(Kernel) Canonical Correlation Analysis

CS-E4830 - Kernel Methods in Machine Learning: Unsupervised Learning Algorithms 2

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Canonical correlation methods find multivariate relations from two-view datasets

relation: a set of ordered pairs (2-tuples)

The set $\{(x, y) : x^2 + y^2 = 1\}$ is the set of all ordered pairs (x, y) for which $x^2 + y^2 = 1$.

multivariate relation: a set of ordered tuples of more than two elements

The set $\{(x, y, z) : x^2 + y^2 + z^2 = 1\}$ is the set of all ordered tuples (x, y, z) for which $x^2 + y^2 + z^2 = 1$.

function: a relation for which every element in the domain maps on a single element in the codomain

Example of a function: $(x, y) : y = x^2$.

Canonical correlation methods find multivariate relations from two-view datasets

view: a matrix in $\mathbb{R}^{n \times p}$ where n and p denote the observations and variables respectively

two-view dataset: every observation is described by $p + q$ variables, that is the dataset consists of two matrices $\mathbf{X}_a \in \mathbb{R}^{n \times p}$ and $\mathbf{X}_b \in \mathbb{R}^{n \times q}$

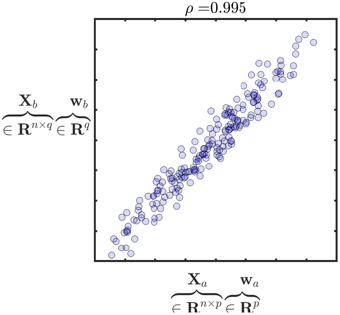
Given a set of $p + q$ variables, or vectors in $\mathbb{R}^n$, canonical correlation methods find subsets of variables that are ordered tuples

Canonical correlation methods find multivariate relations from two-view datasets

Example. Let $\mathbf{X}_a \in \mathbb{R}^{200\times10}$ and $\mathbf{X}_b \in \mathbb{R}^{200\times10}$ denote the two views of the data. Let the first two variables in view $\mathbf{X}_a$ be linearly related with the first two variables of view $\mathbf{X}_b$, that is $\mathbf{x}_b^1 + \mathbf{x}_b^2 = \mathbf{x}_a^1 + \mathbf{x}_a^2 + \boldsymbol{\xi}$ where $\boldsymbol{\xi}$ denotes normal noise.

The related variables are determined from the values of the entries of $\mathbf{w}_a$ and $\mathbf{w}_b$.

Canonical correlation methods find the $\mathbf{w}_a$ and $\mathbf{w}_b$ that maximize the canonical correlation ρ between $\mathbf{X}_a\mathbf{w}_a$ and $\mathbf{X}_b\mathbf{w}_b$.



This lecture covers standard canonical correlation analysis (CCA) and kernel CCA

CCA

$$\boxed{\max_{\mathbf{w}_a,\mathbf{w}_b} \quad \frac{\langle \mathbf{X}_a\mathbf{w}_a, \mathbf{X}_b\mathbf{w}_b\rangle}{||\mathbf{X}_a\mathbf{w}_a||_2||\mathbf{X}_b\mathbf{w}_b||_2}}$$

Kernel CCA

$$\boxed{\max_{\boldsymbol{\alpha},\boldsymbol{\beta}} \quad \frac{\langle \mathbf{K}^x\boldsymbol{\alpha}, \mathbf{K}^y\boldsymbol{\beta}\rangle}{\|\mathbf{K}^x\boldsymbol{\alpha}\|_2\|\mathbf{K}^y\boldsymbol{\beta}\|_2}}$$

$\rightarrow$ How these optimisation problems are solved

$\rightarrow$ How we interpret the solution to the CCA and KCCA problems

$\rightarrow$ When kernel CCA is more useful than CCA

A CCA model is assessed on test data

Training:

- Learn the coefficients
-Tune the hyperparameters

Testing:
Are the learnt relations predictive?

Learning methods:
Standard Eigenvalue Problem (CCA, Kernel CCA)
Generalised Eigenvalue Problem (CCA, Kernel CCA)
Singular Value Decomposition (CCA)

CCA is based on linear transformations

We only know the transformations (the data matrices)

$$\underbrace{\mathbf{X}_a}_{\mathbb{R}^{n\times p}}\underbrace{\mathbf{w}_a}_{\mathbb{R}^{p}} = \underbrace{\mathbf{z}_a}_{\mathbb{R}^{n}} \quad \underbrace{\mathbf{X}_b}_{\mathbb{R}^{n\times q}}\underbrace{\mathbf{w}_b}_{\mathbb{R}^{q}} = \underbrace{\mathbf{z}_b}_{\mathbb{R}^{n}}$$

We want to find the positions $\mathbf{w}_a$ and $\mathbf{w}_b$ and their images $\mathbf{z}_a$ and $\mathbf{z}_b$ such that the cosine of the angle between the images is maximized:

$$\cos\theta_r = \max\langle \mathbf{z}_a^r, \mathbf{z}_b^r\rangle$$

$$||\mathbf{z}_a^r||_2 = 1 \quad ||\mathbf{z}_b^r||_2 = 1$$

$$\langle \mathbf{z}_a^r, \mathbf{z}_a^j\rangle = 0 \quad \langle \mathbf{z}_b^r, \mathbf{z}_b^j\rangle = 0$$

$$\forall j \neq r : j, r = 1, 2, \ldots, \min(p, q)$$

Consecutive pairs of images with greater enclosing angles are found in the orthogonal complements.

The CCA problem can be formulated in terms of the data matrices and $\mathbf{w}_a$ and $\mathbf{w}_b$

Let $\mathbf{C}_{ab} = \frac{1}{n-1}\mathbf{X}_a^\top \mathbf{X}_b$, $\mathbf{C}_{ba} = \frac{1}{n-1}\mathbf{X}_b^\top \mathbf{X}_a$, $\mathbf{C}_{aa} = \frac{1}{n-1}\mathbf{X}_a^\top \mathbf{X}_a$, and $\mathbf{C}_{bb} = \frac{1}{n-1}\mathbf{X}_b^\top \mathbf{X}_b$ denote the empirical between-set and within-set covariance matrices.

We can formulate the CCA problem:

$$\cos\theta = \max_{\mathbf{z}_a, \mathbf{z}_b} \langle \mathbf{z}_a, \mathbf{z}_b \rangle = \max_{\mathbf{w}_a, \mathbf{w}_b} \mathbf{w}_a^\top \mathbf{C}_{ab} \mathbf{w}_b$$

$$||\mathbf{z}_a||_2 = \sqrt{\mathbf{w}_a \mathbf{C}_{aa} \mathbf{w}_a} = 1 \quad ||\mathbf{z}_b||_2 = \sqrt{\mathbf{w}_b \mathbf{C}_{bb} \mathbf{w}_b} = 1$$

The norm constraints are generally expressed in squared form, $\mathbf{w}_a \mathbf{C}_{aa} \mathbf{w}_a = 1$ and $\mathbf{w}_b \mathbf{C}_{bb} \mathbf{w}_b = 1$.

The standard eigenvalue problem is obtained through the Lagrange multiplier technique

Let $L = \mathbf{w}_a^\top \mathbf{C}_{ab}\mathbf{w}_b - \frac{\rho_1}{2}(\mathbf{w}_a^\top \mathbf{C}_{aa}\mathbf{w}_a - 1) - \frac{\rho_2}{2}(\mathbf{w}_b^\top \mathbf{C}_{bb}\mathbf{w}_b - 1)$, where ρ_1 and ρ_2 denote the Lagrange multipliers.

$$\frac{\delta L}{\delta \mathbf{w}_a} = \mathbf{C}_{ab}\mathbf{w}_b - \rho_1 \mathbf{C}_{aa}\mathbf{w}_a = \mathbf{0} \text{ and } \frac{\delta L}{\delta \mathbf{w}_b} = \mathbf{C}_{ba}\mathbf{w}_a - \rho_2 \mathbf{C}_{bb}\mathbf{w}_b = \mathbf{0}$$

$$\mathbf{w}_a^\top \mathbf{C}_{ab}\mathbf{w}_b - \rho_1 \mathbf{w}_a^\top \mathbf{C}_{aa}\mathbf{w}_a = 0 \text{ and } \mathbf{w}_b^\top \mathbf{C}_{ba}\mathbf{w}_a - \rho_1 \mathbf{w}_b^\top \mathbf{C}_{bb}\mathbf{w}_b = 0$$

Since $\mathbf{w}_a^\top \mathbf{C}_{aa}\mathbf{w}_a = \mathbf{w}_b^\top \mathbf{C}_{bb}\mathbf{w}_b = 1$ we have $\rho_1 = \rho_2 = \rho$.

Then $\mathbf{w}_a = \frac{\mathbf{C}_{aa}^{-1}\mathbf{C}_{ab}\mathbf{w}_b}{\rho}$ and $\frac{1}{\rho}\mathbf{C}_{ba}\mathbf{C}_{aa}^{-1}\mathbf{C}_{ab}\mathbf{w}_b - \rho \mathbf{C}_{bb}\mathbf{w}_b = 0.$

If $\mathbf{C}_{bb}^{-1}$ is invertible we have $\mathbf{C}_{bb}^{-1}\mathbf{C}_{ba}\mathbf{C}_{aa}^{-1}\mathbf{C}_{ab}\mathbf{w}_b = \rho^2 \mathbf{w}_b.$

The canonical correlations are the square roots of the eigenvalues of the matrix $\mathbf{C}_{bb}^{-1}\mathbf{C}_{ba}\mathbf{C}_{aa}^{-1}\mathbf{C}_{ab}$, the eigenvectors correspond to $\mathbf{w}_b$ and the $\mathbf{w}_a = \frac{\mathbf{C}_{aa}^{-1}\mathbf{C}_{ab}\mathbf{w}_b}{\rho}$.

The generalised eigenvalue problem is obtained from simultaneous equations

$$\frac{\delta L}{\delta \mathbf{w}_a} = \mathbf{C}_{ab}\mathbf{w}_b - \rho_1 \mathbf{C}_{aa}\mathbf{w}_a = \mathbf{0} \text{ and } \frac{\delta L}{\delta \mathbf{w}_b} = \mathbf{C}_{ba}\mathbf{w}_a - \rho_2 \mathbf{C}_{bb}\mathbf{w}_b = \mathbf{0}$$

$$\mathbf{C}_{ab}\mathbf{w}_b = \rho \mathbf{C}_{aa}\mathbf{w}_a \text{ and } \mathbf{C}_{ba}\mathbf{w}_a = \rho \mathbf{C}_{bb}\mathbf{w}_b$$

$$\begin{pmatrix} \mathbf{0} & \mathbf{C}_{ab} \\ \mathbf{C}_{ba} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{w}_a \\ \mathbf{w}_b \end{pmatrix} = \rho \begin{pmatrix} \mathbf{C}_{aa} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}_{bb} \end{pmatrix} \begin{pmatrix} \mathbf{w}_a \\ \mathbf{w}_b \end{pmatrix}$$

The generalised eigenvalues come in pairs

$$\{\rho_1, -\rho_1, \rho_2, -\rho_2, \ldots, \rho_p, -\rho_p, 0\}$$

where $p < q$.

The positive generalised eigenvalues correspond to the canonical correlations.

The SVD can be applied on a rectangular matrix of covariances

$$\mathbf{C}_{aa} = \mathbf{C}_{aa}^{1/2}\mathbf{C}_{aa}^{1/2} \quad \text{and} \quad \mathbf{C}_{bb} = \mathbf{C}_{bb}^{1/2}\mathbf{C}_{bb}^{1/2}$$

$$\begin{pmatrix} \mathbf{C}_{aa}^{-1/2} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}_{bb}^{-1/2} \end{pmatrix} \begin{pmatrix} \mathbf{C}_{aa} & \mathbf{C}_{ab} \\ \mathbf{C}_{ba} & \mathbf{C}_{bb} \end{pmatrix} \begin{pmatrix} \mathbf{C}_{aa}^{-1/2} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}_{bb}^{-1/2} \end{pmatrix} =$$

$$\begin{pmatrix} \mathbf{I}_q & \mathbf{C}_{aa}^{-1/2}\mathbf{C}_{ab}\mathbf{C}_{bb}^{-1/2} \\ \mathbf{C}_{bb}^{-1/2}\mathbf{C}_{ba}\mathbf{C}_{aa}^{-1/2} & \mathbf{I}_p \end{pmatrix}$$

$$\mathbf{C}_{aa}^{-1/2}\mathbf{C}_{ab}\mathbf{C}_{bb}^{-1/2} = \mathbf{U}^\top\mathbf{S}\mathbf{V}$$

$\rightarrow$ The columns of the matrices $\mathbf{U}$ and $\mathbf{V}$ correspond to the sets of orthonormal left and right singular vectors respectively.

$\rightarrow$ The positions $\mathbf{w}_a$ and $\mathbf{w}_b$ are obtained from

$\mathbf{w}_a = \mathbf{C}_{aa}^{-1/2}\mathbf{U} \quad \mathbf{w}_b = \mathbf{C}_{bb}^{-1/2}\mathbf{V}$

$\rightarrow$ The singular values of matrix $\mathbf{S}$ correspond to the canonical correlations.

Jupyter Exercise 1: canonical correlations through the standard eigenvalue problem

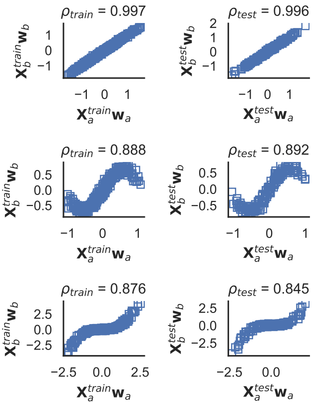
Let $\mathbf{X}_a^{\text{train}} \in \mathbb{R}^{500\times 10}$ and $\mathbf{X}_b^{\text{train}} \in \mathbb{R}^{500\times 10}$ where the columns of both matrices are generated from a random normal distribution with zero mean and unit variance. The following relations are simulated:

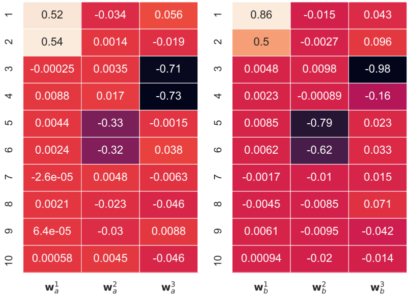
$$\begin{array}{rcl} \mathbf{X}_b^1 + \mathbf{X}_b^2 & = & \mathbf{X}_a^1 + \mathbf{X}_a^2 + \boldsymbol{\xi} \\ \mathbf{X}_b^2 + \mathbf{X}_b^4 & = & (\mathbf{X}_a^2 + \mathbf{X}_4^2)^3 + \boldsymbol{\xi} \\ \mathbf{X}_b^5 + \mathbf{X}_b^6 & = & \sin(\mathbf{X}_a^5 + \mathbf{X}_a^6) + \boldsymbol{\xi} \\ \text{where } \boldsymbol{\xi} & \sim & \mathcal{N}(0, 0.1) \end{array}$$

We compute the square roots of the eigenvalues of the matrix $\mathbf{C}_{bb}^{-1}\mathbf{C}_{ba}\mathbf{C}_{aa}^{-1}\mathbf{C}_{ab}$ and obtain

$$\{\mathbf{0.997}, \mathbf{0.888}, \mathbf{0.876}, 0.172, 0.168, 0.127, 0.1020.094, 0.022, 0.002\}$$

Jupyter Exercise 1: canonical correlations through the standard eigenvalue problem





The score plots show the forms of the relations

The related variables are determined from $\mathbf{w}_a$ and $\mathbf{w}_b$

If there are more variables than examples the within-set covariance matrix becomes singular

$\rightarrow$ The inverses of $\mathbf{C}_{aa}$ and/or $\mathbf{C}_{aa}$ cannot be computed if $p > n$ or $q > n$

$\rightarrow$ This problem is addressed with regularization: we add small positive constants to the diagonal of the within-set covariance matrix.

Regularised standard eigenvalue problem:

$$\left(\mathbf{C}_{bb} + c_b\mathbf{I}\right)^{-1}\mathbf{C}_{ba}\left(\mathbf{C}_{aa} + c_a\mathbf{I}\right)^{-1}\mathbf{C}_{ab}\mathbf{w}_b = \rho^2\mathbf{w}_b.$$

Regularised generalised eigenvalue problem:

$$\begin{pmatrix} \mathbf{0} & \mathbf{C}_{ab} \\ \mathbf{C}_{ba} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{w}_a \\ \mathbf{w}_b \end{pmatrix} = \rho \begin{pmatrix} \mathbf{C}_{aa} + c_a\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}_{bb} + c_b\mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{w}_a \\ \mathbf{w}_b \end{pmatrix}$$

Kernel CCA (KCCA) is CCA on Hilbert Space Objects

The observations are transformed to Hilbert spaces $\mathcal{H}_a$ and $\mathcal{H}_b$ using symmetric positive semi-definite kernels

$$\mathbf{K}_a(\mathbf{x}_a^i, \mathbf{x}_a^j) = \langle \boldsymbol{\phi}_a(\mathbf{x}_a^i), \boldsymbol{\phi}_a(\mathbf{x}_a^j) \rangle_{\mathcal{H}_a} \text{ and } \mathbf{K}_b(\mathbf{x}_b^i, \mathbf{x}_b^j) = \langle \boldsymbol{\phi}_b(\mathbf{x}_b^i), \boldsymbol{\phi}_b(\mathbf{x}_b^j) \rangle_{\mathcal{H}_b}$$

where $i, j = 1, 2, \ldots, n$. In KCCA, the data matrices, $\mathbf{X}_a \in \mathbb{R}^{n \times p}$ and $\mathbf{X}_b \in \mathbb{R}^{n \times q}$, are substituted by the Gram matrices $\mathbf{K}_a \in \mathbb{R}^{n \times n}$ and $\mathbf{K}_b \in \mathbb{R}^{n \times n}$.

Let $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ denote the positions in the kernel space $\mathbb{R}^n$ that have the images $\mathbf{z}_a = \mathbf{K}_a \boldsymbol{\alpha}$ and $\mathbf{z}_b = \mathbf{K}_b \boldsymbol{\beta}$. The KCCA optimisation problem becomes:

$$\max_{\mathbf{z}_a, \mathbf{z}_b \in \mathbb{R}^n} \langle \mathbf{z}_a, \mathbf{z}_b \rangle = \boldsymbol{\alpha}^\top \mathbf{K}_a^\top \mathbf{K}_b \boldsymbol{\beta}$$

$$||\mathbf{z}_a||_2 = \sqrt{\boldsymbol{\alpha}^\top \mathbf{K}_a^2 \boldsymbol{\alpha}} = 1 \quad ||\mathbf{z}_b||_2 = \sqrt{\boldsymbol{\beta}^\top \mathbf{K}_b^2 \boldsymbol{\beta}} = 1$$

Pen-and-Paper Exercise 2: Derive the KCCA problem.

To find non-spurious correlations, kernel CCA needs to be regularised

KCCA is regularised in similar manner as CCA.

Regularised kernelised standard eigenvalue problem:

$$\left(\mathbf{K}_b + c_a \mathbf{I}\right)^{-2} \mathbf{K}_b \mathbf{K}_a \left(\mathbf{K}_a + c_b \mathbf{I}\right)^{-2} \mathbf{K}_a \mathbf{K}_b \boldsymbol{\alpha} = \rho^2 \boldsymbol{\alpha}$$

Regularised kernelised generalised eigenvalue problem:

$$\underbrace{\begin{pmatrix} \mathbf{0} & \mathbf{K}_a \mathbf{K}_b \\ \mathbf{K}_b \mathbf{K}_a & \mathbf{0} \end{pmatrix}}_{\mathbf{A}} \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix} = \rho \underbrace{\begin{pmatrix} \left(\mathbf{K}_a + c_a \mathbf{I}\right)^2 & \mathbf{0} \\ \mathbf{0} & \left(\mathbf{K}_b + c_b \mathbf{I}\right)^2 \end{pmatrix}}_{\mathbf{B}} \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix}$$

The hyperparameters $c_a > 0$ and $c_b > 0$ can be determined through cross-validation. In general, a small positive value, such as 0.02, can be used [1].

Pen-and-Paper Exercise 1: Show that KCCA needs to be regularised.

Linear KCCA is the same as CCA

Canonical correlation: $\rho_{\text{cca}} \quad = \quad \frac{\langle \mathbf{X}_a \mathbf{w}_a, \mathbf{X}_b \mathbf{w}_b \rangle}{||\mathbf{X}_a \mathbf{w}_a||_2 ||\mathbf{X}_b \mathbf{w}_b||_2}.$

Kernel canonical correlation: $\rho_{\text{kcca}} = \frac{\langle \mathbf{K}_a \boldsymbol{\alpha}, \mathbf{K}_b \boldsymbol{\beta} \rangle}{\|\mathbf{K}_a \boldsymbol{\alpha}\|_2 \|\mathbf{K}_b \boldsymbol{\beta}\|_2}$

Let $\mathbf{K}_a = \mathbf{X}_a \mathbf{X}_a^\top$ and $\mathbf{K}_b = \mathbf{X}_b \mathbf{X}_b^\top$.

$$\rho_{\text{kcca}} = \frac{\langle \mathbf{X}_a \mathbf{X}_a^\top \boldsymbol{\alpha}, \mathbf{X}_b \mathbf{X}_b^\top \boldsymbol{\beta} \rangle}{\|\mathbf{X}_a \mathbf{X}_a^\top \boldsymbol{\alpha}\|_2 \|\mathbf{X}_b \mathbf{X}_b^\top \boldsymbol{\beta}\|_2}$$

Denote $\mathbf{w}_a = \mathbf{X}_a^\top \boldsymbol{\alpha}$ and $\mathbf{w}_b = \mathbf{X}_b^\top \boldsymbol{\beta}$.

We obtain $\rho_{kcca} = \rho_{cca}$.

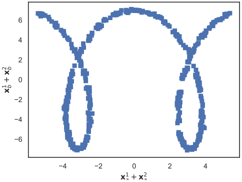
Jupyter Exercise 2: Quadratic KCCA finds non-monotonic trigonometric relations

The homogeneous quadratic polynomial kernel $\mathbf{K} = \langle \mathbf{X}, \mathbf{X} \rangle^2$ finds periodic trigonometric relations.

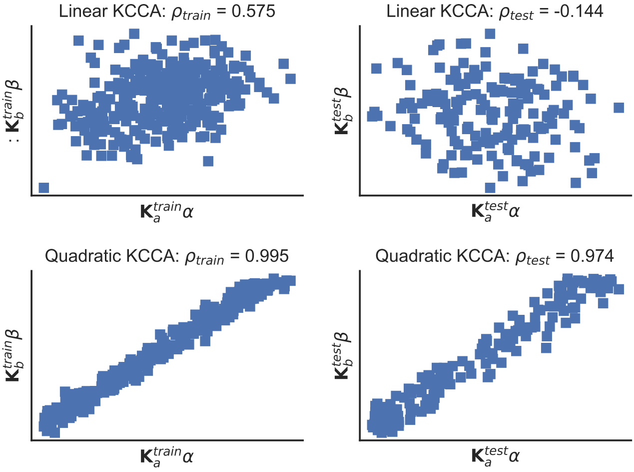
Example simulated data: Let every entry of $\boldsymbol{\theta} \in \mathbb{R}^n \sim U[-2\pi, 2\pi]$.

$$\mathbf{X}_a = \begin{pmatrix} 3 \cdot \sin \frac{\mathbf{x}_a^2}{1} + \boldsymbol{\xi} & \cdots & \boldsymbol{\theta}_p \end{pmatrix}$$

$$\mathbf{X}_b = \begin{pmatrix} 3 \cdot \cos \frac{\mathbf{x}_a^2}{1} + \boldsymbol{\xi} & 6 \cdot \cos \frac{\mathbf{x}_a^2}{0.4} + \boldsymbol{\xi} & \cdots & \boldsymbol{\theta}_q \end{pmatrix}$$



Jupyter Exercise 2: Quadratic KCCA finds non-monotonic trigonometric relations



Exercise: Complete the generalized eigenvalue problem for KCCA and apply it on this dataset.

Wrap-up: CCA is an eigenvalue-based method that finds multivariate relations from two-view datasets

CCA:

$\rightarrow$ we solve the CCA problem through a standard or generalized eigenvalue problem or by applying the SVD.

$\rightarrow$ The related variables are determined from the entries of $\mathbf{w}_a$ and $\mathbf{w}_b$.

$\rightarrow$ The value of the training and test correlation is obtained from $\rho = \frac{\langle \mathbf{X}_a^t \mathbf{w}_a, \mathbf{X}_b^t \mathbf{w}_b \rangle}{||\mathbf{X}_a^t \mathbf{w}_a|| ||\mathbf{X}_b^t \mathbf{w}_b||}$ where t is either train or test data.

$\rightarrow$ Training correlation shows whether learning occurs, test correlation shows if the relation is predictive

$\rightarrow$ The form of the underlying relation is seen from the score plot.

Wrap-up: KCCA is an eigenvalue-based method that finds multivariate relations from two-view datasets

KCCA:

$\rightarrow$ we map the observations to a Hilbert space and solve the CCA problem there, through the standard or generalised eigenvalue problem.

$\rightarrow$ with non-linear kernels, we cannot extract the related variables from the dual coefficient vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$

$\rightarrow$ a high test (non-linear) kernel canonical correlation tells that the data contains non-linear relations

References

- Francis R Bach and Michael I Jordan. "Kernel independent component analysis". In: *Journal of machine learning research* 3.Jul (2002), pp. 1–48.
- Viivi Uurtio et al. "A Tutorial on Canonical Correlation Methods". In: *ACM Comput. Surv.* 50.6 (Nov. 2017), 95:1–95:33. ISSN: 0360-0300. DOI: 10.1145/3136624. URL: http://doi.acm.org/10.1145/3136624.