Comparing different interpolation methods on two dimensional test functions

Thomas Mühlenstädt, Sonja Kuhnt

February 19, 2009

Keywords: Interpolation, computer experiment, Kriging, Kernel interpolation, Thin plate spline, Natural neighbor interpolation.

Abstract

In the context of computer experiments a common way of dealing with expensive simulation models is to evaluate the simulation at a number of well designed input values and to replace the simulation by an easy to calculate surrogate model, which has been fitted to the observations. Then the surrogate model is used for optimization, sensitivity analysis or other applications at hand. As for computer experiments there is usually no random error the surrogate model has to interpolate the observations. In the literature there exist different multivariate interpolation methods which can be applied as surrogate model. The aim of this talk is to provide a comparison of four of these: Kriging, Kernel interpolation, Natural Neighbor interpolation and Thin Plate splines. We give suggestions, when to use which method.

The interpolation method commonly used for modeling computer experiments is *Kriging* [Santner et al. (2003)]. Kriging can be considered as an adaption of least square regression to the interpolation task by assuming a special correlation structure, defined by a parametric correlation function depending on the input points of the computer experiment. The correlation parameters have to be estimated, for example by maximum likelihood approaches. Kriging is applied in many practical situations and is well known for it's high prediction accuracy.

As an alternative [Mühlenstädt and Kuhnt (2009)] just recently suggested *Kernel interpolation*, consisting of two steps: First, a piecewise linear polygon is fitted to the data. As this polygon is not smooth and only defined for points inside the convex hull, the linear functions of the polygon are not

just considered locally for the corresponding simplex but globally. Then the linear functions are weighted in an appropriate way in order to obtain a single prediction value. In one dimension a piecewise linear polygon is uniquely defined. But in higher dimensions the polygon depends on the underlying triangulation used. Here, the Delaunay triangulation is used [Okabe et al. (2000)]. Under certain conditions for the weighting process it can be shown that this results in an interpolation function which is differentiable and not only defined for points inside the convex hull.

Natural neighbor interpolation was proposed by [Sibson (1980)]. It is defined in terms of the Voronoi diagram. The Voronoi diagram defines the natural neighbors of the sample input points for a prediction point. Then for interpolation, a weighted average of the responses of the natural neighbor points is calculated.

Thin plate splines [Micula (2002)] are considered to be a multidimensional extension of the natural cubic spline, which is known to have an optimal smoothness property in one dimension. In two or higher dimensions the solution to the underlying optimization problem is not a piecewise polynomial but a special case of interpolation methods using radial basis functions.

These interpolation methods are compared on a set of two dimensional test functions. The test functions are searched in literature and chosen to represent different typical behavior.

References

Mühlenstädt, T. and Kuhnt, S. (2009). Kernel interpolation. Technical report, Faculty of Statistics, Technische Universität Dortmund, Dortmund, Germany.

Micula, G. (2002). A variational approach to spline functions theory. *General Mathematics*, 10(1):21–50.

Okabe, A., Boots, B., Sugihara, K., and Chiu, S. (2000). *Spatial Tessellations, Concepts and Applications of Voronoi Diagrams.* Wiley Series in Probability and Statistics. Wiley, Chichester.

Santner, T., Williams, B., and Notz, W. (2003). *The Design and Analysis of Computer Experiments.* Springer Series in Statistics. Springer Verlag, New York.

Sibson, R. (1980). A brief description of natural neighbor interpolation. In Barnett, V., editor, *Interpreting multivariate data*, pages 21–36. Wiley.