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 α_x, α_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 θ_x,θ_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 θ_x as a function of the Jacobian matrix $\frac{\partial \phi_x}{\partial \theta_x}$.

Task 1

Task 2

Task 3

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The unconstrained form allows to learn more highly correlated representations, which aren't supposed to be linear. Thus, a kernel for KCCA is learned while the mapping function is not as restricted as in KCCA.

Elaborate

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Solve

$$\frac{\partial}{\partial \theta_x} \max_{\theta_x, \theta_y, w_x, w_y} w_x^T C_{xy} w_y + \alpha [\min(0, 1 - w_x^T C_{xx} w_x) + \min(0, 1 - w_y^T C_{yy} w_y)]$$

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