# Machine Learning 2 – Group ESHG Assignment 01

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auto-correlation. The primal optimization problem is:

Find 
$$w_x \in \mathbb{R}^{d_1}, w_y \in \mathbb{R}^{d_2}$$
 maximizing  $w_x^\top C_{xy} w_y$   
subject to  $w_x^\top C_{xx} w_x = 1$   
 $w_y^\top C_{yy} w_y = 1$ , (1)

where  $C_{xx} = XX^{\top} \in \mathbb{R}^{d_1 \times d_1}$  and  $C_{yy} = YY^{\top} \in \mathbb{R}^{d_2 \times d_2}$  are the auto-covariance matrices of X resp. Y, and  $C_{xy} = XY^{\top} \in \mathbb{R}^{d_1 \times d_2}$  is the cross-covariance matrix of X and Y.

#### Exercise 1: Dual CCA (40 P)

In this exercise, we would like to derive the dual optimization problem, which is more efficient to solve if  $N \ll d_i$ .

(a) Show, that it is always possible to find an optimal solution in the span of the data, that is,

$$w_x = X\alpha_x, w_y = Y\alpha_y. \tag{2}$$

with some coefficient vectors  $\alpha_x \in \mathbb{R}^N$  and  $\alpha_y \in \mathbb{R}^N$ .

(b) Show that the dual optimization problem is equivalent to finding the solution of the generalized eigenvalue problem

$$\left[ \begin{array}{cc} 0 & A \cdot B \\ B \cdot A & 0 \end{array} \right] \left[ \begin{array}{c} \alpha_x \\ \alpha_y \end{array} \right] = \rho \left[ \begin{array}{cc} A^2 & 0 \\ 0 & B^2 \end{array} \right] \left[ \begin{array}{c} \alpha_x \\ \alpha_y \end{array} \right], \tag{3}$$

in  $\alpha_x, \alpha_y$ , where  $A = X^\top X$  and  $B = Y^\top Y$ .

(c) Show how a solution to the original problem can be obtained from a solution of the generalized eigenvalue problem above.

### Exercise 2: Kernelized CCA (30 P)

We consider a kernel  $k_x(x,x')$  and  $k_y(y,y')$  for each modality of the data. We denote by  $K_X \in \mathbb{R}^{N \times N}$  and  $K_Y \in \mathbb{R}^{N \times N}$  the Gram matrices of the respective kernels.

- (a) Describe how the CCA problem and its generalized eigenvalue formulation can be kernelized.
- (b) Explain how the solution of the resulting kernelized CCA are to be interpreted, and under which condition the solution can/cannot be expressed as directions in the input spaces  $\mathbb{R}^{d_1}$  and  $\mathbb{R}^{d_2}$ .

## Exercise 3: Deep CCA (30 P)

We would like to perform CCA on the top layer representation of two neural networks. Abstracting each network as a feature map  $\phi_x(x;\theta_x) \in \mathbb{R}^{h_1}$  and  $\phi_y(y;\theta_y) \in \mathbb{R}^{h_2}$ , with respective parameter vectors  $\theta_x,\theta_y$ , and where x,y are the two input modalities, we consider a relaxed and unconstrained form of CCA given by:

$$\max_{\theta_{x},\theta_{y},w_{x},w_{y}} w_{x}^{\intercal} C_{xy} w_{y} + \alpha \cdot \left[\min\left(0\,,\,1-w_{x}^{\intercal} C_{xx} w_{x}\right) + \min\left(0\,,\,1-w_{y}^{\intercal} C_{yy} w_{y}\right)\right],$$

for  $w_x \in \mathbb{R}^{h_1}$  and  $w_y \in \mathbb{R}^{h_2}$ , where the covariance matrices are defined as

$$C_{xy} = \mathbb{E}[\phi_x \phi_y^\top], \quad C_{xx} = \mathbb{E}[\phi_x \phi_x^\top], \quad C_{yy} = \mathbb{E}[\phi_y \phi_y^\top],$$

where the parameter  $\alpha > 0$  is chosen at hand, and  $\mathbb{E}[\cdot]$  is the expectation with respect to the input distribution.

- (a) Explain how the unconstrained objective above relates to the original CCA objective.
- (b) Express the gradient of the new objective with respect to  $\theta_x$  as a function of the Jacobian matrix  $\frac{\partial \phi_x}{\partial \theta_x}$ .

Task 1

Task 2

Task 3

i

ii