8th. World Congress on Computational Mechanics (WCCM8)
5th European Congress on Computational Methods in Applied Sciences and Engineeering (ECCOMAS 2008)
June 30 –July 5, 2008
Venice, Italy

Radial Basis Functions Performance on Large Scale Problems

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Key Words: *Radial Basis Functions, Metamodels, High Dimensionality Problems.*

ABSTRACT

Radial Basis Functions (RBF) are a powerful tool for multivariate scattered data interpolation. *Scattered* data means that the training points do not need to be sampled on a regular grid: in fact RBF is a proper *meshless* method. Since RBF are *interpolant* response surfaces they pass exactly through training points.

There exists a vast body of literature on both the theoretical and the computational features of RBF: for example refer to [1, 2, 3] for a detailed treatment of the subject.

RBF have an important application in the context of multiobjective optimization. In real case applications, it is not always possible to reduce the complexity of the problem and obtain a model that can be solved quickly. Usually every single simulation can take hours or even days. In these cases, the time to run a single analysis makes running more than a few simulations prohibitive and some other smart approaches are needed. A Design of Experiments (DoE) technique can be implemented in order to perform a reduced number of calculations. After that, these well-distributed results can be used to create an interpolating surface. This surface represents a metamodel of the original problem and can be used to perform the optimization without computing any further analyses.

The aim of this work is to study the RBF performance on large scale problems. In fact very often optimization problems involve a large number of input variables: for this reason it is very important to check the reliability of metamodeling tools in the high dimensionality limit.

In this work three different radial functions have been implemented in the RBF algorithm, all suited for large scale problems.

The scaling parameter determines the shape of the radial function: its value has to be set accordingly to the specific problem one is facing. The minimization of root-mean-square (rms) leave-one-out error is a suitable method for finding the optimum value of the scaling parameter. Therefore this method, proposed by [4], has been implemented as an automatic procedure for determining the proper setting of the scaling parameter.

The Singular Value Decomposition (SVD) algorithm has been used for solving the interpolation equations: SVD is a very powerful technique for solving a linear system of equations, even when dealing with numerically difficult situations.

In the first part of this work the RBF performance has been studied on two families of large scale problems: Sinusoid Family Problems and KUR Problems. Each problem is not fixed but rather belongs to a "family" because its dimensionality can be varied: in this way the effect of the increasing difficulty (as the number of input variables increases) can be studied.

Furthermore, also the size of the training set has been varied, in order to detect the minimum number of points guaranteeing reasonable performance on each problem.

The performance of the trained RBF has been evaluated on a brand new (and sufficiently large) dataset of points, the validation dataset. The measure of accuracy and computing time are reported and discussed.

In the second part of this work the RBF performance in terms of standard measures of accuracy and computational time has been evaluated on a set of standard test cases of both smooth and noisy multidimensional functions taken from [5], allowing to compare RBF with other standard metamodeling techniques.

According to the performed benchmark, RBF show a fair and reasonable performance even on large scale (high dimensionality) problems. Clearly the training set size has to be sufficiently large in order to guarantee a reasonable performance: the minimum size is problem-dependent, and is related to the problem complexity. The general trend is that performance improves as the training set size increases.

When the problem is too complex, clearly RBF cannot overcome that intrinsic difficulty. But probably in that case the problem is too hard to be tackled efficiently by metamodels technique in general.

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