MVA "Kernel methods"
Homework 4

Jean-Philippe Vert

Due March 16, 2011

1 Splines

Let $H = C_2([0,1])$ be the set of twice continuously differentiable functions $f : [0,1] \to \mathbb{R}$, and $H_1 \subset H$ be the set of functions $f \in H$ that satisfy:

$$f(0) = f'(0) = 0.$$

1.1. Show that H_1 endowed with the norm:

$$\| f \|_{H_1}^2 = \int_0^1 f''(t)^2 dt$$

is a reproducing kernel Hilbert space (RKHS), and compute the reproducing kernel K_1.

1.2. Let H_2 be the set of affine functions $f : [0,1] \to \mathbb{R}$ (i.e., the functions that can be written as $f(x) = ax + b$, with $a, b \in \mathbb{R}$). Show that H_2 endowed with the norm:

$$\| f \|_{H_2}^2 = f(0)^2 + f'(0)^2$$

is a RKHS and compute the corresponding kernel K_2.

1.3. Deduce that H endowed with the norm:

$$\| f \|_H^2 = \int_0^1 f''(t)^2 dt + f(0)^2 + f'(0)^2$$

is a RKHS and compute the reproducing kernel K.

1.4. Let $0 < x_1 < \ldots < x_n < 1$ and $(y_1, \ldots, y_n) \in \mathbb{R}^n$. In order to estimate a regression function $f : [0,1] \to \mathbb{R}$, we consider the following optimization problem:

$$\min_{f \in H} \frac{1}{n} \sum_{i=1}^{n} \left(f\left(x_i\right) - y_i\right)^2 + \lambda \int_0^1 f''(t)^2 dt. \tag{1}$$

Show that any solution of (1) can be expanded as:

$$\hat{f}(x) = \sum_{i=1}^{n} \alpha_i K_1(x_i, x) + \beta_1 x + \beta_2,$$

with $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)' \in \mathbb{R}^n$ et $\boldsymbol{\beta} = (\beta_0, \beta_1)' \in \mathbb{R}^2$.

1.5. Let I be the $n \times n$ identity matrix, M be the square $n \times n$ matrix defined by:

$$M_{i,j} = \begin{cases} K_1(x_i, x_j) & \text{si } i \neq j, \\ K_1(x_i, x_j) + n\lambda & \text{si } i = j, \end{cases}$$

T be the $n \times 2$ matrix:

$$T = \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix},$$

and $\mathbf{y} = (y_1, \ldots, y_n)'$.

Show that $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ satisfy:

$$\begin{cases} T'\boldsymbol{\alpha} = 0, \\ M\boldsymbol{\alpha} + T\boldsymbol{\beta} = \mathbf{y}. \end{cases}$$

1.6. Deduce that $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are given by:

$$\begin{cases} \boldsymbol{\alpha} = M^{-1}\left(I - T\left(T'M^{-1}T\right)^{-1} T'M^{-1}\right)\mathbf{y}, \\ \boldsymbol{\beta} = \left(T'M^{-1}T\right)^{-1} T'M^{-1}\mathbf{y}. \end{cases}$$

1.7. Show that

- $\hat{f} \in C_2\left([0,1]\right)$;
- $\hat{f}$ is a polynomial of degree 3 on each interval $[x_i, x_{i+1}]$ for $i = 1, \ldots, n-1$;
- $\hat{f}$ is an affine function on both intervals $[0, x_1]$ and $[x_n, 1]$.

$\hat{f}$ is called a *spline*.

2 More kernels...

Are the following functions positive definite kernels?

$$\forall x, y \in \mathbb{R}^p, \quad K_2(x, y) = \frac{1}{2 - e^{-\| x-y \|^2}}$$

$$\forall x, y \in \mathbb{R}, \quad K_3(x, y) = \max\left(0, 1 - |x - y|\right)$$