Kernel Principal Component Analysis

Exercise 3.1: Kernel PCA: Toy Data (10 points)

(a) Create a dataset of 2-dimensional data points $\underline{\mathbf{x}}^{(\alpha)} = (x_1^{(\alpha)}, x_2^{(\alpha)})^\top$, $\alpha = 1, \ldots, 90$. The points represent iid samples from 3 different distributions with uncorrelated, normally distributed (SD=0.1) coordinate values. Draw 30 samples from each distribution. The only difference between the distributions is their mean:

- The first 30 samples (i.e. $\alpha = 1, \ldots, 30$) should be centered on $\langle \underline{\mathbf{x}}^{(\alpha)} \rangle_1 = (-0.5, -0.2)^\top$.
- The second subset (i.e. $\alpha = 31, \ldots, 60$) should have $\langle \underline{\mathbf{x}}^{(\alpha)} \rangle_2 = (\,0\,, 0.6)^\top$.
- The third subset (i.e. $\alpha = 61, \ldots, 90$) should have $\langle \underline{\mathbf{x}}^{(\alpha)} \rangle_3 = (0.5,\ 0\,)^\top$.

(b) Apply Kernel PCA using an RBF kernel with a suitable value for the width σ of the kernel[1] and calculate the coefficients for the representation of the eigenvectors (PCs) in the space spanned by the transformed data points.

$$k_{RBF}(\underline{\mathbf{x}}, \underline{\mathbf{x}}') = \exp\left(-\frac{\|\underline{\mathbf{x}} - \underline{\mathbf{x}}'\|_2^2}{2\sigma^2}\right)$$

(c) Visualize the first 8 PCs in the original 2-dimensional input space in the following way:

(i) Use equally spaced "test" gridpoints (in a rectangle $[\underline{\mathbf{a}}, \underline{\mathbf{b}}] \times [\underline{\mathbf{c}}, \underline{\mathbf{d}}] \subset \mathbb{R}^2$ which contains all sampled data points from above).

(ii) Determine the PC values of each test point by projecting it onto the first 8 eigenvectors in *feature space*[2].

Hint: Make sure to center the kernel matrix before projecting anything onto the PCs. Furthermore, since most *test* points will differ from the sampled data points, you have to ensure that when calculating the PC projections of these *test* points that you ensure their feature vectors are centered (i.e. the kernel matrix is centered/normalized.

(iii) Plot contour lines in the original 2-dimensional input space. The contours should indicate 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.

[1] You might not be able to assess if one value for σ is better than another until after you've computed the eigenvalues or set up the subsequent visualization step. However, this shouldn't stop you from making an educated guess on what value to start with.

[2] i.e. *after* applying the kernel trick. Which pairs do you select for constructing the kernel matrix?

(iv) Plot the 90 training points in the same plot (e.g. using small gray circles).

(v) How do you interpret the results? What kind of roles do the different PCs play?

(vi) Discuss suitable applications for Kernel PCA.

Total 10 points.