Kernel Principal Component Analysis

4.1 Kernel PCA: Toy Data (10 points)

(a) Create a toy dataset of 2-dimensional data points $\boldsymbol{x}^{(\alpha)} = (x_1^{(\alpha)}, x_2^{(\alpha)})$, $\alpha = 1, \ldots, 90$. The points represent iid samples of 30 points from 3 different distributions with uncorrelated, normally distributed (sd=0.1) coordinate values differing only in their mean value. The first sample ($\alpha = 1, \ldots, 30$) should be centered on $\langle \boldsymbol{x}^{(\alpha)} \rangle_1 = (-0.5, -0.2)$, the second ($\alpha = 31, \ldots, 60$) on $\langle \boldsymbol{x}^{(\alpha)} \rangle_2 = (0, 0.6)$, and the third ($\alpha = 61, \ldots, 90$) on $\langle \boldsymbol{x}^{(\alpha)} \rangle_3 = (0.5, 0)$.

(b) Apply a Kernel PCA using the RBF kernel (see below) with a suitable parameter value for the width σ of the kernel and calculate the coefficients for the representation of the eigenvectors (PCs) in the space spanned by the transformed data points.

(c) Visualize the first 8 PCs in the 2-dimensional input space in the following way: Use equally spaced "test" gridpoints (in a rectangle $[a, b] \times [c, d] \subset \mathbb{R}^2$ containing all sampled data points) and determine their PC values by projecting onto the first 8 eigenvectors in feature space. For example, plot contour lines indicating points that yield the same projection onto the respective PC. You may also use a heat map or pseudo color plot (e.g. `pcolor`) to distinguish the different regions. Plot the 90 data points in the same plot (e.g, using small gray circles). How do you interpret the results?

(d) Discuss for which applications Kernel-PCA might be suitable.

Remark 1: Ensure to center the kernel matrix of the data points before projecting them onto the PCs. Furthermore, since most test points will differ from the sampled data points, you have to ensure that also when calculating the PC projections of these points centered feature vectors are considered.

Remark 2:

RBF kernel: $$k(x^{(\alpha)}, x^{(\beta)}) = \exp\left(-\frac{\|x^{(\alpha)} - x^{(\beta)}\|^2}{2\sigma^2} \right)$$

Total points: 10