Wine Project Report

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Abstract This paper is an analysis of the effectiveness of the various models studied during the course applied to a binary classification model. The dataset is a transformed version of the one provided in *Modeling wine preferences by data mining from physicochemical properties* from *Decision Support Systems, Elsevier* (P. Cortez, A. Cerdeira, F. Almeida, T. Matos and J. Reis.), where grades span from 0 to 10. Grade 6 has been removed, grades above 6 have been mapped to class 1 and grades below 6 to class 0. Due to limited time and computanional power, results may be just close-to or far-from optimal, depending on the time required to train a model.

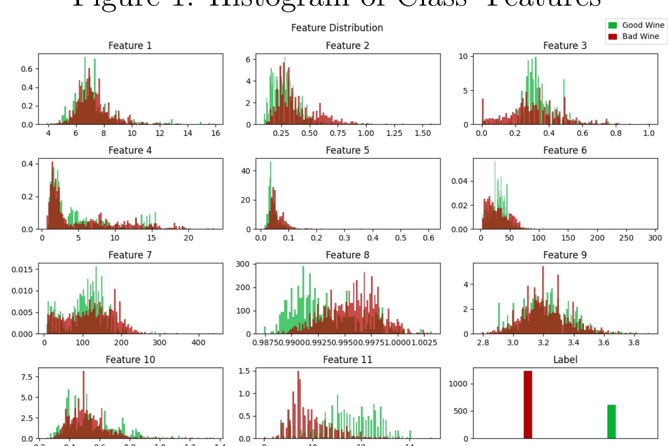
Contents

1 Preliminary Data Analysis

1.1 Feature Distribution

Before discussing the model, their implementation and their effectiveness we briefly take a look at how the features are distributed. For convenience we shall now report the legend just one, but keep in mind that in all pictures red color is associated to class 0 (which we will be referring to as class *Bad*) and green color is associated to class 1 (which will be class *Good*).

Figure 1: Histogram of Class' Features



First of all, our training dataset is unbalanced. In the next pages we will be classifying samples obtained from a K-Fold[1]Validation approach, using a theoretical threshold given by:

$$t = -\log \frac{\pi}{1-\pi}$$

For the threshold to be optimal, we should use the empirical prior $\pi \approx .33$ based on a frequentist approach; Instead we will be using a non-optimal prior $\tilde{\pi} = .5$ as it is the application we are going to be targeting .

Coming back to features distributions, some things are to be noticed. While some features are similar between class Good and class Bad (see feature *1*) others differ substantially and can be very helpful in discriminating samples (see feature *8*).

Moreover, the features are distributed in various ways: while some do look pretty Gaussian (see feature *9*) and others are instead fairly regular (see feature *5*) and could thus be well estimated by Gaussian models[2], other act in a more irregular way.

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To take a closer look we now project the data on the two dimensional plane. We will be using 3 methods to do so: PCA[3], Normalization + PCA, Normalization + Whitening.

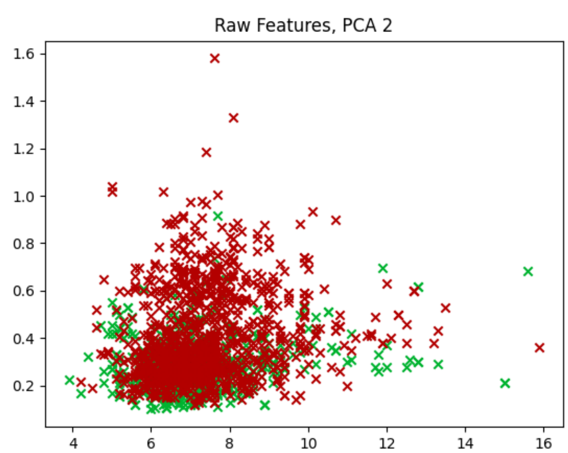

Figure 2: 2D-PCA Projection

[1]K varies through models. For fast ones, 5 or 10 is used. For slower ones, 3 is used.

[2]Meaning both Gaussian Classifiers and Gaussian Mixture Models

[3]Without data centering to appreciate the correlation

The points are very close one another, we thus expect linear models to be not so effective compared to others. The data is pretty *circularly* distributed, so correlation may not play an important role in discriminating samples.

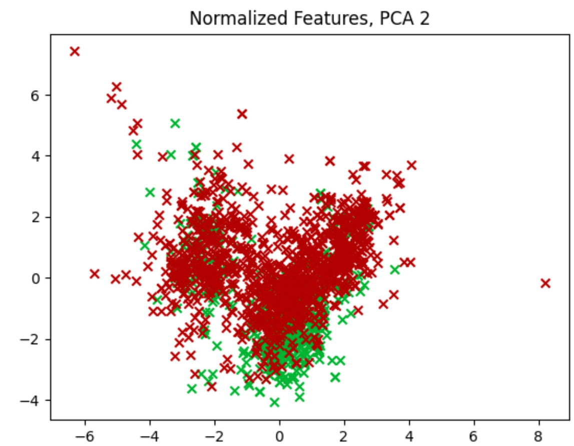

Figure 3: 2D-PCA Projection, Normalized Data

The normalized projection seems to split data in two clusters, each containing some samples of either class, but some points of different class seem to get far apart from the other. So normalization is a technique worth trying.

Note that for Normalization we refer to *Z-Normalization*. From some early tests we found that *Min-Max* normalization was not very effective, and with *Gaussianization* centering and scaling data in the same way as Z while being slower, we decided to use this method.

Lastly we take a look at normalized and whitened data.

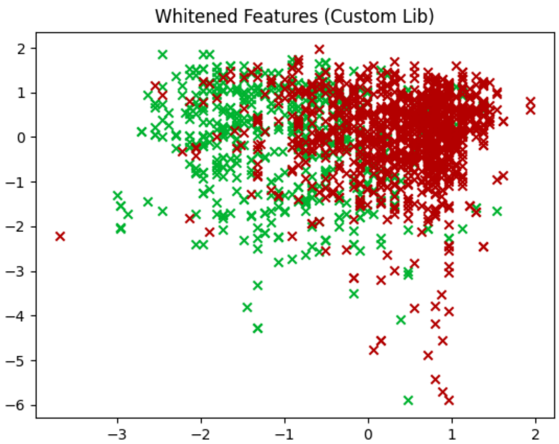

Figure 4: 2D-PCA Projection, Whitened Data

Results do look interesting: points to get much apart, even if we can spot many outliers. With the distribution being this way, we could expect even linear models to achieve decent results.

2 Pre-Processing Analysis

In this section we will run some dummy[4]models to learn how pre-processing affects the models for our task.

Note that we will be discarding combinations or entire models targeting our final application. A discussion about different applications will be made in the ending.

2.1 Pre-Processing MVG Classifiers

Since MVG classifiers are fairly similar, we will now pick the most promising one and discarding the others, while trying to infer its optimal working condition.

Type	PCA	DCF	minDCF
Raw	8	0.375	**0.321**
Raw	9	**0.360**	0.326
Norm.	10	0.419	0.330
Norm.	11	0.424	0.322
Whit.	11	0.424	0.322
Whit.	8	0.392	0.342

Table 1: Full-Covariance MVG - Best Results

Type	PCA	DCF	minDCF
Raw	11	**0.342**	0.332
Norm.	**5**	0.414	**0.330**
Norm.	11	**0.342**	0.332
Whit.	11	**0.342**	0.332

Table 2: Tied-Covariance MVG - Best Results

Type	PCA	DCF	minDCF
Raw	9	0.404	0.365
Raw	7	**0.391**	0.370
Norm.	9	0.428	0.350
Whit.	11	0.460	**0.344**
Whit.	5	0.394	0.374

Table 3: Naive-Bayes MVG - Best Results

The results seem in line with our assumptions. In fact, if we look again at picture 2 we wouldn't expect the Naive Bayes to perform much differently from the Full Covariance one. The best model, with a modest margin, is the tied covariance one so we will keep it, and removing some dimensions seems to be helpful.

Notice that while the Tied Covaraiance model achieved the best DCF[5]of all classifiers, the MVG achieved the lowest Minimum DCF values, hiting that it is actually the one out of the three that could theoretically best separate classes.

Normalization and Whitening look irrelevant so we won't further experiment them.

2.2 Pre-Processing for GMMs

For our dummy GMM model we arbitrairly set the number of components to 4. The starting

[4]Simple model that run with arbitrary, non-optimized hyper-parameters

[5]By DCF we actually mean the *normalized* DCF, considering a prior $\pi_T = .5$ and equal costs

point for our EM algorithm is identity covariance matrices and means placed around the dataset mean.

Type	PCA	DCF	minDCF
Raw	No	0.410	**0.394**
Normalized	9	**0.407**	0.402
Whitened	4	0.429	0.420

Table 4: GMM - Best Results

As for our Gaussian Classifiers, Whitening and Normalization do not look promising. However, as the difference between the Raw and Normalized does not look significant, we will further test both models. This first test shows us that high dimensionality is actually preferred.

2.3 Pre-Processing for Kernel SVMs

Differently for what we did up to now, given the non-probabilistic nature of SVM scores, we will be deciding our optimal model for both types of kernel SVMs on just minimum DCFs values.

2.3.1 Pre-Processing for Polynomial Kernel SVMs

The polynomial kernel function is defined as:

$$\phi(\mathbf{x}_1)^T\phi(\mathbf{x}_2) = k(\mathbf{x_1}, \mathbf{x_2}) = (\mathbf{x}_1^T\mathbf{x}_2 + c)^d + b$$

We proceed to set our parameters arbitrairly for this dummy execution:

$$k(\mathbf{x_1}, \mathbf{x_2}) = (\mathbf{x}_1^T\mathbf{x}_2 + 1)^2 + 0.5$$

Type	PCA	DCF	minDCF
Raw	7	0.554	0.545
Normalized	6	**0.393**	**0.381**
Whitened	11	0.399	0.393

Table 5: Polynomail Kernel SVM - Best Results

While competitiveness with other models has to be made later, when each one will be fully used, here we see an interesting change: normalization greatly improves our classification. While a lower PCA has obtained the lowest DCF, it is not significantly lower than the one obtained with higher dimensionality, so we can say that here it's normalization helping us out. Whitening, again, does not make any difference, as the results are same or close to the ones obtained with normalization only.

Notice also how scores seems well calibration with our theoretical threshold even if they do not have a probabilistic interpretation.

2.4 Pre-Processing for RBF Kernel SVMs

The dummy RBF function used here is the following:

$$k(\mathbf{x_1}, \mathbf{x_2}) = e^{-\gamma||\mathbf{x}_1-\mathbf{x}_2||^2} + b = e^{-0.05||\mathbf{x}_1-\mathbf{x}_2||^2} + 0.05$$

Small values of γ and b were picked to avoid numerical issues when using non-normalized models.

Type	PCA	DCF	minDCF
Raw	10	0.588	0.579
Normalized	11	**0.356**	**0.352**
Whitened	11	**0.356**	**0.352**

Table 6: RBF Kernel SVM - Best Results

Just like polynomial kernel, RBF prefers high dimensionality , so further testing in this direction is required. Again, normalization plays an important role while whitening seems to have no effect whatsoever and scores look extremely well calibrated.

Just like polynomial kernel SVMs, here normalization has no effect whatsoever whilte normalization greatly improves our performance. The RBF Kernel works significantly better when working with all or most components.

We are not yet discussing perfomance in detail but so far, this is our most promising model.

2.5 Pre-Processing for Logistic Regression Model

Regarding the Logistic Regression, we will consider both linear and quadratic model.

2.5.1 Linear Logistic Regression

In the Linear model, dimensionality reduction through PCA and prepocessing through normalization helped to obtain lower minimum DCF compared to raw features. For the whitened features, best results are obtained without applying PCA. As the Gaussian Classifiers, only a small numberof features can be removed.

Only results with already optimized hyperparameters are reported.

Type	PCA	DCF	minDCF
Raw ($\lambda = 0.0001$)	10	0.369	0.342
Normalized ($\lambda = 0.01$)	9	0.369	**0.336**
Whitened ($\lambda = 0.0001$)	11	0.549	0.503

Table 7: Linear Logistic Regression - Best Results

Whitening didn't help so much to improve results, so it won't be considered in further analysis.

2.5.2 Quadratic Logistic Regression

In the Quadratic Logistic Regression, after the preprocessing stage, the features space was expanded through

$$\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} vec\langle \mathbf{x}\mathbf{x}^{\mathbf{T}} \rangle \\ \mathbf{x} \end{bmatrix}$$

In contrast to linear model, whitening helped as well as normalization, PCA was useful in both cases, with and without preprocessing, but with a notable difference in the number of features used to obtain following results.

Type	PCA	DCF	minDCF
Raw ($\lambda = 0.1$)	6	0.385	0.366
Normalized ($\lambda = 0.001$)	10	0.324	**0.307**
Whitened ($\lambda = 0.001$)	10	0.324	**0.307**

Table 8: Quadratic Logistic Regression - Best Results

2.6 Pre-Processing for Linear SVM

The Linear SVM model performed much better with normalization and whitening rather than raw features. Applying PCA was useful to obtain low values of minimum DCF in all cases, even if the model trained with raw features performed worse than models trained with preprocessed features.

Type	K	C	PCA	DCF	minDCF
Raw	0	10.0	6	0.911	0.568
Normalized	10	0.1	9	0.350	**0.330**
Whitened	1.0	1.0	9	0.364	0.331

Table 9: Linear SVM - Best Results

The high difference between minimum DCF and DCF suggests us that scores are miscalibrated, but we will try to optimize it in next chapters.

3 Optimizing Models

3.1 Optimizing Logistic Regression

Now we will try to find the λ that gives us the best (lower) minimum DCF in the validation set, extracted from the training set through a 5-fold cross validation protocol. Several values of λ have been tried, in a range between $[10^{-4}, 10^{3}]$ for both linear and quadratic model.

Model	Type	λ	PCA	DCF	minDCF
Linear	Normalized	0.01	9	0.369	0.336
Quadratic	Normalized	0.001	10	0.324	0.307

Table 10: Best λ values for Logistic Regression

We tried to lower the difference between the DCF and the minimum one, in both linear and and quadratic model. To reduce the DCF, we tried to calibrate the scores:

Model	Type	λ	PCA	DCF	minDCF
Linear	Normalized	0.01	9	0.373	0.336
Quadratic	Normalized	0.001	10	0.312	0.307

Table 11: Calibrated scores for logistic regression

As reported in table 11, calibration helped in the quadratic case, but DCF got worse in linear one.

3.2 Optimizing Gaussian Mixture Models

For GMMs we decided inspect both raw and normalized optimization.

Type	DCF	DCF_{min}	PCA	# Comp.
Raw	**0.347**	**0.308**	No	2
Norm	0.365	0.311	6	3
Norm	0.348	0.317	No	2

Table 12: GMM Optimization Results

As in table 4, raw and normalized version both perform similarly, so both model could be of use, depending on the application.

3.3 Optimizing Kernel SVMs

Diffrently from other models, for SVMs we will choose the best parameter based on only the minimum DCF values, given the non probabilistic nature of the scores generated.

3.3.1 Optimizing Polynomial SVMs

Type	DCF_{min}	PCA
Raw	0.380	9
Norm.	**0.367**	No
Whit.	0.381	No

Table 13: Polynomial K. Optimization Results

As opposed to table 5, we find out that the normalized version is actually better than the raw features one.

3.3.2 Optimizing RBF SVMs

Type	DCF_{min}	PCA
Norm.	0.288	10
Whit	0.00	X

Table 14: RBF K. Optimization Results

Here we determine that whitening has no more benefits than plain normalization, so we ultimately discard it.

4 Experimental Results

After having run our models in order to find the best parameters, we now test them on previously unseen data.

All the parameters here reported have been found through a K-Fold Cross-Validation approach. The value of K used spans from 3 (heavier models, e.g. Kernel SVMs) up to 10 (lighter models, e.g. Gaussian Classifiers).

Model	Calibration	Features	PCA	Hyper-Parameters	DCF	DCF$_{min}$
Linear LogReg	No	Normalized	9	$\lambda = 0.01$	0.303	0.299
Quadratic LogReg	Yes	Normalized	10	$\lambda = 0.001$	0.285	0.274
Linear SVM	Yes	Normalized	9	K = 10, C = 0.1	0.276	0.270
MVG Tied Cov.	No	Normalized	5	-	0.390	0.331
GMM	No	Raw	No	$N_{Comp} = 2$	0.327	0.294

As mentioned earlier, up to now all models have been evaluated considering a balanced application ($pi_T = 0.5$). We now want to discuss how or best models, based on the table above, perform in different conditions.

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