Chapter 16
An Automated Geoprocessing Model for Accuracy Assessment in Various Interpolation Methods for Groundwater Quality

Baskaran Venkatesh and M. A. M. Mannar Thippu Sulthan

Abstract The qualities of different groundwater parameters rely on the sources of groundwater recharge, industrial effluent, urban interactions, agriculture, aquifer pumping, and waste disposal. Domination of any of these factors alters the groundwater quality. GIS enables the tracking of changes throughout time within an area/watershed and correlating changes in water quality with these alterations. Choosing an appropriate GIS-spatial interpolation technique is a critical success element in surface analysis since different interpolation methods might result in different surfaces and, eventually, different outcomes. Though no particular interpolation technique is completely optimum, the best interpolation method for a given circumstance can only be determined by comparing their results. An automated tool has been developed to assess popular interpolation techniques like inverse distance weightage, radial basis function, ordinary kriging, universal kriging, empirical Bayesian kriging, and kernel interpolation in terms of root mean square error and mean absolute error. The model provides researchers and official groundwater quality monitoring and assessment teams with the help to pick the optimal algorithm.

Keywords Groundwater quality · GIS · Spatial interpolation · Geoprocessing model · Automated tool · Accuracy assessment

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16.1 Introduction

The total freshwater available on earth is less than 3%, in which 2.15% of water is trapped in the polar region as a glacier, which is not usable for human consumption. In the earth water resources, less than one percent of water is used for domestic purposes in which 0.32% of water is present in deep below as groundwater, and 0.33% of water is readily available as surface water like in a river, lake, and pond. Groundwater is widely used for domestic, irrigational, and industrial purposes [1, 2]. Urban and industrial activities disturb groundwater's natural infiltration by interventions the surface water movement, which results in sub-standard quality. Groundwater's chemical composition decides the suitability for necessary function [3]. The contamination leads to a decrease in the groundwater quality, which results in potential health problems, avoidance of water withdrawal, and higher remedial costs [4].

Groundwater quality can be improved by monitoring and controlling the external factors which cause risk to it [5]. A prompt monitoring program may identify possible restoration work and determine the harmful external factors [6, 7]. With the interpolation technique in geographic information system (GIS), monitoring and controlling are straightforward to achieve [8]. GIS helps in hydrologic and hydrogeologic-based decision-making through mapping and analyzing appropriate spatial data [9].

Interpolation is the technique to estimate unknown data from known data. These techniques were initially used in mining and further extended to all fields [10]. Spatial interpolation is a scientific way to tell about groundwater's status around the extent, where samples were collected [11, 12]. Deterministic and geostatistical methods are the two interpolation methods based on smoothness and certainity [13, 14]. Generally, geostatistical methods perform better than deterministic methods [15].

Geostatistical interpolation from the GIS technique provides spatial variation within the prescribed environmental setting [16]. Hoover et al. [17] used the GIS technology for dynamic visualization of interpreted water quality detail for unregulated drinking water.

The GIS-based statistical study is efficient in groundwater quality assessment compared to the conventional method. It is also very essential to estimate the accuracy of various geostatistical modeling techniques [18]. The selection of a valid interpolation method is considered a necessary factor for producing an environmental-based spatial variability map [19, 20]. Developing an advanced statistical strategy for spatial analysis in a GIS platform would be challenging [9].

Global polynomial interpolation, Bayesian interpolation, kernel interpolation, radial basis function interpolation, inverse distance weighted interpolation, simple kriging interpolation, ordinary kriging interpolation, and tension spline interpolation are popular geostatistical interpolation methods [21]. The performance of each interpolation technique can be evaluated by cross-validations methods [22] like root mean square, mean absolute error, and mean bias error [18, 23–25].

The geoprocessing model helps in automatic spatial analysis with better data management. ModelBuilder in the GIS platform is a drag-and-drop tool for automating and reusing workflows. In ModelBuilders, the geoprocessing tools are sequenced to set the predecessor output as an input for a successor [26]. This extensive decision support tool solves a knotty problem in a pretty simple way. The framed model can be customized and run multiple times with a single click on the mouse [27].

16.2 Methods

16.2.1 Geostatistical Interpolation

Interpolation is preferred when data availability is limited and operates based on the principle of autocorrection by assuming the objects nearby behave similarly to the thing apart [28]. Geostatistical techniques apply mathematical and stochastic models which perform autocorrelation, while deterministic techniques apply only mathematical models [29]. As the number of steps needs to be followed while executing the different interpolation methods cross-validation, creating a model makes the process easier with performing automatic tasks in a defined sequence [30]. The research work reported using geostatistical modeling techniques in water quality assessment has clinched to the positive trend line since 2000. The effectiveness of the study on modeling the water quality should be measured [31]. As we cannot measure everything to assess the suitability of the techniques, the model with minimal predictive error should be given preference for that particular dataset [32, 33]. Various authors have identified different modeling techniques as the best ones based on cross-validation. The predictive performance depends on sampling design, sample distribution, data quality, and all [34, 35]. The workflow for this automated tool is briefed in Fig. 16.1.

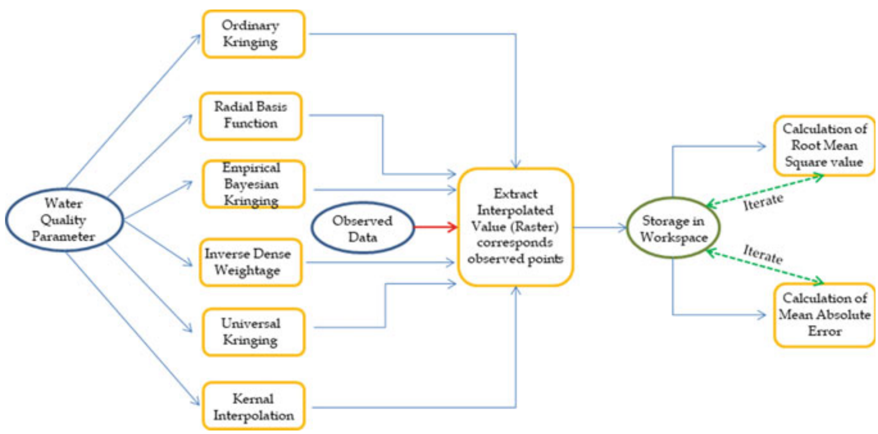


Fig. 16.1 Workflow of automated tool for assessment of different interpolation method

(a) Inverse Distance Weightage

This method creates unknown attribute values by considering certain inverse weightage to known attribute values [36, 37]. The attribute value that is only available at sampled location creates a spatial surface by connecting determined values. The influence of sampled location decreases with greater distance [38].

$$z = \sum_{i=1}^{n} \frac{Z_i}{(d_i)^p} / \sum_{i=1}^{n} \frac{1}{(d_i)^p} \tag{16.1}$$

where

Z the estimated value of the unknown prediction point
Z_i the measured value of know sample point
d_i the distance between prediction point and sample point
p the power weightage parameter, and
n the number of sample points.

(b) Radial Basis Function

RBFs are preferred for a large number of data points to create smooth surfaces. The radial basis function (RBF) predicts values from the generated surface, passing through all the measured sample points. This function minimizing the total curvature of the surface from measured values results in gentle variation in surface [19]. The predicted value shall either be greater than the maximum or lesser than the minimum measured value. This geostatistical method contains five different basis functions: thin-plate spline, spline with tension, completely regularized spline, multi-quadric spline, and inverse multi-quadric spline.

(c) Ordinary Kriging

Ordinary kriging (OK) is a popular kriging model used for the study of water quality mapping. The estimated neighborhood location through variogram estimates the value around any point in the region [39]. Assuming constant mean as unknown, this kriging model is considered flexible and straightforward. OK is preferred for its exactness, where interpolated values or local averages coexist with the known sampled locations [40]. It is an advantage for integrating diverse predicted datasets and used for data with decent trends. Accommodation of modification and changes in the mean value of the surface is possible [41]. OK assumes the model,

$$Z(s) = \mu + \varepsilon(s) \tag{16.2}$$

where

$Z(s)$ the variable of interest
μ unknown constant mean
$\varepsilon(s)$ an error with constant mean.

(d) **Universal Kriging**

The universal kriging model is a generalized version of ordinary kriging [42]. Estimation and prediction are two-step procedures indulged here [43], and it uses either semi-variograms or covariances forms for autocorrection and measurement of error [44]. Here, the error $\varepsilon(s)$ is random and modeled as autocorrelated. The model assumed here is based on a deterministic function and a variation (error) as

$$Z(s) = \mu(s) + \varepsilon(s) \tag{16.3}$$

where

$Z(s)$ the variable of interest
$\mu(s)$ some deterministic function
$\varepsilon(s)$ random variation or error.

(e) **Kernel Interpolation**

Kernel interpolation is a first-order local polynomial interpolation variant in which instability in the calculations is avoided by utilizing an approach similar to that used to estimate the regression coefficients in ridge regression. By introducing a slight degree of bias to the equations, the ridge parameter in the kernel smoothing model corrects the problem of substantial prediction standard errors and dubious predictions [45]. For the output surface type, this interpolation only supports prediction and prediction standard error. The shortest distance between points is used in this model to connect locations on both sides of the given nontransparent (absolute) barrier with a sequence of straight lines.

(f) **Empirical Bayesian Kriging**

EBK is one of the reliable automatic interpolator models classified under geospatial interpolation. It differs from classical kriging methods because the semivariogram model estimation reduces the introduced error [46]. The process is attained by considering various iterative semivariogram models rather than a single semivariogram model. This model is preferred for its fast and reliability in a large set of spatial data interpolation [47, 48]. By not considering uncertain semivariogram estimates, this kriging does not underestimate prediction's standard error.

16.2.2 Qualitative Assessment

The various spatial interpolation techniques use different models and assumptions. The selection of appropriate interpolation depends on accuracy, applicability to large datasets, robustness, and flexibility in defining multiple phenomena, smoothening noisy data, running time, and ease of use [49]. Currently, selecting the suitable interpolation method by considering all these attributes is not an easier task. The selection of inaccurate methods and unsuitable parameters ends with a distorted spatial interpolation model, leading to wrong decisions from this misleading spatial information [19]. The observed and estimated values for different interpolation techniques are compared for various water quality parameters. There are various methods to calculate interpolation error. We have selected root mean square error (RMSE) and mean absolute error (MAE) for this study. Both express average model prediction errors and are widely reported in environmental and climate change literature [50]. The inconsistency between RMSE and MAE shall be due to differing error variance of associated sets [51]. RMSE is sensitive to extreme outliers than MAE. Because of its simplicity in the calculation, these two methods are often used to assess the model's performance [18, 52, 53]. RMSE and MAE are calculated as follows:

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(Z_i - E_i)} \tag{16.4}$$

$$\mathrm{MAE} = \frac{\sum_{i=1}^{n}|(Z_i - E_i)|}{n} \tag{16.5}$$

Where Z_i and E_i are the observed and estimated value of any water quality parameter, respectively, at a point i within our study area.

16.3 Result and Discussion

16.3.1 Automated Geoprocessing Model

A model tool can be built with the set tools arranged in sequence and connected adequately in Arcmap ModelBuilder. The automated tool is accomplished by blending a large processing workflow in ModelBuilder that includes various tools, variables, parameters, and preconditions. This setup automates the tool's performance as per the structure and ends with a single raster or vector file as workflow's output. The ModelBuilder also allows to create, edit, and manage the models [54]. It again allows the user to modify the model as per the reforms in the objective. Generally, the elements in the model are classified into input data, geoprocessing tool, and output data. The shape and color of elements display their functional uniqueness, as shown in Fig. 16.2.

Input (blue-oval shape) is generally geographic data in either raster or vector format before the model is executed. Tools (yellow-rectangular) are the tasks to be performed on the input. A process would be one of the various ready-to-use system tools offered in ArcGIS, which can be easily grabbed from the ArcToolbox and positioned onto the ModelBuilder interface. Output (green–oval shape) is data created when the model runs by the tools or scripts, which does not exist until the

Fig. 16.2 Diagram property and symbology of model elements

process is over [55]. They can be used in another process once they have been created. Raster, vector, and non-geographical values are the possible derived elements created while running a tool [56]. The geoprocessing tools shall be connected in parallel or series, but there should be proper input data to validate the model. Since manually selecting the inputs for the number of tools in the process workflow consumes solid time, the first advantage of any automated geoprocessing model is time-saving [57].

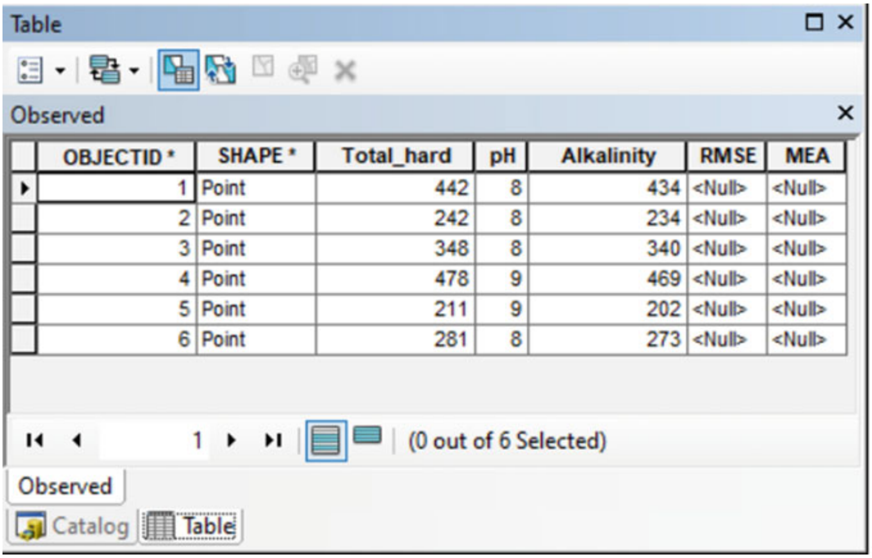
16.3.2 Interpolation Accuracy Assessment Model

The model begins by interpolating the acquired data on water quality. The input attribute table of collected data on water quality must include specifics such as parameter names and their values. By making the parameter name the head of the associated column, the tool's user can select which parameter to examine for accuracy. All six interpolation algorithms mentioned here are parallelized to receive water quality parameter data as a common input vector layer. All of these processing tools produce a raster dataset as their output. The user can specify any folder or geodatabase as the destination for all derived data. The required environmental settings for the entire model, such as processing extent, output coordinates, cell size, mask layer, and compression, can be overridden by the user via the model properties menu bar.

The final goal of this automated model is to determine the accuracy of a widely adopted geostatistical interpolation technique in water quality assessments by comparing the predicted value to observed data within the study area [58]. The observed data should be spatially consistent but contained inside the research area. An additional two empty columns with the names MAE and RMSE should be added to the attribute table of this vector layer to minimize the model steps as shown in Fig. 16.3. The next step is to extract predicted water quality data from an interpolated raster surface at the exact location, where the observation was made.

Specific outputs generated during model processing are required to generate the final output only and are of no value once the model is complete. Such outputs are marked as intermediate data [27]. All six resulting extracted vector datasets will be saved as intermediate data in a specified location. Since MAE and RMSE require only the difference between predicted and actual values, almost all the modeling work is done.

Following that, the model does a basic mathematical computation using MAE and RMSE formulas. Compounded by the fact that Python lacks a direct mathematical



OBJECTID *	SHAPE *	Total_hard	pH	Alkalinity	RMSE	MEA
1	Point	442	8	434	<Null>	<Null>
2	Point	242	8	234	<Null>	<Null>
3	Point	348	8	340	<Null>	<Null>
4	Point	478	9	469	<Null>	<Null>
5	Point	211	9	202	<Null>	<Null>
6	Point	281	8	273	<Null>	<Null>

Fig. 16.3 Attribute table format for observed data

function for MAE and RMSE, the computing steps are a bit long. A single tool cannot do operations such as difference, square, square root, summation, and average in ArcMap. Calculate field and summary statistics are the tools that this model uses to execute simple calculations to furnish the required outcome. If these tools are linked with the output of all six extract values from the point tool as their input, the model may appear to be a cluster of similar tools. Iterating the procedure while evaluating the prediction error will result in a pleasing and straightforward model.

Iteration, commonly called looping, involves repeating a procedure with a certain degree of automation. It is significant since repeated task automation lowers the time and effort necessary to carry out the job. In each iteration, a process can be repeated over and over with changing settings or data. ModelBuilder also gives flexibility in iteration, as it is possible to repeatedly run an entire model or merely a specific tool or process [59]. In this model, the iterate feature class, which iterates across a workspace's or feature dataset's feature classes, is adopted.

Though the similar series of operations to compute MAE and RMSE is curtailed by the iterator tool, the model looks too lengthy, and modifying the settings as per user requirements will be difficult. The entire model is customized to reduce complexity. The first part of the automated tool till extraction of interpolated value to the observed point is modeled as a sub-model.

A sub-model, nested model, or model within another model is an approach that involves embedding and executing one model tool within another model. This model hierarchy is used for two major reasons: simplifying a large, complicated model and enabling more extensive model iterators usages. Whenever an error occurs in one sub-model, just that model should be corrected, and then the single model should be repeated rather than the complete process. The sub-model for the automated tool is shown in Fig. 16.4. The collect values tools are intended to collect iterator output values or combine a list of multi-values into a single input, which helps connect the sub-model to the main model.

Setting precondition in combining sub-model to the main model is mandatory for this automated tool. Preconditions can be used to regulate the sequence of operations in a model deliberately. By making the output of the first process a precondition for

Fig. 16.4 Sub-model: automated tool for interpolation accuracy assessment

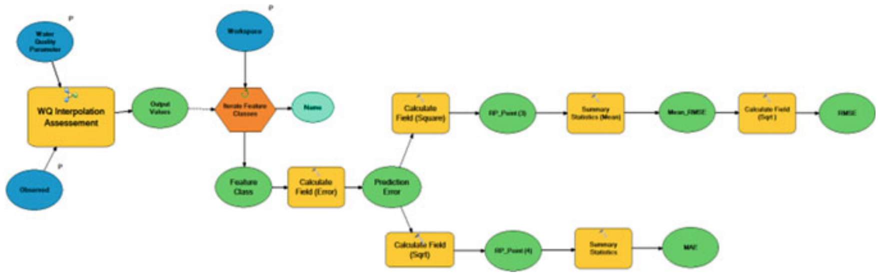


Fig. 16.5 Main model: automated tool for interpolation accuracy assessment

the second process, a process may be made to run only after another. Any variable can be used as a precondition for executing a tool, which can have several preconditions. The complete main model configured with sub-model preconditioning is shown in Fig. 16.5.

Every model variable can be converted into a model parameter. The value of a variable can be provided in the model tool dialog box when it is turned into a model parameter. The letter P displays next to the variable in the model once it is set as a parameter. Creating model parameters are preferred when the model user must specify variable values each time the model is run. Figure 16.6 depicts the automated tool's dialog box for assessing various interpolation techniques. Workspace or geodatabase, water quality parameter for interpolation, and observed data to assess six interpolation techniques are marked as model parameters for this model. The user shall select the appropriate file for all the three variable tabs from the tool dialog box.

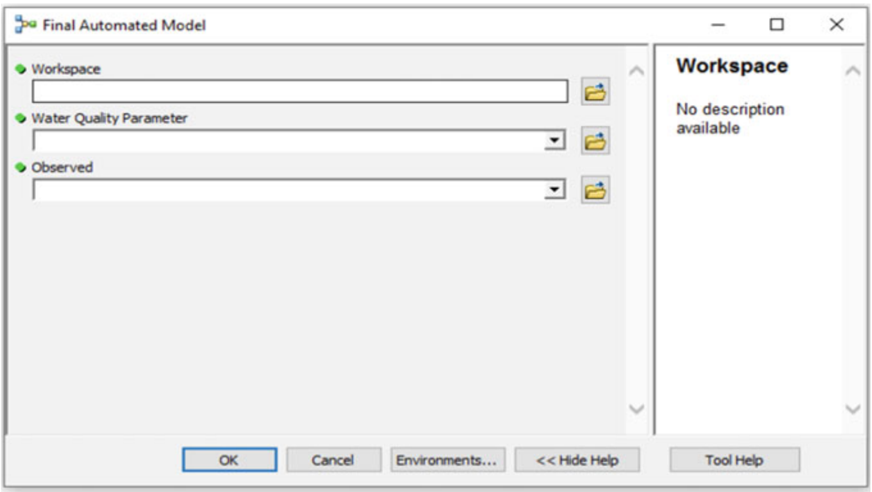


Fig. 16.6 Automated model tool dialog box

The user can run the entire model from the tool dialog box or the run button on the ModelBuilder edit screen. Once the model is finished, a running tab will alert the user that the model is completed, and this automated tool will notify them within a few minutes. If a user manually executes the equivalent set of operations with a clear objective, it will take more than 30 min. Again the performance depends on the processing efficiency of hardware. Remembering the number of tools, the sequence of tools to be used, selecting the correct file as input, storing the output in the desired location, and adjusting the environmental settings for all tools will be challenging in manual operation. After successfully running this automated tool, each six output tables of MAE and RMSE corresponds to six geostatistical interpolations as shown in Fig. 16.7.

A single-rowed table containing either the RMSE or MAE value of these six interpolations will be saved in the desired location as specified in the tool dialog box before executing the model. Combining all the RMSE and MAE values in a single table may make the model intricate and complicate. Finally, the table of any

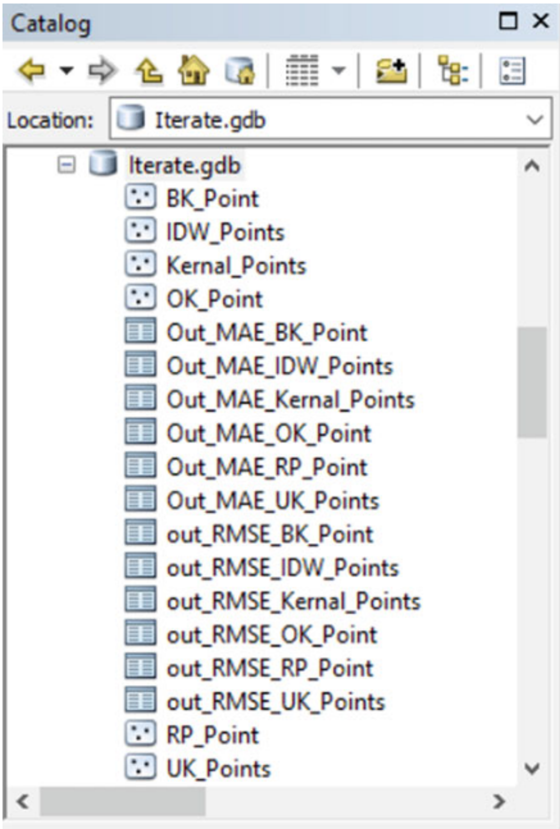


Fig. 16.7 Output table of RMSE and MAE for six interpolations stored in a geodatabase

technique with the most negligible value of compounded error shall be preferred to study water quality parameters.

16.4 Conclusion

The model frameworks and applications outlined in this study demonstrate the potential benefits of utilizing GIS models in evaluating various interpolation mechanisms for water quality spatial mapping. These enable us to save time, develop reusable and shareable tools, depict workflows in an easy-to-understand diagram, and create sophisticated models as per our project objectives, all of which will help us save time and energy. The significant barriers were identified when a user prefers manual operation to accomplish the objectives of determining the best are spatial interpolation techniques. A few are performing workflow in the correct sequence, selecting valid input for all tools, modifying the storage directory for output of any tool, and repeatedly using the calculate field and summary statistics tool.

The recharge and discharge activities shall influence the quality of the groundwater parameter. Modeling any parameter of groundwater quality by taking account of typical external forces is a challenging task. It is challenging to model any groundwater quality parameter accurately. No technique will ever be able to match the genuine reality on the ground. Since each interpolation algorithm's assumptions and expressions are unique, the automated tool can help reduce uncertainty by recommending the best technique with the least prediction error for any water quality parameter. This automated tool helps select the suitable interpolation technique for any research related to the study on a parcel's water quality. The developed tool will allow policymakers and city planners working on water quality restoration and sustainable groundwater management to make evidence-based decisions promptly.

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