The optimal choice of the shape parameter in smooth RBFs

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Abstract. The main purpose of this report is to present concrete and useful criteria for choosing the constant c contained in the famous radial function

$$h(x) := (-1)^{\lceil -\frac{\beta}{2} \rceil}(c^2 + |x|^2)^{\frac{\beta}{2}},\ \beta \in R \backslash 2N_{\geq 0},\ c > 0 \tag{1}$$

which is called multiquadric for $\beta > 0$ and inverse multiquadric for $\beta < 0$, respectively. The optimal choice of c is a longstanding question and has obsessed many experts in the field of radial basis functions(RBFs). Most time what people can do is just making experiments and try to build a model to predict the influence of c, for some special cases. Here, we make a lucid clarification for its influence on the error estimates and show it with a concrete function, denoted by $MN(c)$. The approximated functions lie in a function space which is equivalent to Gaussians' native space, and is denoted by E_σ. Then, $|f(x) - s_f(x)| \leq MN(c) \cdot F(\delta)$, for all $f \in E_\sigma$, where s_f is the frequently used interpolation function constructed by (1) and δ is the fill distance which measures the spacing of the data points. Both $MN(c)$ and $F(\delta)$ contribute to the error bound, but $MN(c)$ is more influential. The constant σ describes the rate of decay for the Fourier transform of f.

We find $MN(c)$ depends on five parameters, β, σ, the dimension n, the domain size, and the fill distance δ. So the optimal choice of c which minimizes the value of $MN(c)$ also depends on the five parameters. There are three cases. We offer two of them here. In the following definitions b_0 controls the domain size of the approximated functions and is roughly speaking the diameter of the domain. The constant ρ depends on n and β and is usually equal to 1 or a bit greater than 1.

Case1. $\boxed{\beta < 0,\ |n+\beta| \geq 1 \text{ and } n+\beta+1 \geq 0}$ Let $f \in E_\sigma$ and h be as in (1). Then

$$MN(c) := \begin{cases} \sqrt{8\rho}c^{\frac{\beta-n-1}{4}} \left\{ (\xi^*)^{\frac{n+\beta+1}{2}} e^{c\xi^* - \frac{(\xi^*)^2}{\sigma}} \right\}^{1/2} \left(\frac{2}{3}\right)^{\frac{c}{24\rho\delta}} & \text{if } c \in [24\rho\delta,\ 12b_0\rho), \\ \sqrt{\frac{2}{3b_0}} c^{\frac{\beta-n+1}{4}} \left\{ (\xi^*)^{\frac{n+\beta+1}{2}} e^{c\xi^* - \frac{(\xi^*)^2}{\sigma}} \right\}^{1/2} \left(\frac{2}{3}\right)^{\frac{b_0}{2\delta}} & \text{if } c \in [12b_0\rho,\ \infty) \end{cases}$$

where

$$\xi^* = \frac{c\sigma + \sqrt{c^2\sigma^2 + 4\sigma(n+\beta+1)}}{4}.$$

Case3. $\boxed{\beta > 0 \text{ and } n \geq 1}$ Let $f \in E_\sigma$ and h be as in (1). Then

$$MN(c) := \begin{cases} \sqrt{8\rho}c^{\frac{\beta-n-1}{4}} \left\{ \frac{(\xi^*)^{\frac{1+\beta+n}{2}} e^{c\xi^*}}{e^{\frac{(\xi^*)^2}{\sigma}}} \right\}^{1/2} \left(\frac{2}{3}\right)^{\frac{c}{24\rho\delta}} & \text{if } c \in [24\rho\delta,\quad 12b_0\rho), \\ \sqrt{\frac{2}{3b_0}} c^{\frac{1+\beta-n}{4}} \left\{ \frac{(\xi^*)^{\frac{1+\beta+n}{2}} e^{c\xi^*}}{e^{\frac{(\xi^*)^2}{\sigma}}} \right\}^{1/2} \left(\frac{2}{3}\right)^{\frac{b_0}{2\delta}} & \text{if } c \in [12b_0\rho,\ \infty), \end{cases}$$

where

$$\xi^* = \frac{c\sigma + \sqrt{c^2\sigma^2 + 4\sigma(1+\beta+n)}}{4}.$$

All the functions $MN(c)$ can be shown by a beautiful curve, called MN curve, whose lowest point corresponds to the optimal value of c. The value of $MN(c)$ reaches 1E-61 when δ is of reasonable size. Since $F(\delta)$ also contributes to the error bound, the actual error is much smaller than 1E-61.