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Neural Network Methods in Surface Modeling. Preliminary Notes

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ABSTRACT. *Surface modeling* consists of estimation of a surface values at any unsampled location, based on a set of samples, which usually have a non-uniform distribution. The problem is also known as *spatial interpolation*. Spatial interpolation is a key feature of *Geographic Information Systems (GIS)*. The surface-modeling problem occurs in many fields: geology, geophysics, meteorology, environmental sciences, agriculture, engineering, economy, medicine, social sciences, etc.
The main current approach in spatial interpolation nowadays is geostatistical. *Geostatistics* is neither the only nor the best spatial interpolation method. Actually there is no "best" method, universally valid. Choosing a particular method implies to make assumptions. The understanding of initial assumption, of the methods used, and the correct interpretation of the interpolation results are key elements of the spatial interpolation process.
A powerful alternative is the application of *soft computing methods*. They offer the potential for a more flexible, less assumption dependent approach. *Artificial Neural Networks (ANNs)* are well suited for this kind of problems, due to their ability to handle non-linear, noisy, and inconsistent data.

1. INTRODUCTION

Surface modeling consists of estimating the values of a surface at any location, based on a set of (x_i, y_i, z_i) samples, which usually have a non-uniform distribution. Input data represent z values samples at (x, y) locations, usually called control points. The problem is also known as spatial interpolation. Spatial interpolation is a key feature of *Geographic Information Systems* (*GIS*). Surface modeling problem occurs in many fields: geology, geophysics, meteorology, environmental sciences, agriculture, engineering, economy, medicine, social sciences, etc. Some typical z variables that require surface modeling in geology are grade of elements, or depths of formation boundary. **Hypersurface modeling** is a generalization of surface modeling, in a 4 (or higher) dimensions space [11], [21], [22], [23].

In order to estimate the value of a variable at a new location, based on known values at the control points, we must assume that there is some relationship between the two types of values. They must not be completely independent. The transformation of isolated data in functional variables is made by interpolation. The interpolation correctness (accuracy) highly depends on the variability of the given z samples. Regardless of the interpolation method we use, better estimations are obtained in areas of low variability. That is why the study of local anomalies of variability is very important.

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The interpolation approach can be:

- *global* – attempts to discover and explain the behavior of a spatial function using all available data, and assuming that its behavior has a certain periodicity,
- *local* – attempts to reconstruct a spatial function only based on knowledge of nearby samples.

The use of a surface modeling software offers many advantages:

- large sets of data can be rapidly process,
- different models can be test,
- interpolation results can be stored and post process,
- a large range of presentation forms can be used.

Two classes of methods are used in surface modeling:

- *triangulation,*
- *gridding.*

Triangulation requires a tessellation by an optimal network of triangles, with control points at all apices. The triangles set represent an approximation of the surface.

A regular array of data is generated by gridding, z parameter being estimated at the grid nodes, based on a set of control points. Gridding offers at least two major advantages over triangulation:

- it is not necessary to sample the extreme points of the surface to be estimated,
- subsequent operations on grid data are facilitated.

Gridding is not an aim by itself; it is a preliminary step in geological data processing. Surface modeling in geology is used in order to obtain geological models, which can finally lead to useful elements reserve estimation [21].

2. Current Surface Modeling Approaches

The main current approach in spatial interpolation nowadays is **geostatistical**. A large number of books, papers, scientific meetings are dedicated to geostatistics and its application. Geostatistical methods have been in use for more than three decades, and a large number of researchers and professionals work in geostatistics.

Geostatistics was originated by the application of statistical methods to the study of geological phenomenon. A complex theory was later developed, being applied not only to earth sciences, but also to many other areas: natural, economic, social phenomenon, among others. Geostatistics uses regionalized variables, which values are not random, but neither are exactly describable by any geometric function. A regional variable may consist of a drift component and residual. Actually a third error component has to be considered [28].

Geostatistical interpolation estimates values by *kriging*. Kriging is an exact interpolator which uses geostatistical techniques to calculate the autocorrelation between data points, and produce a minimum variance unbiased estimate, taking in consideration the spatial configuration of the phenomenon.

Geostatistics is neither the only nor the best spatial interpolation method. Actually there is no "best" method, universally valid [5], [17], [21], [25]. The choice of interpolation method may vary according to:

- the type and nature of the data,
- the aim of modeling.

Choosing of a particular method implies to make assumptions. The understanding of initial assumptions, of the methods used, and the correct interpretation of the interpolation results are key elements of the spatial interpolation process.

Comparison of methods can be made based on criteria as:

- goodness of representation (errors in honoring control points),
- dependence on data distribution,
- number of control points that can be handled,
- ease of implementation,
- speed of computation.

An alternative approach to surface modeling problem, is the application of **soft computing** methods. They offer the potential for a more flexible, less assumption dependent approach.

Currently, **surface modeling software** implement the following spatial interpolation methods:

- *Geostatistics (ordinary kriging, simple kriging, universal kriging),*
- *Inverse Distance Weighting (IDW),*
- *Polynomial Regression,*
- *Local Polynomial,*
- *Moving Average,*
- *Minimum Curvature,*
- *Natural Neighbour,*
- *Radial Basis Function (RBF).*

The range of available methods is much more restricted in the case of hypersurfaces: usually only kriging and IDW are implemented. The only available soft computing method for surface modeling is RBF. Users have little control over RBF techniques using commercial surface modeling software, and practically no explanation (tutorial) is given. None of the soft computing method is available for hypersurfaces modeling, in commercial software products.

3. Soft Computing Methods in Surface Modeling

Soft Computing (*SC*) differs from conventional (hard) computing in that, unlike hard computing, it is **tolerant of imprecision**, **uncertainty**, **partial truth**, and **approximation**. Human mind, unlike present day computers, possesses a remarkable ability to store and process information which is pervasively imprecise, uncertain, and lacking in cathegoricity.

The principal constituents of SC are *Fuzzy Logic* (FL), *Neural Computing* (NC), *Evolutionary Computation* (EC) *Machine Learning* (ML) and *Probabilistic Reasoning* (PR), with the latter subsuming belief networks, chaos theory and parts of learning theory. SC is a partnership in which each of the partners contributes a distinct methodology for addressing problems in its domain. The principal constituent methodologies in SC are complementary rather than competitive. In many cases a problem can be solved most effectively by using FL, NC, GC and PR in combination rather than exclusively [27]. A particularly effective combination is what has come to be known as "*neurofuzzy systems*". SC is not replacing hard computing, it is an alternative more or less appropriate, depending on specificity of the problem to solve. SC is likely to play an especially important role in science and engineering.

Fuzzy logic is basically a superset of conventional (Boolean) logic that has been extended to handle the concept of partial truth values between "completely true" and "completely false".

Evolutionary computation is based on genetic algorithms that use a population of "individuals" competing against one other in relation to a measure of fitness. At each stage of the process some individuals will breed, others will die off, and new individual will arise through combination and mutation.

4. Artificial Neural Networks

Artificial Neural Networks (ANN) are information processors, trained to represent the implicit relationship and processes that are inherent within a data set [1], [8], [9], [18], [19]. Geological data require finding spatial relationship between input, since other areas require the identification of both spatial and temporal relationships (meteorology, environmental sciences, etc.).

The original inspiration for ANN was biological; so much of the terminology of ANN reflects this biological heritage. The basic structure of an ANN consists of a number of simple processing units, also known as neurons (nodes). The basic role of each node is to take the weighted sum of the inputs and process this through an activation function. A connection joins the output of one node to the input of another. Each link has a weight, which represents the strength of the connection.

The values of all the weights in a network represent the current state of learning of the network, in a distributed manner. These weights are altered during the training process to ensure that the inputs produce an output that is close to the desired value.

The arrangement of nodes and interconnecting links is called the *architecture*. In many architectures, nodes are arranged in layers, whereby there are no links between nodes in the same layers. Data enters the network through the inputs units of the input layer, are fed forwards through successive hidden layers and emerge from the output units in the output layer of the network. Because the flow of information is in one direction only, from input to output units, this is called a *feedforward network* (or *Multi-Layer Perceptron – MLP*).

A *learning function or algorithm* is used to adjust the weights of the network during the training phase. Training can be supervised or unsupervised. Hybrid training techniques and reinforcement learning are also used.

There are many learning algorithms for training a MLP, being *backpropagation* (BP) one of the most common. During the learning period both the input and output vector are supplied to the network. The network then generates an error signal based on the difference between the actual output and the target vector. The error is used to adjust the weights of the network adequately. The error for a hidden processing unit is derived from the error that has been passed back from each processing unit in the next forward layer. The total error for a hidden unit is the weighted sum of the error for the error contributions from each individual unit in the next forward layer.

Following training, input data are then passed through the trained network in its non-training (recall) mode, where they are transformed within the hidden layers to provide the modeling output values.

ANN can be implemented in countless way, depending on:

- how neurons are arranged into layers or groups,
- how links joining neurons allow data flow in different directions through the network,
- how neurons activate,
- how network is trained.

5. ANN in Surface Modeling

ANN have emerged as an option for spatial data analysis a decade ago. Training data in an ANN development are the observation samples used to derive the predictive model. The independent (predictor) variables are known as the input variables, and the dependent variables (response) are known as the output variables. In supervised learning, an ANN makes use of the input variables and their corresponding output variables to learn the relationship between them. Once found, the trained ANN is then used to predict values for the output variables given some new input data set. For unsupervised learning, an ANN will only make use of the input variables and attempts to arrange them based on their properties, hopefully in a way that is meaningful to the analyst.

Fuzzy logic was also used in dealing with spatial data analysis problem. Fuzzy systems make use of human knowledge, past experience or detailed analysis of the available spatial data in order to build the fuzzy rules. They have the ability to interpret the analysis model built and to handle vagueness and uncertainty in the data. The data analysis model can be easily changed by modifying the fuzzy rule base.

ANN and fuzzy logic are complementary technologies in designing an intelligent spatial data analysis approach. They have been combined in many different ways, i.e.:

- *Concurrent Neuro-Fuzzy* – ANN and Fuzzy systems work together on the same task, without influence on each other,
- *Fuzzy Neural Networks* – use fuzzy methods to enhance the learning capabilities or performance of ANN,
- *Cooperative Neuro-Fuzzy* – use ANN to extract rules,
- *Hybrid Neuro-Fuzzy* – ANN and Fuzzy are combined into one homogeneous architecture.

Wong and others use a cooperative neuro-fuzzy technique [26]. The technique makes use of the robustness and learning ability of the ANN to sub-divide and generalize from training data, using Self-Organizing Map (SOM), as unsupervised clustering technique, and BPNN. Then the learned underlying function is translated into fuzzy rules. This way a self-learning and self-explained spatial interpolation technique was put forward, and the interpretability and the ability of handling vagueness and uncertainty has enhanced the interpolation model, by using fuzzy rules.

Huang, Wong, and *Gedeon* use a dynamic fuzzy-reasoning-based function estimator [10]. They optimize functional parameters by genetic algorithms. The procedure operates on overlapping partition surfaces, obtained based on expert knowledge and interpretive judgment. The fuzzy-reasoning component extends the extrapolation and interpolation using non-linear weightings for the neighboring values, based on closeness and the directions of the deviation vectors, similar to human reasoning. Such fuzzy concepts can tolerate partial satisfaction of the preconditions and take into account the discrepancy in inferring the function values. It is an assumption-free, model-free and exact interpolator.

Lee, Cho, and *Wong* also work with partition surfaces, but independent, not overlapped [14]. They call this approach simply “divide-and conquer”. Partitions are obtained using interpretive judgment, based on external conditions. They apply then RBF networks on some partitions, and expert knowledge on others.

Demyanov and others combine ANN and geostatistics [3]. They use ANN with supervised learning, in a first step, to estimate large scale structures. The second step is the analysis of residuals, using geostatistics to model local spatial correlation. They also propose an incremental methodology, based an ANN only.

Gilardi and *Bengio* compare different machine learning algorithms applied to spatial data analysis [7]. They remark once again the preponderancy of geostatistical methods instead of machine learning models. They think a possible reason can be the difficulty of tuning the algorithm without a clear methodology and some prior information. This is arguable, as geostatistics' users have to deal with similar complicatedness.

Dubois and *Shibli* analyze the result of the scientific exercise of spatial interpolation SIC 97 [4]. They highlight the clear preference of the contributors for geostatistical methods, followed by soft computing methods. The statistics of the estimates which are the closest to the true values have been obtained by a fuzzy logic-based method, followed by neural networks, and locally adjusted polynomial function. However, geostatistics prove to be robust methods, honoring their large spread. Self-learning methods offer a promising future because of their ease with which multiple secondary variables can be included in the interpolation process, without the need to perform tedious cross-correlation modeling as is required by geostatistical methods.

Luo and *Dimitrakopoulos* underline that a major problem in mineral exploration and mineral resource assessment is the integration of geo-information from multiple sources and diverse nature in developing *mineral favourability indexes* (*MFI*) [15]. They prove that fuzzy logic provides a convenient framework to combine and analyze qualitative and quantitative data independently of their source or characteristics. A data-driven formulation for calculating MFI based on fuzzy analysis is developed. Geo-variables are considered fuzzy sets and their appropiate functions are defined and modeled.

Finally, *Whigham* describes 23 possible areas of research and development in spatial information field, in the 21^{st} century [24]. In the context of the current proposal, we find particularly interesting 3 of these areas: (1) dealing with "fuzzy boundaries", (2) the necessity of integrate global and local pattern detections into a common framework, and (3) spatial systems as integrators of data will further become integrator of technologies.

6. Conclusions

The progress made in spatial interpolation is usually presented only in journals or scientific meetings dedicated to statistics, mining, environmental etc. Users who have a different technical background often do not have in-depth knowledge of spatial interpolation methods. That is why the use of new techniques is often discouraging for newcomers.

When spatial interpolation methods are integrated in software tools, they are often implemented in such a rigid way that users have no real choice in selecting the best possible method, according to the true nature of data to process, and the aim of modeling. Moreover, many required parameters are fixed, without any possible way to modify them.
A major problem is the high cost of software dedicated to surface modeling and spatial data analysis. The cost is exponentially increasing in the case of integrated solutions for geological exploration and mining exploitation. It is definitely prohibitive for small and medium mining companies.

Laffan [13] signalized an important problem: ANN behavior is unpredictable because the training algorithms are not guaranteed to converge on a global solution, possibly ending training in a sub-optimal solution. Overfitting results from overtrained networks, and reduces the generalization of the network as a classifier. If the user can visualize training in a meaningful way, then these problems may be reduced. The visualization could also increase the understanding of the process, and possibly the confidence in the results. This way, ANN will not be used just as a black box. We think that graphic visualization will allow better interaction, and will increase usability. This is an important issue to work on, and a good opportunity to use our training and previous experience in the human-computer interaction field.

The above mentioned arguments are motivating the present research project, which is currently running in *Escuela de Ingeniería Informática* of *Pontificia Universidad Católica de Valparaíso* (Chile). The main objectives of our future work are:

- Developing a problem-oriented methodology for geological reserve estimation, mainly based on inductive learning algorithms,
- Developing a decision support system proposal for environmental monitoring networks.

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