

BOOSTING

COMBINE WEAK LEARNERS THAT WERE TRAINED SEQUENTIALLY AND PREDICTS BASED ON THE WEIGHTS OF EACH MODEL (WEIGHT CALCULATED BASED ON MODEL PERFORMANCE).

GRADIENT BOOSTING

$$dY(0) = Y - \text{MEAN}(Y)$$

for $k=1 : (\# \text{ OF TREES} / \# \text{ OF ITERATIONS}) :$

$$\text{LEARNER}(k) = \text{TRAIN-REGRESSOR}(X, dY(k-1))$$

$$dY(k) = dY(k-1) - \alpha(k) * \text{PREDICT}(\text{LEARNER}(k), X)$$

"TRAIN OVER THE RESIDUAL"

BAGGING

- * GENERATE N DIFFERENT BOOTSTRAP TRAINING SAMPLE WITH REPLACEMENT
- * TRAIN ALGORITHM ON EACH BOOTSTRAPPED SAMPLE
- * COMBINE THEM ALL USING MAJORITY VOTE / MEAN

RELATIVE VARIABLE IMPORTANCE

THE MEASURE IS MADE BASED ON $\#$ TIMES A VARIABLE IS SELECTED FOR SPLITTING AND WEIGHTED BY THE IMPROVEMENT TO THE MODEL AS A RESULT OF EACH SPLIT, THEN AVERAGED OVER ALL TREES.

CONFUSION MATRIX

POSITIVE CLASS = 0

		OBSERVED	
		P	N
PREDICT	P	TP	FP
	N	FN	TN

$$\text{SENSITIVITY} = \frac{TP}{TP + FN} = \text{RECALL}$$

$$\text{SPECIFICITY} = \frac{TN}{TN + FP}$$

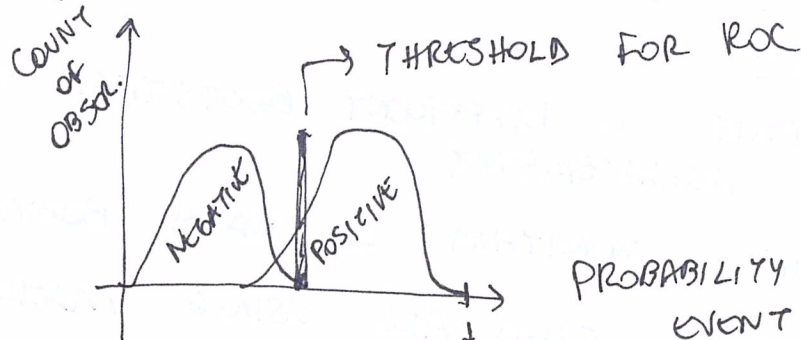
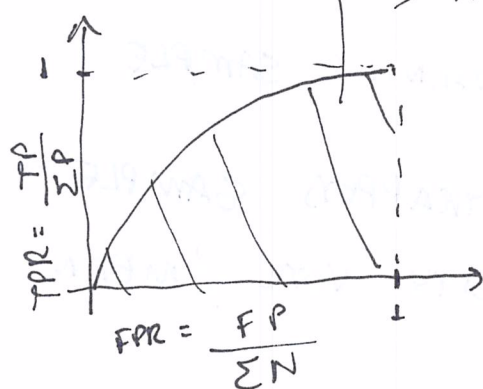
$$\text{PRECISION} = \frac{TP}{TP + FP}$$

$$\text{F1 SCORE} = 2 \cdot \frac{\text{PRECISION} \times \text{RECALL}}{\text{PRECISION} + \text{RECALL}} = \frac{2}{\frac{1}{\text{PRECISION}} + \frac{1}{\text{RECALL}}} \quad \text{"HARMONIC MEAN"}$$

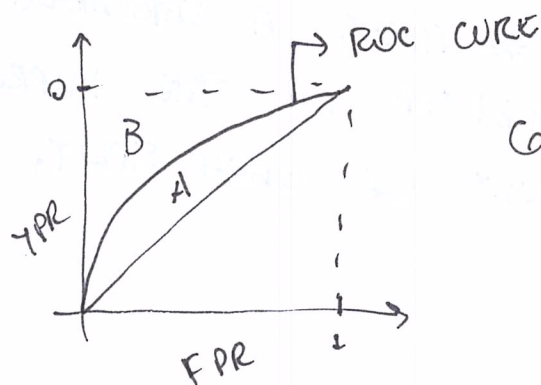
$$\text{ACCURACY} = \frac{TP + TN}{P + N}$$

ROC CURVE

AUC (AREA UNDER THE CURVE)



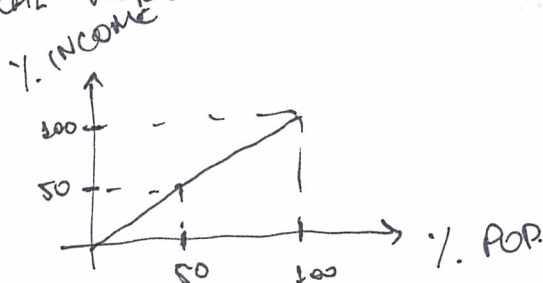
GINI COEFFICIENT (INEQUALITY COEFFICIENT)



$$\text{GINI} = \frac{A}{A + B}$$

HIGHER A \Rightarrow BETTER MODEL
HIGHER INEQUALITY

REAL-WORLD EXAMPLE:



"PERFECT DISTRIBUTION OF MONEY OVER POPULATION"

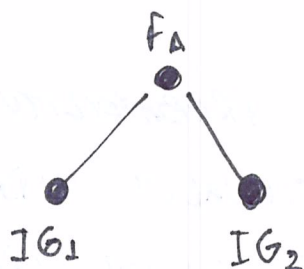
CLASSIFICATION TREES

FOR ALL FEATURES TESTS INFORMATION GAIN USING

ENTROPY:

$$IG = - \sum_{i=1}^J p_i \cdot \log_2 p_i$$

p_i = PROPORTION
OF CLASS i ON
NODE



$$IG_T = IG_1 + IG_2$$

(FOR FEATURE A THE
INFORMATION GAIN WILL
BE THE SUM OF $IG_1 + IG_2$)

REGRESSION TREES

AT EACH ITERATION FOR EACH FEATURE x_k FIND OPTIMAL s :

$$\min_s [MSE(y | x_k < s) + MSE(y | x_k \geq s)]$$

(* s IS THE ~~CUT OFF~~ CUT OFF)

* FOR BOTH METHODS: VARIABLE IMPORTANCE GENERALLY BE
COMPUTED BASED ON CORRESPONDING REDUCTION OF PRE-
DICTIVE ACCURACY WHEN THE PREDICTOR OF INTEREST IS
REMOVED OR SOME MEASURE OF DECREASE OF NODE IMPURITY.

LINEAR REGRESSION

LINEAR APPROACH TO MODELLING RELATIONSHIP BETWEEN
SCALAR RESPONSE TO EXPLANATORY VARIABLES
"ORDINARY LEAST SQUARES"

$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_n x_n$$

LOGISTIC REGRESSION

LOG-ODDS OF PROBABILITY OF AN EVENT IS A
LINEAR COMBINATION OF EXPLANATORY VARIABLES
"MAXIMUM LIKELIHOOD ESTIMATION"

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

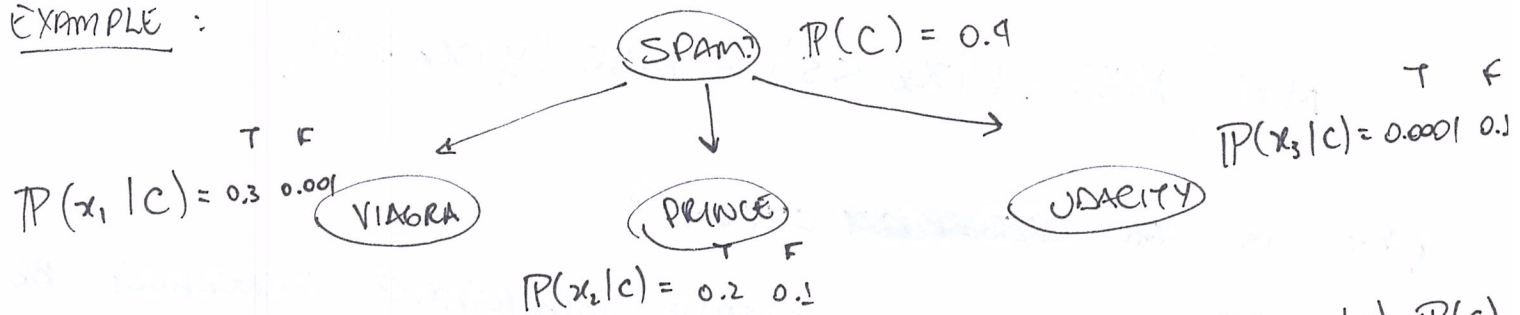
* VARIABLE IMPORTANCE FOR REGRESSION CAN BE SET BASED ON THE COEFFICIENTS ONLY. IF THE FEATURES ARE NORMALIZED (CONTINUOUS) OR THEY ARE DISCRETE.

NAIVE BAYES CLASSIFICATION

BASED ON BAYES THEOREM WITH CONDITIONAL PROBABILITY OF EVENT TO PREDICT. ASSUMES x_i CONDITIONALLY INDEPENDENT OF EVERY OTHER FEATURE x_j ($i \neq j$) GIVEN CATEGORY C_k

$$P(C_k) \Rightarrow \boxed{P(C_k | x_1, \dots, x_n) \propto P(C_k) \cdot \prod_{i=1}^n P(x_i | C_k)}$$

EXAMPLE :



$$P(C | x_1=T, x_2=F, x_3=F) \propto P(x_1=T | C) \cdot P(x_2=F | C) \cdot P(x_3=F | C) \cdot P(C)$$

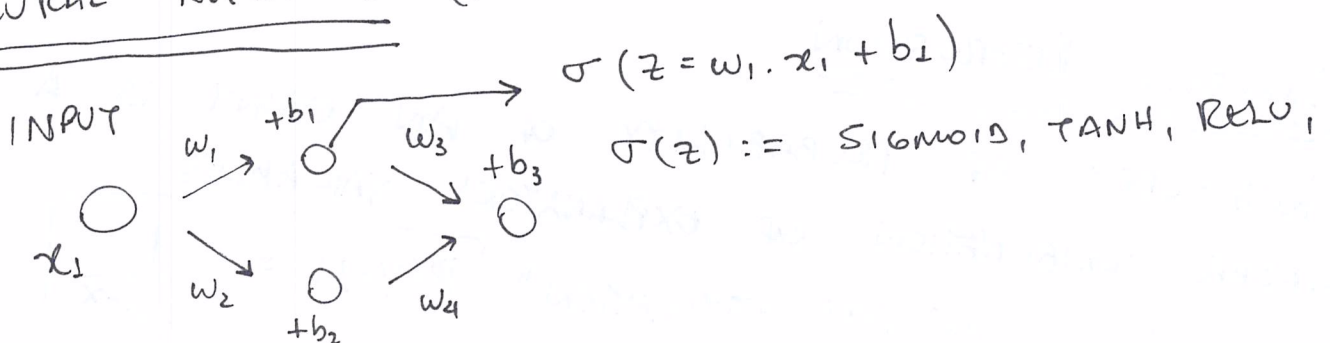
RANDOM FOREST

SELECTING BAGGING SAMPLES FOR EACH TREE CHOOSE

RANDOM FEATURES (\sqrt{D}).

* REDUCES VARIANCE BUT RANGE (AS ALL TREE MODELS) IS LIMITED.

NEURAL NETWORKS (ARTIFICIAL NEURAL NETWORKS)



SIGMOID := $\sigma(z) = \frac{1}{1+e^{-z}}$; $\sigma(z) \in (0,1)$

TANH := $\sigma(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}} = \tanh(z)$; $\sigma(z) \in (-1,1)$

RELU := $\sigma(z) = \max(0, z)$; $\sigma(z) \in [0, \infty)$

SOFT MAX := $\sigma_i(\vec{z}) = \frac{e^{z_i}}{\sum_{j=1}^J e^{z_j}}$, $i = 1, \dots, J$; $\sigma(\vec{z}) \in (0,1)$

K-NN (K - NEAREST NEIGHBORS)

REGRESSION OR CLASSIFICATION OF K NEAREST NEIGHBORS
BASED ON DISTANCE FUNCTIONS:

EUCLIDEAN : $\sqrt{\sum_{i=1}^n (x_i - y_i)^2}$

MANHATTAN : $\sum_{i=1}^n |x_i - y_i|$

MINKOWSKI : $\left(\sum_{i=1}^n (|x_i - y_i|)^q \right)^{1/q}$

K-MEANS

0. PLACE CENTROIDS AT RANDOM LOCATIONS (K CENTROIDS)
1. FIND NEAREST CENTROIDS TO EACH OBSERVATION
2. ASSIGN OBSERVATION TO CLOSER CLUSTER
3. CALCULATE NEW CENTROIDS

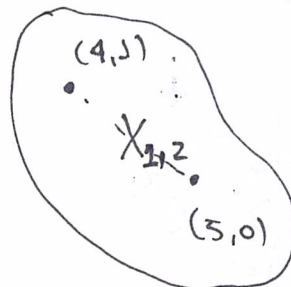
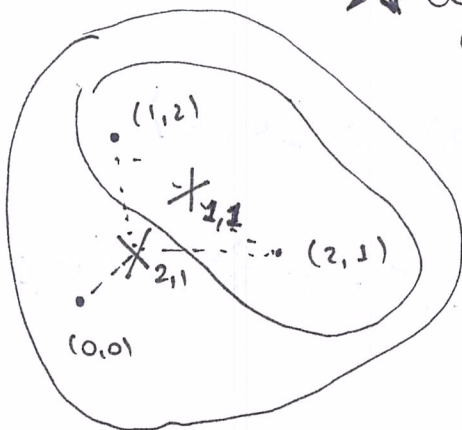
* REPEAT UNTILL DIFF. FROM PREVIOUS CENTROIDS IS MINIMUM (DIFFERENCE FROM DISTANCES)

→ K-MEANS ONLY USES EUCLIDEAN DISTANCE

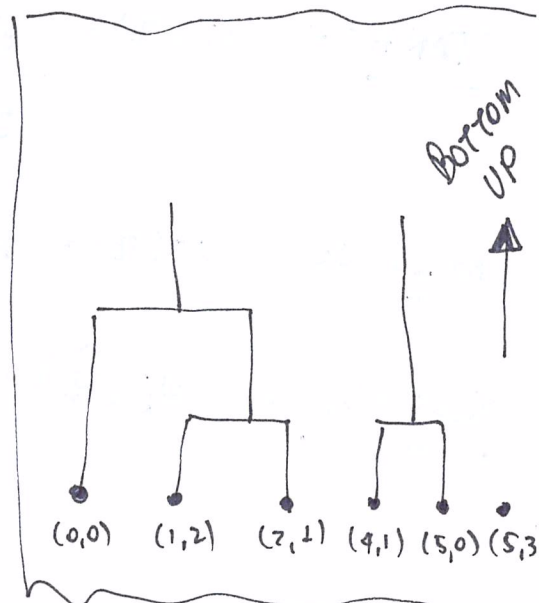
HIERARCHICAL CLUSTERING



CENTROIDS
CLUSTER
DISTANCE
MEASURES



(5,3)



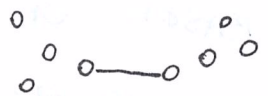
~~CLUSTERS~~ DISTANCES TO BE USED:

EUCLIDEAN, MANHATTAN, MINKOWSKI, MAHALANOBIS := $\sqrt{(a-b)^T S^{-1} (a-b)}$

* S IS THE COVARIANCE MATRIX

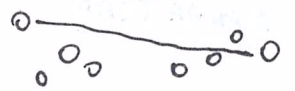
→ SINGLE LINKS: $D(c_1, c_2) = \min D(x_1, x_2)$

DISTANCE BETWEEN CLOSEST ELEMENTS IN CLUSTERS



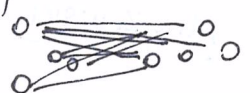
→ COMPLETE LINKS: $D(c_1, c_2) = \max D(x_1, x_2)$

DISTANCE BETWEEN FARTHEST ELEMENTS IN CLUSTERS



→ AVERAGE LINKS: $D(c_1, c_2) = \frac{1}{|c_1|} \frac{1}{|c_2|} \sum_{x_1} \sum_{x_2} D(x_1, x_2)$

AVERAGE OF ALL PAIRWISE DISTANCES



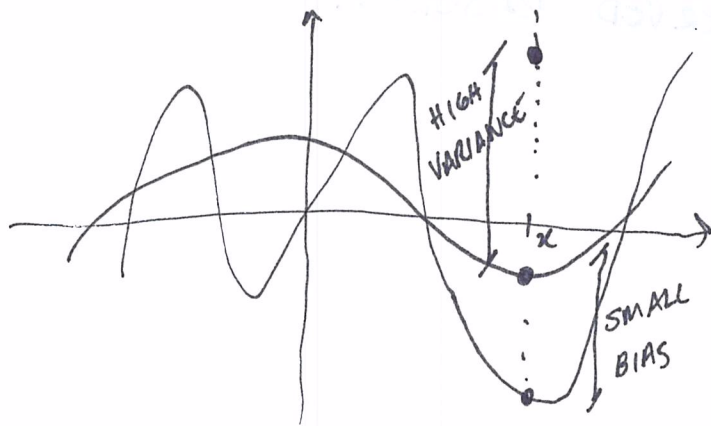
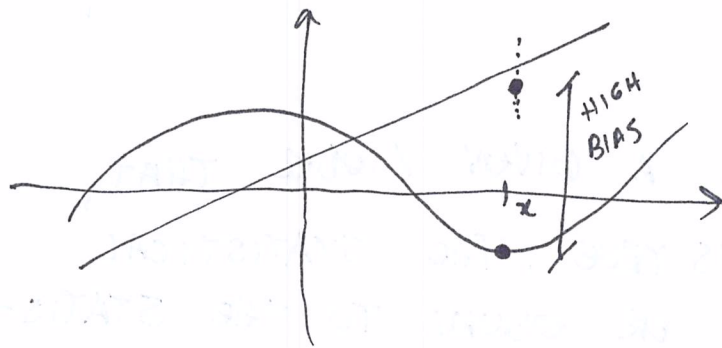
→ CENTROIDS: $D(c_1, c_2) = D\left[\left(\frac{1}{|c_1|} \sum_{x_1} \vec{x}\right), \left(\frac{1}{|c_2|} \sum_{x_2} \vec{x}\right)\right]$



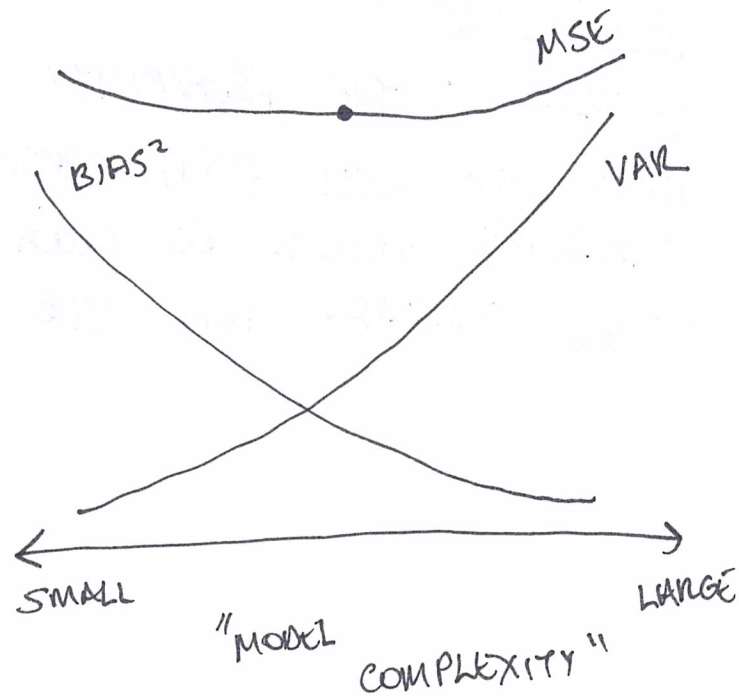
DISTANCE BETWEEN CENTROIDS
(MEANS) OF TWO CLUSTERS

BIAS - VARIANCE DECOMPOSITION

- BIAS IS THE ERROR FROM ERRONEOUS ASSUMPTIONS IN THE MODEL
- VARIANCE IS THE ~~ERR~~OR FROM SENSITIVITY TO SMALL FLUCTUATIONS IN THE TRAINING SET.



$$MSE(\hat{\theta}) = BIAS^2(\hat{\theta}) + VAR(\hat{\theta})$$



$\left\{ \begin{array}{l} BIAS \uparrow = \text{UNDERFITTING} \\ VAR \uparrow = \text{OVERFITTING} \end{array} \right.$

CROSS-VALIDATION

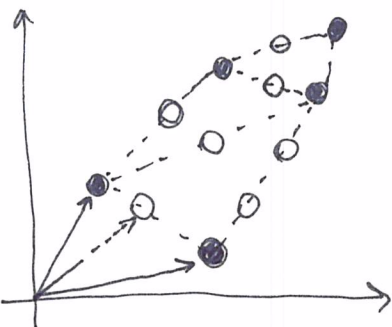
PREVENTS OVERFITTING BECAUSE MODEL THAT FITS RANDOM NOISE ON TRAINING DATA WON'T PERFORM GOOD ON VALIDATION DATASET.

K-FOLD: SEPARATES DATA ON K FOLDS, TRAINING WILL BE K-1 FOLDS AND VALIDATION WILL BE 1

LOOCV: LEAVE-ONE-OUT CROSS-VALIDATION IS THE SAME AS K-FOLD BUT $K = N$.

SMOTE (SYNTHETIC MINORITY OVER-SAMPLING TECHNIQUE)

- CREATES NEW "SYNTHETIC" OBSERVATIONS
- IDENTIFY FEATURE VECTOR AND NEAREST NEIGH.
- TAKE THE DIFF. BETWEEN TWO
- MULTIPLY DIFF. BY RANDOM BETWEEN 0 AND 1
- IDENTIFY NEW POINT ON LINE SEGMENT BY ADDING RANDOM NUMBER TO FEATURE VECTOR
- REPEAT @



P-VALUE

P-VALUE IS THE PROBABILITY FOR A GIVEN MODEL THAT, WHEN THE NULL HYPOTHESIS IS TRUE, THE STATISTICAL SUMMARY WOULD BE GREATER OR EQUAL TO THE STATISTICAL SUMMARY FOR THE OBSERVED RESULTS.

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REGULARIZATION

: REDUCE VARIANCE AT THE COST OF INTRODUCING SOME BIAS

(\uparrow BIAS \Rightarrow UNDERFITTING)
(\uparrow VAR \Rightarrow OVERFITTING)

LINEAR REGRESSION MODEL

$Y = X\beta + \epsilon$, $\epsilon \sim N(0, \sigma^2)$
ORDINARY LEAST SQUARES (OLS) \Rightarrow ESTIMATE $\hat{\beta}$ SUCH A WAY THAT SUM OF SQUARES OF RESIDUALS IS AS SMALL AS POSSIBLE

$$\min L_{OLS}(\hat{\beta}) = \min \sum_{i=1}^n (y_i - x_i^T \hat{\beta})^2 = \min \|y - X\hat{\beta}\|^2$$

IN ORDER TO OBTAIN $\hat{\beta}_{OLS} = (X^T X)^{-1} (X^T Y)$

• RIDGE REGRESSION (L2 PENALTY)

OLS LOSS FUNCTION IS AUGMENTED

IN A WAY WE PENALIZE THE SIZE OF PARAMETER ESTIMATES:

$$L_{RIDGE}(\hat{\beta}) = \sum_{i=1}^n (y_i - x_i^T \hat{\beta})^2 + \lambda \sum_{j=1}^m \hat{\beta}_j^2 = \|y - X\hat{\beta}\|^2 + \lambda \|\hat{\beta}\|^2$$

* ALSO CALLED AS L2 PENALTY

• LASSO REGRESSION (L1 PENALTY)

SIMILAR TO RIDGE REGRESSION BUT LOSS FUNCTION IS:

$$L_{\text{Lasso}}(\hat{\beta}) = \sum_{i=1}^n (y_i - x_i^T \hat{\beta})^2 + \lambda \sum_{j=1}^m |\hat{\beta}_j|$$

* ALSO CALLED L1 PENALTY

• ELASTIC NET

A COMBINATION OF BOTH RIDGE REGRESSION AND LASSO REGRESSION, LOSS FUNCTION IS:

$$L_{\text{ENET}}(\hat{\beta}) = \sum_{i=1}^n \frac{(y_i - x_i^T \hat{\beta})^2}{2n} + \lambda \left(\frac{1-\alpha}{2} \sum_{j=1}^m \hat{\beta}_j^2 + \alpha \sum_{j=1}^m |\hat{\beta}_j| \right)$$

WHERE α IS THE MIXING PARAMETER BETWEEN RIDGE ($\alpha=0$) AND LASSO ($\alpha=1$).

GRID - SEARCH

GRID-SEARCH IS USED TO FIND THE OPTIMAL HYPERPARAMETERS OF A MODEL WHICH RESULTS IN THE MOST 'ACCURATE' PREDICTIONS.

IT CAN BE CHOOSE THE FOLLOWING PARAMETERS:

- PENALTY: L1, L2, ELASTIC NET
- LEARNING RATE
- METRIC: ACCURACY, RECALL, PRECISION, F1-SCORE

* DISCUSSIONS ABOUT RANDOM - SEARCH IS

BETTER (AND FASTER) THAN GRID-SEARCH. SAME CONCEPT BUT INSTEAD OF SETTING SOME VALUES/INPUTS THEY ARE RANDOMLY CHOSEN.

(PROBABILITY / ODDS / LOG ODDS)

PROBABILITY of 80% of RAIN TODAY

ODDS RATIO IS 80% OF CHANCE OF RAIN DIVIDED BY
20% OF CHANCE OF NOT RAIN $\Rightarrow 80\% / 20\% = \boxed{4}$

LOG ODDS IS THE LOGARITHM OF ODDS $\Rightarrow \boxed{\ln(4)}$

$$* \text{ ODDS RATIO} = \frac{IP(A)}{IP(-A)} = \frac{IP(A)}{1 - IP(A)} \quad \therefore \text{LOG ODDS} = \ln\left(\frac{P}{1-P}\right)$$

$$\text{AND } \text{LOG ODDS} = \ln\left(\frac{P}{1-P}\right) = \beta_0 + \sum_{i=1}^m \beta_i x_i$$