# Wissenschaftliches Rechnen II/Scientific Computing II

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**Exercise sheet 11** To be handed in on **Thursday, 07.06.2016**

# Application of PCA and MDS

## 1 Group exercises

**G 1.** (MDS: embedding of out-of-sample data)

Assume you had training data in the form of a centered Gram matrix $G^c = (\langle y^i, y^j \rangle)_{i,j=1}^n = Y^T Y$ or in the form of a Euclidean distance matrix $D = (\|y^i - y^j\|)_{i,j=1}^n$ and learned a $p$-dimensional embedding of the training data using the CMDS algorithm. Now assume there is a new test point $x \in \mathbb{R}^d$, which is different from the $y^i$ but stems from the same data generating source. You cannot observe $x$ directly but only one of the following sets of features:

a) you either observe inner products $x_S = Y^T x$,

b) or you observe squared Euclidean distances $x_E = (\|x - y^i\|_2^2)_{i=1}^n$.

Use the components computed by the CMDS algorithm to construct a $p$-dimensional embedding $\hat{x}$ of $x$ from the given feature representation. Give a geometric interpretation of the constructed embedding $\hat{x}$. Discuss what properties the training data $y^1, \dots, y^n$ must have such that the obtain embedding $\hat{x}$ is reasonable.

**G 2.** (Kernel-MDS)

Discuss how MDS could be generalized to distances and inner products which are induced by a reproducing kernel $k : \Omega \times \Omega \to \mathbb{R}$. Concretely, assume that there are points $x_1, \dots, x_n \in \Omega$ of which you observe $(k(x_i, x_j))_{i,j=1}^n$ and you want to construct embeddings $\hat{x}^1, \dots, \hat{x}^n \in \mathbb{R}^p$ such that

$$k(x_i, x_j) \approx \langle \hat{x}^i, \hat{x}^j \rangle.$$

## 2 Homework

**H 1.** (Optimal $p$-dimensional subspace in a RKHS)

Let $k : \Omega \times \Omega \to \mathbb{R}$ be a reproducing kernel, $\mathcal{H}$ its native Hilbert space and $X = \{x_1, \ldots, x_n\} \subset \Omega$. Consider the kernel matrix $K = (k(x_i, x_j))_{i,j=1}^n$ and the corresponding eigenvalue decomposition $K = V \Lambda V^T$ with $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_m, 0, \ldots, 0)$, where we assume $m \leq n$. Consider for $i = 1, \ldots, m$ the functions

$$f_i := \frac{1}{\sqrt{\lambda_i}} \sum_{j=1}^{n} V_{ij} k(x^j, \cdot) \in \mathcal{H}_X.$$

a) Show that $(f_i)_{i=1}^m$ forms an orthonormal basis of $H_X$. **Hint:** Use that $\Lambda = V^T K V$.

b) Let $p \in \{1, \ldots, m\}$. Show that $(f_i)_{i=1}^p$ is the solution of

$$\min_{(g_i)_{i=1}^n \text{ ONB of } \mathcal{H}_X} \sum_{i=1}^{n} \|k(x_i, \cdot) - \sum_{j=1}^{p} g_j(x_i) g_j\|_k^2.$$

**Hint:** Argue analogously as in Sheet 10, H2 b).

(10 Punkte)

**H 2.** (Programming exercise: pedestrian classification)

See accompanying notebook.

(10 Punkte)