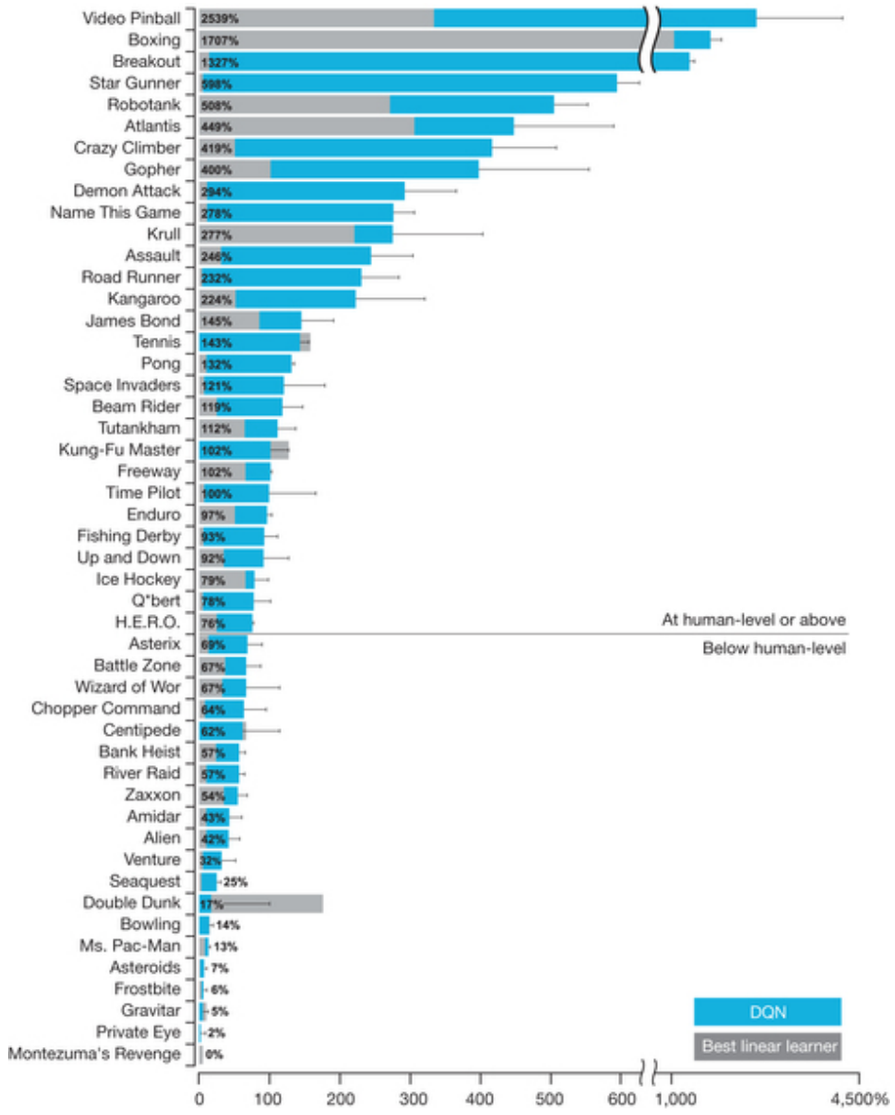


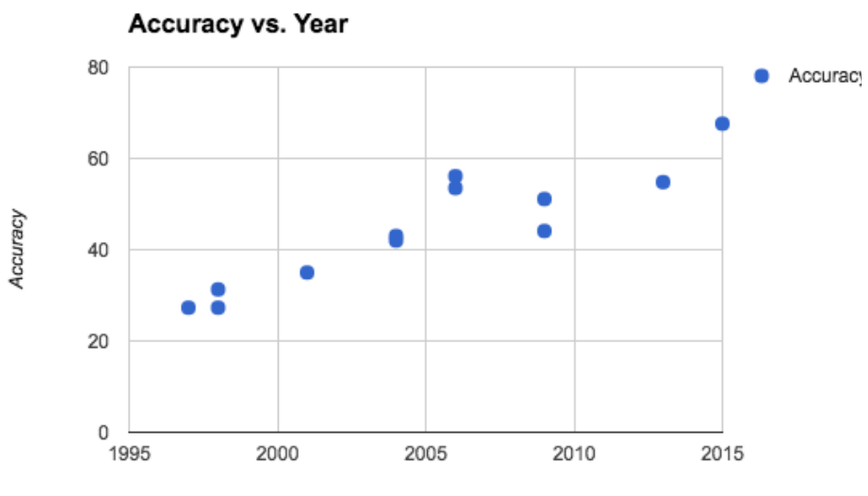
Images from Wikipedia

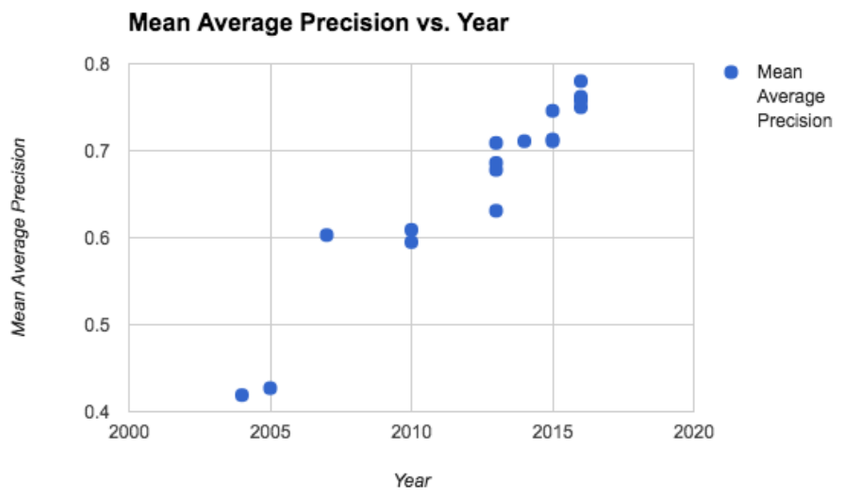


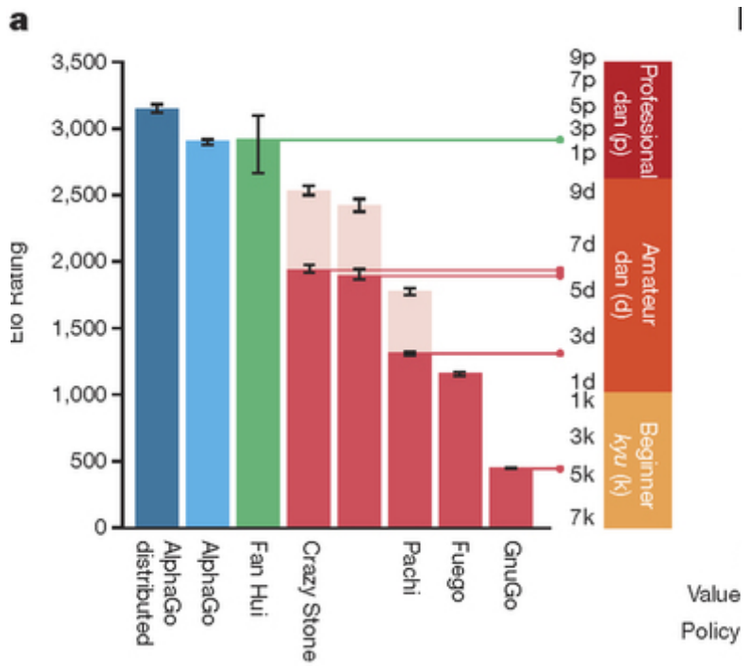


- Continuous server ASR word error rate (WER) reduction ~18% / year: combination of algorithms, data, and computing
- Deep learning (DNNs) is driving recent performance improvements in ASR and meaning extraction



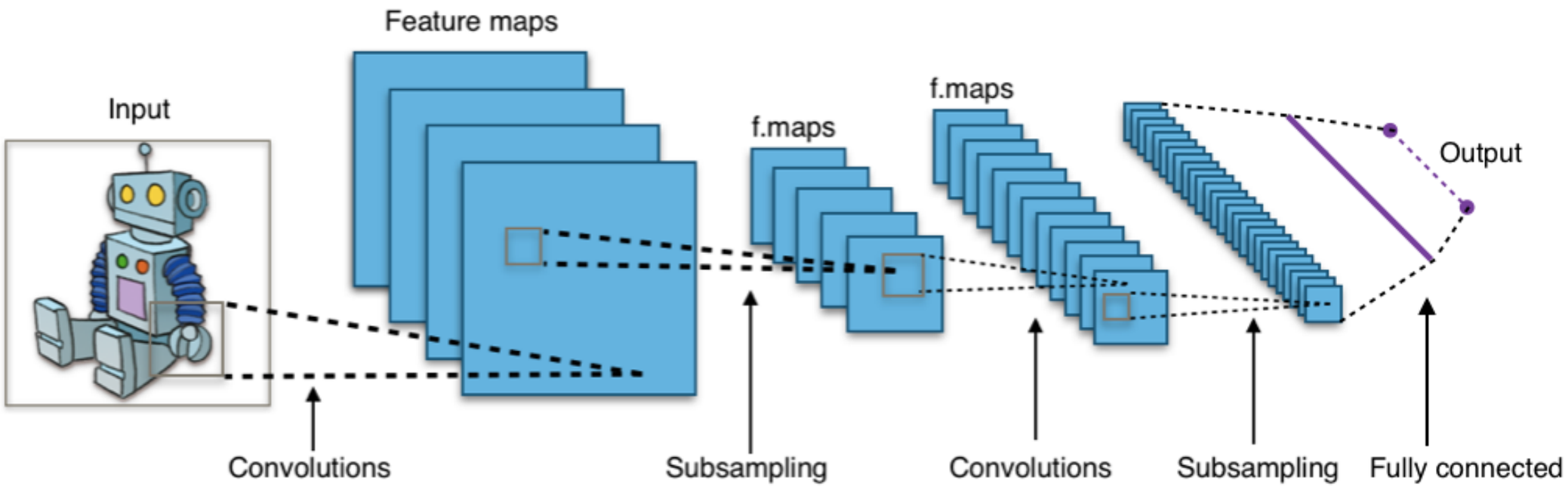


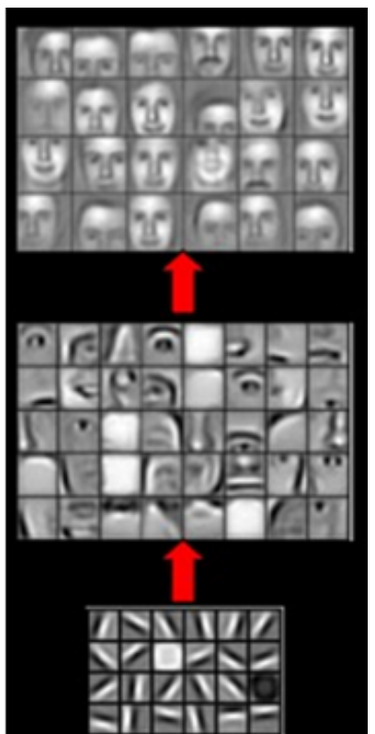




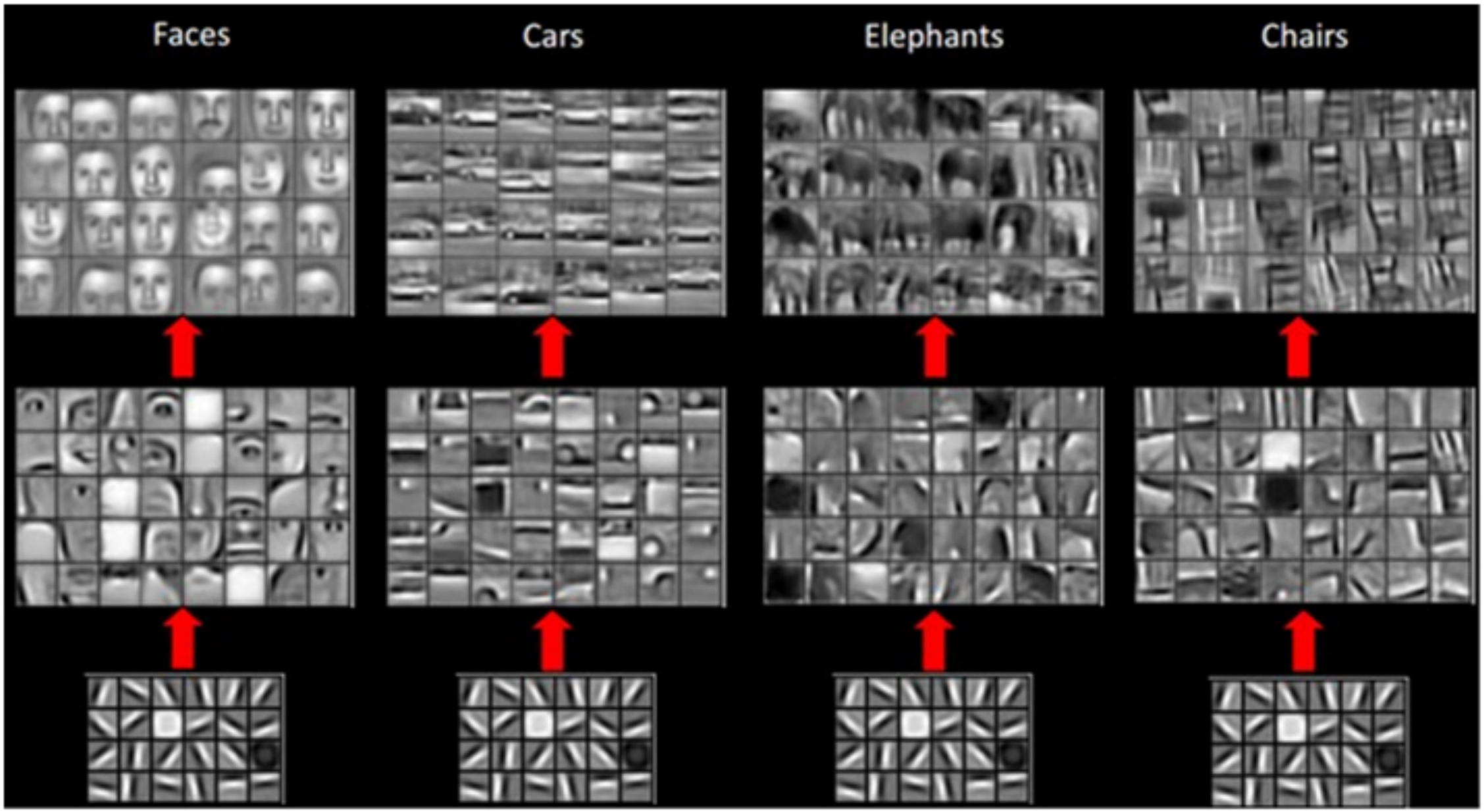
Feature Learning

- ***Feature Engineering***: e.g. Event Reconstruction ~ Feature Extraction, Pattern Recognition, Fitting, …
- Deep Neutral 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.



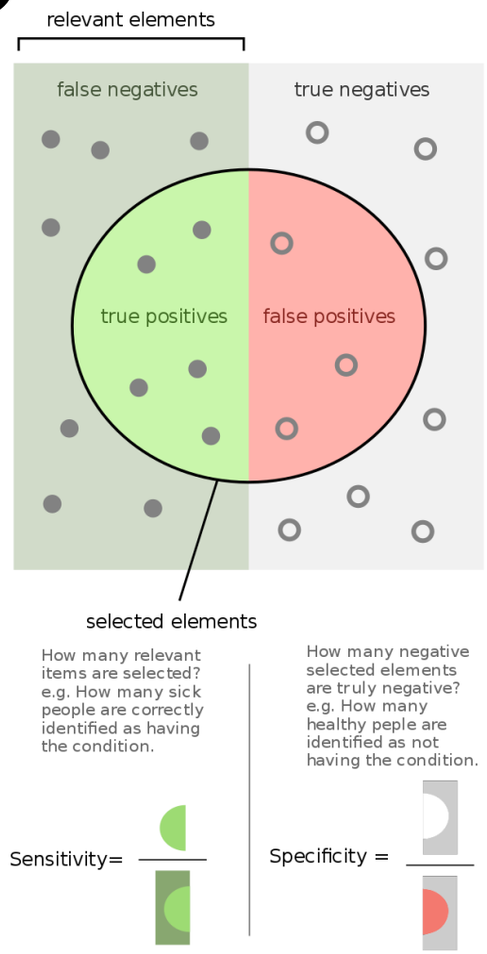


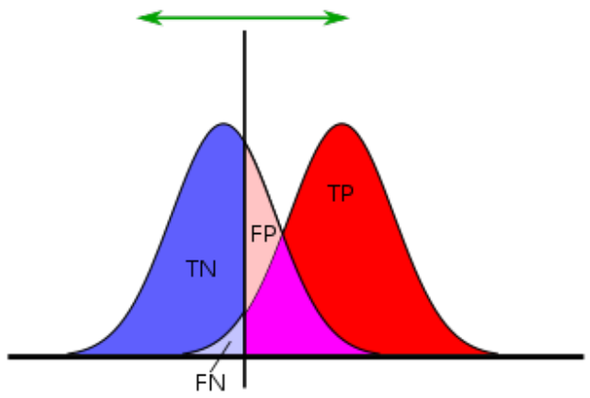
Deep Neutral Networks



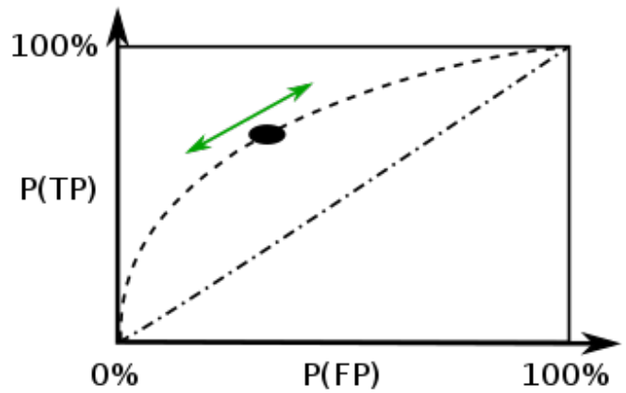
Assessing Performance

- ***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





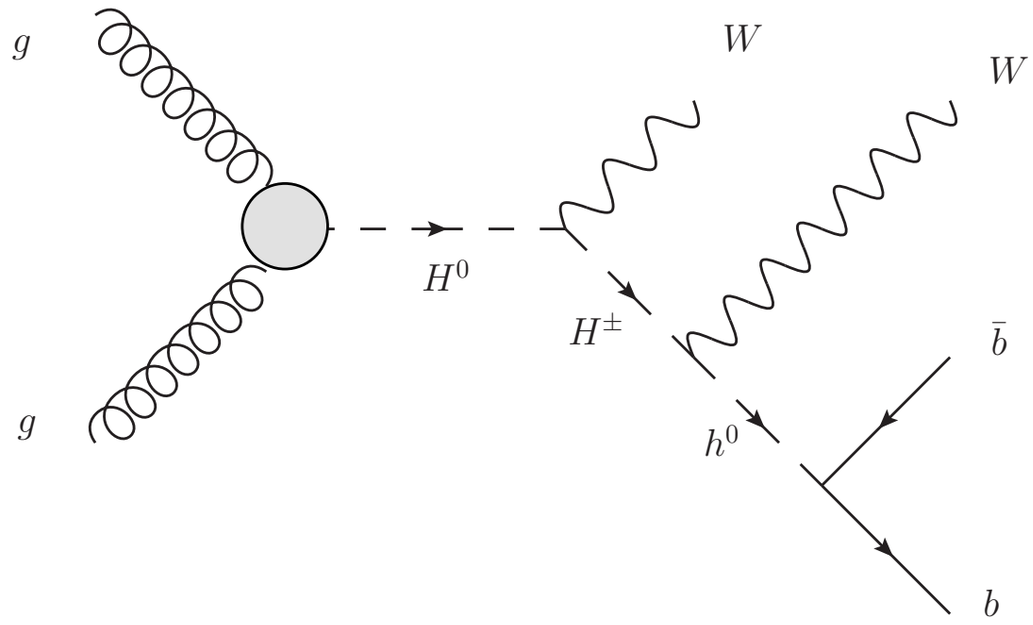
TP	FP
FN	TN

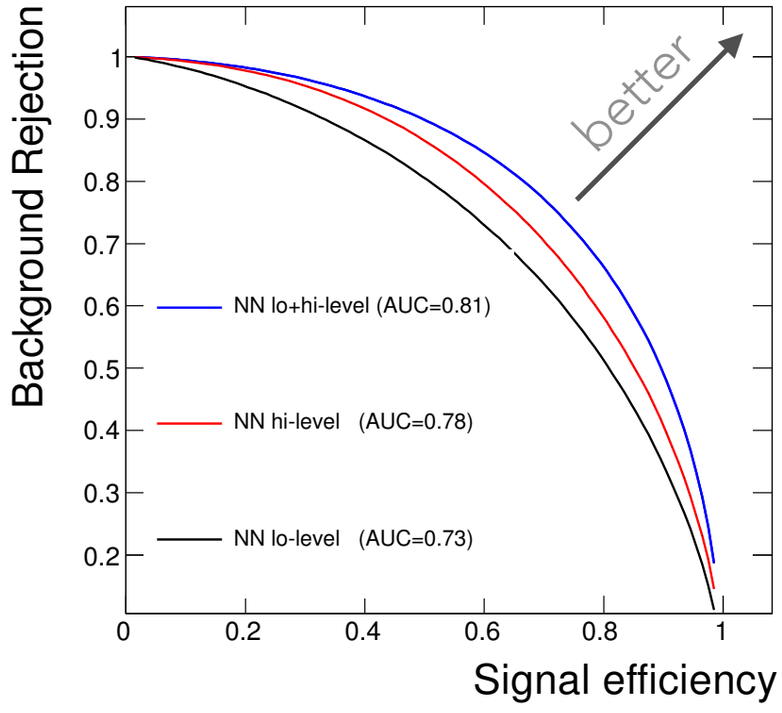


		True condition				
	Total population	Condition positive	Condition negative	Prevalence = $\frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	Accuracy (ACC) = $\frac{\Sigma \text{ True positive} + \Sigma \text{ True negative}}{\Sigma \text{ Total population}}$	
Predicted condition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

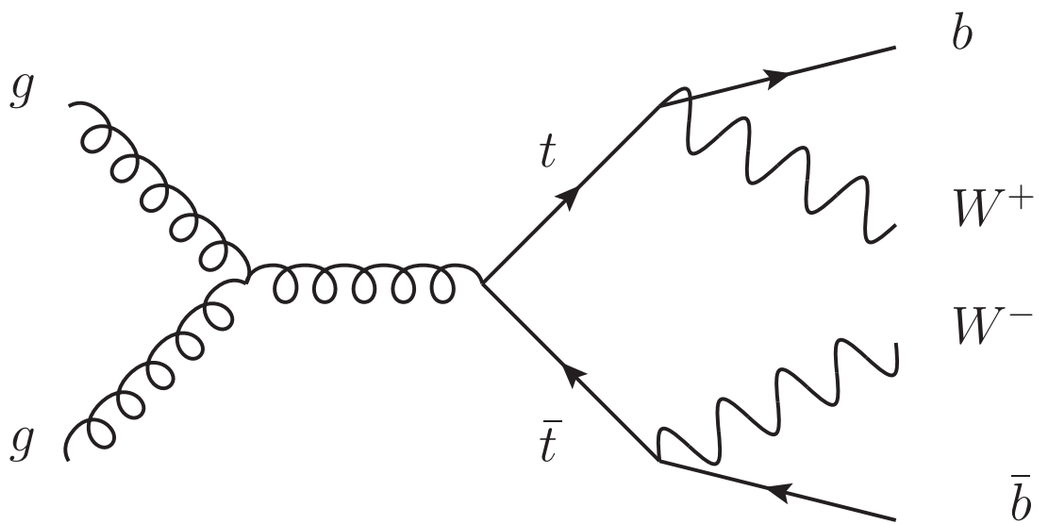
DEEP LEARNING IN HEP

Baldi, Sadowski,Whiteson
arxiv:1402.4735

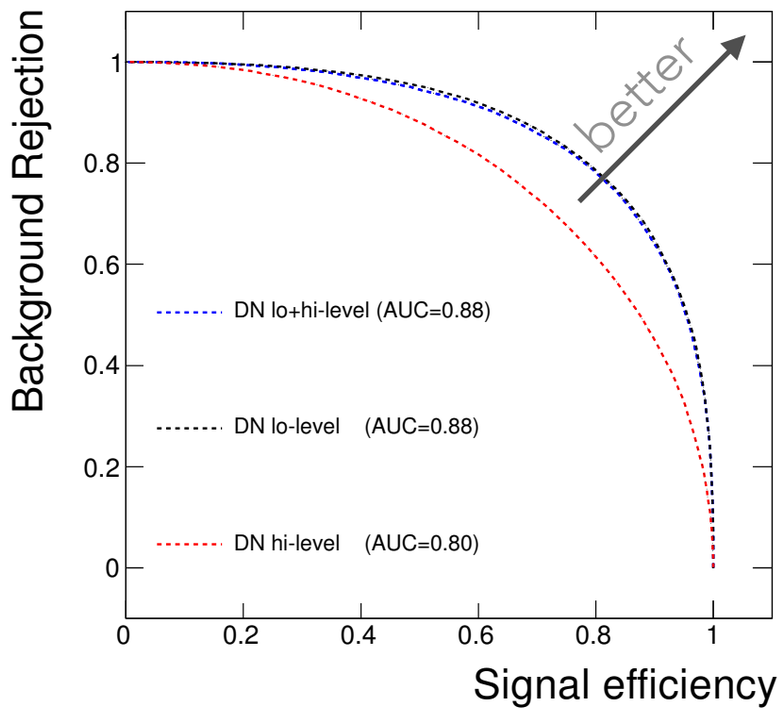




(a)



(b)



Slide from Kyle Cranmer

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 = (N_1, N_2, N_3, …, N_R): 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=3nd 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*:
  - ($\mathbf{X}_{train}$, $\mathbf{Y}_{train}$) = training dataset
  - ($\mathbf{X}_{test}$, $\mathbf{Y}_{test}$) = test dataset
  - ($\mathbf{X}$) = unlabeled data
- Set *Goal*:
  - *Inference* algorithm/function F($\mathbf{X} \mid \boldsymbol{\alpha}$) = $\mathbf{Y}_{predict}$.
    - F can be a heuristic. e.g. if (computer science student) then (student knows python).
    - F can be anything
  - $\boldsymbol{\alpha}$ are parameters of the function, for Neural Networks, these are weights.
    - Note that in a simple classification problem, $\mathbf{Y}_{train}$ can be 0 or 1 for any example. But $\mathbf{Y}_{predict}$ will usually be between 0 and 1.
- *Training*: (for Neural Networks)
  - Optimize (usually a minimization) a *cost function* F($\mathbf{X} \mid \boldsymbol{\alpha}$) = C(F($\mathbf{X}_{train} \mid \boldsymbol{\alpha}$), $\mathbf{Y}_{train}$) w.r.t. $\boldsymbol{\alpha}$
  - For example, C = [F($\mathbf{X} \mid \boldsymbol{\alpha}$) - $\mathbf{Y}_{train}$]^2
  - $\boldsymbol{\alpha}_{trained}$= result of training
- Validation:
  - Compute cost function on test data C(F($\mathbf{X}_{test} \mid \boldsymbol{\alpha}_{trained}$), $\mathbf{Y}_{test}$)
  - Other metrics. For example:
    - Select $\mathbf{Y}_{test}$=1 and see how often F($\mathbf{X}_{test} \mid \boldsymbol{\alpha}_{trained}$) > 0.5
- Inference:
  - $\mathbf{Y}_{predict}$ = F($\mathbf{X} \mid \boldsymbol{\alpha}_{trained}$)