

Complexity of the PSVM

Sepp Hochreiter

Institute of Bioinformatics,
Johannes Kepler Universität Linz
4040 Linz, Austria

hochreit@bioinf.jku.at

$$\mathbf{w}^\top \mathbf{X} \mathbf{X}^\top \mathbf{w} = \|\mathbf{X}^\top \mathbf{w}\|^2 \quad (1)$$

$$\mathbf{K} = \mathbf{X}^\top \mathbf{Z} . \quad (2)$$

The data vectors $(K_{1j}, K_{2j}, \dots, K_{Lj})$ are normalized to zero mean and unit variance:

$$\frac{1}{L} \sum_{i=1}^L (K_{ij} - \bar{K}_j)^2 = 1 \quad \text{and} \quad \bar{K}_j = \frac{1}{L} \sum_{i=1}^L K_{ij} = 0 , \quad (3)$$

$$\mathbf{K}^\top \mathbf{1} = \mathbf{0} \quad \text{and} \quad \text{diag}(\mathbf{K}^\top \mathbf{K}) = L \mathbf{1}. \quad (4)$$

The labels are normalized to zero mean:

$$b = \frac{1}{L} \sum_{i=1}^L y_i = 0 . \quad (5)$$

If the P-SVM is used for classification. Primal:

$$\begin{aligned} \min_{\mathbf{w}, \xi^+, \xi^-} \quad & \frac{1}{2} \|\mathbf{X}^\top \mathbf{w}\|^2 + C \mathbf{1}^\top (\xi^+ + \xi^-) \\ \text{s.t.} \quad & \mathbf{K}^\top (\mathbf{X}^\top \mathbf{w} - \mathbf{y}) + \xi^+ \geq \mathbf{0} \\ & \mathbf{K}^\top (\mathbf{X}^\top \mathbf{w} - \mathbf{y}) - \xi^- \leq \mathbf{0} \\ & \mathbf{0} \leq \xi^+, \xi^- \end{aligned} \quad (6)$$

Lagrangian L :

$$\begin{aligned}
L &= \frac{1}{2} \mathbf{w}^\top \mathbf{X} \mathbf{X}^\top \mathbf{w} + C \mathbf{1}^\top (\boldsymbol{\xi}^+ + \boldsymbol{\xi}^-) \\
&\quad - (\boldsymbol{\alpha}^+)^\top (\mathbf{K}^\top (\mathbf{X}^\top \mathbf{w} - \mathbf{y}) + \boldsymbol{\xi}^+) \\
&\quad + (\boldsymbol{\alpha}^-)^\top (\mathbf{K}^\top (\mathbf{X}^\top \mathbf{w} - \mathbf{y}) - \boldsymbol{\xi}^-) \\
&\quad - (\boldsymbol{\mu}^+)^\top \boldsymbol{\xi}^+ - (\boldsymbol{\mu}^-)^\top \boldsymbol{\xi}^- .
\end{aligned} \tag{7}$$

Dual:

$$\begin{aligned}
\min_{\boldsymbol{\alpha}} \quad & \frac{1}{2} \boldsymbol{\alpha}^\top \mathbf{K}^\top \mathbf{K} \boldsymbol{\alpha} - \mathbf{y}^\top \mathbf{K} \boldsymbol{\alpha} \\
\text{s.t.} \quad & -C \mathbf{1} \leq \boldsymbol{\alpha} \leq C \mathbf{1} ,
\end{aligned} \tag{9}$$

We know that

$$\mathbf{w} = \mathbf{Z} \boldsymbol{\alpha} . \tag{10}$$

P-SVM feature selection primal optimization problem:

$$\begin{aligned}
\min_{\mathbf{w}} \quad & \frac{1}{2} \|\mathbf{X}^\top \mathbf{w}\|^2 \\
\text{s.t.} \quad & \mathbf{K}^\top (\mathbf{X}^\top \mathbf{w} - \mathbf{y}) + \epsilon \mathbf{1} \geq \mathbf{0} \\
& \mathbf{K}^\top (\mathbf{X}^\top \mathbf{w} - \mathbf{y}) - \epsilon \mathbf{1} \leq \mathbf{0} .
\end{aligned} \tag{11}$$

Lagrangian:

$$\begin{aligned}
L &= \frac{1}{2} \mathbf{w}^\top \mathbf{X} \mathbf{X}^\top \mathbf{w} \\
&\quad - (\boldsymbol{\alpha}^+)^\top (\mathbf{K}^\top (\mathbf{X}^\top \mathbf{w} - \mathbf{y}) + \epsilon \mathbf{1}) \\
&\quad + (\boldsymbol{\alpha}^-)^\top (\mathbf{K}^\top (\mathbf{X}^\top \mathbf{w} - \mathbf{y}) - \epsilon \mathbf{1}) ,
\end{aligned} \tag{12}$$

$$\mathbf{w} = \mathbf{Z} \boldsymbol{\alpha} , \tag{13}$$

Dual:

$$\begin{aligned}
\min_{\boldsymbol{\alpha}^+, \boldsymbol{\alpha}^-} \quad & \frac{1}{2} (\boldsymbol{\alpha}^+ - \boldsymbol{\alpha}^-)^\top \mathbf{K}^\top \mathbf{K} (\boldsymbol{\alpha}^+ - \boldsymbol{\alpha}^-) \\
&\quad - \mathbf{y}^\top \mathbf{K} (\boldsymbol{\alpha}^+ - \boldsymbol{\alpha}^-) + \epsilon \mathbf{1}^\top (\boldsymbol{\alpha}^+ + \boldsymbol{\alpha}^-) \\
\text{s.t.} \quad & \mathbf{0} \leq \boldsymbol{\alpha}^+ , \mathbf{0} \leq \boldsymbol{\alpha}^- .
\end{aligned} \tag{14}$$

$$\epsilon \mathbf{1}^\top (\boldsymbol{\alpha}^+ + \boldsymbol{\alpha}^-) \tag{15}$$

$$\boldsymbol{\alpha} = (\boldsymbol{\alpha}^+ - \boldsymbol{\alpha}^-) \tag{16}$$

The Karush-Kuhn-Tucker conditions require:

$$(\boldsymbol{\alpha}^+)^{\top} (\mathbf{K}^{\top} (\mathbf{X}^{\top} \mathbf{w} - \mathbf{y}) + \boldsymbol{\xi}^+) = 0 \quad (17)$$

$$(\boldsymbol{\alpha}^-)^{\top} (\mathbf{K}^{\top} (\mathbf{X}^{\top} \mathbf{w} - \mathbf{y}) - \boldsymbol{\xi}^-) = 0 \quad (18)$$

or

$$(\boldsymbol{\alpha}^+)^{\top} (\mathbf{K}^{\top} (\mathbf{X}^{\top} \mathbf{w} - \mathbf{y}) + \epsilon \mathbf{1}) = 0 \quad (19)$$

$$(\boldsymbol{\alpha}^-)^{\top} (\mathbf{K}^{\top} (\mathbf{X}^{\top} \mathbf{w} - \mathbf{y}) - \epsilon \mathbf{1}) = 0 \quad (20)$$

We know that

$$\frac{\partial L}{\partial \xi_i^+} = C - \alpha_i^+ - \mu_i^+ = 0 \quad (21)$$

$$\frac{\partial L}{\partial \xi_i^-} = C - \alpha_i^- - \mu_i^- = 0 \quad (22)$$

$$(23)$$

KKT conditions require

$$\xi_i^+ \mu_i^+ = 0 \quad (24)$$

$$\xi_i^- \mu_i^- = 0 \quad (25)$$

$$(26)$$

Optimality requires

$$\alpha_i^+ \alpha_i^- = 0 \quad (27)$$

because otherwise the term $\epsilon \mathbf{1}^{\top} (\boldsymbol{\alpha}^+ + \boldsymbol{\alpha}^-)$ can be decreased without changing the other terms in the objective.

$$\alpha_i^+ = 0 \implies \mu_i^+ = C \implies \xi_i^+ = 0 \quad (28)$$

$$\alpha_i^- = 0 \implies \mu_i^- = C \implies \xi_i^- = 0 \quad (29)$$

$$(30)$$

Therefore

$$\alpha_i^+ > 0 \implies \alpha_i^- = 0 \quad \text{and} \quad \xi_i^- = 0 \quad (31)$$

$$\alpha_i^- > 0 \implies \alpha_i^+ = 0 \quad \text{and} \quad \xi_i^+ = 0 \quad (32)$$

It follows that

$$(\alpha_i^+ + \alpha_i^-) (\xi_i^+ + \xi_i^-) = \alpha_i^+ \xi_i^+ + \alpha_i^- \xi_i^- \quad (33)$$

$$\begin{aligned}
\mathbf{w}^\top \mathbf{X} \mathbf{X}^\top \mathbf{w} &= \\
\boldsymbol{\alpha}^\top \mathbf{Z}^\top \mathbf{X} \mathbf{X}^\top \mathbf{w} &= \\
\boldsymbol{\alpha}^\top \mathbf{K}^\top \mathbf{X}^\top \mathbf{w} &= \\
\boldsymbol{\alpha}^\top \mathbf{K}^\top \mathbf{X}^\top \mathbf{w} - \boldsymbol{\alpha}^\top \mathbf{K}^\top \mathbf{y} + \boldsymbol{\alpha}^\top \mathbf{K}^\top \mathbf{y} &= \\
- (\boldsymbol{\alpha}^+)^\top \boldsymbol{\xi}^+ + (\boldsymbol{\alpha}^+)^\top \boldsymbol{\xi}^+ - (\boldsymbol{\alpha}^-)^\top \boldsymbol{\xi}^- + (\boldsymbol{\alpha}^-)^\top \boldsymbol{\xi}^- &= \\
(\boldsymbol{\alpha}^+)^\top (\mathbf{K}^\top (\mathbf{X}^\top \mathbf{w} - \mathbf{y}) + \boldsymbol{\xi}^+) + & \\
(\boldsymbol{\alpha}^-)^\top (\mathbf{K}^\top (\mathbf{X}^\top \mathbf{w} - \mathbf{y}) - \boldsymbol{\xi}^-) + & \\
\boldsymbol{\alpha}^\top \mathbf{K}^\top \mathbf{y} + (\boldsymbol{\alpha}^+)^\top \boldsymbol{\xi}^+ + (\boldsymbol{\alpha}^-)^\top \boldsymbol{\xi}^- &= \\
\boldsymbol{\alpha}^\top \mathbf{K}^\top \mathbf{y} + (\boldsymbol{\alpha}^+)^\top \boldsymbol{\xi}^+ + (\boldsymbol{\alpha}^-)^\top \boldsymbol{\xi}^- &= \\
\boldsymbol{\alpha}^\top \mathbf{K}^\top \mathbf{y} + (\boldsymbol{\alpha}^+ + \boldsymbol{\alpha}^-)^\top (\boldsymbol{\xi}^+ + \boldsymbol{\xi}^-) &= \\
\boldsymbol{\alpha}^\top \mathbf{K}^\top \mathbf{y} + |\boldsymbol{\alpha}|^\top \boldsymbol{\xi}, &
\end{aligned} \tag{34}$$

where

$$|\boldsymbol{\alpha}| = \boldsymbol{\alpha}^+ + \boldsymbol{\alpha}^- \tag{35}$$

$$\boldsymbol{\xi} = \boldsymbol{\xi}^+ + \boldsymbol{\xi}^- \tag{36}$$

We have for the optimal values:

$$\mathbf{w}^\top \mathbf{X} \mathbf{X}^\top \mathbf{w} = \boldsymbol{\alpha}^\top \mathbf{K}^\top \mathbf{y} + |\boldsymbol{\alpha}|^\top \boldsymbol{\xi} \tag{37}$$

Similarly it follows for feature selection

$$\mathbf{w}^\top \mathbf{X} \mathbf{X}^\top \mathbf{w} = \boldsymbol{\alpha}^\top \mathbf{K}^\top \mathbf{y} + \epsilon |\boldsymbol{\alpha}|^\top \mathbf{1}. \tag{38}$$

$$\text{var}(\mathbf{K}) = \frac{1}{L} \text{diag}(\mathbf{K}^\top \mathbf{K}) = \mathbf{1} \tag{39}$$

$$\text{covar}(\mathbf{K}, \mathbf{y}) = \frac{1}{L} \mathbf{K}^\top \mathbf{y} \tag{40}$$

$$\text{var}(\mathbf{y}) = \frac{1}{L} \mathbf{y}^\top \mathbf{y} = \frac{1}{L} \|\mathbf{y}\|^2 \tag{41}$$

$$\text{corel}(\mathbf{K}, \mathbf{y}) = \frac{\text{covar}(\mathbf{K}, \mathbf{y})}{\sqrt{\text{var}(\mathbf{K})} \sqrt{\text{var}(\mathbf{y})}} = \frac{\mathbf{K}^\top \mathbf{y}}{\sqrt{L} \|\mathbf{y}\|} \tag{42}$$

We have

$$\mathbf{K}^\top \mathbf{y} = \sqrt{L} \|\mathbf{y}\| \text{corel}(\mathbf{K}, \mathbf{y}) \tag{43}$$

and

$$\boldsymbol{\alpha}^\top \mathbf{K}^\top \mathbf{y} = \sqrt{L} \|\mathbf{y}\| \boldsymbol{\alpha}^\top \text{corel}(\mathbf{K}, \mathbf{y}) \tag{44}$$

For positive correlation coefficient the α is positive, otherwise it is negative, so that

$$\boldsymbol{\alpha}^\top \mathbf{K}^\top \mathbf{y} = \sqrt{L} \|\mathbf{y}\| |\boldsymbol{\alpha}|^\top |\text{corel}(\mathbf{K}, \mathbf{y})| \quad (45)$$

$$\mathbf{w}^\top \mathbf{X} \mathbf{X}^\top \mathbf{w} = |\boldsymbol{\alpha}|^\top \left(\sqrt{L} \|\mathbf{y}\| |\text{corel}(\mathbf{K}, \mathbf{y})| + \boldsymbol{\xi} \right) \quad (46)$$

and for feature selection

$$\mathbf{w}^\top \mathbf{X} \mathbf{X}^\top \mathbf{w} = |\boldsymbol{\alpha}|^\top \left(\sqrt{L} \|\mathbf{y}\| |\text{corel}(\mathbf{K}, \mathbf{y})| + \epsilon \mathbf{1} \right) \quad (47)$$

The complexity depends on $\|\mathbf{y}\|$ which can be used to bring the model into a canonical form, like scaling y until we have the canonical form of the classical C -SVM.

Then the complexity is the values $|\boldsymbol{\alpha}|$ weighted by correlation coefficient between the features given by \mathbf{K} and the labels/targets \mathbf{y} and the error given by ϵ or $\boldsymbol{\xi}$.

The complexity in the classical SVM is $\boldsymbol{\alpha}^\top \mathbf{1} = |\boldsymbol{\alpha}|^\top \mathbf{1}$ where all components of $\boldsymbol{\alpha}$ are equally weighted.