

On Designing Invertible Pseudo Covariance Matrix for Undersampled Cases in Classification

ABSTRACT

In linear discriminant analysis, determinant and inverse of the covariance matrix are required to be computed. If number of features is greater than the number of available examples, covariance matrix is no longer invertible. A common approach is to reduce dimensionality due to which some features of interest may be lost. When we are not interested in dimensionality reduction, one approach to solve such problems is to take pseudoinverse of covariance matrix which is not always possible. We propose, in such cases, to project covariance matrix onto a highly correlated space to compute pseudoinverse of the matrix. Proposed solution has been tested for classification of microarray gene expression data of colon's tumor.

Keywords: Covariance matrix, dimensionality reduction, pseudoinverse

1. INTRODUCTION

1.1. Technical background

Let $\mathbf{x}_i$ be data points or collection of observations such that $\mathbf{x}_i \in \mathbb{R}^d$ for $1 \leq i \leq n$ and $i \in \mathbb{N}$, where $\mathbb{R}$ is a set of real numbers and number of data points be n . Therefore, $\mathbb{R}^{d \times n}$ is our sample space. In classification, a pattern is a pair of variables $\{\mathbf{x}_i, \mathbf{w}_i\}$ where $\mathbf{w}_i$ is the concept behind the observation. The task is to discriminate examples from different classes with respect to $\mathbf{w}_i$. Examples from the same class should have similar $\mathbf{w}_i$ while examples from different classes have different $\mathbf{w}_i$. The minimum-error-rate classification can be achieved by use of following discriminant functions:

$$g_i(\mathbf{x}) = \ln p(\mathbf{x}|\mathbf{w}_i) + \ln P(\mathbf{w}_i) \quad (1)$$

If $p(\mathbf{x}|\mathbf{w}_i) \sim \mathcal{N}(\mu_i, \Sigma_i)$, we have

$$g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x} - \mu_i)^T \Sigma_i^{-1}(\mathbf{x} - \mu_i) - \frac{d}{2} \ln 2\pi - \frac{1}{2} \ln |\Sigma_i| + \ln P(\mathbf{w}_i) \quad (2)$$

The covariance matrix Σ is always symmetric and positive semi-definite. In the following, we discuss the general case when Σ_i is arbitrary.

In a general multivariate normal case, covariance matrices are different for each category. The only term that can be dropped from Eq. 2 is the $-\frac{d}{2} \ln(2\pi)$ term, and the resulting discriminant functions are inherently quadratic.

$$g_i(\mathbf{x}) = \mathbf{x}^T \mathbf{W}_i \mathbf{x} + \mathbf{w}_i^T \mathbf{x} + w_{i0} \quad (3)$$

28 Where

$$29 \quad W_i = -\frac{1}{2} \Sigma_i^{-1}$$

$$30 \quad w_i = \Sigma_i^{-1} \mu_i$$

31 and

$$32 \quad w_{i0} = -\frac{1}{2} \mu_i^T \Sigma_i^{-1} \mu_i - \frac{1}{2} \ln |\Sigma_i| + \ln P(w_i)$$

33 This shows that computing inverse of covariance matrix (i.e., Σ^{-1}) is essential in discriminant analysis. In
34 this situation, two types of problems arise when relationship between n and d is considered.

- 35 • Case 1 ($n \geq d$): When number of available samples (n -samples) is equal to or greater than the
36 number of dimensions (d -dimensions), the computation of Σ^{-1} is trivial.
- 37 • Case 2 ($n < d$): In most of practical problems (e.g., classification of cardiac signal or detection of
38 tumor from microarray gene expression data), d is large such that $d \gg n$. Such problems are
39 known as undersampled problems (Krzanowski et al., 1995).

40 There are three common approaches to solve these problems when n is smaller than d .

- 41 • Dimensionality reduction is applied such that $d < n$, where d is number of dimensions in reduced
42 space. However, it is possible that some useful features may lose.
- 43 • Eigen values are translated such as none of eigen values is zero. This reshapes the system matrix.
- 44 • Computing pseudoinverse of Σ which is not always possible.

45 In this paper, we propose a solution to problem when Σ does not exist and dimensionality reduction and
46 reshaping the system matrix are to be avoided. The related work is presented in Section 2. The proposed
47 methodology is described in Section 3. Results and discussion are presented in Section 4. Finally, the
48 paper is concluded in Section 5.

49

50 1.2. Related work

51 There are many algorithms developed so far to tackle undersampled problems (Akguna, 2016; Friedman,
52 1986; Yang, 2001; Yuen, 2003; Bensmail, 1995; Baudat, 2000; Raudys, 1998; Hastie, 1995; Howlan,
53 2004; Belhumeur, 1997). Most of the methods are proposed in the context of scatter matrix in classical
54 linear discriminant analysis (LDA). This is because to perform discriminant analysis, the scatter matrix
55 must be non-singular. Depending on nature of pre-processing of scatter matrix, the proposed methods
56 can broadly be categorized in two categories: dimensionality reduction (DR) and matrix transformation

(MT). The DR techniques are applied to reduce the dimensionality such that the features vectors have dimensions smaller than the number of samples. For instance in (Belhumeur, 1997; Swets, 1996; Zhao, 1999), PCA is used and orthogonalization is applied in (Zheng, 2004a; Zheng, 2004b) for reducing the dimensionality. Afterwards, LDA is applied for classification. DR is useful when we have to classify over the dominant features. However, in cases like classification of ventricle diseases using electrocardiogram waveforms or classification of cancerous genes using microarray data, classification may not be carried out using dominant features. Therefore, DR may not be helpful. In this situation, MT techniques can be used to make the scatter matrix invertible. The most notable examples of these techniques include regularized LDA (RLDA) (Friedman, 1986; Sullivan, 1986; Titterington, 1981), penalized LDA (PLDA) (Hastie et al., 1995), pseudo-inverse LDA (Raudys and Duin, 1998) and shrinkage LDA (SLDA) (Cornfield, 1967). In RLDA, all the eigen values of the scatter matrix are given a scalar, constant and equal shift. This replaces zero eigen values with some positive real value. This shift in eigen values makes the scatter matrix invertible (Friedman, 1986). This regularization minimizes within-class variance at the cost of bias. Therefore, we have to play with parameters(s) for optimal tradeoff between variance and bias. In penalized LDA, all values of within class scatter matrix are given a positive scalar shift, i.e., we use $\Sigma + \Omega$ where Σ is a within class scatter matrix and Ω the shift matrix. If $\Omega = \mu I$ for some constant μ and I as identity matrix, penalized LDA converges to the regularized LDA. Therefore, penalized LDA is more general as compared to regularized LDA. A problem with this technique is that there is no single algorithm (Ω) for any set of applications (Hastie, 1995). When the scatter matrix is singular, sometimes its pseudo-inverse is possible. Therefore, we consider pseudo-inverse of the scatter matrix in place of its inverse. The technique is referred as pseudo-inverse LDA. However, pseudo-inverse is not possible when numerical values are very small during computations. Pseudo-inverse is an estimate of the inverse of the matrix using least square estimation (Fukunaga, 1990; Raudys and Duin, 1998). Effect of the sample size and dimension on classification error was studied in (Krzanowski, 1995). Performance of this technique is comparable to PCA + LDA and RLDA (Skurichina and Duin, 1996).

2. METHODOLOGY

Let $\Sigma_b \in \mathbb{R}^{N \times N}$ be a space onto which Σ is projected. We consider that Σ_b is an ideal covariance matrix which is drifted by the covariance matrix of the system, i.e., Σ . We define $\tilde{\Sigma}$ such that it is a projection of Σ on Σ_b .

$$\tilde{\Sigma} = \Sigma \Sigma_b \quad (4)$$

Matrix $\tilde{\Sigma}$ represents a situation (space) between ideal space and real space and possesses all the properties of Σ , like symmetry, Hermitian etc. Some properties of Σ_b are given below.

2.1. Inverse

Let Σ_b be a matrix of size $n \times n$, as it is a symmetric Hermitian matrix, its inverse is computed as follows: Consider that $\mu_d, \gamma_d, d_d \in \mathbb{R}$, where d is the dimensionality and $d \in \mathcal{D}$. Usually, matrix inversion is a computationally heavy task; we have derived simple expressions for its computation.

$$\mu_d = -\beta(\alpha - \beta)^{d-2} \quad (5)$$

$$\gamma_d = (\alpha - \beta)^{d-1} - (d - 1)\mu_d \quad (6)$$

$$\tau_d = \mu_d + \beta(d - 1)\mu_d \quad (7)$$

This τ_d is the determinant of Σ_b .

$$\Sigma_b^{-1} = \frac{1}{\tau_d} [\mu_d \mathbf{O}_d + (\gamma_d - \mu_d) \mathbf{I}_d] \quad (8)$$

where $\mathbf{O}_d$ is defined as a matrix of size $d \times d$ with all elements as 1, and $\mathbf{I}_d$ is an identity matrix of the same size.

2.2. Eigenvalues of Σ_b

We have found that the largest eigenvalue of Σ_b is:

$$\lambda_{\max} = \alpha + (d - 1)\beta \quad (9)$$

Other eigenvalues are:

$$\lambda_i = \alpha - \beta \quad (10)$$

for $i = 2, 3, \dots, D$.

2.3. Eigenvalues of Σ_b^{-1}

As eigenvalues of Σ_b^{-1} are inverse of eigenvalues of Σ_b . Therefore, minimum eigenvalue is:

$$\hat{\lambda}_{\min} = \frac{1}{\alpha + (d - 1)\beta} \quad (11)$$

and other $(d - 1)$ eigenvalues are:

$$\hat{\lambda}_i = \frac{1}{\alpha - \beta} \quad (12)$$

for $i = 2, 3, \dots, D$.

2.4. Eigen Value Decomposition of Σ_b

117 Consider that:

$$118 \quad \Sigma_b = U_b \Lambda_b V_b^T \quad (13)$$

119

120 Λ_b is given by:

$$121 \quad \Lambda_b = \begin{pmatrix} \alpha + (d-1)\beta & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \alpha - \beta \end{pmatrix} \quad (14)$$

122 We have found U_b as:

$$123 \quad U_b = \begin{pmatrix} -\frac{1}{\Delta_1} & -\frac{1}{\Delta_2} & \cdots & 0 & 0 \\ \frac{1}{\Delta_1} & \frac{1}{(d-1)\Delta_2} & \cdots & 0 & 0 \\ -\frac{1}{\Delta_1} & -\frac{1}{(d-1)\Delta_2} & \ddots & \vdots & \\ -\frac{1}{\Delta_1} & \frac{1}{(d-1)\Delta_2} & \cdots & -\frac{1}{\Delta_{d-1}} & 0 \\ \frac{1}{\Delta_1} & \frac{1}{(d-1)\Delta_2} & \cdots & \frac{1}{\Delta_{d-1}} & 1 \\ -\frac{1}{\Delta_1} & -\frac{1}{(d-1)\Delta_2} & \cdots & -\frac{1}{2\Delta_{d-1}} & \frac{1}{\Delta_d} \end{pmatrix} \quad (15)$$

124

$$125 \quad \Delta_1 = \sqrt{d}$$

126

127 and

$$128 \quad \Delta_k = \sqrt{1 + \frac{1}{d-k+1}} \quad (16)$$

129 for $k = 2, 3, \dots, D$.

130 First column of U_b is an eigenvector corresponding to the largest eigenvalue of Σ_b . Matrix V_b is
131 computed as:

132

$$133 \quad V_b = U_b \quad (17)$$

134 **2.5. Eigen Value Decomposition of Σ_h^{-1}**

$$135 \quad \Sigma_b^{-1} = (U_b \Lambda_b V_b^T)^{-1} \quad (18)$$

136

$$= U_b \Lambda_b^{-1} V_b^T \quad (19)$$

138 The matrix Λ_b^{-1} is a diagonal matrix with eigenvalues of Σ_b^{-1} on its diagonal.

139 2.6. Pseudo Inverse of Σ

140 Let us consider that

$$\Sigma = U \Lambda V^T \quad (20)$$

$$\Sigma_b = U_b \Lambda_b V_b^T \quad (21)$$

143 And

$$\begin{aligned} \Sigma &= \Sigma \Sigma_b \\ &= U (\Lambda V^T U_b \Lambda_b) V_b^T \end{aligned} \quad (22)$$

$$= U \hat{\Lambda} V_b^T \quad (23)$$

$$\hat{\Lambda} = \Lambda V^T U_b \Lambda_b \quad (24)$$

148 We have found that under the assumption of $U = U_b$ and $V = V_b$:

$$V^T U_b = I \quad (25)$$

$$\hat{\Lambda} = \Lambda \Lambda_b \quad (26)$$

$$\hat{\Lambda}^{-1} = \Lambda_b^{-1} \Lambda^{-1} \quad (27)$$

152 Therefore

$$\hat{\Sigma}^\dagger = U_b \hat{\Lambda}^{-1} V_b^T \quad (28)$$

154 Where $\Sigma^\dagger$ represents the pseudoinverse of Σ .

155 2.7. Density Function in the Projected Space

156 The general expression for multivariate normal density in d-dimensions, in the projected space is as
157 follows:

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{\frac{d}{2}} |\hat{\Sigma}|^{\frac{1}{2}}} e^{[-\frac{1}{2}(\mathbf{x}-\mu)^T \hat{\Sigma}^\dagger (\mathbf{x}-\mu)]} \quad (29)$$

158

159 Or simply $p(\mathbf{x}) \sim \mathcal{N}(\mu, \Sigma)$. The discriminant function corresponding to Eq. 29 is:

$$g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x} - \mu_i)^T \hat{\Sigma}_i^{-1}(\mathbf{x} - \mu_i) - \frac{d}{2} \ln(2\pi) - \frac{1}{2} \ln|\hat{\Sigma}_i| + \ln P(\omega_i) \quad (30)$$

where Σ_i is arbitrary. We assume that Σ_i is also arbitrary. Therefore,

$$g_i(\mathbf{x}) = \mathbf{x}^T W_i \mathbf{x} + w_i^T \mathbf{x} + \omega_{i0} \quad (31)$$

Where

$$W_i = -\frac{1}{2} \hat{\Sigma}_i^{-1} \quad (32)$$

$$w_i = \hat{\Sigma}_i^{-1} \mu_i \quad (33)$$

And

$$\omega_{i0} = -\frac{1}{2} \mu_i^T \hat{\Sigma}_i^{-1} \mu_i - \frac{1}{2} \ln|\hat{\Sigma}_i| + \ln P(\omega_i) \quad (34)$$

2.8. Classification

Let $x_1^i, x_2^i, \dots, x_N^i \sim (\mu_i, \Sigma)$ be data points from class i . Let d be the length of x_j , for $i \leq j \leq N$.

We compute the mean of the class.

$$\mu_i = \frac{1}{N} \sum_{j=1}^N x_j^i \quad (35)$$

Transforming $\mathcal{N}(\mu_i, \Sigma_i)$ to $\mathcal{N}(0, \Sigma_i)$:

$$x_j^i \leftarrow x_j^i - \frac{1}{d} \sum_{k=1}^d x_j^i[k] \quad \forall j = 1, 2, \dots, N$$

Where $x_j^i[k]$ means k^{th} value of j^{th} sample in i^{th} class.

Let

$$X_i = [x_1^i \ x_2^i \ \dots \ x_N^i]$$

The scatter matrix is:

$$\Sigma_i = \frac{1}{N} X X^T \quad (36)$$

$$\hat{\Lambda}_i = \Lambda_i \Lambda_i^b \quad (37)$$

Pseudo inverse is computed as:

$$\hat{\Sigma}_i^{\dagger} = U_b \hat{\Lambda}_i^{-1} U_b^T \quad (38)$$

The classification algorithm produces μ_i and $\Sigma_i^{\dagger}$.

2.9. Threshold Setting

Eq. 31 is quadratic with d variables where d is large. Therefore, it is very hard to compute the closed form solution or any general expression for the threshold. We suggest that training samples, i.e., $x_1^1, x_2^1, \dots$ for $i = 1, 2, \dots, c$ are used in $g_i(x)$ given by Eq. 31 and human or machine intelligence is used for deciding threshold values, as optimal as possible.

2.10. Testing

Let y be a vector from unknown class. We transform distribution from y from $\mathcal{N}(\mu, \Sigma)$ to $\mathcal{N}(0, \Sigma)$ using:

$$y \leftarrow y - \frac{1}{d} \sum_{j=1}^n y[j]$$

where $y[j]$ is the j^{th} value of the vector y . Compute $g_i(y)$ for $i = 1, 2, \dots, c$ where c is the number of classes. Considering the threshold and $g_i(y)$, we decide the class to which y probably belongs.

3. RESULTS AND DISCUSSION

To analyze the effectiveness of proposed approach, we have taken a cancer gene expression dataset, namely "Colon Tumor", which is collected from Kent Ridge Bio-medical Dataset Repository (Ridge). The dataset contains 62 instances collected from colon-cancer patients. There are 40 tumor biopsies from tumors. Other instances are normal biopsies taken from healthy parts of the same patients. Every sample has expressions from large number of genes and a class label (i.e. normal or cancer). The data has higher number of dimensions as compared to the number of samples, thus making the problem as low sample size problem, i.e., $d \gg n$, where d is dimension and n is the number of samples in the set. In this case, $d = 256$ and $n = 40$ and $n = 22$ for biopsies from sick and normal cells, respectively. As microarray experiments are very expensive, it seems impossible to have $d \leq n$.

This work does not include preprocessing of the raw dataset. Every sample is in the vector form. Such a form of data is the input to the method.

To show the performance of our classifier, standard metrics, namely, sensitivity (S_n), specificity (S_p), positive predicted value (PPV), negative predicted value (NPV) and precision (P) are computed and shown in table 1.

Table 1. Performance analysis of the classifier.

Metric	Measure (%)
S_n	66.67%
S_p	83.33%
PPV	75.00%
NPV	76.92%
P	76.19%

4. CONCLUSION

We have studied a case in classification when dimensionality is larger than the number of samples. This paper discussed when neither the number of dimensions is reduced nor pseudoinverse is possible. We have proposed that in such cases projection of the scatter matrix onto an ideal scatter matrix makes computation of pseudoinverse possible. However, due to the computation of large power (Eq. 5-8), the accuracy of the method can be affected. Moreover, the computational complexity and space complexity of the proposed technique is $O(d^4)$ where d the dimension is and d is very large. Therefore, it is a computationally heavy technique and requires large space, but the same is true for the existing techniques. The proposed classifier is also noise sensitive like existing techniques. However, by gaining a larger dataset and preprocessing, the results may further be improved.

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