Kernel assignment: advanced topics in machine learning

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The assignment must be handed in to Liyuan Xu (Liyuan Xu) on **Friday November 27 2020 by 11:59pm**. The code must be emailed to Liyuan in a text file; the proofs and plots must be submitted electronically (if written by hand, they may be scanned in). The UCL CS policy will apply to late submissions of any part of the assignment.

The final component of the assignment involves teaming up with either one or two additional students, generating a dataset, and running your software on the dataset generated by another team (Section 3). Your datasets for kernel CCA must be emailed to Liyuan by **11:59pm on Friday December 04 2020** (i.e. Liyuan needs to receive by email Python or Matlab code to generate the data, and the plots of the canonical projection functions). Pleease submit this dataset on time, since it will be used by other students in the second part of the assignment. Your assessment of the dataset from another team is due **by 11:59pm Friday 18th December 2020**.

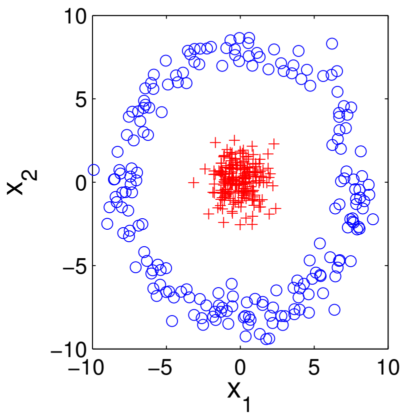
Please contact Liyuan Xu with any questions on the assignment.

1 Feature spaces (30%)

1. Describe a *simple* (finite dimensional) feature space that allows error-free linear classification for the datasets in Figure 1 (the feature space coordinates will be functions of the input space coordinates x_1 and x_2).

2. Consider the case in which the input space $\mathcal{X}$ contains a finite number m of elements. You are given the inner product matrix K between the feature space mapping of every pair of elements x_i, x_j in $\mathcal{X}$, where the i, jth entry in K is written $k(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle_{\mathcal{H}} = (K)_{ij}$. Derive the feature space representation of each element $x_i \in \mathcal{X}$, $i \in \{1 \dots m\}$. Hint: K is positive semidefinite and symmetric - what is its eigendecomposition?

Figure 1: Ring dataset



2 Kernel dependence detection

2.1 Incomplete Cholesky for efficient COCO (20%)

We observe pairs (x_i, y_i) which we arrange in the matrices

$$X = \begin{bmatrix} \phi(\; x_1) & \dots & \phi(x_n) \end{bmatrix} \qquad Y = \begin{bmatrix} \psi(\; y_1) & \dots & \psi(y_n) \end{bmatrix},$$

where $x_i \in \mathcal{X}$, $\phi(x) \in \mathcal{F}$, $\mathcal{F}$ is an RKHS with kernel $k(x, x')$; and $y_i \in \mathcal{Y}$, $\psi(y) \in \mathcal{G}$, $\mathcal{G}$ is an RKHS with kernel $l(x, x')$. Define the Gram matrices K and L such that $k(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle_{\mathcal{F}} = (K)_{ij}$ and $l(y_i, y_j) = \langle \psi(y_i), \psi(y_j) \rangle_{\mathcal{G}} = (L)_{ij}$. The empirical covariance in feature space is

$$\begin{aligned} \widehat{C}_{XY} &= \frac{1}{n} \sum_{i=1}^{n} (\phi(x_i) - \hat{\mu}_x) \otimes (\psi(y_i) - \hat{\mu}_y) \\ &= \frac{1}{n} X H Y^{\top}, \end{aligned} \tag{1}$$

where

$$\hat{\mu}_x = \frac{1}{n} \sum_{i=1}^{n} \phi(x_i) \qquad \hat{\mu}_y = \frac{1}{n} \sum_{i=1}^{n} \psi(y_i).$$

Recall from the lecture notes that the solution to

$$\begin{aligned} &\text{COCO} := \max_{f,g} \left\langle f, \widehat{C}_{XY} g \right\rangle_{\mathcal{G}} \\ &\text{subject to} \quad \|f\|_{\mathcal{F}} = 1 \qquad (2) \\ &\qquad\qquad\quad\; \|g\|_{\mathcal{G}} = 1, \qquad (3) \end{aligned}$$

is written

$$\begin{bmatrix} 0 & \frac{1}{n} \widetilde{K} \widetilde{L} \\ \frac{1}{n} \widetilde{L} \widetilde{K} & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \gamma \begin{bmatrix} \widetilde{K} & 0 \\ 0 & \widetilde{L} \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}.$$

Here

$$f = \sum_{i=1}^{n} \alpha_i \left[\phi(x_i) - \hat{\mu}_x\right] = XH\alpha \qquad g = \sum_{j=1}^{n} \beta_i \left[\psi(y_i) - \hat{\mu}_y\right] = YH\beta,$$

and

$$\widetilde{K} = HKH \qquad \widetilde{L} = HLH, \tag{4}$$

where $H = I - n^{-1}\mathbf{1}_n$, and $\mathbf{1}_n$ is an $n \times n$ matrix of ones.[1]

Using the attached extract on incomplete Cholesky, taken from [1, Section 5.2], derive (i.e., show your working) and implement a more computationally efficient estimate of COCO (the estimate will not be exact). Compare the computational cost of COCO computed exactly, and approximated via incomplete Cholesky (give the number of operations, *not* just runtimes). Implement the incomplete Cholesky-based COCO in Python or Matlab using Gaussian kernels, and test it on the following data (see Figure 2).

$$\begin{aligned} x &= \sin(t) + n_1 \\ y &= \cos(t) + n_2 \\ n_1, n_2 &\sim \mathcal{N}(0, 0.01^2) \\ t &\sim \mathcal{U}([0, 2\pi]) \end{aligned}$$

where $\mathcal{N}(\mu, \sigma^2)$ is a Gaussian random variable with mean μ and variance σ^2, and $\mathcal{U}([a,b])$ is a uniform random variable on the interval $[a,b]$. The random variables t, n_1, n_2 are to be mutually independent. Plot f and g when a Gaussian kernel is used. Plot the mapping of (x,y) via these projections, and compute the correlation of the mapped variables.

2.2 Kernel CCA (20%)

The canonical correlation is defined as

$$\arg\max_{f,g} \left(\mathrm{cov}[f(x), g(y)]\right) = \left\langle f, \widehat{C}_{XY} g \right\rangle_{\mathcal{G}}, \tag{5}$$

subject to the constraints

$$\mathrm{var}(f(x)) = \left\langle f, \widehat{C}_{XX} f \right\rangle_{\mathcal{F}} = 1, \tag{6}$$

$$\mathrm{var}(g(y)) = \left\langle g, \widehat{C}_{YY} g \right\rangle_{\mathcal{G}} = 1, \tag{7}$$

where $\widehat{C}_{XY}$ is given in (1), and

$$\widehat{C}_{XX} = n^{-1} XHX^{\top} \qquad \widehat{C}_{YY} = n^{-1} YHY^{\top}.$$

[1] You can use that $H = HH$, and that XH is a matrix from which each column has had its mean subtracted: these are simple results, so you do not need to show working for them.

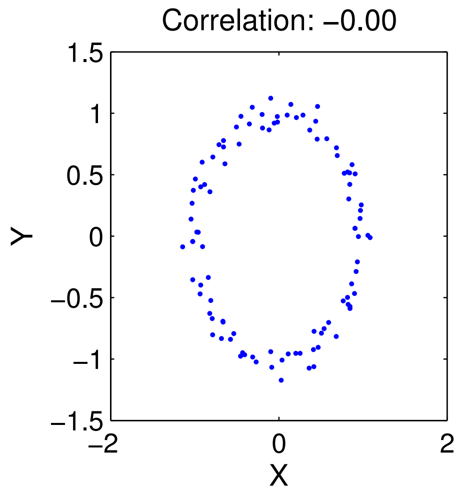


Figure 2: Data to be used for kernel CCA.

Write a kernelized solution to the canonical correlation problem (5) in terms of the Gram matrices $\widetilde{K}$ and $\widetilde{L}$ defined in (4), as a generalized eigenvalue problem $Ua_i = \lambda_i V a_i$ (U and V are matrices, a_i is the eigenvector, λ_i is the eigenvalue). Hints: **(1)** you may assume that

$$f = \sum_{i=1}^{n} \alpha_i \left[\phi(x_i) - \hat{\mu}_x\right] = XH\alpha \qquad g = \sum_{j=1}^{n} \beta_i \left[\psi(y_i) - \hat{\mu}_y\right] = YH\beta.$$

(2) don't forget to keep track of the centring matrices H. Assume a Gaussian kernel, and that the points are also non-pathologically distributed so that K and L have full rank. What went wrong? By adding suitable regularizing terms to (6) and (7), show you can obtain the solution

$$\begin{bmatrix} 0 & \frac{1}{n}\widetilde{K}\widetilde{L} \\ \frac{1}{n}\widetilde{L}\widetilde{K} & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \lambda \begin{bmatrix} \widetilde{K}^2 + \varkappa\widetilde{K} & 0 \\ 0 & \widetilde{L}^2 + \varkappa\widetilde{L} \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}, \tag{8}$$

where $\widetilde{K}$ and $\widetilde{L}$ are defined in (4). Implement kernel CCA as above in Python or Matlab, using Gaussian kernels, and test it on the dataset in Figure 2. Compare functions f and g to those you got with COCO.

3 Dataset design for kernel CCA (15% for your dataset, 15% for results on other dataset)

Teaming up with either one or two other students, design a dataset for kernel CCA. Create variables (perhaps in more than one dimension) which have a nonlinear relationship, and plot the largest kernel canonical projections. You are encouraged to be creative in the choice of domain, even if this means that one of the canonical correlation functions f, g can't be plotted (though at least one projection function must be plottable, hence defined on $\Re$ or $\Re^2$). For instance, one of the domains might contain strings, or vectors of dimensionality greater than two. **Due 11:59pm on Friday December 04 2020.**

Finally, we will assign your team a dataset generated by another team of students. Find and plot the largest canonical projection directions in this case. **Due 11:59pm Friday 18th December 2020.**

References

[1] J. Shawe-Taylor and N. Cristianini. *Kernel Methods for Pattern Analysis*. Cambridge University Press, Cambridge, UK, 2004.