

MODELLING OF 3 DIMENSIONAL SCALAR FIELDS REPRESENTED BY FUNCTION VALUES IN SCATTERED POINTS*

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Abstract

The phenomena of the real world exist in three dimensional space. The authors in the former years performed a research aiming at modelling the undersurface solids, cavities and strata. The present paper is the first publication concerning the continuation of this research. In this new activity, an attempt will be made to model scalar fields of different properties under and over the surface of the Earth.

The modelling process is influenced by the character of the source data which depends on the conditions of the data acquisition.

Especially in undersurface models

- it is very expensive to capture new data;
- there is no possibility to measure in the places of maximum and minimum;
- the values of arguments as well as of functions are determined with several types of uncertainties.

The methods to be applied should take into account the properties of the source data as well as the problems to be solved by the model.

After sketching the methods to be examined in the future, the method of local polynomials worked out by the authors is explained in detail. The gist of this approach is to divide the set of nodal points into M "units", composed by help of Voronoi polyhedrons. Each unit represents a polynomial of k -th degree (where k depends on the accuracy of the source data). The interpolation of a function value for a point P in the competency of the i -th unit's polynomial can be calculated as a weighted average of all the M polynomials for the argument x_P, y_P, z_P . The weight is growing when the distance of the unit is decreasing.

Keywords: spatial modelling, approximation, interpolation.

1. Introduction

As a result of our five year research activity in the fields of modelling subsurface solids and strata (in the last case, of course, we did not exclude the modelling of the Earth surface itself) (SÁRKÖZY 1989), (SÁRKÖZY 1990) on the basis of our theoretical contributions we worked out a program

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system suitable for three dimensional modelling of solids given by scattered points, cavities given by quasi-profiles, two and half dimensional modelling of strata given by their boundary surface points.

The initial conditions of our former studies, namely the assumption of homogeneity of bodies and strata given by their boundary points can be accepted in many practical cases but not generally. One step closer to the reality is the case when we suppose that the parameters of the material filling up the space are building scalar fields, which can be continuous in global sense or only locally. Although these conditions are more general than the former ones, even in this new phase of our research we do not aim to reach the complete generality, which would be the modelling of vector fields instead of scalar ones.

The demand on modelling of scalar fields is not a new idea in the geosciences. As examples we can hint at two classical problems: the determination of potential function of the gravity field of the Earth, or the modelling of temperature distribution in the toposphere. These two examples as methodological counterpoints very well illustrate the limits of suitability of scalar models. While the assumption of relative unchangeability in relation to the potential function from practical point of view is quite acceptable, the consideration of the dynamics of the atmosphere is demanded almost by all the problems. Hence the scalar modelling of potential function provides final results for the practice while the scalar model of the temperature is only an element of the vector field demanded by the practical tasks.

2. The Specific Character of the Modelling Process Considered

Both the undersurface and toposphere models rely on function values measured in randomly located points. These points are commonly characterized by uncertainties in the locations as well as in the function values. This statement is especially true in the case of undersurface models.

The undersurface data as a rule can be obtained as a result of drilling, which is a very expensive process and therefore in a lot of cases the models should be composed using relatively few input data.

A meaningful difference should be pointed out between the tasks to be solved and the interpolation problem well known and worked out in detail in the surveyors' practice: the creation of digital elevation models. The good-quality DEM is built up on the basis of such not regularly (but also not randomly) located points, which truly reflect the features of the terrain. The surveyors or photogrameters really see the places of maximum or

minimum values of the "function", i. e., the tops of hills, the bottoms of valleys etc. and the well measured input data should contain these values.

We can encounter a completely different situation in the case of input data for the scalar field models in question. The places of extremal values of the functions are invisible, consequently, there is no reason to regard the measured maxima and minima as the extremal values of the function. With other words there is a certain probability that in the not measured places we can meet greater or smaller values than the measured maximum or minimum.

This fact should be underlined because of our conclusion which can be drawn from it: *such interpolation methods which determine the interpolated values as some weighted average of the measured values can not be used correctly in the tasks we have to solve.*

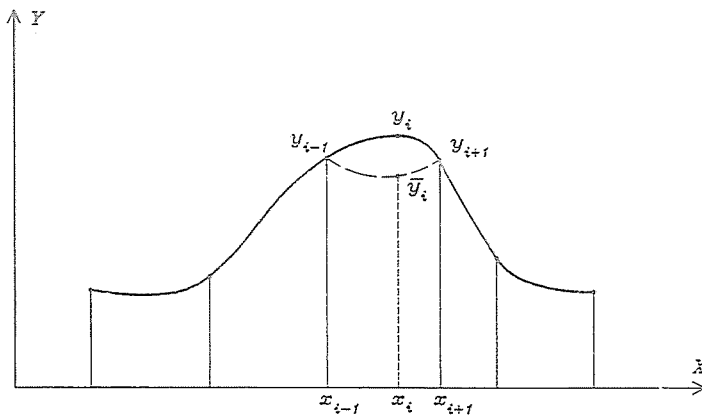


Fig. 1.

Fig. 1 illustrates our statement for the one-dimensional case. If the interpolated function value in point x_i , computed by some kind of average building, is denoted by \bar{y}_i then $\bar{y}_i \leq y_{i-1}$, $\bar{y}_i \leq y_{i+1}$ because of the nature of the average. If we fit a polynomial to the nodal points we get $y_i > y_{i-1} = y_{i+1}$. In our opinion, the scalar fields built up by the natural processes in most cases coincide with the latter approximation.

Let us once again dwell on the interpolation methods using average building. In the case of known extremal function values some of those can give excellent results, for example, the method of 'stolen territories'

(GOLD 1991). This method is based on the building of *Voronoi* polygons (polyhedrons in the three-dimensional case) around the nodal points. If we want to interpolate the function value of a new point, we should construct its *Voronoi* polygon based on the connection of the new point with the old neighbouring ones. The new polygon cuts out territories from the original polygons belonging to the nodal points which were connected with the new point. The weights related to these nodal point heights are the "stolen" or cut out territories. From geometrical point of view the method of *Voronoi* cells is suitable for 3D modelling, too. However, in this case it is also true that the use of *Voronoi* cells for interpolation by means of simple weighted averages can give good results only in the case when we know the extremal values of the function. Similar remarks can be made on the kriging (STEINER, 1990), the probably most popular interpolation method in geostatistics. Our misgivings in relation of averages by missing extrema henceforward stay in force and would be diminished only if the possibility of unlimited densification of the measured points could be easily realizable. But in the field of undersurface investigations there exists an opposing situation: the drillings are very expensive and the modelling should be effectively fulfilled on the basis of incomplete information. In such circumstances we can not accept the kriging as a universal tool for undersurface modelling.

For a part of the problems considered (e.g. for spreading of contaminating concentrations in undersurface spaces) we can find physical-mathematical models which describe under certain conditions for a constant time the iso-surfaces of the phenomenon in question. The finding of such laws (if they exist) can significantly improve the quality of interpolation.

All physical points situated under or over the surface of the Earth are arguments (places) of an infinite number of scalar fields. A lot of practical tasks demand the analysis of interaction of several fields. Our methods should be suitable for fulfilling the quantitative analysis of these interactions. For example we can consider the task of oil investigation. The decision about the location and volume of the oil should be based on the comparison and correlation of the fields of porosity, permeability, temperature, pressure etc.

The common analysis of several fields at the same time should call our attention to the uncertainties in each model and their influences on the result.

We can distinguish global fields (as that of the temperature) and local fields (as that of the sulphur concentration of a coal bed). In the case of local fields assuming that the samples are spread over the object, first of

3. The Methods to be Applied

After the determination of natural (in local case) or artificial (in global case) boundaries the interpolation of the function describing the scalar field can take place.

In the computational mathematics we can find three principal methods of interpolation (DANILINA 1988):

- interpolation by polynomials,
- interpolation by trigonometric functions,
- interpolation by exponential functions.

As the general solution our choice fell on the interpolation by polynomials, paying special attention to the degree of the polynomials and the grouping of the neighbouring nodal points. We will return later to the explanation of this method .

Our further aim is to use the series composed from exponential functions for modelling of physical phenomena. We can suppose that the natural circumstances produce bias in the boundary conditions which in turn produces local distortions in the shape of phenomenon in relation to the modelling function. In such cases the modelling process can be performed in two steps: first we describe the global model by "regular" functions, secondly the discrepancies by superposing proper series.

The great challenge of interpolation by functions is in the reduction of the number of parameters to be stored. Although if we take anomalies into consideration the demand in storage places can grow significantly, in many cases we can find tasks of lower resolution which are satisfactorily modelled by the properly parametrized original interpolating function. At the same time it is unquestionable that the compilation of an expert system with a great number of interpolating functions is a very hard work.

Whatever approach will be chosen for the modelling of scalar fields, in most of the practical tasks there is a demand to interpolate the model values in the nodes of a regular grid. While in the case of interpolation by functions the grid system is only a temporary one, making the use of different application programs possible, in the case of interpolation by polynomials the grid structure can play the role of storage structure, too.

For engineering purposes the visualization of the models is especially important. The perspective display of the iso-surfaces built up by points of equal function values and the bodies bounded by these surfaces can be of significant interest.

Our scalar models can be used also for modelling dynamic phenomena if we have measured function values related to different points of time. In these cases we should display the "moving" surfaces and by their help the trend of the process.

The uncertainties in modelling the bodies bounded by iso-surfaces appear especially significantly when similar bodies originated from other scalar fields intersect. For determination of uncertainties in the resulting section we plan to use the tools of the fuzzy sets' theory.

4. Approaching our First Method

The values u_i of the space scalar function $f(\mathbf{r})$ are given in the points \mathbf{r}_i ($i = 1, 2, \dots, M$). Our task is the approximate determination of the $f(\mathbf{r})$ function values in the not measured points \mathbf{r} . Let us designate the approximating function in general as f_M

$$f(\mathbf{r}) \approx f_M(\mathbf{r}, \mathbf{a}), \quad \mathbf{a} \in \mathbb{R}^n, \quad (1)$$

where the parameters \mathbf{a} are traced back to the known data u_i, \mathbf{r}_i . In the books on computational mathematics e.g. (DANILINA 1988, DEMIDOVICH 1987) we can find a lot of methods of different properties for the one dimensional case. We can easily generalize most of these methods for the three-dimensional case, however, most of them will not work effectively enough. The solution of multidimensional problems is much more difficult because of the extended sizes, they can produce storage shortages even in the process of computations. The effective methods are based as a rule on the special properties of the task (e.g. the given points have a regular spatial arrangement, the type of the function $f(\mathbf{r})$ is known, etc.).

When choosing our method of approximation we should consider the errors in the given function values. In several cases, as mentioned earlier, the location vectors \mathbf{r}_i can be affected by errors, too. These facts indicate that the choice of a smoothing approximation is more advantageous in most of the cases than that of an interpolating one. The smoothing function which only approximates the measured values of the field is more advantageous even if the latter are errorless but taken too sparsely in relation to the changeability of the function. In such cases the smoothing expresses better the main characteristics of the field than the interpolation does.

We should decide whether a global or a local method will be more appropriate for the first experiment (do not confuse the notions global and local methods with global and local fields). The global methods have the advantages of handling the task as a whole. The global approximating functions provide the continuity, unbrokenness and proper smoothness for the entire model space. However, these methods have the drawback that they demand the solution of very large systems which can cause several

numerical and computational problems, furthermore without the knowledge of the characteristic features of the field it is very difficult to select the proper, most effective basic functions for the approximating expression (DETREKÖI 1991). In the case of local methods we have to solve a lot of small tasks which is very easy to do even if we consider a high level of accuracy. The problems occur by the linkage of the elementary models, it is not so easy to assure the continuity and the unbrokenness. These methods do not yield a proper smoothness in many cases.

By proper combination of local and global methods we can get procedures of rather nice behaviour. As an example we can refer to the well-known method of splines which can be used both for smoothing and for interpolation. The use of splines by regularly located nodes, even if the sizes are large, is very efficient but in the case of scattered points one can face significant computational difficulties.

The locally independent interpolating methods (STEINER 1990) are very simple and can easily be used when the nodal points are located in a regular grid. The main computational advantage of these methods is the small number of input data in model building and interpolation. The criteria of continuity, unbrokenness or the continuity of second derivatives can be realized by the selection of a proper weighting function. In case of irregularly located nodal points the method is difficult to use.

Also in the case of spatial scattered nodal points one can build up a usable method by means of estimation on the basis of local models.

For each point \mathbf{r}_i in which the value u_i of the in general unknown function $f(\mathbf{r})$ is given we can construct a $G_i(\mathbf{r})$ approximating function which is properly near to the original function in the neighbourhood of the point. The function should be defined everywhere over the global model and give good approximation at least for the neighbouring points.

In a random point \mathbf{r} we can compute the approximating values from each local function

$$u_{i,r} = G_i(\mathbf{r}), \quad (i = 1, 2, \dots, M). \quad (2)$$

The values $u_{i,r}$ approximate the value of $f(\mathbf{r})$ in different measure. The accuracy of the approximation depends on the distance of the point \mathbf{r} from the central point \mathbf{r}_i of the function $G_i(\mathbf{r})$.

We can consider the $u_{i,r}$ values the estimations of the function value $f(\mathbf{r})$ by the local model G_i and therefore they are random variables. The distribution of these variables is unknown, but some of their statistical characteristics (e.g. dispersion) can be estimated. The dispersion can be estimated on the basis of the discrepancies at the point \mathbf{r}_j

$$\delta_{ij} = G_i(\mathbf{r}_j) - u_j. \quad (3)$$

If we know the probability characteristics of the values $u_{i,r}$, out of them (their number is M) we can compute the estimate of the mathematical expectation of the function value $f(\mathbf{r})$, denoted by \hat{u}_r , using some method of estimation. In the simplest case this estimate can be expressed by means of weighted average building:

$$\hat{u}_r = \frac{\sum_{i=1}^M s_i \cdot u_{i,r}}{\sum_{i=1}^M s_i}, \quad (4)$$

where the s_i weights are computed from the $\sigma_{i,r}$ dispersions

$$s_i = \sigma_{i,r}^{-2}. \quad (5)$$

Of course instead of the estimate (4) we can also use other methods of estimation; for example the robust estimation can be used.

4.1 The Local Modelling

For the construction of local models the usual methods of function approximation can be applied. The simplest is the use of polynomials with three unknowns:

$$P_n(x, y, z) = \sum_{i=0}^n \sum_{j=0}^{n-i} \sum_{k=0}^{n-i-j} a_{ijk} \cdot x^i \cdot y^j \cdot z^k. \quad (6)$$

Mostly the use of third degree polynomials seems to be expedient, they have twenty coefficients, that means at least the same number of nodal points should be available for their computation.

To determine the function $G_i(\mathbf{r})$ approximating in the neighbourhood of point \mathbf{r}_i , the necessary number of nodal points should be selected from the same region. The simplest way of selection is the choice of a proper distance or that of coordinate-intervals. In this case we should consider the equal distribution of nodal points taken into account. We can get an improved but much more complicated method of selection using the neighbouring and second neighbouring nodal points indicated by the *Voronoi* polyhedrons (BOWYER 1981).

We usually apply smoothing methods for determining approximating functions, but possibly we can enforce the fulfillment of the $u_i = G_i(\mathbf{r}_i)$ condition in the point \mathbf{r}_i . The coefficients of the function G_i should be

computed by some kind of adjustment, mostly by method of least squares. In the adjustment by choice we can use weights, which depend on the distances.

The locally approximating $G_i(\mathbf{r})$ function approximates the $f(\mathbf{r})$ well inside the region determined by the nodal points used. Outside this region the error of approximation grows. By polynomial approach the error of approximation in the extrapolation region grows rapidly and tends to the infinity.

4.2 Computation of Dispersions and Weights

After the construction of the $G_i(\mathbf{r})$ functions we can compute the δ_{ij} discrepancies and the respective d_{ij} distances according to (3). If we divide the greatest distance into intervals, we can estimate the σ_d^2 dispersion square related to the average of distances in one interval:

$$\sigma_d^2 = \frac{1}{K} \sum_{i=1}^K \delta_i^2, \tag{7}$$

where K is the number of distances in the particular interval. If we draw the graph of the d, σ_d^2 pairs we can get the average dispersion of the $u_{i,r}$ values estimated by the $G_i(\mathbf{r})$ functions in terms of the distance.

In general, the $\sigma_d^2(d)$ function can be well estimated by the expression

$$\sigma_d^2(d) \approx \sigma_m^2 + a \cdot d^b + c \quad , \quad a, b, c \geq 0, \tag{8}$$

where σ_m is the dispersion of the known function values in the nodal points, the parameters a, b, c can be computed from the related pairs d, σ_d^2 . If by the construction of local models we prescribe the equality $G_i(\mathbf{r}) = u_i$ in the point \mathbf{r}_i then $c = 0$.

It sometimes occurs that in different directions we get different dispersions. In such cases we should introduce a new distance notion instead of the Euclidian one according to the following expression:

$$d_{ij} = [(\mathbf{r}_j - \mathbf{r}_i)' \mathbf{D} (\mathbf{r}_j - \mathbf{r}_i)]^{\frac{1}{2}}. \tag{9}$$

In this case the elements of the matrix \mathbf{D} should be determined together with the remaining parameters. Now, we can eliminate the use of distance intervals and we can estimate the dispersion from the discrepancies δ_{ij} and δ_{ji} belonging to the distances $d_{ij} = d_{ji}$:

$$\sigma_{d_{ij}}^2 = \frac{1}{2} (\delta_{ij}^2 + \delta_{ji}^2). \tag{10}$$

If the spatial distribution of the \mathbf{r}_i nodal points is highly unequal, then instead of a global $\sigma_d^2(d)$ function, we may apply separate dispersion functions $\sigma_{id}^2(d)$ for each local model.

We can compute the weights from the dispersions by the following expression:

$$s(d) = \frac{\sigma_0^2}{\sigma_d^2}. \quad (11)$$

4.3 Compilation of the Global Model

On the basis of local models we can compute the different values of $u_{i,r}$ in any space point \mathbf{r} and for each of them determine the dispersion and the weight by means of formulas (8) and (11). The series

$$u_{i,r}; \quad \sigma_{i,r}, \quad (i = 1, 2, \dots, M) \quad (12)$$

can be considered as indirect observations of different accuracy for the quantity $f(\mathbf{r})$. Consequently, the mathematical expectation \hat{u}_r and its dispersion $\sigma_{\hat{u}}$ can be determined by some method of parameter estimation. In general the correlation of the quantities $u_{i,r}$ can be neglected. The simplest method for estimation of \hat{u}_r is the weighted average

$$\hat{u}_r = \frac{\sum_{i=1}^M s_i \cdot u_{i,r}}{\sum_{i=1}^M s_i}, \quad (13)$$

which corresponds to the estimation by the least squares method. Among the quantities $u_{i,r}$ values with large errors can occur though they have small weights in general, nevertheless it can be reasonable to apply robust estimation methods (HAMPEL 1986).

The models $G_i(\mathbf{r})$ located far from the point \mathbf{r} have only a very small influence on the value of (13) which can be neglected introducing a distance of influence T interpreted as (9). The local models which are further as T should not be taken into account in the estimation of \hat{u}_r . This fact increases the efficiency of the computations.

The global approximating function $f_M(\mathbf{r})$ compiled using our method is continuous and unbroken over the complete region of definition, in the case of using a proper estimation method (e.g. (13)) the second derivatives are also continuous and the approximating function is smooth enough.

4.4 Numerical Illustration

For illustration we have chosen a very simple one-dimensional example. Let us consider the function $\sin x$ as unknown in respect of the task to be solved. The measurements will be substituted by values of $\sin x$ computed in 25 points, randomly selected in the interval $(0, 10)$. The computed function values are considered as errorless and the method will be used for interpolation.

For local models we have determined third-order polynomials in the way that besides the points P_i the neighbouring four points have been involved into the computations. On the basis of these five points we have calculated four coefficients for each polynomial by means of least squares method using weights reciprocal to the distances. This weighting results in the fitting in the local model $G_i(x)$ at the point P_i , while in the neighbouring points the "measurements" are only approximated by $G_i(x)$. In *Fig. 2* we display two local models belonging to two neighbouring points. It is visible that moving away from the nodal points the local model can produce significant discrepancies.

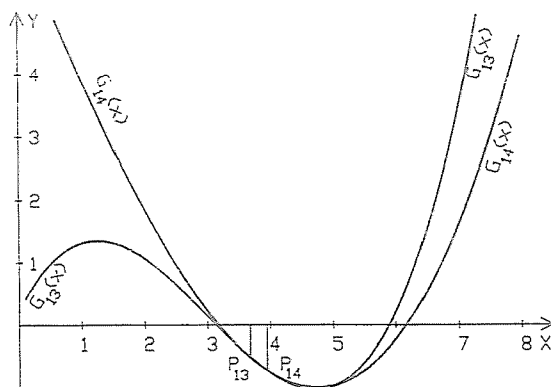


Fig. 2.

The variances in terms of distances have been computed by formula (10) and the coefficients a and b of formula (8) have been determined by means of least squares. *Fig. 3* shows the suitability of the chosen weighting function rather well.

The global model and the 25 nodal points have been shown in *Fig. 4*.

The average accuracy of the estimated $f_{25}(x)$ values was characterized by the dispersion computed from the differences $f_{25}(x) - \sin x$ taken over

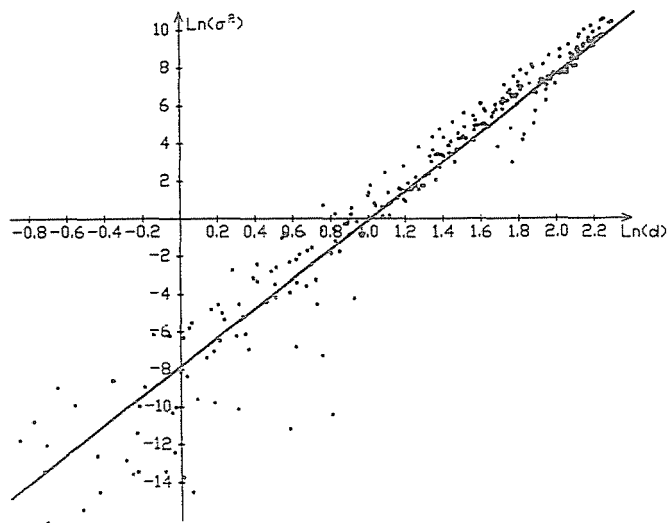


Fig. 3.

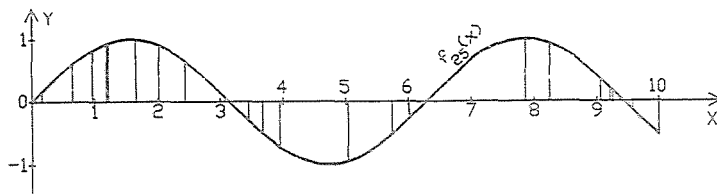


Fig. 4.

the whole interval in 0.1 steps. The result is

$$\sigma_{f_{25}} = 0.0068.$$

Because of the unequal distribution of nodal points the largest errors origin around $x = 7$ where the nodal points are far from each other. We compared our results with the interpolation by splines constructed at the same nodal points. In average our method gives a slightly better result than the spline interpolation, but in the case of few nodal points our results are much better (see Fig. 5).

Similarly to the global method, the dispersion of the spline function has been computed:

$$\sigma_{\text{spline}} = 0.0308,$$

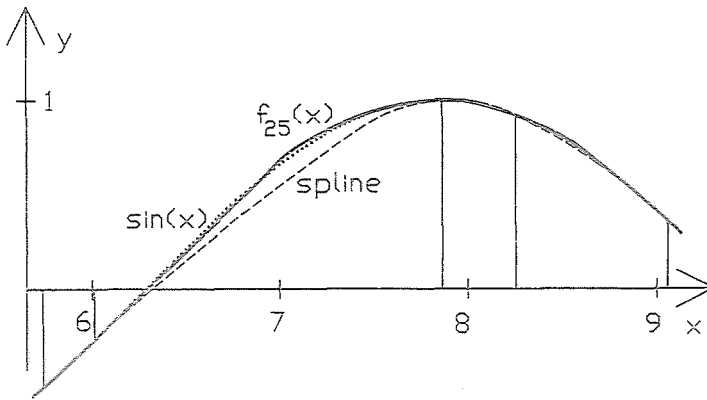


Fig. 5.

which is more than four times larger than the dispersion of the global method.

Of course from this small example we cannot draw decisive conclusions, but we can state the usability of the method, which can be applied first of all for construction of grids with adequate density.

5. Conclusions

The numerical experiment shows that our method, the global model building from local ones is suitable for the realization of 3 D modelling.

On the basis of our first experiences we have found that further investigations are necessary to answer the following questions:

- a) what other kind of approximating functions (in addition to the polynomials) can be used efficiently for the local modelling;
- b) whether there is a reason to apply weights by fitting the local functions to the nodes, if the answer is yes what kind of weights should be taken into account;
- c) how does the distance of influence depend on the type of the local functions, on the weighting functions applied for the global approximation and on the characteristics of the scalar field;
- d) what characteristics can the general features of the scalar field describe and what their influence is on the desirable density of samples?

Even if we can give only partial answers on these questions our method becomes suitable for practical applications.

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