Distance Weighted Discrimination

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Given two sets of points in a matrix $\mathbf{X} \in \mathcal{R}^n$ with associated class variables [-1,1] in $\mathbf{Y} = diag(\mathbf{y})$, distance weighted discrimination ([1]) seeks to classify the points into two distinct subsets by finding a hyperplane between the two sets of points. Mathematically, the distance weighted discrimination problem seeks a hyperplane defined by a normal vector, $\boldsymbol{\omega}$, and position, β , such that each element in the residual vector $\bar{\mathbf{r}} = \mathbf{Y}\mathbf{X}^{\mathsf{T}}\boldsymbol{\omega} + \beta \mathbf{y}$ is positive and large. Since the class labels are either 1 or -1, having the residuals be positive is equivalent to having the points on the proper side of the hyperplane.

Of course, it may be impossible to have a perfect separation of points using a linear hyperplane, so an error term ξ is introduced. Thus, the perturbed residuals are defined to be

$$\mathbf{r} = \mathbf{Y}\mathbf{X}^{\mathsf{T}}\boldsymbol{\omega} + \beta\mathbf{y} + \boldsymbol{\xi}$$

Distance Weighted Discrimination solves the following optimization problem to find the optimal hyperplane[1].

$$\begin{array}{ll} \underset{\mathbf{r}, \boldsymbol{\omega}, \boldsymbol{\beta}, \boldsymbol{\xi}}{\text{minimize}} & \sum_{i=1}^{n} (1/r_i) + C \mathbf{1}^{\mathsf{T}} \boldsymbol{\xi} \\ \text{subject to} & \\ \mathbf{r} &= \mathbf{Y} \mathbf{X}^{\mathsf{T}} \boldsymbol{\omega} + \beta \mathbf{y} + \boldsymbol{\xi} \\ \boldsymbol{\omega}^{\mathsf{T}} \boldsymbol{\omega} &\leq 1 \\ \mathbf{r} &\geq \mathbf{0} \\ \boldsymbol{\xi} &> \mathbf{0} \end{array}$$

where C > 0 is a penalty parameter to be chosen.

The function dwd takes as input two $n \times p$ matrices X1 and X2 containing the points to be separated, as well as a penalty term $C \ge 0$ penalizing the movement of a point on the wrong side of the hyperplane to the proper side, and returns the optimal solution using sqlp to the distance weighted discrimination problem.

R> out <- dwd(X1,X2,C)</pre>

Numerical Example

Consider two point configurations - An and Ap - which we would like to classify using distance weighted discrimination. Each point configuration is a matrix containing 50 points in three dimensional space.

```
R> data(Andwd)
R> data(Apdwd)
R> d <- ncol(Andwd)
R> head(Andwd)
```

V1 V2 V3 [1,] 0.214 -1.577 -1.525

0.480	0.624	-0.501
0.088	0.330	-1.213
0.444	-0.398	-0.630
-0.363	-1.081	-1.447
0.123	-0.077	-0.167
	0.480 0.088 0.444 -0.363 0.123	0.480 0.624 0.088 0.330 0.444 -0.398 -0.363 -1.081 0.123 -0.077

R> head(Apdwd)

	V1	V2	٧З
[1,]	-0.687	0.192	0.726
[2,]	0.444	0.782	0.887
[3,]	2.360	-1.114	0.089
[4,]	2.230	1.428	1.369
[5,]	1.555	-0.142	2.138
[6,]	0.259	0.163	1.818

Distance weighed discrimination is used to separate these two configurations by specifying an appropriate penalization term. Here, we will take a value of 0.5.

```
R> out <- dwd(Apdwd,Andwd,0.5)
```

The information defining the separating hyperplane (ω and β) is stored in the X output vector.

```
X <- out$X
```

```
omega <- X[[1]][2:(d+1)]
beta <- X[[1]][d+3]
```

omega

[,1] [1,] 0.6567689 [2,] 0.4857645 [3,] 0.5767907

beta

[1] -0.7520769

References

[1] James Stephen Marron, Michael J Todd, and Jeongyoun Ahn. Distance-weighted discrimination. Journal of the American Statistical Association, 102(480):1267–1271, 2007.