

Derivation of the expressions for λ_{\max}

The shrunken centroid for all shrunken centroid based classifiers considered in the paper is defined as

$$\bar{x}_{kj} = \bar{x}_j + \hat{d}_{kj} \cdot m_k \cdot (s_j + s_0). \quad (1)$$

The class-centroid for variable j for class k will be equal to the overall centroid when $\hat{d}_{kj} = 0$.

PAM

In PAM \hat{d}_{kj} is defined as

$$\hat{d}_{kj} = \text{sgn}(d_{kj})(|d_{kj}| - \lambda)_+, \quad (2)$$

so we need to find a solution to

$$\text{sgn}(d_{kj})(|d_{kj}| - \lambda)_+ = 0, \quad (3)$$

which is $\lambda = |d_{kj}|$. In order to effectively remove variable j from the calculation of the discriminant score, we must set the threshold parameter to $\lambda = |d_{kj}|$, for each k . Setting λ to $\max_k(|d_{kj}|)$ will therefore remove the variable j from the calculation of the discriminant score. It is then obvious that when $\lambda = \max_{k,j}(|d_{kj}|)$, all class-centroids will be shrunken to the overall centroid for each variable.

ALP-NSC

According to Theorem I in Wang and Zhu (2007) the numerical solutions to p minimization problems

$$\min_{\tilde{d}_{kj}} \frac{1}{2} \sum_{i=1}^n \sum_{k=1}^K \frac{z_{ik}}{n_k} (\tilde{x}_{ij} - \tilde{d}_{kj})^2 + \lambda \cdot w_j \cdot \max_k(|\tilde{d}_{1j}|, \dots, |\tilde{d}_{Kj}|), \quad (4)$$

$j = 1, \dots, p$, if there exists an indices set $C = \{k_1, \dots, k_r\}$, such that

$$|\hat{d}_{k_1j}| = \dots = |\hat{d}_{k_rj}| > |\hat{d}_{kj}|, \text{ for } k \notin C \quad (5)$$

are

$$\hat{d}_{kj} = \begin{cases} d_{kj} & k \notin C \\ \text{sgn}(d_{kj}) \left(\frac{1}{r} \sum_{s=1}^r |d_{k_sj}| - \frac{\lambda w_j}{r} \right)_+ & k \in C \end{cases}. \quad (6)$$

In order to put all class centroids to the overall centroid for variable j then $C = \{1, \dots, K\}$ and the eq. 6 simplifies to

$$\hat{d}_{kj} = \text{sgn}(d_{kj}) \left(\frac{1}{K} \sum_{k=1}^K |d_{kj}| - \frac{\lambda w_j}{K} \right)_+. \quad (7)$$

λ that puts \hat{d}_{kj} to zero for all k is then a solution to

$$\text{sgn}(d_{kj}) \left(\frac{1}{K} \sum_{k=1}^K |d_{kj}| - \frac{\lambda w_j}{K} \right)_+ = 0, \quad (8)$$

which yields

$$\lambda = \frac{1}{w_j} \sum_{k=1}^K |d_{kj}|. \quad (9)$$

In order to put all class centroids to the overall centroid for each $j = 1, \dots, p$, then

$$\lambda_{\max} = \max_j \left(\frac{1}{w_j} \sum_{k=1}^K |d_{kj}| \right). \quad (10)$$

AHP-NSC

In Wang and Zhu (2007) the authors propose an iterative approach to estimate γ_j and θ_{kj} by using

$$\hat{\gamma}_j = I_{(\exists k, \theta_k \neq 0)} \cdot \left(\sum_{k=1}^K \frac{\theta_{kj}}{\sum_{k=1}^K \theta_{kj}^2} d_{kj} - \frac{\lambda_\gamma w_j^\gamma}{\sum_{k=1}^K \theta_{kj}^2} \right)_+ \quad \text{and} \quad (11)$$

$$\hat{\theta}_{kj} = I_{\gamma_j > 0} \text{sgn}(d_{kj}) \left(\frac{|d_{kj}|}{\gamma_j} - \frac{\lambda_\theta w_{kj}^\theta}{\gamma_j^2} \right)_+, \quad (12)$$

and therefore it is necessary only to tune one of the shrinkage parameters, say λ_θ , and setting λ_γ to zero. In this case $\hat{\gamma}_j^1$ at the first step is

$$\hat{\gamma}_j^1 = I_{(\exists k, \theta_k \neq 0)} \cdot \left(\sum_{k=1}^K \frac{\theta_{kj}}{\sum_{k=1}^K \theta_{kj}^2} d_{kj} \right), \quad (13)$$

which after setting $\theta_{kj}^1 = \text{sgn}(d_{kj})$ as proposed by the authors, yields to

$$\hat{\gamma}_j^1 = \sum_{k=1}^K \frac{|d_{kj}|}{K}. \quad (14)$$

and the λ_θ that sets $\hat{\theta}_{kj}^1$ to zero (and in the second step then also $\hat{\gamma}_j^2$ to zero) is then a solution to

$$\text{sgn}(d_{kj}) \left(\frac{|d_{kj}|}{\hat{\gamma}_j^1} - \frac{\lambda_\theta w_{kj}^\theta}{\hat{\gamma}_j^{1^2}} \right)_+ = 0. \quad (15)$$

It is then straightforward to show that the solution to the above expression is

$$\lambda_\theta = \frac{1}{w_{kj}^\theta} \frac{1}{K} \sum_{k=1}^K d_{jk}^2. \quad (16)$$

This will then set the centroid for class k and variable j to the overall centroid for variable j . Setting

$$\lambda_\theta = \max_{k,j} \left(\frac{1}{w_{kj}^\theta} \frac{1}{K} \sum_{k=1}^K d_{jk}^2 \right), \quad (17)$$

will set all class centroids to the overall centroid for all variables.