Interpolating Normal Hermite Splines

Consider the following interpolation problem:

Problem: Given points $\{p_i, p_i \in R^n\}_{i=1}^{n_1}$, $\{s_j, s_j \in R^n\}_{j=1}^{n_2}$ and a set of unit vectors $\{e_j, e_j \in R^n\}_{j=1}^{n_2}$ find a function f such that

$$f(p_i) = u_i\,, \quad i = 1, 2, \ldots, n_1\,,$$
$$\frac{\partial f}{\partial e_j}(s_j) = v_j\,, \quad j = 1, 2, \ldots, n_2\,, \tag{1}$$
$$n_1 > 0\,, \quad n_2 \geq 0\,.$$

where $\frac{\partial f}{\partial e_j}(s_j) = \nabla f(s_j) \cdot e_j = \sum_{k=1}^{n} \frac{\partial f}{\partial x_k}(s_j)e_{jk}$ is a directional derivative of f at the point s_j in the direction of e_j.

We assume that function f is an element of the Bessel potential space $H_\varepsilon^s(R^n)$ which is defined as:

$$H_\varepsilon^s(R^n) = \left\{ \varphi | \varphi \in S', (\varepsilon^2 + |\xi|^2)^{s/2}\mathcal{F}[\varphi] \in L_2(R^n) \right\}, \quad \varepsilon > 0,\ s > \frac{n}{2} + r, \quad r = 1, 2, \ldots\,.$$

where $|\cdot|$ is the Euclidean norm, $S'(R^n)$ is space of L. Schwartz tempered distributions, parameter s may be treated as a fractional differentiation order and $\mathcal{F}[\varphi]$ is a Fourier transform of the φ. The parameter ε can be considered as a "scaling parameter", it allows to control approximation properties of the normal spline which usually are getting better with smaller values of ε, also it can be used to reduce the ill-conditioness of the related computational problem (in traditional theory $\varepsilon = 1$).

Theoretical properties of spaces H_ε^s at $\varepsilon > 0$ are identical — they are Hilbert spaces with inner product

$$\langle \varphi, \psi \rangle = \int (\varepsilon^2 + |\xi|^2)^s \mathcal{F}[\varphi]\overline{\mathcal{F}[\psi]}\, d\xi$$

and norm

$$\|\varphi\| = (\langle \varphi, \varphi \rangle)^{1/2} = \|(\varepsilon^2 + |\xi|^2)^{s/2}\mathcal{F}[\varphi]\|_{L_2}\,.$$

It is easy to see that all these norms are equivalent. It means that space $H_\varepsilon^s(R^n)$ is equivalent to $H^s(R^n) = H_1^s(R^n)$ ([3], [5]).

Hilbert space $H_\varepsilon^s(R^n)$ ($s = n/2 + 1/2 + r$, $r \geq 1$) is continuously embedded in Hölder space $C_b^r(R^n)$ ([3],[17],[20]) of functions continuous and bounded with their first r derivatives, it means function f can be treated as an element of function class $C^r(R^n)$ of functions continuous with their first r derivatives. Therefore functionals F_i and F_j'

$$F_i(\varphi) = \varphi(p_i), \quad F_j'(\varphi) = \frac{\partial \varphi}{\partial e_j}(s_j), \quad \forall \varphi \in H_\varepsilon^s(R^n), \; s = n/2 + 1/2 + r, \; r \geq 1, \quad p_i, \, s_j \in R^n,$$

$$i = 1, 2, \ldots, n_1, \; j = 1, 2, \ldots, n_2,$$

are linear continuous functionals in H_ε^s.

We also assume that all points $\{p_i\}$ are different and in a case when among points $\{s_j\}$ there are coincident ones, we stipulate that the corresponding unit vectors defining the directions of the directional derivatives at such points are linearly independent. Note that some points $\{p_i\}$ may coincide with some $\{s_j\}$. Under these restrictions all functionals F_i, F_j' are linearly independent.

In accordance with Riesz representation theorem [1] these linear continuous functionals can be represented in the form of inner product of some elements $h_i, h_j' \in H_\varepsilon^s$ and $\varphi \in H_\varepsilon^s$, for any $\varphi \in H_\varepsilon^s$:

$$F_i(\varphi) = \langle h_i, \varphi \rangle, \quad F_j'(\varphi) = \langle h_j', \varphi \rangle, \quad \forall \varphi \in H_\varepsilon^s,$$

$$i = 1, 2, \ldots, n_1, \; j = 1, 2, \ldots, n_2.$$

Elements h_i and h_j' are continuously differentiable functions. Thereby the original system of constraints (1) can be written in form:

$$f(p_i) = F_i(f) = \langle h_i, f \rangle = u_i,$$

$$\frac{\partial f}{\partial e_j}(s_j) = F_j'(f) = \langle h_j', f \rangle = v_j, \tag{2}$$

$$h_i, \, h_j', \, f \in H_\varepsilon^s, \quad i = 1, 2, \ldots, n_1, \; j = 1, 2, \ldots, n_2.$$

here all functions h_i and h_j' are linear independent and system of constrains (2) defines a nonempty convex and closed set (as an intersection of hyper-planes in the Hilbert space H_ε^s).

Problem of reconstruction of function f satisfying system of constraints (2) is undetermined. We reformulate it as a problem of finding solution of this system of constraints that has minimal norm:

$$\sigma = \arg\min\{\|f - z\|^2 : (2), z \in H_\varepsilon^s, \forall f \in H_\varepsilon^s\}, \tag{3}$$

where $z \in H_\varepsilon^s$ is a "prototype" function. Solution of this problem exists and it is unique ([6], [16]) as a projection of element z on the nonempty convex closed set in Hilbert space H_ε^s. Element σ is an interpolating normal spline.

In accordance with generalized Lagrange method ([13], [16]) solution of the problem (3) can be presented as:

$$\sigma = z + \sum_{i=1}^{n_1} \mu_i h_i + \sum_{j=1}^{n_2} \mu_j' h_j', \tag{4}$$

where coefficients μ_i and μ_j' are defined by system of linear equations

$$\sum_{l=1}^{n_1} g_{il}\mu_l + \sum_{j=1}^{n_2} g'_{ij}\mu'_j = u_i - \langle h_i, z \rangle, \quad 1 \le i \le n_1,$$

$$\sum_{i=1}^{n_1} g'_{ij}\mu_i + \sum_{m=1}^{n_2} g''_{jm}\mu'_m = v_j - \langle h'_j, z \rangle, \quad 1 \le j \le n_2, \tag{5}$$

Matrix of system (5) is the positive definite symmetric Gram matrix of the set of linearly independent elements $\{h_i\}, \{h'_j\}$ and coefficients $g_{il}, g'_{ij}, g''_{jm}$ are defined as follows:

$$g_{il} = \langle h_i, h_l \rangle, \quad g'_{ij} = \langle h_i, h'_j \rangle, \quad g''_{jm} = \langle h'_j, h'_m \rangle. \tag{6}$$

Space $H^s_\varepsilon(R^n)$ is a reproducing kernel Hilbert space ([5],[18],[19],[20]). We denote its reproducing kernel as $V(\eta, \xi)$.

Recall the definition of the reproducing kernel ([4], [7]). The reproducing kernel of space H^s_ε is a such function $V(\eta, \xi)$ that

- for every $\xi \in R^n$, $V(\eta, \xi)$ as function of η belongs to H^s_ε
- for every $\xi \in R^n$ and every function $\varphi \in H^s_\varepsilon$

$$\varphi(\xi) = \langle V(\eta, \xi), \varphi(\eta) \rangle \tag{7}$$

Reproducing kernel is a symmetric function:

$$V(\eta, \xi) = V(\xi, \eta),$$

also in the considered case ($s = n/2 + 1/2 + r, \, r \ge 1$) it is a continuously differentiable function. Differentiating the identity (7) allows to get the identities for derivatives:

$$\frac{\partial \varphi(\xi)}{\partial \xi_k} = \left\langle \frac{\partial V(\cdot, \xi)}{\partial \xi_k}, \varphi \right\rangle \tag{8}$$

which holds for any $\varphi \in H^s_\varepsilon$ and $\xi \in R^n$, it means that function $\frac{\partial V(\cdot, \xi)}{\partial \xi_k}$ represents a point-wise functional defined as value of function $\frac{\partial \varphi(\cdot)}{\partial \xi_k}$ at a point ξ.

Now it is possible to express functions h_i and h'_j via the reproducing kernel V. Comparing (2) with (7) and (8) we receive:

$$h_i(\eta) = V(\eta, p_i), \qquad\qquad\qquad i = 1, 2, \ldots, n_1$$

$$h'_j(\eta) = \frac{\partial V(\eta, s_j)}{\partial e_j} = \sum_{k=1}^{n} \frac{\partial V(\eta, s_j)}{\partial \xi_k} e_{jk}, \quad j = 1, 2, \ldots, n_2. \tag{9}$$

The coefficients (6) of the Gram matrix can be presented as ([7], [8], [10]):

$$g_{il} = \langle h_i, h_l \rangle = \langle V(\cdot, p_i), V(\cdot, p_l) \rangle = V(p_i, p_l),$$

$$g'_{ij} = \langle h_i, h'_j \rangle = \left\langle V(\cdot, p_i), \frac{\partial V(\cdot, s_j)}{\partial e_j} \right\rangle = \frac{\partial V(p_i, s_j)}{\partial e_j} =$$

$$= \sum_{k=1}^{n} \frac{\partial V(p_i, s_j)}{\partial \xi_k} e_{jk}.$$

(10)

With the help of (7) and (10), we can also calculate g''_{jm} ([8], [10]):

$$g''_{jm} = \langle h'_j, h'_m \rangle = \left\langle \frac{\partial V(\cdot, s_j)}{\partial e_j}, \frac{\partial V(\cdot, s_m)}{\partial e_m} \right\rangle = \frac{\partial^2 V(s_j, s_m)}{\partial e_j \partial e_m} =$$

$$= \sum_{r=1}^{n} \sum_{k=1}^{n} \frac{\partial^2 V(s_j, s_m)}{\partial \eta_r \partial \xi_k} e_{jk} e_{mr}.$$

(11)

Further

$$\langle h_i, z \rangle = \langle V(\cdot, p_i), z \rangle = z(p_i),$$

$$\langle h'_j, z \rangle = \frac{\partial z(s_j)}{\partial e_j} = \sum_{k=1}^{n} \frac{\partial z(s_j)}{\partial x_k} e_{jk}.$$

(12)

Normal hermite splines will be constructed in Bessel potential spaces $H_\varepsilon^{s_1}(R^n)$, $s_1 = n/2 + 3/2$ and $H_\varepsilon^{s_2}(R^n)$, $s_2 = n/2 + 5/2$. Elements of space H^{s_1} can be treated as continuously differentiable functions and elements of space H^{s_2} can be treated as twice continuously differentiable functions. Note, the spline is infinitely differentiable everywhere in R^n exepting the knots p_i and s_j.

Reproducing kernel of Bessel potential space was presented in [5] and its simplified form was given in [14], [18], [19], [20]. For space $H_\varepsilon^s(R^n)$, $s = n/2 + 1/2 + r$, $r \geq 0$ it can be written as:

$$V(\eta, \xi) = \exp(-\varepsilon|\eta - \xi|) \sum_{k=0}^{r} \frac{(r+k)!}{2^k k!(r-k)!} (\varepsilon|\eta - \xi|)^{r-k},$$

(a constant multiplier is omitted here.)

This reproducing kernel is known as the Matérn kernel [23].

Therefore for space $H_\varepsilon^{s_1}(R^n)$ with accuracy to constant multiplier we get:

$$V(\eta, \xi) = \exp(-\varepsilon|\eta - \xi|)(1 + \varepsilon|\eta - \xi|).$$

(13)

and for space $H_\varepsilon^{s_2}(R^n)$:

$$V(\eta, \xi) = \exp(-\varepsilon|\eta - \xi|)(3 + 3\varepsilon|\eta - \xi| + \varepsilon^2|\eta - \xi|^2).$$

(14)

Let's write down expressions of $h_i, h'_j, g_{il}, g'_{ij}, g''_{jm}$ for space $H_\varepsilon^{s_1}(R^n)$:

$$h_i(\eta) = \exp(-\varepsilon|\eta - p_i|)(1 + \varepsilon|\eta - p_i|)\,, \qquad\qquad i = 1, 2, \ldots, n_1\,,$$

$$h'_j(\eta) = \varepsilon^2 \exp(-\varepsilon|\eta - s_j|) \sum_{k=1}^{n} (\eta_k - s_{jk})e_{jk}\,, \quad j = 1, 2, \ldots, n_2\,,$$

$$g_{il} = \exp(-\varepsilon|p_i - p_l|)(1 + \varepsilon|p_i - p_l|)\,, \quad i = 1, 2, \ldots, n_1\,, \ \ l = 1, 2, \ldots, n_1\,,$$

$$g'_{ij} = \varepsilon^2 \exp(-\varepsilon|p_i - s_j|) \sum_{k=1}^{n} (p_{ik} - s_{jk})e_{jk}\,, \quad i = 1, 2, \ldots, n_1\,, \ \ j = 1, 2, \ldots, n_2\,,$$

$$g''_{jm} = \sum_{r=1}^{n} \sum_{k=1}^{n} \frac{\partial^2 V(s_j, s_m)}{\partial \eta_r \partial \xi_k} e_{jk} e_{mr}$$

$$j \neq m\,, \quad j = 1, 2, \ldots, n_2\,, \ \ m = 1, 2, \ldots, n_2\,, \tag{15}$$

where

$$\frac{\partial^2 V(s_j, s_m)}{\partial \eta_r \partial \xi_r} = \varepsilon^2 \exp(-\varepsilon|s_j - s_m|)\left(1 - \varepsilon \frac{(s_{jr} - s_{mr})^2}{|s_j - s_m|}\right)\,,$$

$$\frac{\partial^2 V(s_j, s_m)}{\partial \eta_r \partial \xi_k} = -\varepsilon^3 \exp(-\varepsilon|s_j - s_m|) \frac{(s_{jr} - s_{mr})(s_{jk} - s_{mk})}{|s_j - s_m|}\,, \quad r \neq k\,,$$

$$g''_{jj} = \varepsilon^2 \sum_{r=1}^{n} (e_{jr})^2 = \varepsilon^2\,, \quad j = 1, 2, \ldots, n_2\,,$$

and for space $H_\varepsilon^{s_2}(R^n)$:

$$h_i(\eta) = \exp(-\varepsilon|\eta - p_i|)(3 + 3\varepsilon|\eta - p_i| + \varepsilon^2|\eta - p_i|^2))\,, \qquad\qquad i = 1, 2, \ldots, n_1\,,$$

$$h'_j(\eta) = \varepsilon^2 \exp(-\varepsilon|\eta - s_j|)(1 + \varepsilon|\eta - s_j|) \sum_{k=1}^{n} (\eta_k - s_{jk})e_{jk}\,, \quad j = 1, 2, \ldots, n_2\,,$$

$$g_{il} = \exp(-\varepsilon|p_i - p_l|)(3 + 3\varepsilon|p_i - p_l| + \varepsilon^2|p_i - p_l|^2))\,,$$
$$i = 1, 2, \ldots, n_1\,, \ \ l = 1, 2, \ldots, n_1\,,$$

$$g'_{ij} = \varepsilon^2 \exp(-\varepsilon|p_i - s_j|)(1 + \varepsilon|p_i - s_j|) \sum_{k=1}^{n} (p_{ik} - s_{jk})e_{jk}\,,$$
$$i = 1, 2, \ldots, n_1\,, \ \ j = 1, 2, \ldots, n_2\,,$$

$$g''_{jm} = \sum_{r=1}^{n} \sum_{k=1}^{n} \frac{\partial^2 V(s_j, s_m)}{\partial \eta_r \partial \xi_k} e_{jk} e_{mr} \tag{16}$$

$$j \neq m\,, \quad j = 1, 2, \ldots, n_2\,, \ \ m = 1, 2, \ldots, n_2\,,$$

where

$$\frac{\partial^2 V(s_j, s_m)}{\partial \eta_r \partial \xi_r} = \varepsilon^2 \exp(-\varepsilon|s_j - s_m|)(1 + \varepsilon|s_j - s_m| - \varepsilon^2(s_{jr} - s_{mr})^2)\,,$$

$$\frac{\partial^2 V(s_j, s_m)}{\partial \eta_r \partial \xi_k} = -\varepsilon^4 \exp(-\varepsilon|s_j - s_m|)(s_{jr} - s_{mr})(s_{jk} - s_{mk})\,, \quad r \neq k\,,$$

$$g''_{jj} = \varepsilon^2 \sum_{r=1}^{n} (e_{jr})^2 = \varepsilon^2\,, \quad j = 1, 2, \ldots, n_2\,,$$

In a case when there is no information of function f derivatives the Problem (1) is reducing to the simplest interpolation problem:

Problem: Given points $\{p_i, p_i \in R^n\}_{i=1}^{n_1}$ find a function f such that

$$f(p_i) = u_i, \quad i = 1, 2, \ldots, n_1,$$
$$n_1 > 0. \tag{17}$$

We assume that f is a continuous function. It can be treated as an element of Bessel potential space $H_\varepsilon^{s_0}(R^n)$, $s_0 = n/2 + 1/2$, this space is continuously embedded in Hölder space $C_b(R^n)$ of continuous and bounded functions.

Reproducing kernel of Bessel potential space $H_\varepsilon^{s_0}(R^n)$ can be written as:

$$V(\eta, \xi) = \exp(-\varepsilon|\eta - \xi|).$$

(with accuracy to a constant multipliler), and expressions for h_i, g_{il} are defined by:

$$h_i(\eta) = \exp(-\varepsilon|\eta - p_i|), \quad i = 1, 2, \ldots, n_1,$$
$$g_{il} = \exp(-\varepsilon|p_i - p_l|)), \quad i = 1, 2, \ldots, n_1, \ \ l = 1, 2, \ldots, n_1. \tag{18}$$

When value of the parameter ε is small this normal spline is similar to multivariate generalization of the one dimensional linear spline.

We now consider the choice of value for parameterd ε. In a case when value of this parameter is small the normal spline is similar to Duchon's D^m-spline [12]. Approximating properties of the normal spline are getting better with smaller values of ε, however with decreasing value of ε the condition number of the corresponding Gram matrix is increasing. Therefore, when choosing the value of parameter ε, a compromise is needed. In practice, it is necessary to choose such value of the ε that condition number of Gram matrix is small enough. Numerical procedures of the matrix condition number estimation are well known.

As well, it is useful to preprocess the source data of the problem by transforming the domain where interpolation knots are located into the unit hypercube.

The normal splines method for one-dimensional function interpolation and linear ordinary differential and integral equations was proposed in [8] and [9] and developed in [10]. Multivariate generalization of the normal splines method was developed for two-dimensional problem of low-range computerized tomography in [15] and applied for solving a mathematical economics problem in [11]. Further results were reported on seminars and conferences [14,21,22].

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