Report : Operational Feature Selection in Gaussian Mixture Models

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1. Introduction

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2. Non linear parsimonious features selection

In the remaining, the following notations are used. $\mathcal{S} = \{\mathbf{x}_i, y_i\}_{i=1}^n$ is the training set where $\mathbf{x}_i \in \mathbb{R}^d$ is the vector of features of the ith sample, $y_i = 1, ..., C$ the associated label, C the number of labels, n the number of samples and n_c the number of samples of class c.

2.1. Gaussian Mixture Models

The hypothesis of Gaussian mixture models (GMM) is that the distribution of a given sample is a mixture (convex combination) of several class conditioned distribution:

$$p(\mathbf{x}) = \sum_{c=1}^{C} \pi_c f_c(\mathbf{x}|\theta) \tag{1}$$

where π_c is the prior i.e. the proportion of class c. The Gaussian model assumes that each f_c is , conditionally to c, a Gaussian distribution of parameters $\boldsymbol{\mu}_c$ and $\boldsymbol{\Sigma}_c$ ($f_c(\mathbf{x}|\theta) = \mathcal{N}_c(\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$) and so $f_c(\mathbf{x}|\theta)$ can be written

$$f_c(\mathbf{x}|\theta) = \frac{1}{(2\pi)^{\frac{d}{2}}|\boldsymbol{\Sigma}_c|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_c)^t \boldsymbol{\Sigma}_c^{-1}(\mathbf{x} - \boldsymbol{\mu}_c)\right)$$

Such a model is used in the case of supervised learning and the class parameters $\boldsymbol{\mu}_c$ and $\boldsymbol{\Sigma}_c$ can be estimated using the training samples. In our work, we choose to compute them with the following unbiased empirical estimator

$$\hat{\pi}_c = \frac{n_c}{n} \tag{2}$$

$$\hat{\boldsymbol{\mu}}_c = \frac{1}{n_c} \sum_{\{i|y_i=c\}} \mathbf{x}_i \tag{3}$$

$$\hat{\boldsymbol{\Sigma}}_c = \frac{1}{(n_c - 1)} \sum_{\{i|y_i=c\}} (\mathbf{x}_i - \boldsymbol{\mu}_c)(\mathbf{x}_i - \boldsymbol{\mu}_c)^t \tag{4}$$

To determine the class of a samples using the Bayes' law, the maximum a posteriori (MAP) estimate is used and thus the decision rule can be written as

$$\mathbf{x} \text{ belongs to } c \Leftrightarrow c = \arg\max_{c \in C} p(c|\mathbf{x})$$

$$\Leftrightarrow c = \arg\max_{c \in C} \frac{p(c)p(\mathbf{x}|c)}{p(x)}$$

$$\Leftrightarrow c = \arg\max_{c \in C} p(c)p(\mathbf{x}|c)$$

By taking the log, a simplified decision formula is obtained

$$Q_c(\mathbf{x}) = 2\log\left(p(c)p(\mathbf{x}|c)\right)$$

$$= 2\log\left(\pi_c \frac{1}{(2\pi)^{\frac{d}{2}}|\mathbf{\Sigma}_c|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_c)^t \mathbf{\Sigma}_c^{-1}(\mathbf{x}-\boldsymbol{\mu}_c)\right)\right)$$

$$= 2\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_c)^t \mathbf{\Sigma}_c^{-1}(\mathbf{x}-\boldsymbol{\mu}_c)\right) + 2\log\left(\frac{1}{(2\pi)^{\frac{d}{2}}|\mathbf{\Sigma}_c|^{\frac{1}{2}}}\right) + 2\log(\pi_c)$$

$$= -(\mathbf{x}-\boldsymbol{\mu}_c)^t \mathbf{\Sigma}_c^{-1}(\mathbf{x}-\boldsymbol{\mu}_c) - \log((2\pi)^d|\mathbf{\Sigma}_c|) + 2\log(\pi_c) \tag{5}$$

It is interesting to notice the covariance and its inverse are a key element of the decision function and that the estimation of these elements suffer from the curse of dimensionality. More precisely, the number of parameters to estimate (means, covariance matrices, proportions) increases quadratically relatively to the number of features and we need at least as many samples as parameters to make an estimation which can be an issue. For example, with hyperspectral data, we face high dimensional samples but very few samples are available.

A lack of samples induces ill-conditioned covariance matrices and so unstable inversion. There are two major solutions to this problem. The first option is to use a regularization method to stabilize the inversion of the covariance matrices. The second option is to use a features extraction method in order to reduce the dimensionality of the samples.

In our study based on GMM, a Ridge regularization method described in Section 3 is implemented but we mainly focus on a feature selection method named sequential forward features selection presented in Section 4.1 and an amelioration of this algorithm the sequential floating forward features selection introduced in Section 4.2.

In order to evaluate the benefits of such methods for classification, we introduce in the next section several functions called criterion functions. These functions aim either to evaluate a criterion of good classification or either to evaluate the separability/similarity of class distributions. The choice of one of these criterion functions is up to the user and can depend on the specificity of the task. We purposely choose to present only some of possible functions among the most used. It is also to be noticed that the criterion function is not only use for evaluation in the case of the features selection algorithm presented hereafter but is indeed a parameter of the algorithm.

2.2. Criterion function

2.2.1. Measures of good classification

All this measures of good classification are based on an error matrix M called confusion matrix which is defined so that M_{ij} is the number of samples of class i classified as class j. The confusion matrix allows the computation of several interesting values relatively to each class the number of True Positive (TP) corresponding to good prediction, True Negative (TN) corresponding to good classification of the other class, False Negative (FN) corresponding to the samples of the class labeled

as an other class and the False Positive (FP) corresponding to the samples wrongly classified as part of of this class. Figure 1 illustrates the definition of this values.

Prediction outcome

		p	n
Actual value	p′	True Positive	False Negative
	n′	False Positive	True Negative

Figure 1: Confusion matrix

The overall accuracy is simply the rate of the number of samples with the correct predicted label over the number of samples. This metric is easy to interpret but is biased in the case of unbalanced classes.

The Cohen's kappa is a statistic which measure the probabilities of agreement between predictions and ground-truth. This metric tends to give an equal importance to each class but is hard to interpret.

The mean F1 score is the average of the F1 score for each class and the F1 score is the harmonic mean of the precision (number of True Positive over True Positive plus False Positive) and the recall (number of True Positive over True Positive plus False Negative).

$$\text{Overall Accuracy} = \frac{\text{TP}}{n} \tag{6}$$

$$\text{Kappa} = \frac{pa - pr}{1 - pr} \tag{7}$$

$$\text{F1 Mean} = \frac{2\text{TP}}{2\text{TP} + \text{FN} + \text{FP}} \tag{8}$$

where TP stands for True Positive, FN for False Negative, FP for False Positive, pa is the probability of agreement defined by $pa = Overall Accuracy$ and pr the probability of random agreement defined by $pr = \sum_{c=1}^{C} \frac{TP_c}{FP_c} \frac{TP_c}{FN_c}$.

In order to compute these metrics, the predicted labels are needed and so we need to compute the decision function (Equation 5). Moreover to estimate this measures of good classification, a cross-validation method is used which reduces both bias and variance of the estimation.

2.2.2. Measures of similarity between distributions

The Kullback–Leibler divergence is a measure of distance between two distributions. It actually measures the amount of information lost when the first distribution is approximated by the second one. The formal definition is

$$\text{Div}_{KL}(c_i, c_j) = \int_{\mathbf{x}} p(\mathbf{x}|c_i) \ln(\frac{p(\mathbf{x}|c_i)}{p(\mathbf{x}|c_j)}) d\mathbf{x} \tag{9}$$

And in the case of Gaussian model, it can be rewritten as follows

$$\text{Div}_{KL}(c_i, c_j) = \frac{1}{2}\left(\text{Tr}(\boldsymbol{\Sigma}_{c_i}^{-1}\boldsymbol{\Sigma}_{c_j}) + (\boldsymbol{\mu}_{c_i} - \boldsymbol{\mu}_{c_i})^t \boldsymbol{\Sigma}_{c_i}^{-1}(\boldsymbol{\mu}_{c_i} - \boldsymbol{\mu}_{c_i}) - d + \log\left(\frac{|\boldsymbol{\Sigma}_{c_i}|}{|\boldsymbol{\Sigma}_{c_j}|}\right)\right) \tag{10}$$

where Tr is the trace operator and k the dimension of the distribution.

It can be noticed that the KL divergence is not symmetric and so the symmetrized version is used to compute the criterion function. In the case of Gaussian model, the symmetrization induces the following simplification of the formula

$$\begin{aligned}\text{SKL}_{ij} &= \text{Div}_{KL}(c_i, c_j) + \text{Div}_{KL}(c_j, c_i) \\ &= \frac{1}{2}\left(\text{Tr}(\boldsymbol{\Sigma}_{c_i}^{-1}\boldsymbol{\Sigma}_{c_j} + \boldsymbol{\Sigma}_{c_j}^{-1}\boldsymbol{\Sigma}_{c_i}) + (\boldsymbol{\mu}_{c_i} - \boldsymbol{\mu}_{c_i})^t(\boldsymbol{\Sigma}_{c_i}^{-1} + \boldsymbol{\Sigma}_{c_j}^{-1})(\boldsymbol{\mu}_{c_i} - \boldsymbol{\mu}_{c_i}) - 2d\right)\end{aligned} \tag{11}$$

Moreover, the divergence is computed between two classes and to obtain a unique value the weighted mean of divergence measures is taken

$$C_{SKL} = \sum_{i=1}^{C}\sum_{j=i+1}^{C} \pi_{c_i}\pi_{c_j}\text{SKL}_{ij} \tag{12}$$

The Bhattacharyya distance is an other measure of similarity between two distributions. In fact, we do not discuss the efficiency of this measure in our work and simply used it to compute the next measure. The Bhattacharyya distance is computed as follows

$$B_{ij} = -\ln\left(\int_{\mathbf{x}}\sqrt{p(\mathbf{x}|c_i)p(\mathbf{x}|c_j)}d\mathbf{x}\right) \tag{13}$$

And in the case of Gaussian model:

$$B_{ij} = \frac{1}{8}(\boldsymbol{\mu}_i - \boldsymbol{\mu}_j)^t\left(\frac{\boldsymbol{\Sigma}_i + \boldsymbol{\Sigma}_j}{2}\right)^{-1}(\boldsymbol{\mu}_i - \boldsymbol{\mu}_j) + \frac{1}{2}\ln\left(\frac{|\boldsymbol{\Sigma}_i + \boldsymbol{\Sigma}_j|}{\sqrt{|\boldsymbol{\Sigma}_i||\boldsymbol{\Sigma}_j|}}\right) \tag{14}$$

The Jeffries–Matusita distance is a measure based on the Bhattacharyya distance but transform in a way that the distance saturate if the separability between the two distribution increases. The JM distance is defined according to

$$\text{JM}_{ij} = \sqrt{\int_{\mathbf{x}}\left[\sqrt{p(\mathbf{x}|c_i)} - \sqrt{p(\mathbf{x}|c_j)}\right]^2 d\mathbf{x}} \tag{15}$$

And the Jeffries–Matusita distance can be rewritten according to the Bhattacharyya distance

$$\text{JM}_{ij} = \sqrt{2\{1 - \exp[-B_{ij}]\}} \tag{16}$$

As for the KL divergence, a weighted mean of the distance between two classes is computed to aggregate the measures in a single value.

According to [1], it is interesting to notice that the KL divergence increases quadratically with respect to the distance between the mean vectors of the class distributions whereas the measures of good classification we used asymptotically tends to one when distributions are perfectly separable. On the contrary, the JM distance tends to saturate as these measures of good classification.

3. Ridge Regularization

3.1. Principe of Ridge Regularization

As introduced in the previous section, the aim of a regularization method is to stabilize the inversion of the covariance matrix in the context of high dimensionality which often imply a ill-conditioned matrix. In particular, the Ridge regularization proposes to solve the problem in adding a small value τ to each eigenvalues of the covariance matrix. In our case, we choose to add the same constant to each eigenvalues but it is not compulsory in a general case.

Thus, to perform the regularization, the covariance matrix is decomposed with a diagonalization algorithm for symmetric matrices s.t. $\mathbf{\Sigma} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^t$ where $\mathbf{Q}$ is the matrix of eigenvectors and $\mathbf{\Lambda}$ is the diagonal matrix of eigenvalues. When the decomposition is available, the regularization almost finish and the decision function is simply rewritten as follow

$$Q_c(\mathbf{x}) = -(\mathbf{x} - \boldsymbol{\mu}_c)^t\mathbf{Q}_c(\mathbf{\Lambda}_c + \tau\mathbf{I})^{-1}\mathbf{Q}_c^t(\mathbf{x} - \boldsymbol{\mu}_c) - \log((2\pi)^d|\mathbf{\Sigma}_c + \tau\mathbf{I}|) + 2\log(\pi_c) \qquad (17)$$

where $\mathbf{I}$ is the identity matrix. It is to be noticed that $(\mathbf{\Lambda} + \tau\mathbf{I})$ is also a diagonal matrix and so the inverse is easily obtained in inverting each element of the matrix.

3.2. Implementation

The main steps of the training algorithm when using Ridge regularization are summarized in Algorithm 1. Indeed, before training the GMM model, a preliminary step is needed in order to determine a good value for the parameter τ and to do so, a gridsearch is performed with a set of values $\mathcal{P}$ given by the user. Moreover, to have a good estimation of the quality of the classification with a given τ a cross-validation method is used. Thus, the training set is divided in k folds, then, the training is done with $(k-1)$ folds and the performances are estimated with the remaining fold.

A particularity of this regularization method is used to accelerate the gridsearch. More precisely, the two computationally costly step are the computation of the inverse and the determinant of the regularized covariance matrices and it is important to see that these operations can be performed only once to test all τ. The covariance matrix is diagonalized before selecting τ and the eigenvalues and eigenvectors are stored and used to test all τ using Equation 17.

Algorithm 1 Ridge Regularization training steps

Require: $\mathcal{S}, k, \mathcal{P}$

  1: Randomly cut $\mathcal{S}$ in k subsets such as $\mathcal{S}_1 \cup ... \cup \mathcal{S}_k = \mathcal{S}$ and $\mathcal{S}_i \cap \mathcal{S}_j = \varnothing$

  2: **for all** $\mathcal{S}_i$ **do**

  3:     Learn GMM with $\mathcal{S} \setminus \mathcal{S}_i$

  4:     Compute decomposition of covariance matrices of each classes s.t. $\mathbf{\Sigma}_c = \mathbf{Q}_c\mathbf{\Lambda}_c\mathbf{Q}_c^t$

  5:     **for all** $\tau \in \mathcal{P}$ **do**

  6:         Estimate classification rate on $\mathcal{S}_i$ using Equation 17

  7:     **end for**

  8: **end for**

  9: Average the classification rate over the k folds

10: Compute $\arg\max_\tau$ of the classification rates to get the best parameter τ^*

11: Learn GMM with the whole training set $\mathcal{S}$ and parametrize the GMM with τ^*

Finally, another trick could used to optimize the gridsearch. As explained in the next section, it is possible to avoid the learning step on the $(k-1)$ fold and instead learn the model with the whole dataset and deduce the submodel used for cross-validation from the complete model and the mean vector and covariance matrix of the kth fold.

As stated before, we choose to implement a basic Ridge regression method and only the small improvement explained herebefore as been proposed. To the contrary, we choose in our study to focus more on a feature selection method named sequential forward features selection described in following section.

4. Features selection

We remains that the aim of feature selection method is to select a subset of variables to described each samples and so to get rid of high dimensionality and its curse. It is also important to underline that the proposed method is a *selection* method and not an *extraction* method. It means the subset of variables obtained at the end is composed of actual variables of the original set and not variables built as combination of several others as it is the case for example with PCA. This choice is made to assure an easier interpretation by the user of the obtained subset of variables.

Two selection algorithms are presented the sequential forward features selection method (Section 4.1) and the sequential floating forward feature selection method (4.2) the second being a more complex variation of the first.

4.1. Sequential forward features selection

The Sequential Forward Selection (SFS) starts with an empty set of selected features. Then it tests at each step for all the remaining features the value of a criterion function J chosen by the user among the ones presented in Section 2.2 when the feature is added to the pool of selected features. The feature that maximizes the criterion function is definitively added to the pool of selected features and it moves to the next iteration. The choice of the criterion function is discussed afterward in Section 2.2. The algorithm stops when a given number of variables maxVar has been selected.

To summarize, the features are selected one by one and the set of selected features are never put into questions. It results in a reasonable computational time but a suboptimal solution to the selection problem.

Algorithm 2 Sequential forward features selection

Require: $\mathcal{S}, J, \text{maxVar}$
1: $S = \varnothing$
2: $F = \{\text{all variables}\}$
3: **while** Repeat till S contained maxVar variables **do**
4:     **for all** $f_i \in F$ **do**
5:         $R_i = J(\{S + f_i\})$
6:     **end for**
7:     $j = \arg\max_i R_i$
8:     $S = \{S + f_j\}$
9:     $F = F \setminus f_j$
10: **end while**
11: **return** S

4.2. Sequential floating forward feature selection

The Sequential Floating Forward Selection (SFFS) is actually based on two algorithms: the SFS described above and the Sequential Backward Selection (SBS). The SBS is the backward equivalent of SFS. The difference is that it starts with every features in the pool of selected features and tries at each step to remove the less significant one in term of the given criterion function.

The SFFS works as the SFS but between each step of the SFS algorithm a backward selection is operated. At the end of the SBS step, the value of the criterion function is compared to the best value ever obtained with a set of features of the same size and if the new value is better the feature puts into question is effectively taken away and the next step is again a SBS but if the new value is not better the SBS step is forgotten and it moves to the next SFS step. The algorithm stops when a given number of features has been selected.

This SFFS algorithm eventually tests more solutions than the SFS algorithm. The results are expected to be better but the trade-off is an increased computational time which is dependent of the complexity of the dataset.

Algorithm 3 Sequential floating forward features selection

Require: $\mathcal{S}, J, \text{maxVar}$
 1: $S = \varnothing$
 2: $F = \{\text{all variables}\}$
 3: $k = 0$
 4: **while** Repeat till S contained maxVar variables **do**
 5:     **for all** $f_i \in F$ **do**
 6:         $R_i = J(\{S(k) + f_i\})$
 7:     **end for**
 8:     $j = \arg\max_i R_i$
 9:     **if** $R_j \geq J(S^{(k+1)})$ **then**
10:         $k = k + 1$
11:     **else**
12:         $S^{(k+1)} = \{S(k) + f_i\}$
13:         $k = k + 1$
14:         $\text{flag} = 1$
15:         **while** $k > 2$ and flag $= 1$ **do**
16:             **for all** $f_i \in S^{(k)}$ **do**
17:                 $R_i = J(\{S(k) \setminus f_i\})$
18:             **end for**
19:             $j = \arg\max_i R_i$
20:             **if** $R_j < J(S^{(k-1)})$ **then**
21:                 $S^{(k-1)} = \{S(k) \setminus f_i\}$
22:                 $k = k - 1$
23:             **else**
24:                 $\text{flag} = 0$
25:             **end if**
26:         **end while**
27:     **end if**
28: **end while**
29: **return** S

4.3. Implementation

In term of computational efficiency, the main issue is to find an efficient way to compute the mean vector and the covariance matrix and its inverse and to do it only when it is absolutely necessary. More specifically, we develop an optimized way to derive the submodel for cross-validation from the full model and we minimize the number of costly operations during a step of the selection algorithm.

4.3.1. Update for cross validation

Based on [2], a method to accelerate the k-fold cross-validation process in the case of criterion functions based on correct classification measures was implemented. The idea is to estimate the GMM model with the whole training set and then, instead of training a model on $(k-1)$ folds, the complete model and the mean vector and the covariance matrix of the kth fold is used to derive the corresponding submodel.

The following formulae can be obtained (details of calculation in Appendix A)

$$\boldsymbol{\mu}_c^{n_c-\nu_c} = \frac{n_c\boldsymbol{\mu}_c^{n_c} - \nu_c\boldsymbol{\mu}_c^{\nu_c}}{n_c - \nu_c} \tag{18}$$

$$\boldsymbol{\Sigma}_c^{n_c-\nu_c} = \frac{1}{n_c - \nu_c - 1}\left((n_c-1)\boldsymbol{\Sigma}_c^{n_c} - (\nu_c-1)\boldsymbol{\Sigma}_c^{\nu_c} - \frac{n_c\nu_c}{(n_c-\nu_c)}(\boldsymbol{\mu}_c^{\nu_c}-\boldsymbol{\mu}_c^{n_c})(\boldsymbol{\mu}_c^{\nu_c}-\boldsymbol{\mu}_c^{n_c})^t\right) \tag{19}$$

where ν_c is the number of samples of class c removed from the set.

Additionally, the update of the GMM model is the occasion to precompute and store the constant $2\log(\pi_c)$ which is a term of the decision function constant for a given training set.

4.3.2. Criterion function computation

As explained earlier, at each iteration the SFS and SFFS algorithms compute the value of a criterion function for every possible set of features composed of the selected ones augmented by one of the remaining features. One of the main achievements of this work is to reduce the computational time needed to compute the criterion function of augmented sets.

We note $\boldsymbol{\Sigma}^{(k-1)}$ the covariance matrix of the $k-1^{th}$ iteration, i.e., the covariance of the selected features and $\boldsymbol{\Sigma}^{(k)}$ the covariance matrix of the kth iteration, i.e., the covariance of the augmented set. Then, the inverse of the covariance matrix $(\boldsymbol{\Sigma}^{(k)})^{-1}$, the quadratical term $(\mathbf{x}^{(k)})^t(\boldsymbol{\Sigma}^{(k)})^{-1}\mathbf{x}^{(k)}$ and the determinant $\log|\boldsymbol{\Sigma}^{(k)}|$ can be expressed in function of terms of the $(k-1)^{th}$ iteration. These calculi use the fact that the covariance matrix is a positive definite symmetric matrix to simplify formulae using matrices defined by blocks. These update rules are summed up hereafter and are available in [3] (chapter 9.2).

As $\boldsymbol{\Sigma}^{(k)}$ is a positive definite symmetric matrix, we can use the following notation

$$\boldsymbol{\Sigma}^{(k)} = \left[\begin{array}{cc} \boldsymbol{\Sigma}^{(k-1)} & \mathbf{u} \\ \mathbf{u}^t & \sigma_{kk} \end{array}\right]$$

where $\mathbf{u}$ is the kth column of the matrix without the diagonal element i.e. $\mathbf{u}_i = \boldsymbol{\Sigma}_{i+1,k}^{(k)}$ with $i \in [1, k-1]$.

Using the formula of the inverse of a block matrix, the following formula expressing $(\boldsymbol{\Sigma}^{(k)})^{-1}$ in function of $(\boldsymbol{\Sigma}^{(k-1)})^{-1}$ is obtained

$$\boxed{(\boldsymbol{\Sigma}^{(k)})^{-1} = \left[\begin{array}{cc} (\boldsymbol{\Sigma}^{(k-1)})^{-1} + \frac{1}{\alpha}(\boldsymbol{\Sigma}^{(k-1)})^{-1}\mathbf{u}\mathbf{u}^t(\boldsymbol{\Sigma}^{(k-1)})^{-1} & -\frac{1}{\alpha}(\boldsymbol{\Sigma}^{(k-1)})^{-1}\mathbf{u} \\ -\frac{1}{\alpha}\mathbf{u}^t(\boldsymbol{\Sigma}^{(k-1)})^{-1} & \frac{1}{\alpha} \end{array}\right]} \tag{20}$$

where $\alpha = \sigma_{kk} - \mathbf{u}^t(\boldsymbol{\Sigma}^{(k-1)})^{-1}\mathbf{u}$.

In the case of a backward step in SFFS algorithm, we need to invert the formula in order to compute $(\boldsymbol{\Sigma}^{(k-1)})^{-1}$ knowing $(\boldsymbol{\Sigma}^{(k)})^{-1}$. Then, if we use the following notation for the previous matrix

$$(\boldsymbol{\Sigma}^{(k)})^{-1} = \left[\begin{array}{cc} \mathbf{A} & \mathbf{v} \\ \mathbf{v}^t & \frac{1}{\alpha} \end{array}\right]$$

with $\mathbf{A} = (\boldsymbol{\Sigma}^{(k-1)})^{-1} + \frac{1}{\alpha}(\boldsymbol{\Sigma}^{(k-1)})^{-1}\mathbf{u}\mathbf{u}^t(\boldsymbol{\Sigma}^{(k-1)})^{-1}$ and $\mathbf{v} = -\frac{1}{\alpha}(\boldsymbol{\Sigma}^{(k-1)})^{-1}\mathbf{u}$, we can calculate

$$\mathbf{A} - \alpha\mathbf{v}\mathbf{v}^t = (\boldsymbol{\Sigma}^{(k-1)})^{-1} + \frac{1}{\alpha}(\boldsymbol{\Sigma}^{(k-1)})^{-1}\mathbf{u}\mathbf{u}^t(\boldsymbol{\Sigma}^{(k-1)})^{-1} - \alpha(-\frac{1}{\alpha}(\boldsymbol{\Sigma}^{(k-1)})^{-1}\mathbf{u})(-\frac{1}{\alpha}\mathbf{u}^t(\boldsymbol{\Sigma}^{(k-1)})^{-1}))$$

$$= (\boldsymbol{\Sigma}^{(k-1)})^{-1}$$

$$\boxed{(\boldsymbol{\Sigma}^{(k-1)})^{-1} = \mathbf{A} - \alpha\mathbf{v}\mathbf{v}^t} \tag{21}$$

A formula can also be deduced for the quadratical term of the decision function. If we note $(\mathbf{x}^{(k)})^t = \begin{bmatrix} (\mathbf{x}^{(k-1)})^t & x^{(}k) \end{bmatrix}$,

$$(\mathbf{x}^{(k)})^t(\boldsymbol{\Sigma}^{(k)})^{-1}\mathbf{x}^{(k)} = \begin{bmatrix} (\mathbf{x}^{(k-1)})^t & x_k \end{bmatrix} \begin{bmatrix} \mathbf{A} & \mathbf{v} \\ \mathbf{v}^t & \frac{1}{\alpha} \end{bmatrix} \begin{bmatrix} \mathbf{v} \\ x_k \end{bmatrix}$$

$$= \begin{bmatrix} (\mathbf{x}^{(k-1)})^t\mathbf{A} + x_k\mathbf{v}^t & (\mathbf{x}^{(k-1)})^t\mathbf{v} + \frac{x_k}{\alpha} \end{bmatrix} \begin{bmatrix} \mathbf{v} \\ x_k \end{bmatrix}$$

$$= (\mathbf{x}^{(k-1)})^t\mathbf{A}\mathbf{x}^{(k-1)} + x_k\mathbf{v}^t\mathbf{x}^{(k-1)} + (\mathbf{x}^{(k-1)})^t\mathbf{v}x_k + \frac{(x_k)^2}{\alpha}$$

$$= (\mathbf{x}^{(k-1)})^t((\boldsymbol{\Sigma}^{(k-1)})^{-1} + \frac{1}{\alpha}(\boldsymbol{\Sigma}^{(k-1)})^{-1}\mathbf{u}\mathbf{u}^t(\boldsymbol{\Sigma}^{(k-1)})^{-1})\mathbf{x}^{(k-1)} + 2x_k\mathbf{v}^t\mathbf{x}^{(k-1)} + \frac{(x_k)^2}{\alpha}$$

$$= (\mathbf{x}^{(k-1)})^t((\boldsymbol{\Sigma}^{(k-1)})^{-1} + \alpha\mathbf{v}\mathbf{v}^t)\mathbf{x}^{(k-1)} + 2x_k\mathbf{v}^t\mathbf{x}^{(k-1)} + \frac{(x_k)^2}{\alpha}$$

$$= (\mathbf{x}^{(k-1)})^t(\boldsymbol{\Sigma}^{(k-1)})^{-1}\mathbf{x}^{(k-1)} + \alpha((\mathbf{x}^{(k-1)})^t\mathbf{v}\mathbf{v}^t\mathbf{x}^{(k-1)} + 2\frac{x_k}{\alpha}\mathbf{v}^t\mathbf{x}^{(k-1)} + \frac{(x_k)^2}{\alpha^2})$$

$$= (\mathbf{x}^{(k-1)})^t(\boldsymbol{\Sigma}^{(k-1)})^{-1}\mathbf{x}^{(k-1)} + \alpha((\mathbf{x}^{(k-1)})^t\mathbf{v} + \frac{x_k}{\alpha})^2$$

$$= (\mathbf{x}^{(k-1)})^t(\boldsymbol{\Sigma}^{(k-1)})^{-1}\mathbf{x}^{(k-1)} + \alpha(\begin{bmatrix} \mathbf{v}^t & \frac{1}{\alpha} \end{bmatrix}\mathbf{x}^{(k)})^2$$

$$\boxed{(\mathbf{x}^{(k)})^t(\boldsymbol{\Sigma}^{(k)})^{-1}\mathbf{x}^{(k)} = (\mathbf{x}^{(k-1)})^t(\boldsymbol{\Sigma}^{(k-1)})^{-1}\mathbf{x}^{(k-1)} + \alpha(\begin{bmatrix} \mathbf{v}^t & \frac{1}{\alpha} \end{bmatrix}\mathbf{x}^{(k)})^2} \tag{22}$$

Finally, using the formula of the determinant of a block matrix and after taking the log, we obtain

$$\boxed{\log\left(|\boldsymbol{\Sigma}^{(k)}|\right) = \log\left(|\boldsymbol{\Sigma}^{(k-1)}|\right) + \log\alpha} \tag{23}$$

To give an example, if a measure of good classification is used, we need to compute the decision rule and with the update rules, it can be rewritten as follow

$$Q(\mathbf{x}) = -(\mathbf{x}^{(k-1)} - \boldsymbol{\mu}^{(k-1)})^t(\boldsymbol{\Sigma}^{(k-1)})^{-1}(\mathbf{x}^{(k-1)} - \boldsymbol{\mu}^{(k-1)})$$
$$+ \alpha(\begin{bmatrix} \mathbf{v}^t & \frac{1}{\alpha} \end{bmatrix}(\mathbf{x}^{(}k) - \boldsymbol{\mu}^{(k)}))^2$$
$$- \log\left(|\boldsymbol{\Sigma}^{(k-1)}|\right) + \log\alpha + 2\log(\pi)$$

It can be noticed that this new formula allow us to precompute the computationally heavy terms because they are the same for all possible augmented sets at a given iteration of the selection. The Figure 2 illustrates the optimization of the selection algorithm.

Nevertheless, during an iteration of the selection algorithm, it still needs to invert the covariance matrix of the previous iteration. In order to so, we choose to perform a decomposition in eigenvalues and eigenvectors using algorithm specific for symmetric matrices. In other words, we find $\boldsymbol{\Lambda}$ the diagonal matrix of eigenvalues and $\mathbf{Q}$ the matrix of eigenvectors s.t. $\boldsymbol{\Sigma} = \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^t$.

This decomposition has several advantages. First, it is very simple to compute the determinant once the eigenvalues are available because the determinant is equal to the product of these values.
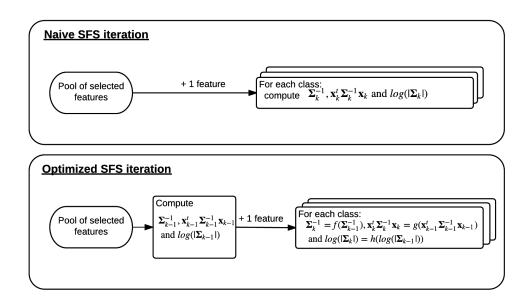
Naive SFS iteration

Pool of selected features — + 1 feature → For each class: compute $\boldsymbol{\Sigma}_k^{-1}$, $\mathbf{x}_k^t \boldsymbol{\Sigma}_k^{-1} \mathbf{x}_k$ and $log(|\boldsymbol{\Sigma}_k|)$

Optimized SFS iteration

Pool of selected features → Compute $\boldsymbol{\Sigma}_{k-1}^{-1}$, $\mathbf{x}_{k-1}^t \boldsymbol{\Sigma}_{k-1}^{-1} \mathbf{x}_{k-1}$ and $log(|\boldsymbol{\Sigma}_{k-1}|)$ — + 1 feature → For each class: $\boldsymbol{\Sigma}_k^{-1} = f(\boldsymbol{\Sigma}_{k-1}^{-1})$, $\mathbf{x}_k^t \boldsymbol{\Sigma}_k^{-1} \mathbf{x}_k = g(\mathbf{x}_{k-1}^t \boldsymbol{\Sigma}_{k-1}^{-1} \mathbf{x}_{k-1})$ and $log(|\boldsymbol{\Sigma}_k|) = h(log(|\boldsymbol{\Sigma}_{k-1}|))$

Figure 2: Iteration of sequential forward features selection.

Secondly, it is possible to check the eigenvalues and so to assure a better computational stability. Due to the curse of dimensionality, the covariance matrix is sometimes ill-estimated and the results is that some eigenvalues are really small (below computational precision) and the decomposition helps us to check their actual values and if they are below EPS_FLT which the machine maximum precision for a float, we set these eigenvalues to EPS_FLT.

A. Update for cross validation (calculation)

A.1. Mean update

$$\boldsymbol{\mu}_c^{n_c} = \frac{1}{n_c} \sum_{j=1}^{n_c} \mathbf{x}_j$$

$$= \frac{1}{n_c} \sum_{j=1}^{n_c-v_c} \mathbf{x}_j + \frac{1}{n_c} \sum_{j=n_c-v_c+1}^{n_c} \mathbf{x}_j$$

$$= \frac{n_c - v_c}{n_c} \boldsymbol{\mu}_c^{n_c-v_c} + \frac{v_c}{n_c} \boldsymbol{\mu}_c^{v_c}$$

$$= \boldsymbol{\mu}_c^{n_c-v_c} + \frac{v_c}{n_c} (\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})$$

$$\boxed{\boldsymbol{\mu}_c^{n_c} = \boldsymbol{\mu}_c^{n_c-v_c} + \frac{v_c}{n_c} (\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})} \tag{24}$$

$$\boxed{\boldsymbol{\mu}_c^{n_c-v_c} = \frac{n_c \boldsymbol{\mu}_c^{n_c} - v_c \boldsymbol{\mu}_c^{v_c}}{n_c - v_c}} \tag{25}$$

A.2. Covariance matrix update

$$\boldsymbol{\Sigma}_c^{n_c} = \frac{1}{n_c - 1} \sum_{j=1}^{n_c} (\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c})(\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c})^t$$

$$= \frac{1}{n_c - 1} \sum_{j=1}^{n_c} (\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c} - \frac{v_c}{n_c}(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c}))(\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c} - \frac{v_c}{n_c}(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c}))^t$$

$$= \frac{1}{n_c - 1} \sum_{j=1}^{n_c} (\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})(\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})^t$$

$$+ \frac{v_c^2}{n_c^2} (\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})^t$$

$$- \frac{v_c}{n_c} (\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})^t$$

$$- \frac{v_c}{n_c} (\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})(\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})^t$$

- $(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})^t = \frac{n_c^2}{(n_c-v_c)^2} (\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})^t$

- $\frac{1}{n_c} \sum_{j=1}^{n_c} (\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})^t = \frac{n_c v_c}{(n_c-v_c)^2} (\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})^t$

- $\frac{1}{n_c} \sum_{j=1}^{n_c} (\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})(\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})^t = \frac{n_c v_c}{(n_c-v_c)^2} (\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})^t$

$$\mathbf{\Sigma}_c^{n_c} = \frac{1}{n_c - 1} \sum_{j=1}^{n_c} (\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})(\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})^t - \frac{v_c^2}{(n_c - v_c)^2}(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})^t$$

$$= \frac{1}{n_c - 1} \sum_{j=1}^{n_c-v_c} (\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})(\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})^t + \frac{1}{n_c - 1} \sum_{j=n_c-v_c+1}^{n_c} (\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})(\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})^t$$

$$- \frac{n_c v_c^2}{(n_c-1)(n_c-v_c)^2}(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})^t$$

$$= \frac{n_c - v_c - 1}{n_c - 1}\mathbf{\Sigma}_c^{n_c-v_c} + \frac{1}{n_c - 1} \sum_{j=n_c-v_c+1}^{n_c} (\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})(\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})^t$$

$$- \frac{n_c v_c^2}{(n_c-1)(n_c-v_c)^2}(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})^t$$

$$\sum_{j=n_c-v_c+1}^{n_c} (\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})(\mathbf{x}_j - \boldsymbol{\mu}_c^{n_c-v_c})^t = \sum_{j=n_c-v_c+1}^{n_c} (\mathbf{x}_j - \boldsymbol{\mu}_c^{v_c} + \boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})(\mathbf{x}_j - \boldsymbol{\mu}_c^{v_c} + \boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})^t$$

$$= (v_c - 1)\mathbf{\Sigma}_c^{v_c} + v_c(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})^t$$

$$+ \sum_{j=n_c-v_c+1}^{n_c} (\mathbf{x}_j - \boldsymbol{\mu}_c^{v_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})^t$$

$$+ \sum_{j=n_c-v_c+1}^{n_c} (\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c-v_c})(\mathbf{x}_j - \boldsymbol{\mu}_c^{v_c})^t$$

$$= (v_c - 1)\mathbf{\Sigma}_c^{v_c} + \frac{n_c^2 v_c}{(n_c - v_c)^2}(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})^t$$

$$\boxed{\mathbf{\Sigma}_c^{n_c} = \frac{n_c-v_c-1}{n_c-1}\mathbf{\Sigma}_c^{n_c-v_c} + \frac{v_c-1}{n_c-1}\mathbf{\Sigma}_c^{v_c} + \frac{n_c v_c}{(n_c-1)(n_c-v_c)}(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})^t} \tag{26}$$

$$\boxed{\mathbf{\Sigma}_c^{n_c-v_c} = \frac{1}{n_c-v_c-1}\left((n_c - 1)\mathbf{\Sigma}_c^{n_c} - (v_c - 1)\mathbf{\Sigma}_c^{v_c} - \frac{n_c v_c}{(n_c-v_c)}(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})(\boldsymbol{\mu}_c^{v_c} - \boldsymbol{\mu}_c^{n_c})^t\right)} \tag{27}$$

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