A bottom-up strategy for uncertainty quantification in complex geo-computational models

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1. Introduction

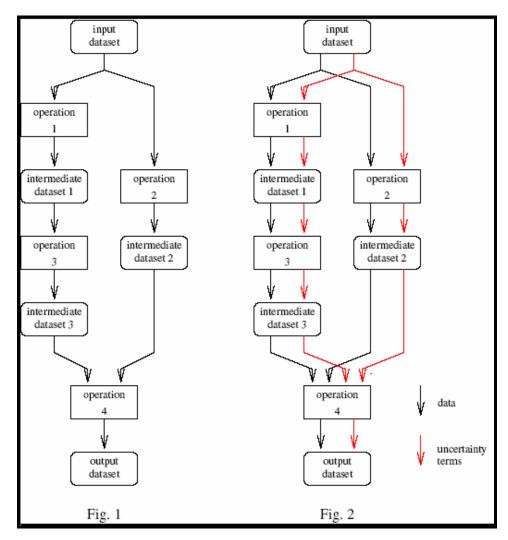
The reliable quantification of uncertainty in complex geo-computational models is an outstanding theoretical and practical problem within geographical information systems (Chiles and Delfiner, 1999; Lowell and Jaton, 1999; Zhang and Goodchild, 2002; Couclelis, 2003; Gertner et al., 2004; Kardos et al., 2005). A commonly used approach for uncertainty quantification in relatively simple geospatial models is due to Openshaw (1989). This approach relies on estimation techniques of errors caused by individual operations and has been used successfully in the context of map algebra operations (Heuvelink, 1998). Recent advances in geospatial uncertainty estimation include new approaches in spatial statistics (Cressie, 1993; Ripley, 2004), refinement Kalman filtering techniques for geospatial data (Wikle and Cressie, 1999), as well as methods for spatial data mining (Ester et al., 2000; Shekhar et al., 2001; Miller and Han, 2001; Shi and Wang, 2002; Hanning and Shuliang, 2004). In the context of specific domains, geo-scientists have developed special methods for spatial and spatio-temporal uncertainty estimation (e.g., Ganguly, 2002; Ganguly and Bras, 2003). However, these approaches have not been applied to, nor have they been designed for, large-scale and complex geo-computational models.

2. Approach

This paper addresses an important gap in the geospatial sciences by proposing a new and generic framework for uncertainty quantification for complex geo-computational models. Within this framework, we propose a "bottom-up strategy" whereby the uncertainties from the individual operations and the input-dependent uncertainties are combined to yield estimates of the overall uncertainty in a complex geo-computational model. This strategy would allow us to develop a systematic approach towards classification of geospatial operations and uncertainty estimation techniques for each geospatial operation or an entire class of such operations.

Geospatial uncertainty can be expressed in various ways, and can be expected to be a function of auto- and cross-correlations in space or time; spatial, temporal or spatio-temporal outliers; spatial and spatio-temporal stationarity; as well as spatial, temporal and attribute error structures. Our approach to problem decomposition and input-

dependent or component-based uncertainty relies on recent developments in time series analysis and complex systems. In our framework, complex, hierarchical geospatial models are viewed as being comprised of chains of simple operations at or between various levels of detail or granularity (Fig. 1). Each such operation transforms not only the data themselves *but also the uncertainty associated with the data*. As a result, even under stationary assumptions, uncertainty "propagates" through complex geospatial models. In the proposed framework uncertainty can be estimated as it "propagates" through a chain of geospatial operations (Fig. 2).



The proposed approach ultimately requires uncertainty estimation methodologies for each and every geospatial operation. However, while the number of such operations may be rather large (e.g., GRASS GIS 6.0 includes about three hundred different data processing and analytical commands: Neteler and Mitasova, 2004), the majority of GIS operations is reduced to a relatively small number of universal operations (e.g., Albrecht, 1996, lists twenty such operations). Our goal is to develop accurate and robust methods for uncertainty estimation for these universal operations.

The methods for uncertainty quantification utilized in this paper are capable of considering the uncertainty in the input data (or input dependent uncertainty in space and time) as well as the uncertainty caused by the individual geospatial operations and

their concatenations (or geospatial model/operation dependent uncertainty). Specifically, the methods in this paper are based on a couple of broad techniques: (i) spatially-weighted linear regression formulations (Cressie, 1993), and (ii) extensions and further development of the "Ensemble Neural Network" (ENN) formulation developed by Ganguly and Bras (2003) and Ganguly (2002), which in turn was developed based on the Bayesian Neural Network approaches proposed by MacKay (1995) and the NARMA formulation of Connor et al. (1994). The regression-based and ENN methodologies are utilized to estimate the uncertainty resulting from individual geospatial operations as well as a chain of such operations. The paper also utilizes the concepts of input-dependent uncertainty, originally developed for time series data (e.g., the ARMA-ARCH and GARCH formulations: see Engle, 1982 and Mills, 1990), in the context of geospatial data and the spatially-weighted regression or the ENN formulations.

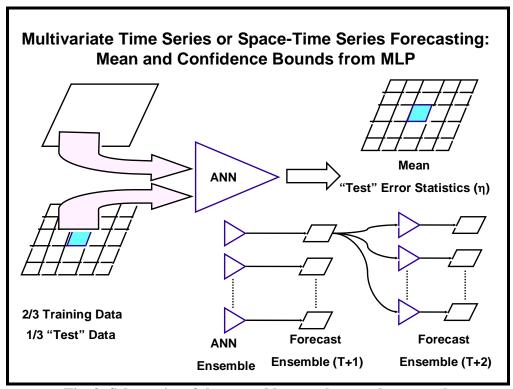


Fig. 3: Schematics of the ensemble neural network approach (ANN: Artificial Neural Networks; MLP: Multi-Layer Perceptrons)

The new contribution of this paper is to bring together these techniques (e.g., the ENN formulation depicted in Fig. 3) into the "bottom-up strategy" schematically illustrated in Figs. 1 and 2. Specifically, this implies a consistent evaluation of both the input-dependent and the model- (or geospatial operation) dependent uncertainty within a common generic framework, in the context of complex geo-computational models.

4. Results

We illustrate the applicability of the proposed framework using two geospatial models comprised of a chain of relatively simple operations. The models simulate a representative set of commonly used geospatial operations and their combinations. Specifically, we utilize geospatial datasets available at ORNL in the areas of population distribution and meteorology. For population, we develop regression-

based approaches for distributing population estimates available from low-resolution census counts or other estimates to high-resolution grid cells through the use of ancillary variables like nighttime lights and land-cover. The overall uncertainty estimates derived from the uncertainty in the constituent geospatial operations are validated by comparing with available high-resolution population datasets. For meteorology, we develop multi-scale relationships between observed variables and develop uncertainty formulations based on the constituent operations. Validation is performed using "held-out" data. Our results demonstrate the validity of our bottom-up strategy for uncertainty formulations.

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