



Multivariate Analysis Report: Breast Cancer Diagnosis With Supervised and Unsupervised Classification (Wisconsin Dataset)

Multivariate Analysis

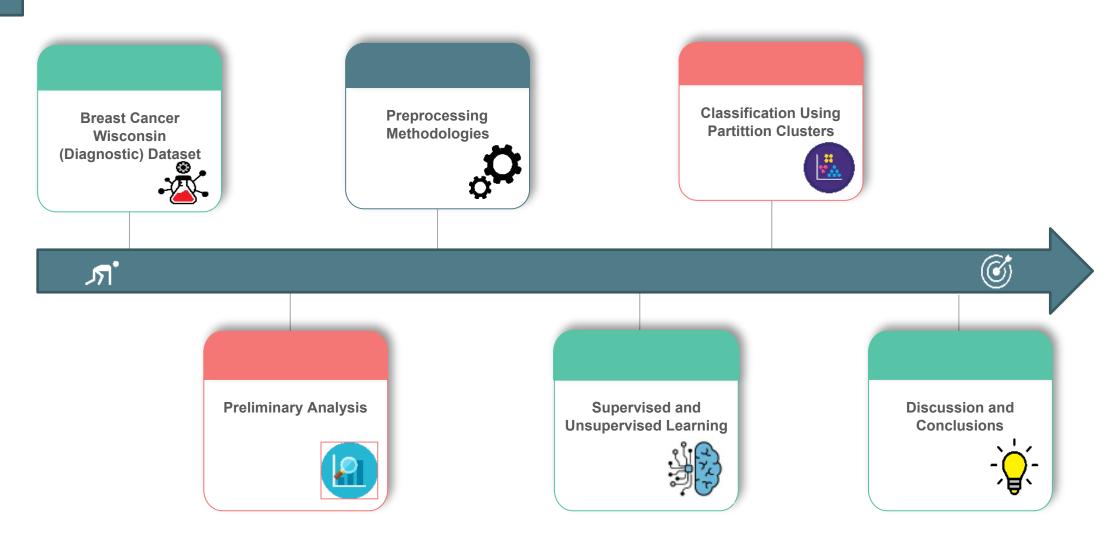
Maria Rosário Oliveira, PhD on Mathematics

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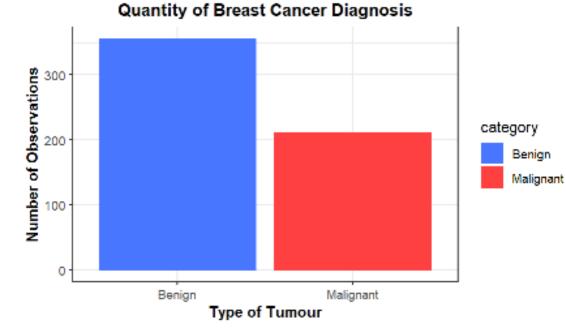
STRUCTURE AND METHODOLOGY



BREAST CANCER WISCONSIN (DIAGNOSTIC) DATASET

Attributes of Breast Cancer Wisconsin (Diagnostic) Dataset

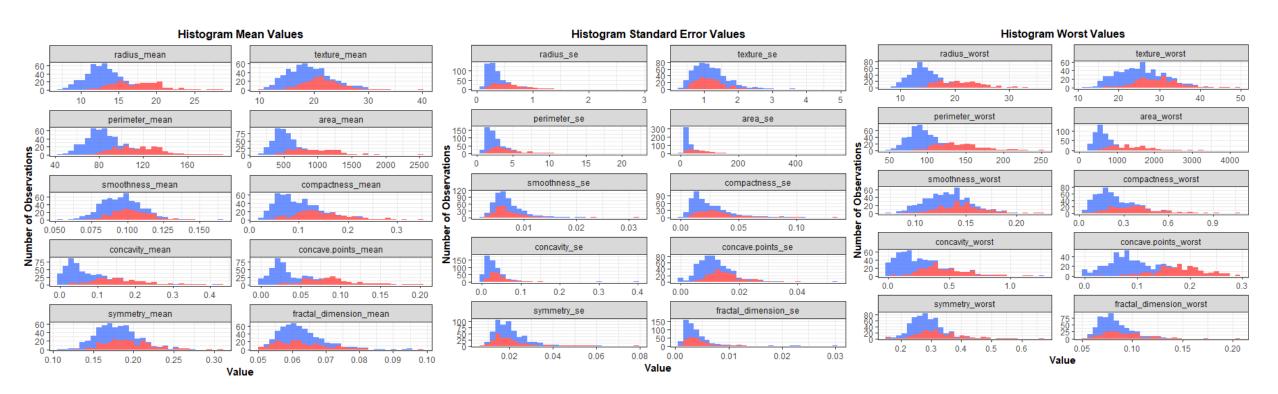
- ID-Number;
- Diagnosis;
- Ten-real values features computed for each nuclear cell:
 - o Radius;
 - o Texture;
 - o Perimeter;
 - o Area;
 - o Smoothness;
 - o Compactness;
 - o Concavity;
 - o Concave points;
 - o Symmetry;
 - Fractal Dimension.



Quantity of the cancer cases in Breast Cancer Wisconsin (Diagnostic) Dataset (Benign=357, Malignant=212).

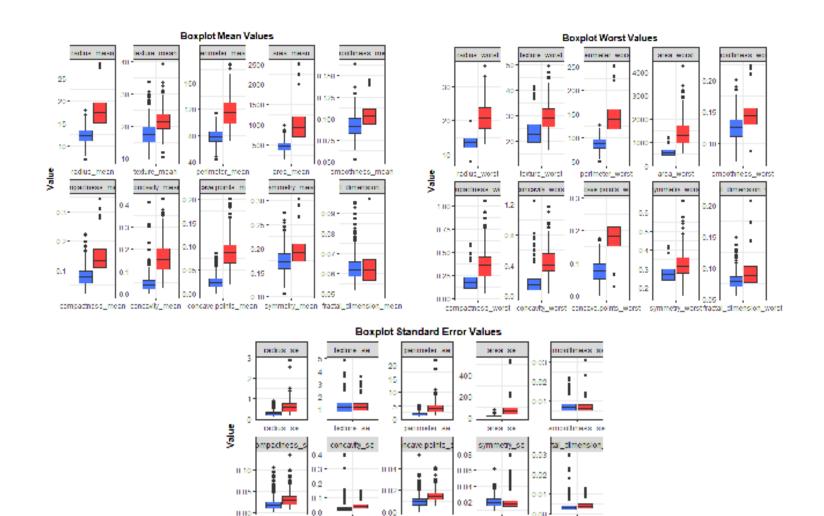
The mean, the standard error and the "worst" (mean of the three largest values) of these features were computed for each image, yielding in 30 features.

PRELIMINARY ANALYSIS



All components mean, standard error and worst values according to the diagnosis (Benign=Blue, Malignant=Red).

PRELIMINARY ANALYSIS

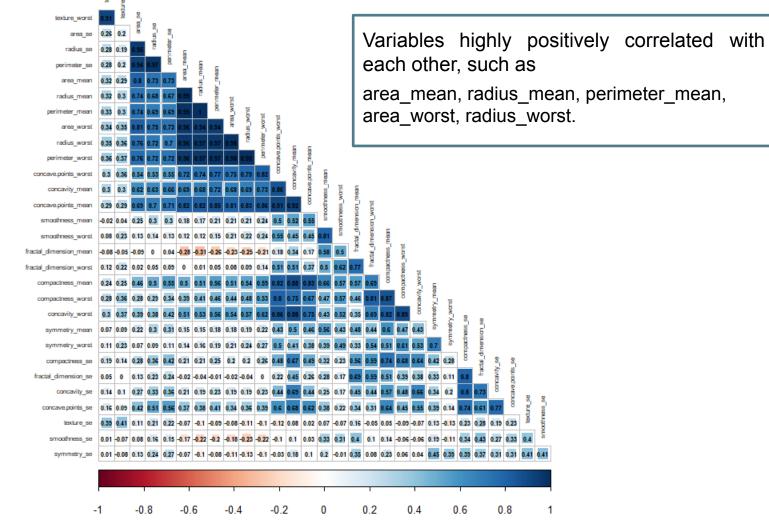


symmetry_se

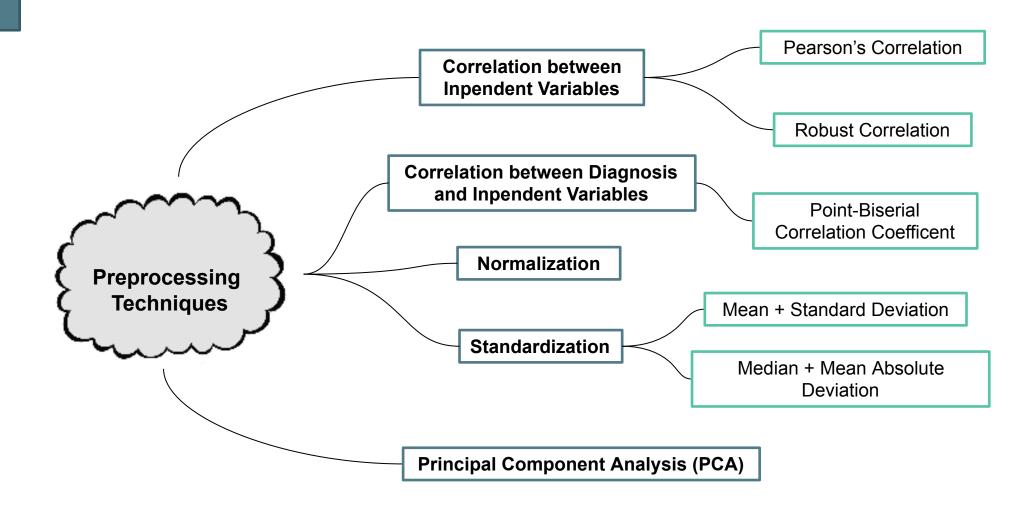
concave.points_se

PRELIMINARY ANALYSIS

Correlation Matrix

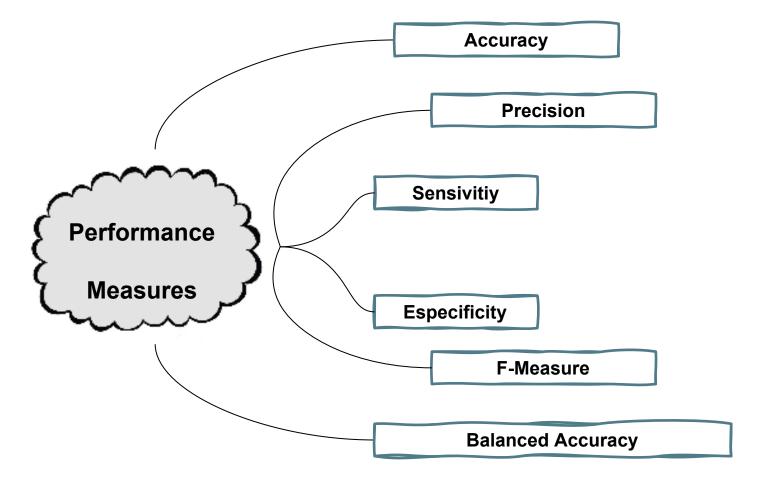


PREPROCESSING METHODOLOGIES



SUPERVISED AND UNSUPERVIDED LEARNING

Validation and Confusion Matrix



SUPERVISED AND UNSUPERVIDED LEARNING Naive Bayes (NB) Random Forest (RF) **Supervised Learning** K-Nearest Neighbors (KNN) **XGBoost Linear Discriminant Analysis** (LDA) Machine Learning Hierarchical Clustering K-Means **Unsupervised Learning** K-Medoids

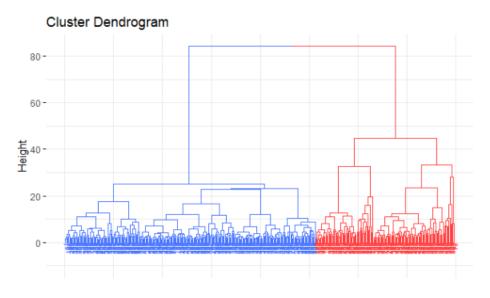
Hierarquical Clustering



TABLE 1: CONFUSION MATRICES USING HIERARCHICAL CLUSTERING (SINGLE LINKAGE, COMPLETE LINKAGE, AVERAGE LINKAGE AND WARD'S METHOD) PERFORMED IN THE TRAIN SET, FOR THE STANDARDIZED DATASET.

Hierarquical Clustering									
Method	hod Single Linkage Complete Linkage Average Linkage						Ward's Method		
Classes	В	M	В	M	В	M	В	M	
Cluster 1	245	152	246	150	246	150	228	28	
Cluster 2	1	0	0	2	0	2	18	124	





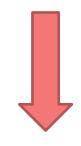
Dendogram for the Standardized Dataset with Ward's Method

The Best Method



TABLE 2: HIERARQUICAL CLUSTERING, K-MEANS AND K-MEDOIDS FOR THE TRAINING STANDARDIZED DATASET.

Best Clustering Method - train data									
Method	Hiera	rquical Clustering	K-M	eans	K-Medoids				
Classes	В	M	В	M	В	M			
Cluster 1	228	28	240	28	238	33			
Cluster 2	18	124	6	124	8	119			
Accuracy	0.8844		0.9146		0.8970				
Sensitivity	0.9268		0.9756		0.9674				



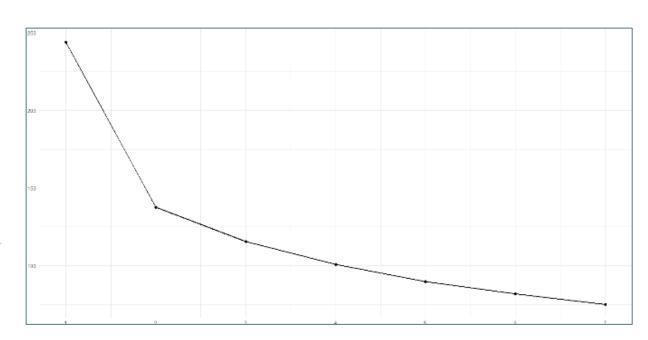
K-Means

The Best Method



TABLE 3: PERFORMANCE MEASURES FOR THE NORMALIZED PCA DATASET, WITH 5 VARIABLES

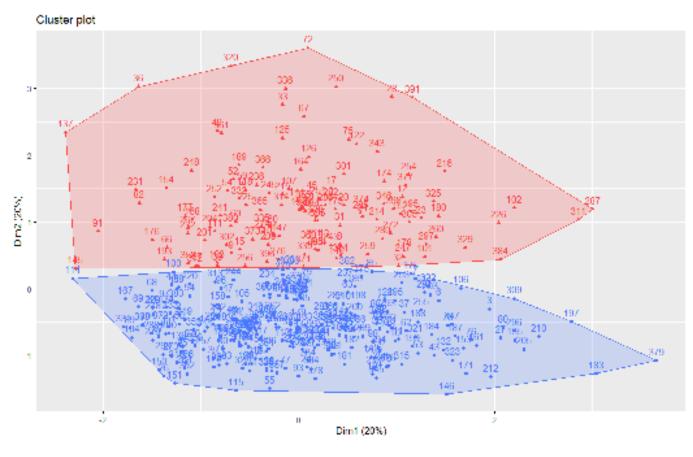
Performance Measures - 5 variables									
Normalization+PCA	Train data		Test	data					
Classes	В	M	B	M					
Cluster 1	237	29	109	8					
Cluster 2	9	123	2	52					
Accuracy	0.9	045	0.94	115					
Sensitivity	0.9	634	0.98	320					
Specificity	0.8	092	0.86	667					
Balanced Accuracy	0.8	863	0.92	243					
Precision	0.8	910	0.93	316					
F1-Score	0.9	258	0.95	661					



Cluster Plot for the Normalized+PCA dataset

The Best Method





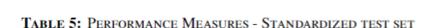
Cluster Plot

TABLE 4: CONFUSION MATRICES - STANDARDIZED TEST SET

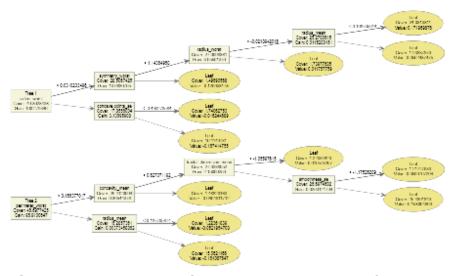


Method	kN	N	N	В	XGB	oost	R	F	LD	A
Classes	В	M	В	M	В	M	В	M	В	M
\boldsymbol{B}	110	4	107	5	110	1	110	3	110	4
M	1	56	4	55	1	59	110 1	57	1	56

The Best Method



Method	kNN	NB	XGBoost	RF	LDA
Accuracy	0.9707	0.9415	0.9883	0.9766	0.9707
Sensitivity	0.9909	0.9549	0.9909	1.000	0.9909
Specificity	0.9333	0.9166	0.9833	0.9333	0.9333
Balanced Accuracy	0.9621	0.9358	0.9871	0.9666	0.9621
Precision	0.9649	0.9549	0.9909	0.9652	0.9649
F1-Measure	0.9777	0.9549	0.9909	0.9823	0.9777



XGBoost results trees for the dataset arising from the analysis of the correlation between independent features and diagnosis variable, comprising three variables.

TABLE 4: CONFUSION MATRICES - STANDARDIZED TEST SET

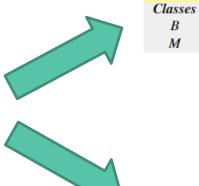
0.958

0.956

0.954

0.952

XGBoost



Method

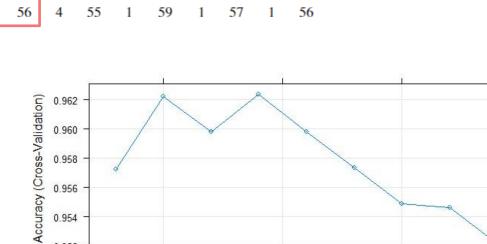
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The Best	
Method	

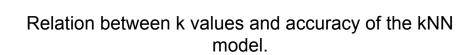
Method

TABLE 5: PERFORMANCE MEASURES - STANDARDIZED TEST SET

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Precision	0.9649	0.9549	0.9909	0.9652	0.9649
F1-Measure	0.9777	0.9549	0.9909	0.9823	0.9777



LDA



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#Neighbors

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REPETITION USING CLUSTERS

The Best Method

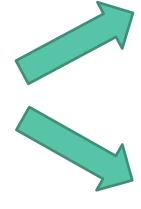


TABLE 6: CONFUSION MATRIX USING CLUSTERS RESULTS

Method	XGBoost				kNN			
Dataset	No	rm	PCA	(norm)	No	rm	PCA	(norm)
Classes	\boldsymbol{B}	M	\boldsymbol{B}	M	\boldsymbol{B}	M	\boldsymbol{B}	M
\boldsymbol{B}	110	10	110	7	110	7	110	7
M	1	50	1	53	1	53	1	53

TABLE 7: PERFORMANCE MEASURES USING CLUSTERS RESULTS

Method	X	GBoost	kNN		
Dataset	Norm	PCA (norm)	Norm	PCA (norm)	
Accuracy	0.9356	0.9532	0.9532	0.9532	
Sensivity	0.9909	0.9909	0.9909	0.9909	

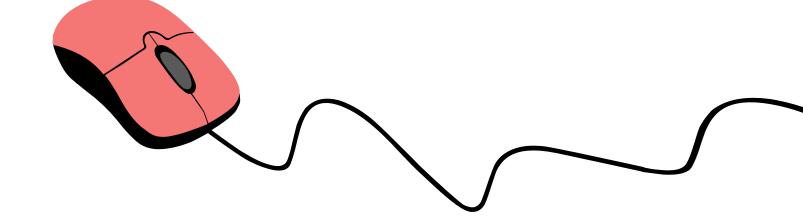
DISCUSSION AND CONCLUSIONS

- XGBoost can obtain predictive models around 98% and kNN around 97%;
- The dataset with 3 variables: radius_worst, perimeter_worst and concave. points_worst presented an accuracy of 95% when predicted by XGBoost;



It's possible to stipulate that these three variables are essential and sufficient to classify if a tumour if either benign or malignant.

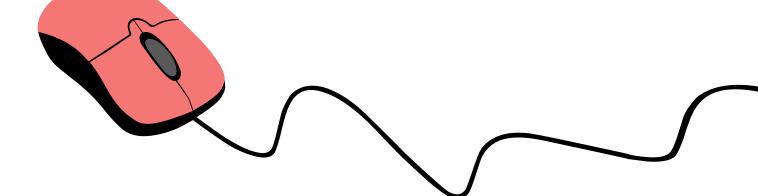




DISCUSSION AND CONCLUSIONS

- Very good results were achieved with the ward's method, and a almost perfect separation of the observations was achieved with a sensitivity of 93%;
- However the best unsupervised method was the K-means because it's vital to have a high sensitivity;
- This way, the K-Means approach not only presented the highest sensitivity (98%), but also the best accuracy (91%);
- When observing both supervised and unsupervised methods, the best results were obtained in datasets that suffered transformations, namely variable reduction.





REFERENCES

• W. N. S. Dr. William H. Wolberg and O. L. Mangasarian. (September 2016) Breast cancer wisconsin (diagnostic) dataset. (accessed: 27.12.2021). [Online]. Available: https://www.kaggle.com/uciml/breast- cancer-wisconsin-data. Studio

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Thank you for your attention!





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