

Implementation in MATLAB of the Partial Least Squares algorithm for classification

Case study: fault detection and diagnosis on steel plates

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Outline

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Introduction to the PLS technique

Partial least squares (PLS), as known as **projection to latent structures**, is a dimensionality reduction technique for maximizing the **covariance** between the predictor (independent) matrix $X \in \mathbb{R}^{n \times m}$ and the predicted (dependent) matrix $Y \in \mathbb{R}^{n \times p}$ for each component of the reduced space \mathbb{R}^α with $\alpha \leq m$, where:

- n = number of observations;
- m = number of covariates (input variables);
- p = number of dependent variables (output variables);
- α = dimension of the reduced space in which X is projected.

Popular application of PLS

This technique is often used in **fault detection** and **isolation**. With PLS is possible to treat both regression and classification problems. The matrix X always contains the process variables (e.g. diameter and thickness of a gasket), while the matrix Y only (quantitative) quality variables (e.g. its mechanical seal) in the regression case, whereas in pattern classification the predicted variables are dummy variables (1 or 0) such as:

$$Y = [\mathbf{y}_1 \quad \mathbf{y}_2 \quad \mathbf{y}_3] = \begin{bmatrix} 1 & \dots & 1 & 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & \dots & 0 & 1 & \dots & 1 & 0 & \dots & 0 \\ 0 & \dots & 0 & 0 & \dots & 0 & 1 & \dots & 1 \end{bmatrix}^T \quad p = 3$$

where each column of Y corresponds to a *fault class*. The first n_j elements of column j are filled with a 1, which indicates that the first n_j rows of X are data from fault j . In classification case PLS is named **discriminant**.

NIPALS algorithm

The most popular algorithm used in PLS to compute the model parameters is known as **non-iterative partial least squares (NIPALS)**. There are two versions of this technique:

- **PLS1**: each of the p predicted variables is modeled separately, resulting in one model for each class;
- **PLS2**: all predicted variables are modeled simultaneously.

The first algorithm is more accurate than the other, however it requires more computational time than PLS2 to find the α eigenvectors into which project the m covariates.

Data structures

Before starting with the description of the algorithm, we recall that:

- the matrix $X \in \mathbb{R}^{n \times m}$ is decomposed into a **score matrix** $T \in \mathbb{R}^{n \times \alpha}$ and a **loading matrix** $P \in \mathbb{R}^{m \times \alpha}$ such that $X = \hat{X} + E = T \cdot P^\top + E$, where $E \in \mathbb{R}^{n \times m}$ is the (true) **residual matrix** for X ;
- the matrix $Y \in \mathbb{R}^{n \times p}$ is decomposed into a **score matrix** $U \in \mathbb{R}^{n \times \alpha}$ and a **loading matrix** $Q \in \mathbb{R}^{p \times \alpha}$ such that $Y = \hat{Y} + \tilde{F} = U \cdot Q^\top + \tilde{F}$, where $\tilde{F} \in \mathbb{R}^{n \times p}$ is the (true) **residual matrix** for Y .
- the matrix $B \in \mathbb{R}^{\alpha \times \alpha}$ is the **diagonal regression matrix** such that $\hat{U} = T \cdot B$.

Therefore:

$$Y = \hat{U} \cdot Q^\top + F = T \cdot B \cdot Q^\top + F$$

where F is the **prediction error matrix**; B is selected such that the induced 2-norm of F is minimized.

MATLAB code

The following MATLAB code implements the PLS2 algorithm:

```

E = X; % residual matrix for X
F = Y; % residual matrix for Y
[~, idx] = max(sum(Y.*Y));
% search of the j-th eigenvector
for j = 1:alpha
    u = F(:, idx);
    tOld = 0;
    for i = 1:maxIter
        w = (E'*u)/norm(E'*u); % support vector
        t = E*w; % j-th column of the score matrix for X
        q = (F'*t)/norm(F'*t); % j-th column of the...
            % loading matrix for Y
        u = F*q; % j-th column of the score matrix for Y
    end
end

```

```

    if abs(tOld - t) < exitTol
        break;
    else
        tOld = t;
    end
end
p = (E'*t)/(t'*t); % j-th column of the...
    % loading matrix of X
% scaling
t = t*norm(p);
w = w*norm(p);
p = p/norm(p);
% calculation of b and the error matrices
b = (u'*t)/(t'*t); % j-th column of the...
    % coefficient regression matrix
E = E - t*p'; % update of the residuals for matrix X
F = F - b*t*q'; % update of the residuals for matrix Y

```



```

% calculation of W, P, T and B2
W(:, j) = w;
P(:, j) = p;
T(:, j) = t;
B2 = W*(P'*W)^-1*(T'*T)^-1*T'*Y;
end
Y_hat = X*B2; % computation of predictions

```

For each row of Y_hat the fault class is chosen by assigning 1 to the column whose value is greater than that of the others, 0 otherwise.

Moreover, to increase the performances of PLS it is necessary **normalize** both X and Y before running the algorithm.

Dataset description

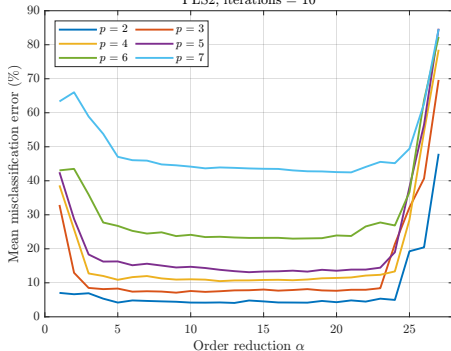
The steel plates faults dataset comes from research by Semeion, Research Center of Sciences of Communication. The aim of the research was to correctly classify the type of surface defects in stainless steel plates. Below is some information about the dataset:

- number of fault classes: $6 + 1$ (no faults);
- number of attributes: 27;
- number of instances: 1941;
- absence of missing values.

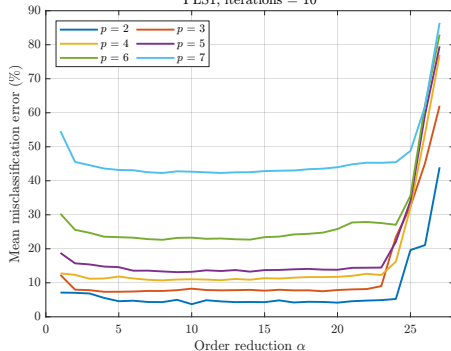
Unfortunately, no further details on the covariates are available.

Preliminary analysis

Mean test CV MCE as function of α and p
PLS2, iterations = 10



Mean test CV MCE as function of α and p
PLS1, iterations = 10



As the number of fault classes p taken into consideration increases, the mean test CV MCE also increases. Both algorithms show a similar behaviour in case of overfitting, while PLS1 underfits less than PLS2.

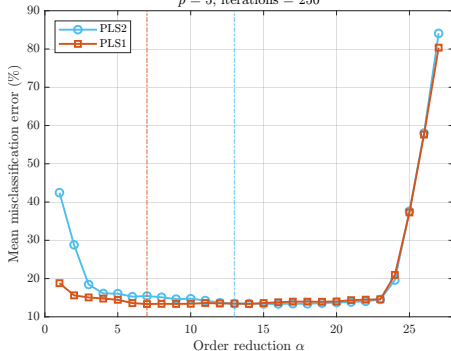
Methodology

To reduce the dependency on a specific dataset randomization during the 10-folds cross-validation, we decided to iterate this procedure n times (10 in preliminary analysis). We used the CV technique to make inference on the model parameters, especially to choose the best model reduction α . As we can see from graphs in the previous frame, with $p = 5$ we obtain a model that is a good compromise between complexity and cross-validation performances, therefore we decided to make our in-depth analysis with this model.

In-depth analysis with $p = 5$

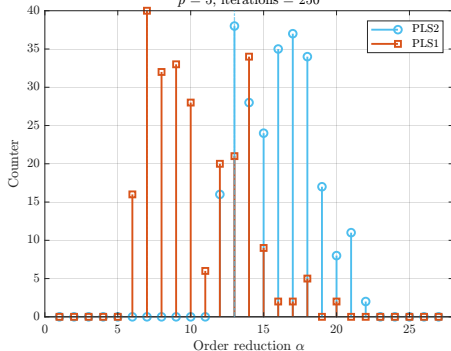
Mean test CV MCE as function of α

$p = 5$, iterations = 250

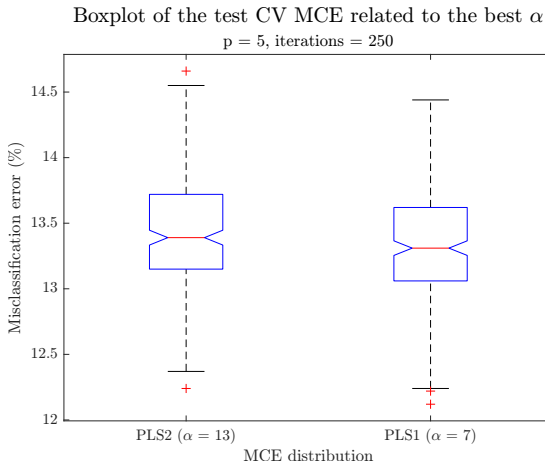


Counters of how many times α was the best order

$p = 5$, iterations = 250

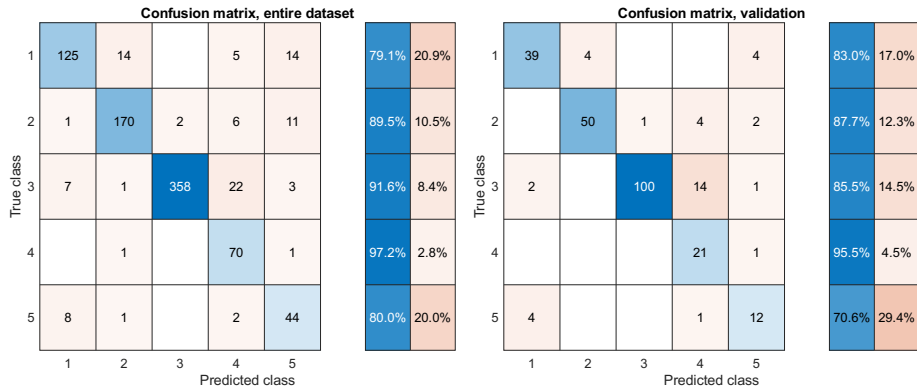


In the right figure we can note that PLS2 tends to advise more complex models than PLS1. This behaviour is confirmed by the left graph: PLS2 goes underfit faster than the other algorithm.



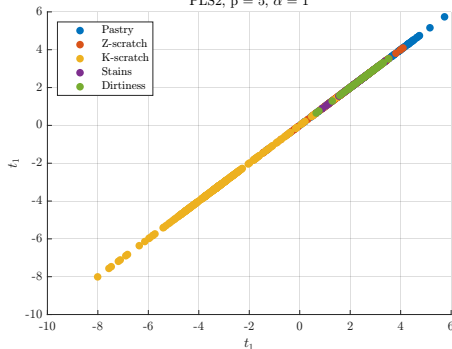
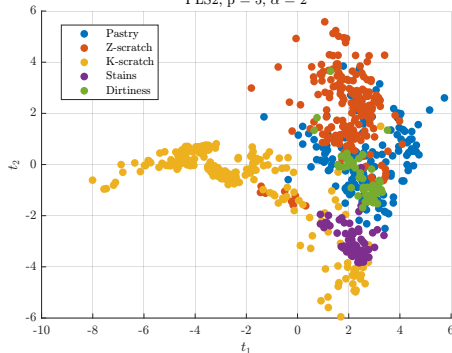
Although PLS1 performs slightly better on average than PLS2, we decided to use the latter one for the following analyses because it is the model with the shortest estimation time.

Validation 70 – 30 of the PLS2 model with $\alpha = 13$

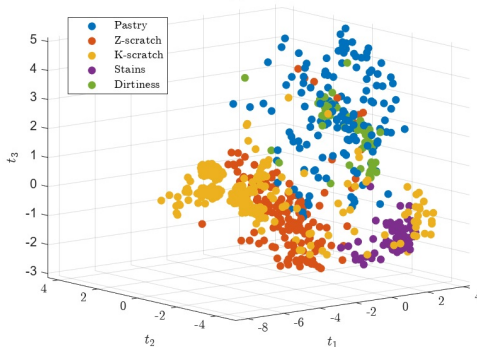


We can see that in validation there is a natural decrease in the predictive capabilities of the model. In particular, the fault classes on which PLS2 struggles the most are classes 1 and 5.

Score matrix T with $\alpha = 1, 2$ and 3

Scatter plot of the score matrix T PLS2, $p = 5$, $\alpha = 1$ Scatter plot of the score matrix T PLS2, $p = 5$, $\alpha = 2$ 

Scatter plot of the score matrix T

PLS2, $p = 5$, $\alpha = 3$ 

α	Pastry	Z-scratch	K-scratch	Stains	Dirtiness	Average
1	1.27%	100%	11.76%	100%	100%	42.15%
2	77.85%	8.95%	12.53%	1.39%	100%	28.29%
3	15.82%	10%	14.58%	1.39%	100%	18.13%

TO DO