A regression model describes a relation between a vector of d real valued input variables (features) $x = (x_1, x_2, ..., x_d)$ and a single real valued output variable y. Using a finite number n of training observations (data cases or data points) $(x_{(i)}, y_{(i)})$, $i = 1,2,...,n$ one wants to build a model F that allows predicting the output value for yet unseen input values as closely as possible.

Radial Basis Function interpolation

RBF was originally developed for scattered multivariate data interpolation (Hardy 1971). It uses a series of basis functions that are symmetric and centred at each sampling point. Radial basis functions are a special class of functions with their main feature being that their response decreases (or increases) monotonically with distance from a central point (Queipo et al. 2005). The centre, the distance scale, and the precise shape of the radial function are parameters of the model. RBF interpolation can be expressed as follows (Jin et al. 2002):

$$F(x) = \mu + \sum_{i=1}^{n} \lambda_i \phi\left(\left\| x - x_{(i)} \right\|\right) \tag{1}$$

where μ is either a polynomial model or a constant value; λ are coefficients calculated by solving linear equations; ϕ is a basis function, for which there are many different choices, such as biharmonic, multiquadric, inverse multiquadric, thin plate spline, Gaussian, etc. Detailed review on RBF methods can be found in (Powell 1987, Gutmann 2001).

For biharmonic basis functions

$$\phi(dist) = dist\,, \tag{2}$$

for multiquadric basis functions

$$\phi(dist) = \sqrt{dist^2 + c^2}\,, \tag{3}$$

for inverse multiquadric basis functions

$$\phi(dist) = 1\Big/\sqrt{dist^2 + c^2}\,, \tag{4}$$

and for polyharmonic basis functions

$$\phi(dist) = \left(dist^2 + c^2\right)\ln\left(\sqrt{dist^2 + c^2}\right) \tag{5}$$

where the shape parameter c is kept constant, e.g. as 1 (Acar & Rais-Rohani 2009) or as $1/n$ (Colaco et al. 2007). And the μ is defined as a constant value – mean of y:

$$\mu = \frac{1}{n}\sum_{i=1}^{n} y_i\,. \tag{6}$$

Gaussian basis functions are defined as follows

$$\phi(dist) = \exp\left(-\frac{dist^2}{2\delta^2}\right) \tag{7}$$

where δ is the radius (also called smoothing parameter).

In some cases in order to avoid matrix singularity the RBF may be augmented by including a polynomial function such that

$$\mu = \sum_{j=1}^{m} b_j\, p_j(x)\,, \tag{8}$$

where m is the total number of terms in the polynomial and b_j, $j = 1,2,\ldots,m$ is the corresponding coefficient. A detailed discussion on the polynomial functions that may be used can be found in (Krishnamurthy 2003).

As now the equation (1) is underdetermined (there are more parameters to be solved than the number of equations created), the orthogonality condition is further imposed on coefficients λ as

$$\sum_{i=1}^{n} c_i p_j(x_{(i)}) = 0, \quad for\ j = 1,2,...,m. \tag{9}$$

Combining equations (1) and (9) in matrix form gives

$$\begin{bmatrix} A & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} \lambda \\ b \end{bmatrix} = \begin{bmatrix} y \\ 0 \end{bmatrix}, \tag{10}$$

where $A_{ij} = \phi\left(\left\| x_{(i)} - x_{(j)} \right\|\right), i = 1,2,...,n,\ j = 1,2,...,n,$ $P_{ij} = p_j(x_{(i)}), i = 1,2,...,n,\ j = 1,2,...,m,$ $\lambda = [\lambda_1 \lambda_2 ... \lambda_n]^T$, and $b = [b_1 b_2 ... b_n]^T$. Equation (10) consists of (n + m) equations and its solution gives coefficients λ and b for the RBF in the form of (1).

References

1. Acar E., Rais-Rohani M. Ensemble of metamodels with optimized weight factors, Structural and Multidisciplinary Optimization, Vol. 37, No. 3, Springer, 2009, pp. 279-294
2. Colaco M.J., Dulikravich G.S., Sahoo D. A comparison of two methods for fitting high dimensional response surfaces, Inverse Problems, Design and Optimization Symposium, Miami, Florida, USA, 2007, 8 p.
3. Gutmann H.-M. A radial basis function method for global optimization, Journal of Global Optimization, Vol. 19, 2001, pp. 201-227
4. Hardy R.L. Multiquadratic equations of topography and other irregular surfaces. Journal of Geophysical Research, Vol. 76, 1971, pp. 1905-1915
5. Jin R., Chen W., Sudjianto A. On sequential sampling for global metamodeling in engineering design. Proceedings of ASME Design Engineering Technical Conferences and Computers and Information in Engineering Conference, Montreal, Canada, ASME, 2002, 10 p.
6. Krishnamurthy T. Response surface approximation with augmented and compactly supported radial basis functions. The 44th AIAA/ASME/ASCE/AHS/ASC structures, structural dynamics, and materials conference, Norfolk, VA, 2003
7. Powell M.J.D. Radial basis functions for multivariable interpolation: a review, Algorithms for Approximation, Mason J.C., Cox M.G. (eds.), London, Oxford University Press, 1987
8. Queipo N.V., Haftka R.T., Shyy W., Goel T., Vaidyanathan R., Tucker P.K. Surrogate-based analysis and optimization. Progress in Aerospace Sciences, Vol. 41, Elsevier, 2005, pp. 1-28