HASM-AD Algorithm Based on the Sequential Least Squares

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Abstract  The HASM (high accuracy surface modeling) technique is based on the fundamental theory of surfaces, which has been proved to improve the interpolation accuracy in surface fitting. However, the integral iterative solution in previous studies resulted in high temporal complexity in computation and huge memory usage so that it became difficult to put the technique into application, especially for large-scale datasets. In the study, an innovative model (HASM-AD) is developed according to the sequential least squares on the basis of data adjustment theory. Sequential division is adopted in the technique, so that linear equations can be divided into groups to be processed in sequence with the temporal complexity reduced greatly in computation. The experiment indicates that the HASM-AD technique surpasses the traditional spatial interpolation methods in accuracy. Also, the cross-validation result proves the same conclusion for the spatial interpolation of soil PH property with the data sampled in Jiangxi province. Moreover, it is demonstrated in the study that the HASM-AD technique significantly reduces the computational complexity and lessens memory usage in computation.

Keywords  surface modeling; HASM; spatial interpolation; sequential least squares

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Introduction

Spatial interpolation has been widely applied to surface modeling in GIS and CAD, such as Kriging, IDW, Spline and Natural Neighbor methods. Effort has been concentrated on the accuracy of the interpolation methods. In recent studies, Vincent Chaplot found that irrespective of the surface area, landscape morphology and sampling density, few differences existed between the employed interpolation techniques if the sampling density was high. At lower sampling densities, in contrast, the performance of techniques tended to vary. [1] Robinson also found in the study, that out of four spatial interpolation methods used, no one single interpolator could produce the best result for the generation of continuous data distribution all the time, particularly with a dataset that had not been designed with one particular interpolator in mind. [2] Classical spatial interpolation methods originated from the geostatistical theory or the hypothesis of neighbor correlation, without accounting for the surface intrinsic factors. Therefore, it becomes difficult for the methods to control error and produce the result in accordance with the actual surface. In contrast, the HASM (high accuracy surface modeling) technique performs surface fitting according to the first and the second surface basic parameters with the restrictions from Gauss-Codazzi equations, based on the theory of differential geometry. [11, 12, 13]
In the past 20 years, HASM has developed into an integral system and solved in theory the error and the multi-scale effect in surface fitting. The accomplished studies illustrated that HASM surpasses the classical spatial interpolation methods in accuracy. The restriction of Gauss-Codazzi surface equations and data precision have not been taken into account in the former HASM computational model, so that the defects resulted in deviation from the true surface. In addition, the iterative algorithm adopted in the former HASM technique resulted in high computational complexity and huge memory usage, usually exceeding the PC capacity, i.e., processing power.

The main objective of the study is to develop a new model for HASM in view of the impacts of the sampled data precision and Gauss-Codazzi surface equations on surface fitting. Simultaneously, sequential division is applied to computation in the new algorithm, based on the sequential least squares technique, in order to improve the efficiency and reduce memory usage in computation.

1 HASM-AD model based on the restriction from surface equations

According to the fundamental theory of surfaces, a surface is uniquely defined by the first and the second fundamental coefficients, and their coefficients satisfy the Gauss-Codazzi equations.

The finite difference of Gauss-Codazzi equations can be formulated as:

\[
\begin{align*}
\frac{f_{ijkl} - 2f_{ijkl}^* + f_{i,jl}}{h^2} &= (I^1_{i,j})_{ijkl}f_{ijkl} - f_{i,jl}^* - (I^1_{i,jl})_{ijkl}f_{ijkl}^* - f_{i,jl}^* \\
&+ \frac{L_{ij}}{\sqrt{E_{ij} + G_{ij} - 1}} \\
\frac{f_{ijkl} - 2f_{ijkl}^* + f_{ijkl}^*}{h^2} &= (I^2_{ijkl})_{ijkl}f_{ijkl} - f_{ijkl}^* - (I^2_{ijkl})_{ijkl}f_{ijkl}^* - f_{ijkl}^* \\
&+ \frac{N_{ij}}{\sqrt{E_{ij} + G_{ij} - 1}} \\
\frac{f_{ijkl} - f_{ijkl}^* + f_{ijkl}^*}{4h^2} &= (I^3_{ijkl})_{ijkl}f_{ijkl} - f_{ijkl}^* - (I^3_{ijkl})_{ijkl}f_{ijkl}^* - f_{ijkl}^* \\
&+ \frac{M_{ij}}{\sqrt{E_{ij} + G_{ij} - 1}}
\end{align*}
\]

The Lagrange function is:

\[
F(V) = V^T P V - 2 \cdot K^T (A V + W)
\]

where the first derivative of the function \(F(V)\) is equal to 0, \(F(V)\) bears the minimum value. The formula is:

\[
\frac{dF}{dV} = 2 \cdot P V - 2 \cdot K^T A = 0
\]

where \(E, F, G\) are the first fundamental coefficients; \(L, M, N\) are the second fundamental coefficients; \(f_{ijkl}^*\) is the approximate value for grid cell; and \(\Gamma_{ij}^k\) is the Christoffel symbol of the metric matrix for the surface. The HASM technique is a method of surface modeling established based on the Gauss-Codazzi equations. In the previous study, sampling points are used as a constraint so that HASM is transformed into a constraint least squares approximation, which can be formulated as:

\[
\begin{align*}
\text{min} & \; / / A F - B / /_2 \\
\text{s.t.} & \; C F = D
\end{align*}
\]

where \(A\) is the coefficient matrix of the Gauss-Codazzi equations, \(B\) is the right-hand vectors of equation, \(F\) is the vector of the estimated points in computational area, \(C\) is the matrix of sampled points and \(D\) is the constant vector. With the iterative algorithm adopted in the previous HASM technique, an optimal solution is calculated to the surface defined by sampling points. However, the solution obtained could fit the mathematical surface defined by sampling points fairly well, not ensuring a good fit to the real surface, due to a lack of relative constraint.

Therefore, a new model, HASM-AD, is developed, in which not only sampling points, but also Gaussian-Codazzi equations are used as constraints to produce the optimal estimates to the real surface by least squares, based on adjustment theory.

The model is fitted:

\[
A V + W = 0
\]

where \(A\) is restriction equations, including Gauss-Codazzi surface equations and sampling point conditional expressions, and \(V\) is correction vector to the estimation points, \(W\) is constant matrix. With the aid of a Lagrange multiplier, the solution of conditional expressions can be transformed into the solution of conditional extreme value.

The Lagrange function is:

\[
F(V) = V^T P V - 2 \cdot K^T (A V + W)
\]
\[ V^T P = K^T A \]

where \( P \) is weight matrix in relation to data precision, and \( V \) is correction vector to the estimation points.

\[ V = P^{-1} A^T K \] (6)

\[ A P^{-1} A^T K = -W \] (7)

Let \( N = A P^{-1} A^T \), the normal Eq. (4) is expressed:

\[ N K = -W \] (8)

where \( N \) is a matrix of full rank, and rank \( N \) = rank \( K \). Therefore, the solution of Eq. (8) is unique, and \( V \) is calculated according to Eq.(6).

The rank of matrix \( N \) in normal Eq. (8) will increase rapidly with the scale of computational area enlarged, which results in huge memory usage and heavy load of computation.

In the HASM-AD model, restrictions are composed of two kinds of equations: Gauss-Codazzi surface equations and conditional equations satisfied with sampling points, which can be expressed as:[16]

\[
\begin{align*}
\frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{h^2} &= \left( \Gamma_{11}^i \right)_{i,j} f_{i+1,j} - f_{i-1,j} \\
\frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{h^2} &= \left( \Gamma_{22}^i \right)_{i,j} f_{i,j+1} - f_{i,j-1} \\
\frac{f_{i+1,j+1} - f_{i+1,j-1} + f_{i-1,j+1} - f_{i-1,j-1}}{4h^2} &= \left( \Gamma_{12}^i \right)_{i,j} f_{i+1,j+1} - f_{i-1,j-1} \\
\end{align*}
\]

\[ f_{m,n} = \tilde{f}_{m,n} \] (9)

However, according to Gauss-Codazzi surface equations in a five-point finite differential scheme, there are \( 3 + U \) conditional equations in a 5×5 grid unit, where \( U \) is the number of sampling points in the computational area, and its maximum is 9. The corrections of the 9 points are estimated in the 5×5 unit in the procedure of surface fitting, while the points on the boundary are only used to calculate the basic parameters of the surface. It is shown in Fig.1.

![Fig.1 Points calculated in a unit and its boundary](image)

As is shown in Fig.1, the white circles represent the points to be estimated in computation, while the black ones symbolize the points on the boundary in the 5×5 unit.

The correction vector is an \( n \times 1 \) row vector, which is composed of the estimates to the 9 points, with its transposed matrix of \( V^T = [v_0, v_1, \ldots, v_8] \).

The corresponding relation between grid coordinates and serial number in the correction vector is described:

\[
\begin{bmatrix}
V_{i-1,j-1} & V_{i+1,j-1} & V_{i,j-1} & V_{i,j+1} & V_{i+1,j+1} & V_{i+1,j+1} & V_{i+1,j+1} & V_{i+1,j+1} & V_{i+1,j+1} \\
\end{bmatrix}^T
\rightarrow [v_0, v_1, v_2, v_3, v_4, v_5, v_6, v_7]_i^n
\]

where \( i \) and \( j \) are coordinates of the calculated points in the independent unit.

Via correction vector \( V \), constraint equations can be transformed into the following conditional equation,

\[
\begin{align*}
\frac{(f_{i+1,j} + v_i) - 2(f_{i,j} + v_i) + (f_{i-1,j} + v_i)}{h^2} &= \left( \Gamma_{11}^i \right)_{i,j} f_{i+1,j} + v_i - f_{i-1,j} - v_i \\
\frac{(f_{i,j+1} + v_i) - 2(f_{i,j} + v_i) + (f_{i,j-1} + v_i)}{h^2} &= \left( \Gamma_{22}^i \right)_{i,j} f_{i,j+1} + v_i - f_{i,j-1} - v_i \\
\frac{(f_{i+1,j+1} + v_i) - 2(f_{i+1,j} + v_i) + (f_{i-1,j+1} + v_i)}{4h^2} &= \left( \Gamma_{12}^i \right)_{i,j} f_{i+1,j+1} + v_i - f_{i-1,j-1} - v_i \\
\end{align*}
\]

\[ f_{m,n} = \tilde{f}_{m,n} \] (10)
where \( A \) is coefficient matrix, \( V \) is correction vector, \( W \) is constant vector.

The matrix \( A \) can be decomposed into two partial matrixes and written as:

\[
A = \begin{bmatrix}
0 & \frac{(2 + h(G^1_{1i,j}))}{2h^2} & 0 & \frac{(G^2_{1i,j})}{2h} \\
0 & \frac{(G^2_{1i,j})}{2h} & 0 & \frac{(2 + h(G^2_{2i,j}))}{2h^2} \\
1 & \frac{(G^2_{1i,j})}{2h} & 0 & \frac{(G^2_{1i,j})}{4h^2} \\
\frac{1}{4h^2} & \frac{(G^2_{1i,j})}{2h} & \frac{1}{4h^2} & \frac{(G^2_{1i,j})}{2h}
\end{bmatrix}
\]

and \( M \) is the coefficient matrix from the conditional equation satisfied by sampling points in the following form:

Rows in \( M \) are determined by the sum of sampling points \( k (k \leq 9) \), and the coefficient in each row corresponds with the position of the sampled points.

It is expressed as:

\[
M = \begin{bmatrix}
\cdots & a_{1i} & \cdots \\
\cdots & a_{2i} & \cdots \\
\cdots & a_{9i} & \cdots \\
\cdots & a_{1i} & \cdots \\
\cdots & a_{2i} & \cdots \\
\cdots & a_{9i} & \cdots \\
\cdots & a_{1i} & \cdots \\
\cdots & a_{2i} & \cdots \\
\cdots & a_{9i} & \cdots
\end{bmatrix}, \quad (a_{1i}, \ldots, a_{9i} = 1)
\]  \( \quad (12) \)

Likely, the constant vector is:

\[
W = \begin{bmatrix}
f_{i+1,j} - f_{i,j} \\
\frac{1}{2h} (f_{i+1,j} - f_{i,j}) + \frac{1}{2h} (f_{i,j+1} - f_{i,j-1}) \\
\sqrt{E_{ij} + G_{ij}} - \frac{1}{h} f_{i,j} - \frac{1}{2h} f_{i+1,j} + \frac{1}{2h} f_{i,j+1}
\end{bmatrix}
\]

where the elements of zero are constant terms in the conditional equations for the sampled points.

The order is not more than 12 for the normal equations in an independent unit, and all units formed in the surface fitting area are to be calculated in the process. The sum of equations is estimated in formula:

\[
N = 15 \times (n - 1) \times (m - 1) + n \times m = 16n \times m
\]

where \( n \) is the sum of independent units in the row direction and \( m \) is for the column direction. With the scale of the area expanding, the sum of equations will increase sharply, so that the computation will exceed the PC capacity.

### 2 Division in equations based on sequential least squares

With the sum of equations increasing, it will become very difficult to compute the integral solution of correction vector \( V \). Therefore, it is not suitable to use the iterative algorithm to fit a large scale area, because the heavy workload will make the procedure too time-consuming to endure. It has been proved to be a feasible method to adopt the division technique to the solution of a large linear system of equations. Sequential least squares is just the method, with which linear equations are divided into two or more groups to compute sequentially, according to the principle of block-matrix factorization.\(^{[22]}\) In computation, the solution to the previous group is taken as virtual observations to initialize the next, that is, the result of the previous group implies influence on the next. Also, the process is to be continued until all groups are calculated in order to obtain the final solution to the linear equations.

It is known from the HASM-AD model that there is linear independence among solutions to the non-overlapped units with the space interval of four grid coordinate units in a row or column direction, and these units are included in a group. On account of
characteristics of the equations above mentioned, the linear equations in computation can be divided into 16 groups completely according to the central position of the origin unit and the offset in every group.

As is shown in Fig.2 above, the positions of the origin unit for 16 groups are marked with red circles. There are only non-overlapped units in each group, whose solutions are linearly independent of each other. Consequently, the coefficient matrix $N_{\text{rr}}$ in normal equation must be a diagonally symmetrical matrix, and it is expressed as:

$$N_{\text{rr}} = \begin{bmatrix} \begin{bmatrix} n_1 \end{bmatrix} \\ \begin{bmatrix} n_2 \end{bmatrix} \\ \vdots \\ \begin{bmatrix} n_k \end{bmatrix} \end{bmatrix}$$

where $[n_1], [n_2], [n_3], \ldots$ and $[n_k]$ are partitioned matrices for all calculated units in the group, which distribute on the diagonal of the matrix of $N_{\text{rr}}$. Therefore, the inverted matrix of $N_{\text{rr}}$ is also diagonally symmetrical distributed, and is expressed as:

$$N^{-1}_{\text{rr}} = \begin{bmatrix} [n_1]^{-1} \\ [n_2]^{-1} \\ \vdots \\ [n_k]^{-1} \end{bmatrix}$$

where $[n_1]^{-1}, [n_2]^{-1}, [n_3]^{-1}, \ldots$ and $[n_k]^{-1}$ are the inverted matrices of the corresponding matrices. As a result, the integral iterative solution to the linear equations in surface fitting is transformed to the repeated solution to the independent units of $5 \times 5$ area in 16 groups with the algorithm used in HASM-AD. All units are to be calculated in sequence, so the time cost of the new algorithm HASM-AD is described as:

$$T = \sum_{i=1}^{n} t_i$$

where $n$ is the count of the independent units in the fitting area, with the estimator of $n = 16 \times n \times m$, and $t_i$ is the time cost of $i$. In contrast to the temporal complexity of $O(n^3)$ for the integral iterative solution in HASM, it is only $O(n)$ for the new model of HASM-AD, with time cost reduced greatly in surface fitting. Moreover, the new algorithm has simplified the computation and reduced memory usage and CPU workload so that it is possible to deal with large-scale datasets in application.

3 Testing for HASM-AD technique

3.1 Test of accuracy

To access the model performance, we compared the algorithm of HASM-AD with the interpolation techniques commonly used in GIS, which included inverse distance weighting (IDW), ordinary kriging, regularized spline with tension and natural neighbor. In the study, we used a mathematical function to define a standard surface in normalized area $[0,1] \times [0,1]$. The function is expressed as:

$$z(x, y) = 3 + 2 \sin(2\pi x) \sin(2\pi y) + \exp(-15(x-1)^2 -15(y-1)^2) + \exp(-10x^2 -15(y-1)^2)$$

and the 3D plot of the reference surface is shown in Fig.3.
The statistics of the simulated error are listed in Table 1, indicating that few differences existed among the classical techniques with high sampling density, but HASM-AD yielded the best result with the least RMSE.

|               | Minimum | Maximum | ME   | RMSE  |
|---------------|---------|---------|------|-------|
| IDW           | −0.138  | 0.134   | 0.005| ±0.058|
| Spline        | −0.138  | 0.141   | 0.006| ±0.059|
| Natural neighbor | −0.131 | 0.137   | 0.006| ±0.058|
| Kriging       | −0.182  | 0.185   | 0.005| ±0.065|
| HASM-AD       | −0.138  | 0.180   | 0.000| ±0.017|

Fig.4 shows the histogram of the error, depicting that the techniques all yielded unbiased estimations. Though error definition is similar to each other, the errors from HASM-AD technique distribute symmetrically with better convergence.

Fig.5 presents the spatial distribution of errors, suggesting that all the techniques yielded unbiased estimations, but lower predicted errors were obtained by using HASM-AD. In the area with high absolute Z values, the surface was systematically underestimated by the methods in comparison (i.e., IDW, kriging, spline and natural neighbor), whereas HASM-AD performed well, revealing that unlike other methods, there no systematical effects resulted from the model.

### 3.2 Cross-validation in the interpolation of soil PH value

In the study, we also tested the accuracy of HASM-AD and the selected spatial interpolation techniques for predicting soil PH in Jiangxi Province. The literature suggests that some 100-150 is the minimum requirement to achieve a stable variogram. In the research of soil PH, 150 soil samples were collected, geo-referenced using a GPS receiver and analyzed for soil PH, as is shown in Fig.6. The quota is satisfied in the case, with 150 data available for soil PH.

It is common practice to use cross-validation to validate the accuracy of an interpolation. Cross-validation is achieved by eliminating information, usually one observation made, estimating the value at the location with the remaining data, and then computing the difference between the actual and estimated value. The cross-validation is used to choose the best variogram model among the candidate models. In the process, we selected randomly 120 sample points of the data to interpolate with the space interval of 500 m, with 30 points left for computing predicted error to compare the selected methods.
The statistical summary of the PH value for the sampled data is listed in Table 2.

Table 2  Summary statistics for the PH soil property of sampled data

| N  | Min    | Max    | Mean  | Range | Variance | Skewness | Kurtosis |
|----|--------|--------|-------|-------|----------|----------|----------|
| 120| 4.50   | 6.18   | 5.08  | 1.68  | 0.136    | 0.951    | 0.287    |

To compare different interpolation techniques, we examined the difference between the known value and the predicted data using the minimum error, the maximum error, the mean error (ME) and the root mean square error (RMSE).

The statistical summary of the difference for the compared interpolation techniques in cross-validation is listed in Table 3. Obviously, the statistics above indicate that HASM-AD surpassed the classical methods in comparison with the least RMSE and ME. In the classical methods, natural neighbor method yielded the best estimates, with the same error range as that of HASM-AD (from −0.67 to 0.42). IDW and Kriging also provided good fits to the experimental variogram, but the kriging method predicted the values with bigger ME. In the case, the biggest RMSE and ME is found in the result interpolated by spline method.

The maps of soil PH value in Jiangxi Province produced by the compared spatial interpolation methods can be seen in Fig. 7. As is shown, there is little difference between the estimates of natural neighbor and HASM-AD techniques, due to the similar. Fig.5 (a) shows the result interpolated by IDW technique, which depicts the integral trend of the spatial distribution with some scattering holes, revealing the inability to deal with the impact of the points with bigger intervals on the whole spatial trends, due to the used weighting method. As is presented in Fig. 7 (b), the soil PH values were underestimated in the east of
the study area so that some patches of high PH values diminished. The estimates yielded by spline method cannot provide a good fit to the known data in the case, probably because the elastic mechanics of regular tension is not suitable to the variogram in the soil PH value.

Fig.7  Interpolated maps of soil PH

4 Discussion

In our study, we tested the accuracy of the selected techniques with high sampling density to decrease the impact of the spatial characteristics of the dataset on the estimations. For the classical interpolation techniques, no prominent differences were found in terms of accuracy, given that the sampling density was high. The result is in accordance with those of Vincent Chaplot et al., Borge and Vizzaccaro, and Lazzaro and Montefusco. Generally, kriging technique is thought to perform well with broad applicability. The fact that kriging has a lower performance in the study compared to other methods may be explained from the high sampling density used in the computation. The sampling density used is so high that the impact of the spatial structure is less than that of the adjacent data points on the estimates in surface modeling. As a result, the interpolation techniques performed well with low RMSE, which take into account only points in the neighborhood (i.e., IDW, spline and natural neighbor). Though these methods produced a better result in the example, they are suitable for some specific conditions due to their inability to model the spatial characteristics of data.

Surprisingly, the fact is found that HASM-AD technique surpassed the other methods with the least accuracy (RMSE=0.017) at the same sampling density. This can be explained from the computational model used in the method, which is based on the differential geometry and error adjustment theory. Unlike the geostatistical theory or the hypothesis of neighbor correlation, Gauss surface equations depict the correlations between the estimators and the adjacent points and take into account the impact of all points in the area. Simultaneously, via error adjustment theory, differences in restriction conditions are eliminated and modified to yield the result to fit the actual surface well. Moreover, data precision is considered in the model so that the impact of the initial dataset on the estimates is quantified. All the factors make up for the mechanical decrease of space between the known
values, and thus HASM-AD excelled in accuracy in spite of high sampling density.

5 Conclusion

The study presents a new surface modeling technique, HASM-AD, and compared its accuracy and the commonly used methods in GIS (IDW, Kriging, spline, natural neighbor).

Without regard to the surface morphology and the surface area, none of the classical interpolation techniques excelled in accuracy if the sampling density was high. Kriging inherently accounts for the arrangement of sampling points, and thus did not provide a better result than the methods based on the hypothesis of neighbor correlations when the spatial structure was weak with the high sampling density. Overall, no appreciable differences existed in the classical methods in comparison. In contrast, the HASM-AD technique yielded better estimates than the classical techniques with the least RMSE, even though the sampling density was high. It is mainly because the technique is based on the differential geometry and error adjustment theory, which offers the optimum result to the actual surface in spatial prediction. Because of the division for linear equations used in computation, the complexity of the algorithm of HASM-AD was reduced significantly. As a result, the large-scale dataset can be solved effectively with much less usage of memory and CPU time.

Extra effort has to be made to plan the division series reasonably in 16 groups of equations. It is indicated by our study that the solution to some divisions had no appreciable impact on the final result. Consequently, excluding these groups from computation will contribute to reduce time cost and improve the efficiency of the algorithm.

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