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Data.arrff
x +
File Edit View

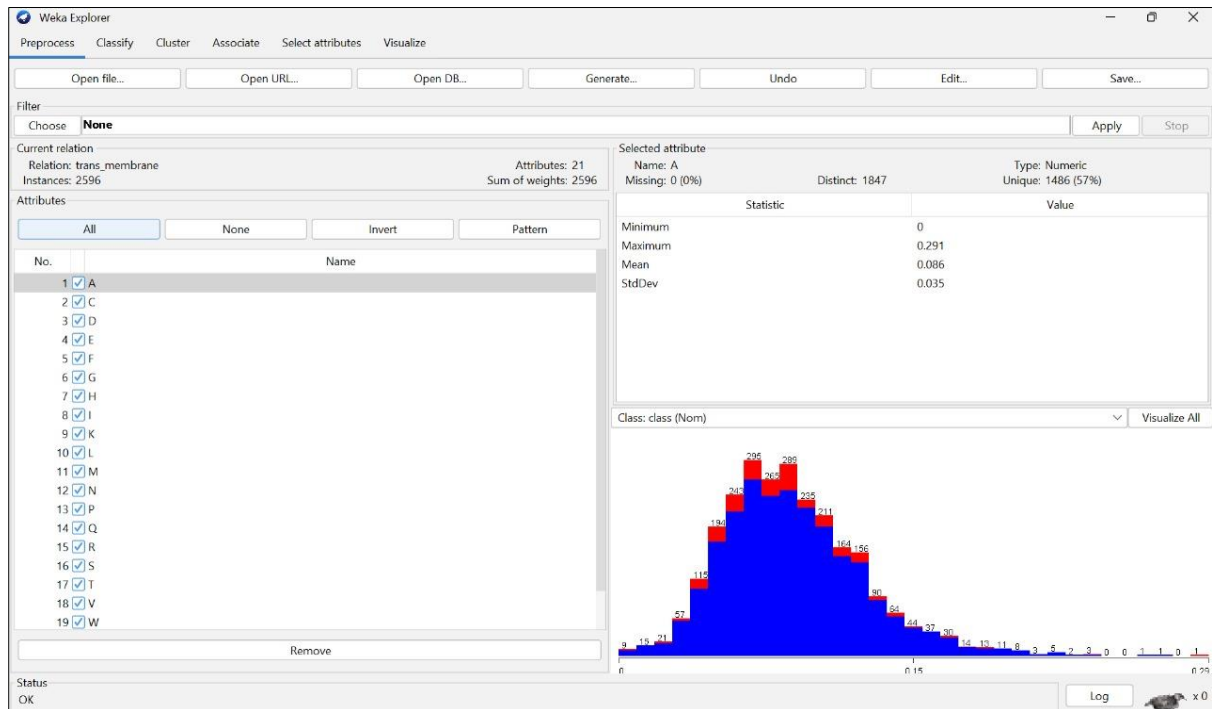
@RELATION trans_membrane

@ATTRIBUTE A numeric
@ATTRIBUTE C numeric
@ATTRIBUTE D numeric
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@ATTRIBUTE F numeric
@ATTRIBUTE G numeric
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@ATTRIBUTE I numeric
@ATTRIBUTE K numeric
@ATTRIBUTE L numeric
@ATTRIBUTE M numeric
@ATTRIBUTE N numeric
@ATTRIBUTE P numeric
@ATTRIBUTE Q numeric
@ATTRIBUTE R numeric
@ATTRIBUTE S numeric
@ATTRIBUTE T numeric
@ATTRIBUTE V numeric
@ATTRIBUTE W numeric
@ATTRIBUTE Y numeric
@ATTRIBUTE class {Alpha,Beta}

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```

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The data file was opened in Weka.



4 and 5

10 different machine learning algorithms were used to perform the classification problem and tested for their performance on the training data alone.

	Training set						
	TP	TN	FP	FN	Sensitivity	Specificity	Accuracy
Logistic	2315	141	102	38	0.98385	0.580247	0.94607
Decision Stump	2353	0	243	0	1	0	0.90639
Random Tree	2353	242	1	0	1	0.995885	0.99961
Random Forest	2353	242	1	0	1	0.995885	0.99961
MultilayerPerceptron	2348	190	53	5	0.997875	0.781893	0.97766
OneR	2338	42	201	15	0.993625	0.17284	0.9168
KStar	2353	242	1	0	1	0.995885	0.99961
Naive Bayes	2211	185	58	142	0.939652	0.761317	0.92296
AdaBoostM1	2278	131	112	75	0.968126	0.539095	0.92797
SGD	2310	152	91	43	0.981725	0.625514	0.94838

Result list (right-click for options)	Correctly Classified Instances Incorrectly Classified Instances Kappa statistic Mean absolute error Root mean squared error Relative absolute error Root relative squared error Total Number of Instances	Result list (right-click for options)	Correctly Classified Instances Incorrectly Classified Instances Kappa statistic Mean absolute error Root mean squared error Relative absolute error Root relative squared error Total Number of Instances
13:25:40 - functions.Logistic 13:28:51 - trees.DecisionStump 13:29:25 - trees.RandomTree 13:29:54 - trees.RandomForest 13:30:27 - functions.MultilayerPerceptron 13:31:23 - rules.OneR 13:31:52 - lazy.KStar 13:35:16 - bayes.NaiveBayes 13:35:52 - meta.AdaBoostM1 13:36:27 - misc.InputMappedClassifier 13:36:44 - misc.SerializedClassifier 13:36:56 - functions.SGD 13:42:12 - functions.Logistic 13:42:49 - trees.DecisionStump 13:43:05 - trees.RandomTree 13:43:37 - trees.RandomForest 13:44:04 - functions.MultilayerPerceptron 13:44:54 - rules.OneR 13:45:23 - lazy.KStar 13:47:01 - bayes.NaiveBayes 13:47:30 - meta.AdaBoostM1	==== Detailed Accuracy By Class ====	13:25:40 - functions.Logistic 13:28:51 - trees.DecisionStump 13:29:25 - trees.RandomTree 13:29:54 - trees.RandomForest 13:30:27 - functions.MultilayerPerceptron 13:31:23 - rules.OneR 13:31:52 - lazy.KStar 13:35:16 - bayes.NaiveBayes 13:35:52 - meta.AdaBoostM1 13:36:27 - misc.InputMappedClassifier 13:36:44 - misc.SerializedClassifier 13:36:56 - functions.SGD 13:42:12 - functions.Logistic 13:42:49 - trees.DecisionStump 13:43:05 - trees.RandomTree 13:43:37 - trees.RandomForest 13:44:04 - functions.MultilayerPerceptron 13:44:54 - rules.OneR 13:45:23 - lazy.KStar 13:47:01 - bayes.NaiveBayes 13:47:30 - meta.AdaBoostM1	==== Detailed Accuracy By Class ====
	TP Rate FP Rate		TP Rate FP Rate
	0.968 0.461		0.982 0.374
	0.539 0.032		0.626 0.018
	Weighted Avg. 0.928 0.421		Weighted Avg. 0.948 0.341
	==== Confusion Matrix ====		==== Confusion Matrix ====
	a b <-- classified as		a b <-- classified as
	2278 75 a = Alpha		2310 43 a = Alpha
	112 131 b = Beta		91 152 b = Beta

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	5-fold CV						
	TP	TN	FP	FN	Sensitivity	Specificity	Accuracy
Logistic	2308	137	106	45	0.980875	0.563786	0.941834
Decision Stump	2353	0	243	0	1	0	0.906394
Random Tree	2211	105	138	142	0.939652	0.432099	0.892142
Random Forest	2340	107	136	13	0.994475	0.440329	0.942604
MultilayerPerceptron	2278	144	99	75	0.968126	0.592593	0.932974
OneR	2298	37	206	55	0.976626	0.152263	0.899461
KStar	2272	127	116	81	0.965576	0.522634	0.924114
Naive Bayes	2216	179	64	137	0.941776	0.736626	0.922573
AdaBoostM1	2280	107	136	73	0.968976	0.440329	0.919492
SGD	2310	143	100	43	0.981725	0.588477	0.944915

	10-fold CV						
	TP	TN	FP	FN	Sensitivity	Specificity	Accuracy
Logistic	2307	133	110	46	0.98045	0.547325	0.939908
Decision Stump	2353	0	243	0	1	0	0.906394
Random Tree	2221	119	124	132	0.943901	0.489712	0.901387
Random Forest	2337	114	129	16	0.9932	0.469136	0.944145
MultilayerPerceptron	2291	149	94	62	0.973651	0.613169	0.939908
OneR	2303	35	208	50	0.978751	0.144033	0.900616
KStar	2271	127	116	82	0.965151	0.522634	0.923729
Naive Bayes	2208	179	64	145	0.938377	0.736626	0.919492
AdaBoostM1	2278	115	128	75	0.968126	0.473251	0.921803
SGD	2313	138	105	40	0.983	0.567901	0.944145

	20-fold CV						
	TP	TN	FP	FN	Sensitivity	Specificity	Accuracy
Logistic	2310	137	106	43	0.981725	0.563786	0.942604
Decision Stump	2353	0	243	0	1	0	0.906394
Random Tree	2214	115	128	139	0.940926	0.473251	0.897149
Random Forest	2336	110	133	17	0.992775	0.452675	0.942219
MultilayerPerceptron	2274	146	97	49	0.978907	0.600823	0.943102
OneR	2302	23	220	51	0.978326	0.09465	0.895609
KStar	2272	128	115	81	0.965576	0.526749	0.924499
Naive Bayes	2207	181	62	146	0.937952	0.744856	0.919877
AdaBoostM1	2280	120	123	73	0.968976	0.493827	0.924499
SGD	2313	137	106	40	0.983	0.563786	0.94376

	66% split						
	TP	TN	FP	FN	Sensitivity	Specificity	Accuracy
Logistic	792	41	36	14	0.98263	0.532468	0.943375
Decision Stump	806	0	77	0	1	0	0.912797
Random Tree	763	28	49	43	0.94665	0.363636	0.89581
Random Forest	801	32	45	5	0.993797	0.415584	0.943375
MultilayerPerceptron	791	46	31	15	0.98139	0.597403	0.947905
OneR	788	3	74	18	0.977667	0.038961	0.89581
KStar	780	40	37	26	0.967742	0.519481	0.928652
Naive Bayes	760	58	19	46	0.942928	0.753247	0.926387
AdaBoostM1	784	38	39	22	0.972705	0.493506	0.930917
SGD	797	41	36	9	0.988834	0.532468	0.949037

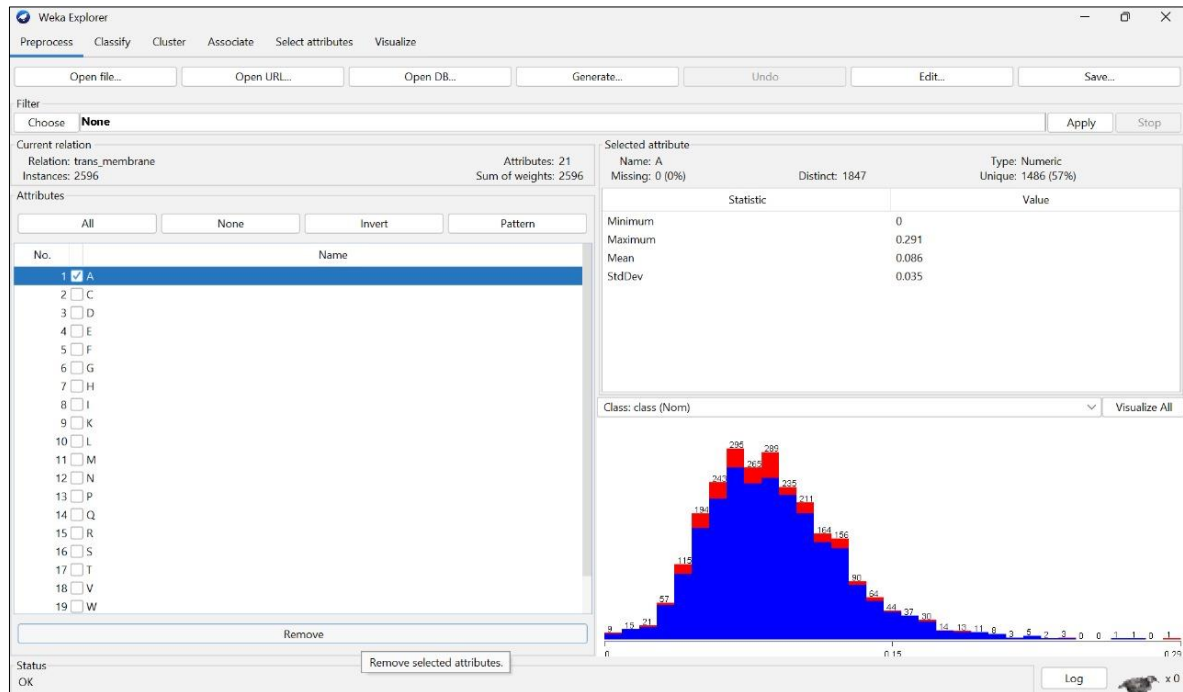
- Most of the models have similar sensitivities and accuracies.
- However, their specificities differ.
- This arises due to the imbalanced nature of the dataset, which has fewer instances of negatives (Beta).
- Thus, using the sensitivity to decide the best model is the appropriate approach.
- Based on this, the **Naive Bayes** classifier has the best performance.

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The best model, Naive Bayes, was tested with different train-test splits.

	TP	TN	FP	FN	Sensitivity	Specificity	Accuracy
70%	667	55	18	39	0.944759	0.753425	0.926829
60%	883	72	18	65	0.931435	0.8	0.920039
50%	1103	94	29	72	0.938723	0.764228	0.922188

Residues were iteratively eliminated to determine their importance. Performance was evaluated using the best model (Naive Bayes) with a 70% train-test split.

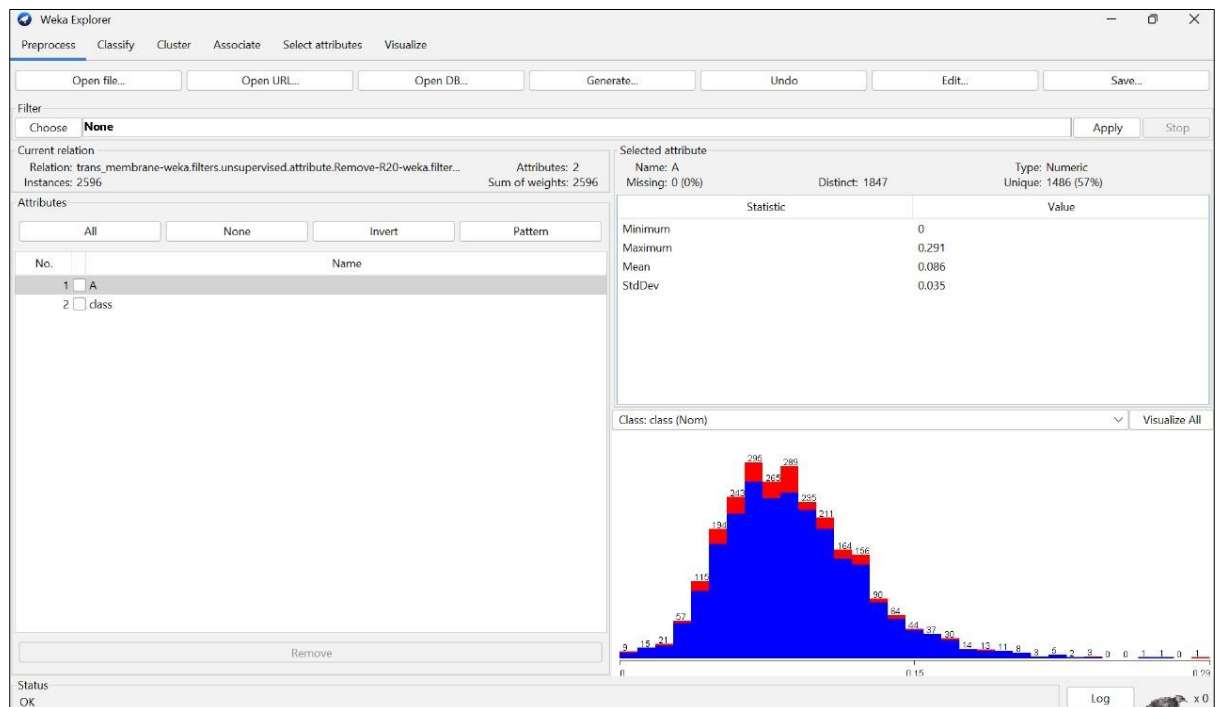


	TP	TN	FP	FN	Sensitivity	Specificity	Accuracy
A	668	55	18	38	0.946176	0.753425	0.928113
C	669	56	17	37	0.947592	0.767123	0.93068
D	669	54	19	37	0.947592	0.739726	0.928113
E	668	55	18	38	0.946176	0.753425	0.928113
F	675	54	19	31	0.956091	0.739726	0.935815
G	661	58	15	45	0.936261	0.794521	0.922978
H	665	55	18	41	0.941926	0.753425	0.924262
I	669	54	19	37	0.947592	0.739726	0.928113
K	666	55	18	40	0.943343	0.753425	0.925546
L	678	54	19	28	0.96034	0.739726	0.939666
M	672	53	20	34	0.951841	0.726027	0.93068
N	660	48	25	46	0.934844	0.657534	0.908858
P	664	54	19	42	0.94051	0.739726	0.921694
Q	667	52	21	39	0.944759	0.712329	0.922978
R	668	54	19	38	0.946176	0.739726	0.926829
S	663	56	17	43	0.939093	0.767123	0.922978
T	666	53	20	40	0.943343	0.726027	0.922978
V	666	56	17	40	0.943343	0.767123	0.926829
W	668	54	19	38	0.946176	0.739726	0.926829
Y	664	59	14	42	0.94051	0.808219	0.928113

- From this, we can see that the sensitivities and accuracies do not change much.
- However, the specificity drops appreciably when Asn (N), Gln (Q), Met (M), or Thr (T) are eliminated.
- N and Q are amino acids with an amide side chain.
- Their compositions may have an important role in discriminating alpha and beta transmembrane proteins.

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The same analysis was performed by using only the composition of a single amino acid as a feature.



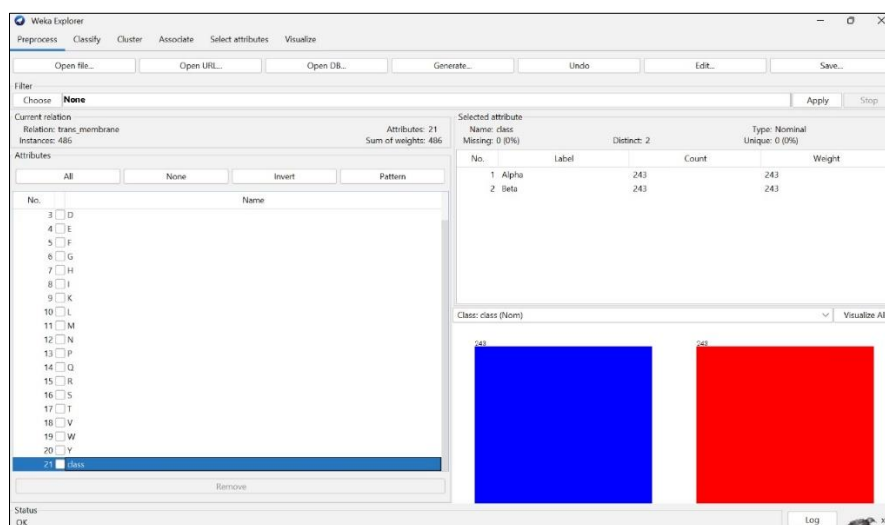
	TP	TN	FP	FN	Sensitivity	Specificity	Accuracy
A	706	0	73	0	1	0	0.90629
C	706	0	73	0	1	0	0.90629
D	700	0	73	6	0.991501	0	0.898588
E	706	0	73	0	1	0	0.90629
F	706	0	73	0	1	0	0.90629
G	696	0	73	10	0.985836	0	0.893453
H	706	0	73	0	1	0	0.90629
I	706	0	73	0	1	0	0.90629
K	706	0	73	0	1	0	0.90629
L	706	0	73	0	1	0	0.90629

M	706	0	73	0	1	0	0.90629
N	693	9	64	13	0.981586	0.123288	0.901155
P	706	0	73	0	1	0	0.90629
Q	706	0	73	0	1	0	0.90629
R	706	0	73	0	1	0	0.90629
S	706	0	73	0	1	0	0.90629
T	706	0	73	0	1	0	0.90629
V	706	0	73	0	1	0	0.90629
W	706	0	73	0	1	0	0.90629
Y	704	0	73	2	0.997167	0	0.903723

From this we can see that the specificity is non-zero only when Asn (N) composition is considered,

10 and 11

A balanced dataset was constructed by considering only the first 243 sequences from ‘Alpha’.



The performance of the Naive Bayes model was evaluated on this with 5-fold cross-validation.

TP	185
TN	209
FP	34
FN	58
Sensitivity	0.761317
Specificity	0.860082
Accuracy	0.8107

The model maintains its good performance.