Wissenschaftliches Rechnen II/Scientific Computing II

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Exercise sheet 8

To be handed in on **Thursday, 16.06.2016**

G 1. Provide the proof details for Lemma 51 given in the lecture.

Solution. For $t \in \Omega$ let $\tilde{k}(x,y) = k(x,y) - k(x,t) - k(t,y) + k(t,t)$.

1. We first show the direction $\tilde{k}$ psd $\Rightarrow$ k cspd. Let $a \in \mathbb{R}^n$ such that $\sum_{i=1}^n a_i = 0$ and let $x \in \Omega^n$. Then

$$0 \leq \sum_{i,j} a_i a_j \tilde{k}(x_i, x_j) = \sum_{i,j} a_i a_j k(x_i, x_j).$$

Thus k is cpsd.

2. For the direction k cpsd $\Rightarrow$ $\tilde{k}$ psd, let $a \in \mathbb{R}^n$, $x \in \Omega^n$. Put $x_0 = t$ and $a_0 = -\sum_{i=1}^n a_i$. Then

$$0 \leq \sum_{i,j=0} a_i a_j k(x_i, x_j) = \sum_{i,j=1} a_i a_j \tilde{k}(x_i, x_j).$$

Thus $\tilde{k}$ is psd.

□

G 2. Let $R(x,y)$ and $R_1(x,y)$ be the kernels defined in Sheet 5, H2. Imitating the approach given in the lecture notes on p. 35/36, derive the system of linear equations which determines the solution $\hat{f}$. Then show that you can replace R_1 by R in the kernel matrix which appears in the derived linear system. **Hint:** Choose as the first two elements of your ONB the functions $\phi_1(x) = 1$, $\phi_2(x) = x$.

Solution. Let $\phi_0(x) = 1$, $\phi_1(x) = x$, and $(\phi_i)_{i=2}^\infty$ be an ONB of $W_0^2([0,1])$. Then we can write any potential solution as $f(x) = \sum_{i=0}^\infty \alpha_i \phi_i(x)$ and we can rewrite $R_{\ell_2,\mathrm{reg}}(f)$ in terms of the coefficient vector $\alpha = (\alpha_0, \alpha_1, \dots)$: $R_{\ell_2,\mathrm{reg}}(f) = R_{\ell_2,\mathrm{reg}}(\alpha)$. Computing $\nabla R_{\ell_2,\mathrm{reg}}(\alpha) = 0$ yields

$$\sum_{i=1}^N (y_i - f(x_i)) = 0, \tag{1}$$

$$\sum_{i=1}^N x_i (y_i - f(x_i)) = 0, \tag{2}$$

$$\frac{1}{n\lambda} \sum_{i=1}^N \phi_j(x_i)(y_i - f(x_i)) = \alpha_j, \qquad j \geq 2. \tag{3}$$

The last line yields

$$f(x) = \alpha_0 + \alpha_1 x + (N\lambda)^{-1} \sum_{i=1}^{N} z_i R_1(x_i, x), \tag{4}$$

where $z_i = y_i - f(x_i)$ for $i = 1, \dots, N$. Substituting $f(x_i)$ in $z_i = y_i - f(x_i)$ by (4) leads to the system of linear equations

$$\begin{pmatrix} I_N + (\lambda N)^{-1} K & \overline{\phi}_0 & \overline{\phi}_0 \end{pmatrix} \begin{pmatrix} z \\ \alpha_0 \\ \alpha_1 \end{pmatrix} = y. \tag{5}$$

where $\overline{\phi}_0 = (1, \dots, 1)^T$, $\overline{\phi}_1 = (x_1, \dots, x_n)^T$, and $K = (R_1(x_i, x_j))_{i,j=1,\dots,N}$. Next, we substitute the $f(x_i)$ by (4) and the y_i by the left-hand side of (5) in (1) and (2) and compare coefficients to obtain the additional conditions

$$\overline{\phi}_0^T z = 0, \qquad \overline{\phi}_0^T z = 0. \tag{6}$$

This finally leads to the system of linear equations

$$\begin{pmatrix} I_N + (\lambda N)^{-1} K & \overline{\phi}_0 & \overline{\phi}_1 \\ \overline{\phi}_0^T & 0 & 0 \\ \overline{\phi}_1^T & 0 & 0 \end{pmatrix} \begin{pmatrix} z \\ \alpha_0 \\ \alpha_1 \end{pmatrix} = \begin{pmatrix} y \\ 0 \end{pmatrix}. \tag{7}$$

Obviously, $\sum_{i=1}^N z_i R(x, x_i) = \sum_{i=1}^N z_i + x \sum_{i=1}^N z_i x_i + \sum_{i=1}^N z_i R_1(x, x_i)$. $\square$

G 3. Choose two arbitrary distinct points t_1, t_2 from the set of sample points $\{x_1, \dots, x_n\}$, say w.l.o.g. $t_1 = x_1$, $t_2 = x_2$. Let p_1, p_2 be the unique polynomials of degree 1 which solve $p_i(t_j) = \delta_{ij}$ for $i, j \in \{1, 2\}$, where δ_{ij} denotes the Kronecker delta (p_1, p_2 form a so-called *Lagrange basis* of $\Pi_1 = \operatorname{span}\{\phi_1, \phi_2\}$). As you have proved in G2 the smoothing spline has the form

$$\hat{f}(x) = \underbrace{\alpha_0 + \alpha_1 x}_{\text{affine part}} + \underbrace{\sum_{j=1}^{N} z_j R_1(x, x_j)}_{\text{kernel part}} \tag{8}$$

a) Show that the conditions $\sum_{i=1}^N z_i = \sum_{i=1}^N z_i x_i = 0$, which you have derived in G2, are equivalent to $\sum_{i=1}^N z_i p_1(x_i) = \sum_{i=1}^N z_i p_2(x_i) = 0$.

b) Use a) to show that the kernel part is contained in the set $P_1(V_0)$, where

$$V_0 := \{f \in W^2 : f(t_1) = f(t_2) = 0\}.$$

Solution.

a) Since both ϕ_1, ϕ_2 and p_1, p_2 form a basis of Π_1, we can represent one via the other. For instance $p_1 = \mu_{11}\phi_1 + \mu_{12}\phi_2$ and $p_2 = \mu_{21}\phi_1 + \mu_{22}\phi_2$, and

$$\sum_{i=1}^N z_i p_j(x_i) = \mu_{j1} \sum_{i=1}^N z_i \phi_1(x_i) + \mu_{j2} \sum_{i=1}^N z_i \phi_2(x_i) = 0.$$

b) Since $p_1(t_1) = p_2(t_2) = 1$, $p_1(t_2) = p_2(t_1) = 0$, we obtain

$$z_1 = -\sum_{i=3}^N z_i p_1(x_i), \qquad z_2 = -\sum_{i=3}^N z_i p_2(x_i).$$

Hence, we can rewrite $\hat{f}(x)$ as follows:

$$
\begin{aligned}
f(x) &= \alpha_0 + \alpha_1 x + \sum_{i=3}^{N} z_i \big(R_1(x_i, x) - p_1(x_i) R_1(t_1, x) - p_2(x_i) R_1(t_2, x) \big) \\
&= \alpha_0 + \alpha_1 x + \sum_{i=3}^{N} z_i F_x(x_i),
\end{aligned}
$$

where $F_x(x_i) = R(x, x_i) - I_{(t_1,t_2)}[R_1(x, \cdot)](x_i)$ and $I_{(t_1,t_2)}[f] = p_1 f(t_1) + p_2 f(t_2)$ is the linear interpolation in t_1, t_2. It remains to observe $F_x(t_1) = R(x, t_1) - R(x, t_1) = 0$ and $F_x(t_2) = R(x, t_2) - R(x, t_2) = 0$.

$\square$