Exercise 7

Fundamentals of Machine Learning 8 ECTS Heidelberg University WiSe 20/21

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2 Proof - Ridge Regression - Primal vs. Dual (10 pts)

In the primal formulation, the ridge regression problem takes the following form

$$\widehat{\beta} = \operatorname{argmin}_{\beta} \|\mathbf{y} - X\beta\|_{2}^{2} + \tau \|\beta\|_{2}^{2}, \tag{1}$$

where X is an $N \times D$ matrix, β is a D-dimensional vector and \mathbf{y} is an N-dimensional vector. As you saw in the lecture, the optimal $\widehat{\beta}$ is given by

$$\widehat{\beta} = \left(X^T X + \tau \mathbb{1}_D \right)^{-1} X^T \mathbf{y}. \tag{2}$$

Here $\mathbb{1}_D$ is the D -dimensional unit matrix. You also know that the dual formulation of the problem is given by

$$\widehat{\alpha} = \operatorname{argmax}_{\alpha} - \alpha^{T} (XX^{T} + \tau \mathbb{1}_{N}) \alpha + 2\alpha^{T} \mathbf{y}, \tag{3}$$

with the solution for $\widehat{\alpha}$

$$\widehat{\alpha} = \left(X X^T + \tau \mathbb{1}_N \right)^{-1} \mathbf{y}. \tag{4}$$

For each feasible α , a corresponding feasible β is given by

$$\beta = X^T \alpha. \tag{5}$$

Prove that the optimal $\widehat{\beta}$ corresponds to the optimal $\widehat{\alpha}$

$$\widehat{\beta} = X^T \widehat{\alpha}. \tag{6}$$

Hint: Prove the following lemma (e.g. using the SVD of X), which will be useful in your derivation

$$(X^{T}X + \tau \mathbb{1}_{D})^{-1}X^{T} = X^{T}(XX^{T} + \tau \mathbb{1}_{N})^{-1}.$$
 (7)

To prove the relation in Eq.(6), we use the individually derived expressions for the optimal $\hat{\beta}$ and $\hat{\alpha}$ in Eq.(2) and Eq.(4) and substitute these into Eq.(6), obtaining

$$(X^{T}X + \tau \mathbb{1}_{D})^{-1}X^{T}y = X^{T}(XX^{T} + \tau \mathbb{1}_{N})^{-1}y,$$
(8)

where we can simplify the equation by removing the response vector y from each side, yielding

$$\left(X^{T}X + \tau \mathbb{1}_{D}\right)^{-1} X^{T} = X^{T} \left(XX^{T} + \tau \mathbb{1}_{N}\right)^{-1}, \tag{9}$$

which is the same equation as the one given in the hint, Eq.(7). To prove that this equality holds, we left-multiply Eq.(9) with $(X^TX + \tau \mathbb{1}_D)$ and right-multiply with $(XX^T + \tau \mathbb{1}_N)$, which then gives

$$X^{T} (XX^{T} + \tau \mathbb{1}_{N}) = (X^{T}X + \tau \mathbb{1}_{D}) X^{T}.$$

$$(10)$$

By finally multiplying the X^T :s into each parenthesis, we can trivially see that

$$LHS = X^T X X^T + \tau X^T = X^T X X^T + \tau X^T = RHS, \tag{11}$$

for any training set X and any regularization parameter τ . We have thus shown that the relation in Eq.(6) holds true, given the expressions Eq.(2) and Eq.(4) for the optimal $\widehat{\beta}$ and $\widehat{\alpha}$ of the ridge regression problem. \square

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