Spatial variable prediction problem of synergistic kriging optimization based on FMM Summary

When studying the spatial variation of spatial variables, Co-Kriging collaborative estimation method shows excellent local detail capturing ability and spatial correlation advantages. In this paper, a cooperative Kriging model based on FMM optimization is established to solve the problem of covariance calculation, and the change mode of spatial variables is deeply studied.

For problem 1, after normalization and 2D meshing of Annex 1 data, random uniform resampling is adopted to ensure fairness and randomness, and then linear interpolation and Kriging interpolation models are constructed. The fit of the models is verified by 3D and contour maps, and the global hierarchical, local peak characteristics and spatial correlation of F1_target are analyzed. Secondly, for the second question, python is used to solve the RMSE error analysis model established, and the conclusion is drawn: the RMSE error of Kriging interpolation decreases rapidly with the increase of sample size and tends to be stable, while the linear interpolation decreases slowly and is difficult to convergence.

For problem 2, the correlation between variables is studied, and two cooperative variables are selected comprehensively. First, the initial trend of variables was drawn by scatterplot and density histogram, and then the Jarque-Bera test was combined to confirm the non-normal distribution of data. Spearman correlation coefficient analysis was adopted, and SPSS software was used to calculate the correlation between target variables and co-variables. The results show that covariate 1 and covariate 4 have strong correlation with the target variable in 99% of cases. Therefore, Collaborative1 and Collaborative4 are selected as co-variables.

For problem 3, based on problem 2 Kriging model, the FMM optimization co-Kriging model is established by introducing fast multipole method, and the anisotropy of F1_target space variable is revealed by two-dimensional contour map. Secondly, on the basis of the first question, the second question establishes the optimized RMSE, R² and MAPE models, and obtains the line graph through the python visual model. The results show that the error is reduced rapidly, the convergence is faster when the sample size is increased, and the global and local prediction accuracy is significantly improved under high sample size. At the same time, the advantages of the co-Kriging model in spatial correlation and interpolation accuracy were verified by comparing the random forest model and quantifying the performance of the two models combined with multi-index radar map and local high-value thermal map. Conclusion: The optimization model has significant advantages in capturing spatial correlation, balancing global and local fluctuations and improving accuracy, and is suitable for F1_target spatial variables.

For problem 4, it is necessary to ensure that the trend of the target variable (F2_target) is estimated in an optimal way. Based on the data in Attachment 2, this paper conducts Jarque-Bera normal distribution test and Spearman correlation coefficient solution, and selects the optimal covariate. On the basis of problem 3 model, a collaborative Kriging model based on FMM optimization is established to interpolate the unsampled points and reveal the trend of target variable (F2_target).

Keywords: Co-kriging; Fast Multipole Method; Jarque-Bera Statistic; Spearman; Random forest

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1. Introduction

1.1 Background

Things and other technologies and the improvement of computing power, spatial data acquisition is more convenient and large-scale, which promotes the development of spatial statistics. However, in practical applications, high-precision measurement samples are scarce due to cost and technical limitations, while low-cost measurement has a wide coverage but low precision, so it is necessary to improve the estimation accuracy of target variables by combining multi-source data with collaborative estimation technology.

The traditional Co-Kriging algorithm can jointly estimate multiple variables, but its application in large-scale and high-dimensional scenarios is limited due to the complexity of covariance and cross covariance functions. Therefore, we propose to construct a collaborative Kriging model based on fast multipole method (FMM) optimization to effectively solve the computational complexity under large-scale data and improve the inference accuracy of spatial variation patterns of target variables. This is the core task of our current research.

1.2 Work

In order to comprehensively analyze and predict the spatial distribution of target variables, we build and optimize the model step by step based on questions 1 to 4.

Firstly, the F1_target data is normalized and meshing in two dimensions, and the linear interpolation and Kriging interpolation models are constructed by random uniform resampling. The spatial distribution characteristics and the relationship between sample size and error are analyzed.

Secondly, through scatterplot, density histogram and Jarque-Bera test, combined with Spearman correlation coefficient and thermal map to quantify the correlation between target variables and covariate, the covariate with the strongest correlation was finally selected.

Then, the FMM optimization co-Kriging model is introduced to improve the efficiency of covariance calculation. Combined with the random forest model, the performance is evaluated by radar map and local hot spot error thermal map, and the spatial variation pattern is revealed.

Finally, in question 4, based on the results of the first three questions, co-variable selection was optimized, and FMM was used to optimize co-Kriging model for interpolation prediction of unsampled points, so as to accurately reveal the spatial variation trend of target variables and provide scientific basis for subsequent research.

2. Problem analysis

2.1 Data analysis

In Annex 1 and Annex 2 provided by the title, the data of each spatial variable file is in three-dimensional mode, and the amount of data is huge. We found that the magnitude gap between data files is relatively large, which brings great trouble to our

data analysis and processing. Therefore, after reducing the three-dimensional data to two-dimensional data, we eliminate the magnitude gap by normalization, and then interpolate and smooth the remaining values. These data are used for correlation analysis to study the change pattern of target variables.

2.2 Analysis of question one

According to question 1, we need to comprehensively analyze the spatial distribution characteristics and influencing factors of F1_target. For the first part of problem 1, on the basis of data normalization and two-dimensional meshing, we adopted random uniform resampling to ensure the fairness and randomness of spatial points, established linear interpolation and Kriging interpolation models, and drew three-dimensional maps and contour maps to analyze the adaptability of the two models, and intuitively presented the spatial change pattern of F1_target. In the second part, the RMSE error analysis model is established based on the interpolation model, and its influence on the prediction error is studied by adjusting the sample size.

2.3 Analysis of question two

In order to analyze the correlation between F1_target and co-variables, we first drew a scatter plot to visually analyze the relationship between target variables and co-variables (Collaborative1, 2, 3, and 4), and then obtained the correlation trend between target variables and each co-variable. Then the density histogram was drawn and the normal distribution curve was fitted. After the normal trend of the data was preliminarily judged, the normality of the variables was quantitatively analyzed through Jarque-Bera test. Spearman's correlation coefficient was finally used to analyze the correlation between the target variable and the co-variable, and heat map was drawn to show it. The two covariables were identified by visual analysis and statistical test.

2.4 Analysis of question three

Based on the model of problem two, we need to select the cooperative variable with the strongest correlation with the target variable, and further study the spatial variation pattern of the target variable F1_target. Because covariance is difficult to be calculated by cokriging algorithm, the fast multipole method is used to calculate covariance function, and a cokriging model based on FMM optimization is established to improve the interpolation accuracy, and a two-dimensional contour map is drawn to show the spatial variation. The relationship between sample size and estimation error is shown by MRSE, R² and MAPE line plots. At the same time, a random forest model is established as a comparison, and the global prediction performance of the two models is quantified by multiple index radar map and local high value heat map.

2.5 Analysis of question four

Problem 4 is a synthesis of the previous three questions, which requires selecting the best method to estimate the trend of the target variable (F2_target). Before the estimation, the synergistic effect of the co-variable on the target variable is also considered, the normal distribution test is carried out and the correlation coefficient is solved, and the variable with the strongest Spearman correlation coefficient is found as the co-variable. On the basis of problem 3, a collaborative Kriging model based on FMM optimization is established, and the remaining unsampled points are interpolated to estimate the trend of target variables.

3. Symbol and Assumptions

3. 1 Symbol Description

Symbol	Description
$\gamma(h)$	Semivariance at a given distance h
C(h)	Covariance at a given distance h
R^2	goodness-of-fit
FMM(h)	Fast Multipole Method-based covariance function
$R_{hotspot}$	Region of detected hotspots above the quantile threshold q
c	Maximum correlated variance
c_0	Minimum variance
$ ho_s$	Correlation coefficient

3. 2 Fundamental assumptions

- 1. Target variables and covariates change gradually in space.
- 2.Mean values are constant regionally, with covariance depending only on point distance.
- 3.Prediction errors are spatially independent, driven by sample size and model features.

4. Modeling and Answering of Question 1

4.1 Data preprocessing

In view of the magnitude difference of the data in Annex 1, Python normalization is adopted to eliminate the impact, and the target variable F1_target is reduced to a two-dimensional grid form, which is convenient for subsequent spatial interpolation and visualization. The two-dimensional grid is shown as follows:

$$\begin{bmatrix} 0.330256 & 0.330729 & \dots & 0.197680 & 0.196259 \\ 0.332623 & 0.332860 & \dots & 0.200758 & 0.199337 \\ \dots & \dots & \dots & \dots & \dots \\ 0.414299 & 0.405066 & \dots & 0.405066 & 0.399148 \\ 0.415009 & 0.417377 & \dots & 0.400331 & 0.394413 \end{bmatrix}$$

$$(1)$$

4.2 The establishment of linear interpolation model

4.2.1 Random uniform resampling

For the first small question of question 1, in order to ensure the fairness of space coverage and simulate sampling randomness, random uniform resampling method is adopted to randomly extract sample points of a specified proportion from target variables through Python to obtain their coordinates and values, so as to achieve unbiased and uniform coverage of the entire space.

4.2.2 Linear interpolation model

The above analysis shows that the resampling points are distributed randomly without fixed rules. To simplify the model, a linear interpolation model was constructed using Python to estimate the values of unsampled spatial variables, where the weight ω between sampling points and interpolation points is correlated:

$$\omega_i = \frac{\frac{1}{d_i}}{\sum_{j=1}^n \frac{1}{d_j}} \tag{2}$$

Where, di is the interpolation point and sampling (x_i, y_i) point spacing, according to the Euclid formula can be obtained:

$$d_i = \sqrt{(x - x_i)^2 + (y - y_i)^2}$$
 (3)

Considering that in the linear interpolation method, the F_target target variable shows a linear change trend among several sampling points (x_i, y_i) in the two-dimensional grid, a linear interpolation model is established:

$$z(x,y) = \sum_{i=1}^{n} \omega_i z_i \tag{4}$$

Where z_i is the known value of the sampling point (x_i, y_i) .

4.3 The establishment of Kriging model

Linear interpolation does not consider the spatial correlation of the target variables. Based on random uniform sampling, we further establish Kriging interpolation model:

$$h_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$$
 (5)

For the spatial relationship between sampling points, the correlation of spatial variables can be described by semi-variance function, and the definition formula is as follows:

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [z(x_i) - z(x_i + h)]^2$$
(6)

In order to calculate the semi-variance of arbitrary distance, a linear model is selected to fit the relationship between distance and semi-variance, and its expression is as follows:

$$\gamma(h) = c_0 + c \cdot h \tag{7}$$

c0 represents the minimum variance; c represents the variance of the variable with the greatest correlation. Based on the geometric relationship between the sampling points, variance function is introduced to calculate the correlation, and the covariance matrix is constructed with the aim of optimal linear unbiased estimation:

$$r_{ij} = c - \gamma(h_{ij}) \tag{8}$$

Where, c = c0 + c presents the maximum covariance, h_{ij} is the distance between sampling points i and j, therefore, the covariance matrix is:

$$C = \begin{bmatrix} r_{11} & r_{12} & \dots & r_{1n} \\ r_{21} & r_{22} & \dots & r_{2n} \\ \dots & \dots & \dots & \dots \\ r_{n1} & r_{n2} & \dots & r_{nn} \end{bmatrix}$$
(9)

According to the correlation formula between interpolation points and known points, the covariance vector can be obtained as follows:

$$c = \begin{bmatrix} r_1 \\ r_2 \\ \dots \\ r_n \end{bmatrix} \tag{10}$$

To sum up, the Kriging interpolation model obtains the weights by solving the equations (11), which not only realizes the optimal linear unbiased estimation of the spatial variables, but also quantifies the uncertainty of the interpolation results.:

$$\begin{bmatrix} r_{11} & r_{12} & \dots & r_{1n} & 1 \\ r_{21} & r_{22} & \dots & r_{2n} & 1 \\ \dots & \dots & \dots & \dots & \dots \\ r_{n1} & r_{n2} & \dots & r_{nn} & 1 \\ 1 & 1 & \dots & 1 & 0 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \dots \\ \lambda_n \\ \phi \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ \dots \\ r_n \\ 1 \end{bmatrix}$$

$$(11)$$

In system (11), \emptyset is the Lagrange multiplier, an auxiliary variable ensuring the weight λi satisfies the unbiased constraint. Using the calculated λi , the optimal coefficient method computes the weighted sum of known points zi, yielding the interpolated value z0:

$$z_0 = \sum_{i=1}^n \lambda_i z_i \tag{12}$$

4.4 The establishment of RMSE model

In order to quantitatively analyze the relationship between sample size and interpolation error, reveal the convergence process and change rule of error, and establish the RMSE model in the range of sampling ratio [0.01,0.05,0.1,0.2].

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (z_i - z_j)^2}{n}}$$
 (13)

The smaller the RMSE value, the better the prediction ability of the model.

4.5 Model solving

(1) Interpolation model 3D diagram

First, the linear interpolation and Kriging interpolation models established in Figure 1 were used to draw the three-dimensional interpolation graphs of F1_target variable before and after sampling, as shown in figures 1 below:

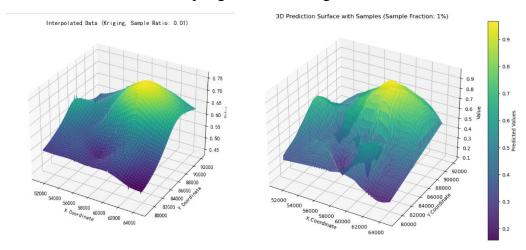


Figure 1 three-dimensional interpolation graphs of F1 target

As can be seen from the figure, Kriging interpolation models spatial correlation to achieve smooth and consistent results with global trends, while linear interpolation relies on resampling point distribution and is difficult to capture the overall trend. In order to further analyze the spatial distribution of F1_target and the influence of interpolation, the 3D diagram of the original data is drawn as follows:

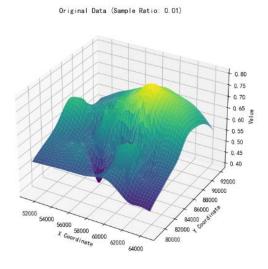


Figure 2 three-dimensional graph of original data

As can be seen from figures 1, 2, the variation of F1_target space variable has the following characteristics:

- (1)Global hierarchy: From low value (blue) to high value (yellow) changes, showing a significant spatial gradient, high value concentration, low value widely distributed.
- (2)Local peak characteristics: the overall change is gentle, the local fluctuation is significant, the high value area is accompanied by obvious local peak, and is significantly affected by local factors.
- (3)Spatial correlation: the changes of adjacent regions are smooth and similar, and the aggregation of high and low values is strong, reflecting the correlation of spatial variables..

(2) Interpolation model detour graph

Python implements linear interpolation, Kriging interpolation, and devious plotting of the original data (Graphs 3), and the original F1_target variable shows significant spatial correlation, showing local peaks and scattered low value regions.

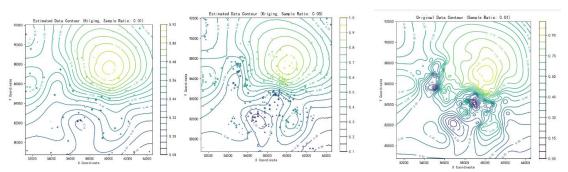


Figure 3 original data Contour

The Kriging interpolation model has high adaptability, accurately portrays the global trend and local details of F1_target, and shows strong prediction ability in sparse regions. The results of the roundabout map are highly consistent with those of the three-dimensional map. The roundabout map reveals the boundary of the high-value hot spot, and the three-dimensional map highlights the peak shape, which verifies the transition of F1_target from low value to high value and the concentration of the high-value region. In summary, F1_target has both global gradient and local fluctuation characteristics, and Kriging interpolation fully reflects its rule, providing reliable support for subsequent analysis.

(3) Error analysis of RMSE

Compared with MSE, RMSE can more directly reflect the difference of prediction performance in sparse regions. The RMSE of the interpolation method was analyzed with Python as the sample size changed, and the sample volume-error relationship graph was drawn (Figure 4, 5).:

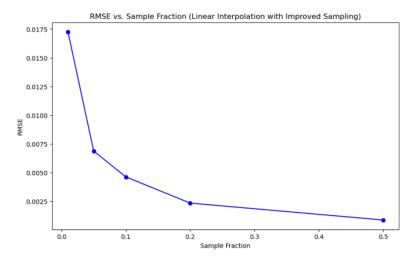


Figure 4 RMSE vs Sample Fraction(Linear)

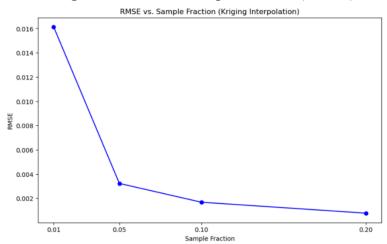


Figure 5 RMSE vs Sample Fraction(Kriging)

As can be seen from Figures 4 and 5, RMSE of Kriging interpolation decreases rapidly with the increase of sample size and becomes stable soon, while RMSE of linear interpolation decreases slowly with the increase of sample size and is difficult to converge.

(4) Result analysis

(1) Overall trend:

RMSE decreases nonlinearly with the increase of sample size. The error is significant at low sample size and decreases rapidly after increasing sample size, but the marginal benefit decreases and eventually becomes stable.

② Low sample size:

The error of linear interpolation is large, it only relies on local information, and it is difficult to capture the global trend. Kriging interpolation uses spatial correlation modeling, with significantly lower errors and more accurate predictions.

3 Sample size increase:

When the sample size of linear interpolation is 10%-20%, the error gradually decreases but does not converge, and the dependence is strong. Kriging interpolation can be stable with 10%-20% sample size, and has high precision under low sample size.

4 High sample size:

The error of linear interpolation decreases slowly and its ability is limited. Kriging interpolation error is stable, high precision display, especially suitable for sparse data scenarios.

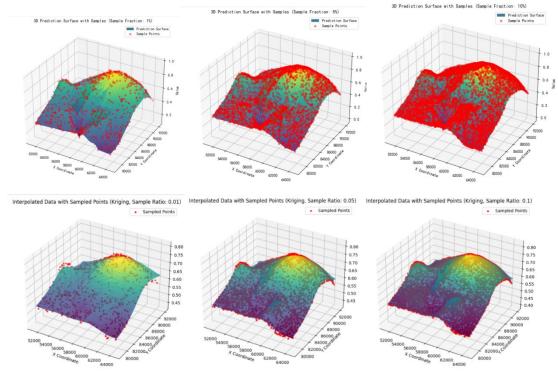
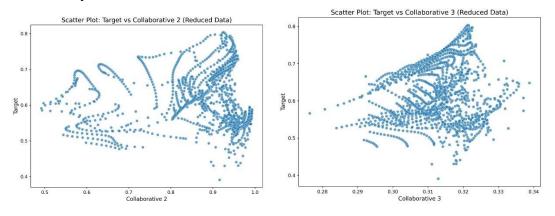


Figure 6 sample size variation

5. Modeling and Answering of Question 2

5.1 Scatter plot analysis

Problem 2 requires us to analyze the correlation between the target variable and the auxiliary variable.



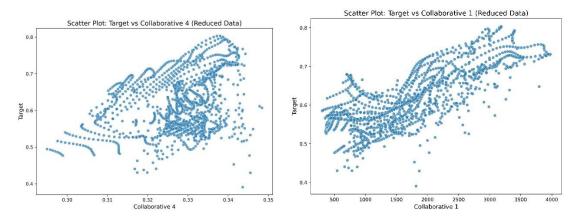


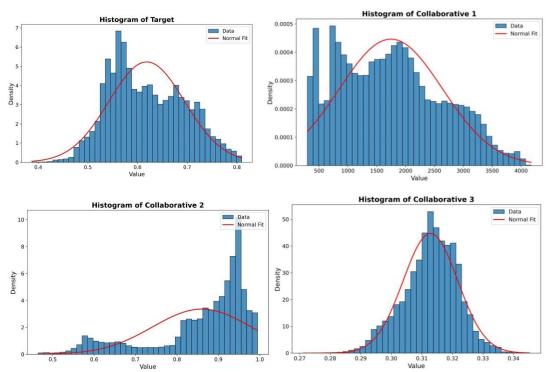
Figure 7 Scatter plot analysis

From the above figure, it can be found that the correlation between Target variable and co-variable (Collaborative1, 2, 3, and 4) is limited. Except for some correlation trends between Target and Collaborative1, the scatter distribution between other relevant variable-co-variable pairs is relatively irregular.

5.2 Correlation analysis

5.2.1 Density - normal graph

In order to explore whether the five spatial variables conform to the normal distribution characteristics, the density histogram is drawn for each variable in turn, and the normal distribution curve is superimposed for preliminary fitting analysis.



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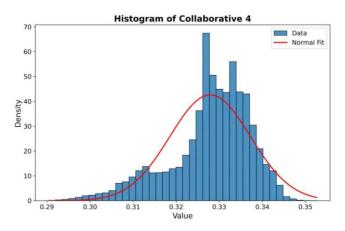


Figure 8 Density - normal graph(all)

- (1)F1_target data is nearly symmetric as a whole, but the tail is deviated and the right tail is biased, which does not fully conform to the normal distribution.
- (2)F1_Collaborative1 has a significant right-sided, left-sided multimodal feature, far from normality.
- (3)F1_Collaborative2 presents a bimodal distribution with a large peak interval and a serious deviation from normality.
- (4)F1_Collaborative3 is symmetrical, and the peak value fits normally, but the right tail is slightly heavier, and the normality is not fully satisfied.
- (5)F1_Collaborative4 is close to the normal distribution shape, but slightly skewed to the right and has poor tail fitting, which does not fully conform to normal.

5.3 Jarque-Bera Normal distribution test

The histogram and line chart show that there is a limited correlation between variables. In order to further verify the correlation between the target variable and the co-variable, the Jarque-Bera test was used for quantitative analysis of normality based on sufficient sample size (>30), providing a reliable basis for statistical analysis.

5.3.1 Calculation of skewness S and kurtosis K

To infer the normality of the data and provide support for correlation coefficient analysis, hypothesis is set:

- (1) Null hypothesis H_0 : data follows a normal distribution
- (2) Alternative hypothesis H_1 : The data does not follow normal distribution

The skewness S and kurtosis K statistics are calculated, where S measures the symmetry of distribution and reveals the trend of spatial migration. K reflects the frequency of volatility and extreme values, and the specific expression is as follows:

$$S = \frac{\frac{1}{n} \sum_{i=1}^{n} (x_i - \overline{x})^3}{\left(\frac{1}{n} \sum_{i=1}^{n} (x_i - \overline{x})^2\right)^{\frac{3}{2}}}$$
(14)

In formula (14), x_i represents the i th sample value in the data; The x digit represents the sample mean.

$$K = \frac{\frac{1}{n} \sum_{i=1}^{n} (x_i - \overline{x})^4}{\left(\frac{1}{n} \sum_{i=1}^{n} (x_i - \overline{x})^2\right)^2}$$
(15)

5.3.2 Jarque-Bera model

Secondly, the relation between skewness S and kurtosis K is established through the Jarque-Bera test formula:

$$JB = n \left(\frac{S^2}{6} + \frac{(K-3)^2}{24} \right) \tag{16}$$

According to the obtained JB value, we can calculate its corresponding p-value through the chi-square distribution to judge the normality of the spatial variable value:

$$p - value = P(\chi^2 \geqslant JB) \tag{17}$$

 χ represents a Chi-square distribution of 2 degrees of freedom. If p-value>0.05, H0 is accepted, and the variable values conform to normal distribution; If p-value \leq 0.05, H0 is rejected, and the variable values do not conform to the normal distribution.

Draw the distribution diagram of skewness and kurtosis of variables in Annex 1 through Python, and calculate JB test values as shown in Table 1 below:

Table 1. 3D test values				
variable	JB Statistic	S	K	p-value
Target	2421.6	0.2648	2.2645	0.0
Collaborative 1	3055.9	0.3471	2.5520	0.0
Collaborative 2	22024.2	-1.3189	3.7160	0.0
Collaborative 3	1606.1	-0.3506	3.2305	0.0
Collaborative 4	10823.9	-0.8973	3.6714	0.0

Table 1: JR test values

As can be seen from Table 1 above, the large sample size amplified the slight skew and tail characteristics of the data, and the P-values of Jarque-Bera (JB test) were all lower than 0.05 level, so the null hypothesis was rejected and the samples were considered not to meet the requirements of normal distribution.

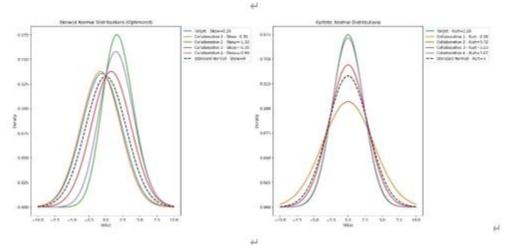


Figure 9 skewness and kurtosis results

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Python visualizations of skewness and kurtosis showed deviations from normality, confirming the invalidity of the normal hypothesis. Thus, Spearman correlation was applied to assess the relationship between the target and cooperative variables..

5.3.3 Spearman Correlation coefficient model

Through Python programming, four two-dimensional matrix data is flattened into a single column vector, and then the entire spatial variable data file is treated as a complete variable:

$$\rho_s = 1 - \frac{6\sum_{i=1}^n d_i^2}{n(n^2 - 1)} \tag{18}$$

Where ρ_s represents the Spearman correlation coefficient between the target variable X and Y (four covariables), which has the following relationship expression:

$$d_i = r_{x_i} - r_{y_i} \tag{19}$$

SPSS software was used to calculate each group of variables to obtain phase relation table 2, and the numerical values were visualized in the bar chart:

Table 2: Spearman correlation

combination	ho	Significance(p)
Target- Collaborative 1	0.750**	<0.01
Target- Collaborative 2	-0.081**	<0.01
Target- Collaborative 3	0.279**	<0.01
Target- Collaborative 4	0.381**	<0.01

Note: ** is at 0.01 level (double tail), the correlation is significant

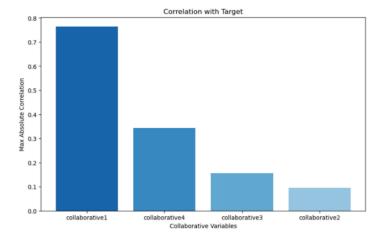


Figure 10 correlation results

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At a 99% confidence level, the correlation results were statistically significant. Collaborative1 and Collaborative4 showed strong positive correlations with the target (ρ =0.750 and ρ =0.381), Collaborative3 was weakly correlated (ρ =0.279), and Collaborative2 was weakly negatively correlated (ρ =-0.081). Thus, Collaborative1 and Collaborative4 are suitable as collaboration variables.

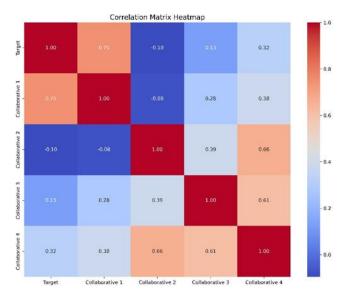


Figure 11 correlation Heatmap

The thermal map still shows that Target has a high correlation with Collaborative 1 and Collaborative 4, especially the strongest correlation with Collaborative 1. Therefore, Collaborative 1 and Collaborative 4 are selected as co-variables.

6. Modeling and Answering of Question 3

Target shows the highest correlation with Collaborative1. Using random sampling and grid data, the normalized Kriging model is extended. Fast multipole method (FMM) optimizes covariance calculation, enhancing interpolation accuracy and spatial prediction.

6.1 Sampling point processing

In order to ensure the spatial correlation and improve the reliability of covariance function fitting, a sampling point set containing the values of the cooperation variable and the target variable is constructed by associating the changes of both.

$$(X_i, Y_i, T_i, C_{1i}) \tag{20}$$

Further analyze the covariance and cross-covariance between target and cooperative variables, establishing a joint distribution model that assumes sampling at the same spatial location and satisfies multivariate normality:

$$Z(s) = \begin{bmatrix} F1_{target}(s) \\ Collaborative_1(s) \end{bmatrix} \sim N \left(\begin{bmatrix} \mu_{target} \\ \mu_{collab1} \end{bmatrix}, \sum \right)$$
 (21)

The expression of covariance matrix can be obtained as follows:

$$\sum = \begin{bmatrix} \sigma^2_{target} & \sigma_{target-collab1} \\ \sigma_{target-collab1} & \sigma^2_{collab1} \end{bmatrix}$$
 (22)

6.2 Covariance function

The fast multipole method (FMM) uses hierarchical grouping and recursion for precise covariance calculation of adjacent points, while reducing time complexity from O(nlogn) or O(n) for distant points, effectively lowering computation cost while maintaining accuracy.

$$C_{ij}(h) = \begin{cases} C_0 + C \cdot FMM(h), h \leq a \\ C_0 + C, & h > a \end{cases}$$
 (23)

Where, FMM (h) represents two covariance function calculations optimized by fast multipole method, $I,j \in \{\text{target,collab1}\};$

6.2.1 Variance function

In the cooperative Kriging interpolation model based on FMM optimization to be established in this problem, the spherical variation function which is more suitable for data complexity is adopted to eliminate the spatial distribution of high value concentration or low value diffusion of target variables and cooperative variables which are difficult to solve by linear variation function in problem 1.

$$\gamma(h) = \begin{cases} C_0 + C \left[1.5 \frac{h}{a} - 0.5 \left(\frac{h}{a} \right)^3 \right], h \leq a \\ C_0 + C, & h > a \end{cases}$$

$$(24)$$

In formula (24), C0 is the small scale error value, C represents the growth amplitude of the variance function, and a is the distance between the correlated variable and the covariate.

6.3 Collaborative Kriging interpolation model based on FMM optimization

Collaborative kriging is widely used in the spatial prediction of high cost variables such as geological exploration and mineral estimation, but the implementation is complicated. To solve this problem, FMM optimization covariance calculation is introduced, co-Kriging model is constructed, and collaborative variables are integrated into the interpolation process to accurately restore the spatial variation trend and reduce the prediction error.

6.3.1 Cokriging interpolation formula

The predicted value of the spatial variable at the unsampled point s:

$$\hat{T}(s) = \sum_{i=1}^{n} \lambda_i^{target} T_i + \sum_{j=1}^{m} \lambda_j^{collab1} C_{1j}$$
(25)

The co-Kriging equations based on FMM optimization can be obtained as:

$$\begin{bmatrix} C_{target-target} & C_{target-collab1} & 1 \\ C_{collab1-target} & C_{collab1-collab1} & 1 \\ 1^{T} & 1^{T} & 0 \end{bmatrix} \begin{bmatrix} \lambda_{target} \\ \lambda_{collab1} \\ \phi \end{bmatrix} = \begin{bmatrix} C_{target}(s) \\ C_{collab1}(s) \\ 1 \end{bmatrix}$$
(26)

The fast multipole method optimizes the covariance calculation, makes the cokriging model complete the large-scale interpolation efficiently, and visually displays the spatial distribution of the target variables through the two-dimensional contour map.

6.4 Error analysis model

Due to insufficient sampling of discontinuous spatial variables such as rainfall and pollutant concentration, the interpolation accuracy is easy to decrease. In order to quantify the relationship between sample size and estimation error and evaluate the performance of the FMM optimized collaborative Kriging model, RMSE, R² and MAPE were used to analyze the absolute error, goodness of fit and relative error from multiple dimensions, providing a reference for the prediction of high-cost spatial variables.

(1) RMSE Model

In order to restore the absolute value of the target variable, the RMSE model in question 1 was used to measure the prediction accuracy under different sampling ratios, and the performance of the model in sparse regions and outliers was evaluated:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (T_i - \hat{T}_i)^2}$$
 (27)

(2) R² Model

An R² determination coefficient model was established to explain the influence of sample size on model performance through goodness of fit:

$$R^{2} = 1 - \frac{\sum_{i=1}^{n} (T_{i} - \hat{T}_{i})^{2}}{\sum_{i=1}^{n} (T_{i} - \hat{T}_{i})^{2}}$$
(28)

When the sample size is low, the R^2 may be low; As the sampling ratio increases, the R^2 change curve quantifies the asymptotic fitting ability of the model.

(3) MAPE Model

When the spatial variable values are small, RMSE may be ignored, while MAPE highlights the relative prediction error in the low-value region. Combining RMSE and R², the error analysis model of MAPE was established to reveal the difference between the global and local performance of the model.

$$MAPE = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{T_i - \hat{T}_i}{T_i} \right| \times 100\%$$
 (29)

6.5 Random forest interpolation model

Through the FMM-optimized co-Kriging model, its ability to improve the prediction accuracy and make up for the information deficiency under different

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sampling ratios is verified. In order to analyze the relationship between sample size and error and the spatial model of target variables, a flexible random forest model is introduced.

6.5.1 Prediction of a single decision tree

Each decision tree makes partition predictions for the target variable Ti based on the input feature xi:

$$f_t(x) = \sum_{l=1}^{L_t} \omega_l f(x \in R_l)$$
(30)

6.5.2 Stochastic forest integrated prediction

In order to reduce the overfitting risk of single decision tree and improve the robustness of prediction. A random forest is constructed by integrating N decision trees, and the predicted value T(x) is obtained by averaging the results of multiple sub-models.

$$\hat{T}(x) = \frac{1}{n} \sum_{t=1}^{n} f_t(x)$$
(31)

6.6 Multivariate contrast model

6.6.1 Global performance comparison model based on multiple indicators

On the basis of question 2 and Question 2, the analysis of EVS, prediction time and training time is added, a multi-index model is established, and the global performance is compared and analyzed.

(1) EVS

Test the interpretation ability of the model to the change of the target variable, the value range [0,1], the larger the value, the better the prediction performance of the model.

$$EVS = 1 - \frac{Var(T_i - \hat{T}_i)}{Var(T_i)}$$
(32)

(2) Forecast time

The calculation time required by the measurement model to predict the unsampled points reflects the efficiency of the algorithm.

(3) Training time

Measure the time it takes to build a model to estimate the computational overhead of the model.

6.6.2 Robustness evaluation model

The multi-index comparison model has analyzed the prediction ability of low-value regions. In order to evaluate the performance of the co-Kriging model of random forest and FMM optimization in high-value regions, a local hotspot prediction error model is constructed, and the quantile q defines the part of the target variable value range higher than q as the hotspot region:

$$T_{threshold} = Quantile(T(s), q)$$
 (33)

Next, sample the hotspot area and obtain the sampling point $s \in R$ hotspot. The expression for calculating the prediction error is as follows:

$$\begin{cases} Error_{RF}(s) = |T_{true}(s) - \hat{T}_{RF}(s)| \\ Error_{CK}(s) = |T_{true}(s) - \hat{T}_{CK}(s)| \end{cases}$$
(34)

Finally, the average error over the entire hot spot region is:

$$\begin{cases} MAE_{RF} = \frac{1}{|R_{hotspot}|} \sum_{s \in R_{hotspo}} Error_{RF}(s) \\ MAE_{CK} = \frac{1}{|R_{hotspot}|} \sum_{s \in R_{hotspot}} Error_{CK}(s) \end{cases}$$
(35)

6.7 Model solving

(1) FMM optimized cokriging 2D contour map

According to the research results of problem 2, Problem 3 adds the determination of covariate and extends the Kriging interpolation model on the basis of problem 1. Similarly, the two-dimensional contour map achieved by the Kriging interpolation model optimized by FMM is shown in Figure 12:

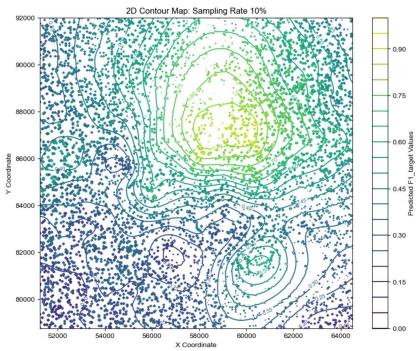


Figure 12 FMM optimized cokriging 2D contour map

Compared with the ordinary Kriging model in problem 1, the collaborative Kriging model based on FMM optimization not only maintains the global hierarchy, local peak characteristics and spatial correlation, but also presents more delicate gradient transitions, high-value hot spot fluctuations and more coherent high-low value regions. At the same time, the anisotropy of F1_target is revealed, which shows the difference of change rate and trend in different directions.

(2) Sample size - error analysis

The interpolation results were brought into RMSE, R square and MAPE models for solving, and the error analysis line diagram under different sample sizes and the error point distribution diagram of the two algorithms were obtained, as shown in Figure 13 below:

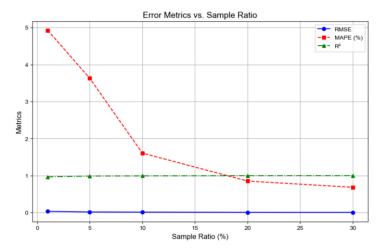


Figure 13 Sample size - error analysis

On the basis of problem 1, the FMM-optimized co-Kriging interpolation model is significantly better than the Kriging model in comparison of sample size and error relation. In the case of low sample size, the spatial correlation modeling ability is enhanced by cooperative variables, and the error is quickly reduced. When the sample size increases, the convergence rate is faster. With a high sample size, both the global and local prediction accuracy of the model are significantly improved. This advantage makes the co-Kriging model more suitable for sparse sampling and complex spatial change scenarios.

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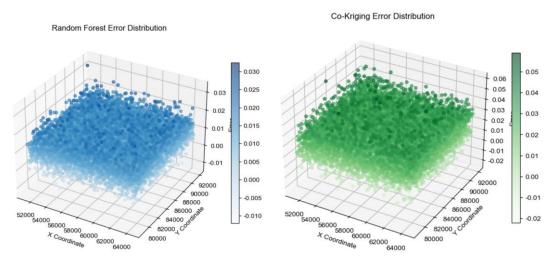


Figure 14 Error Distribution

(3) Two-dimensional contour map of random forest

First of all, the random forest interpolation model established in xxx uses python coding to conduct random forest integrated prediction for target variable and covariable 1, and obtains a two-dimensional contour map as shown in Figure 15:

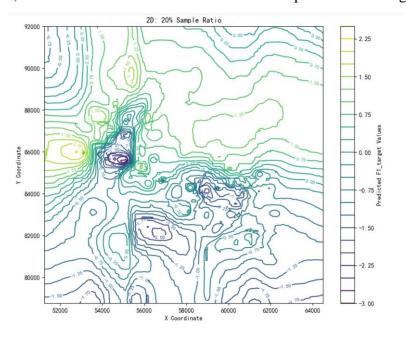


Figure 15 Two-dimensional contour map of random forest

Comparative analysis shows that the FMM optimized co-Kriging model is superior to random forest in global gradient capture, local peak performance and spatial correlation processing, and can more accurately describe the distribution characteristics of F1_target, especially for spatial variable change patterns in local hot spots and sparse sampling scenes.

(4) Multivariate error analysis

According to the established global performance comparison model for a number of indicators, the radar map for a number of indicators and the thermal map for robustness evaluation are obtained through python coding, as shown in Figure 16 and 17:

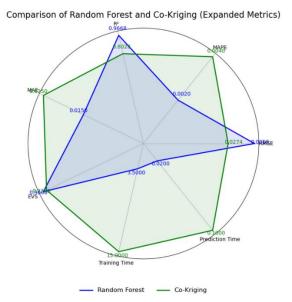


Figure 16 Multivariate error analysis(1)

Radar map analysis shows that although random forest has advantages in nonlinear relationship and multi-dimensional feature processing, it is not enough to capture spatial correlation and has limited performance in high-value region interpolation and sparse data prediction. Compared with the FMM optimization co-Kriging model, it is verified that it has significant advantages in capturing spatial correlation, balancing global and local fluctuations, and using cooperative variables to improve interpolation accuracy. It is suitable for high spatial dependence scenarios such as F1_target.

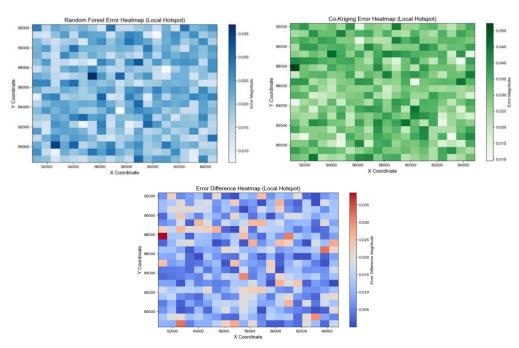


Figure 17 Multivariate error analysis(2)

(1) Random forest error: the error is uniform in the hot spot area but larger near the high value, and the detail capture is limited.

- (2) Co-Kriging error: accurate modeling of spatial correlation, error distribution in line with local characteristics, better restore the complex changes in hot spots.
- (3) Error difference: Cokriging performs better at the hot spot center (red), while random forest performs slightly better at the edge (blue), but the local improvement is limited.

Conclusion: FMM optimization with Kriging is significantly better than random forest in capturing hot spot fluctuations, spatial correlation and detail restoration, and is more suitable for complex spatial variable prediction.

7. Modeling and Answering of Question 4

7.1 Data preprocessing

Following the Annex 1 process, the 3D data is converted to a 2D table using Python and normalized to eliminate level differences. Covariable values corresponding to the 2D coordinates in the F2_target_variable table (Annex 2) are extracted and saved as an xlsx file for correlation analysis and interpolation.

7.2 Correlation analysis

7.2.1 Jarque-Bera Normal distribution test

To account for the synergistic effect of other variables on the target variable, the Jarque-Bera normality test was conducted, followed by a correlation analysis. As the process is similar to Problem 2, details are omitted, and the results are shown in the table below:

Table 3: JB Statistic and p-value

variable	JB Statistic	p-value
Target	99.2	0.0
Collaborative 1	520.3	0.0
Collaborative 2	254.1	0.0
Collaborative 3	66.9	0.0
Collaborative 4	62.1	0.0

As shown in Table 3, similar to Annex 1, the large sample size amplifies slight skewness and tail characteristics, leading to Jarque-Bera (JB test) p-values below 0.05. Thus, the null hypothesis is rejected, indicating non-normality. Therefore, Spearman correlation was used to evaluate the relationship between the target and cooperative variables.

7.2.2 Spearman correlation coefficient model

On the basis of the normality test, the Spearman correlation coefficient model is established, and the correlation coefficient table is calculated by using python code to calculate each group of variables, and the results are presented as a heat map.

Table	4.	Snearman	correlation
Iabic	т.	Spearman	coi i ciation

combination	ho	
Target- Collaborative 1	0.20**	
Target- Collaborative 2	0.20**	
Target- Collaborative 3	0.71**	
Target- Collaborative 4	0.05**	

Note: ** is at the 0.01 level (two-tailed), and the correlation is significant

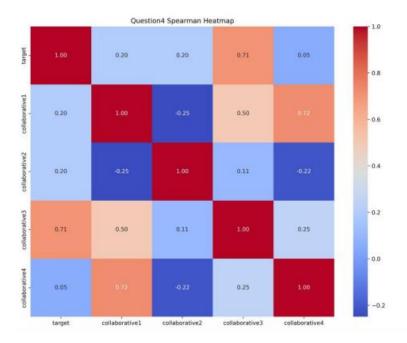


Figure 18 heat map

According to the Spearman correlation coefficient between the target variable and the other variables, the collaborative3 variable with a correlation coefficient of 0.71 was selected as the covariate and brought into the subsequent model estimation. Other variables, such as collaborative4, were not considered as covariates due to their low correlation coefficient (<0.3).

7.3 Collaborative kriging interpolation model based on FMM optimization is solved

Based on the comparative analysis in Problem 3, the FMM-optimized collaborative kriging model was selected to estimate unsampled target variable points in Problem 4. The model from Problem 3 is reused, with results summarized in the table below and presented as a contour plot.:

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Table 5:predict data

	24620 COP2 CHILD HAVE				
coordinate	51250	•••	64450	64500	
78750	0.516105834		0.344097693	0.344871099	
78800	0.515929444		0.345237449	0.345983718	
•••		•••			
91950	0.66968675	•••	0.337693351	0.338263229	
92000	0.652298536	•••	0.335793758	0.336472185	

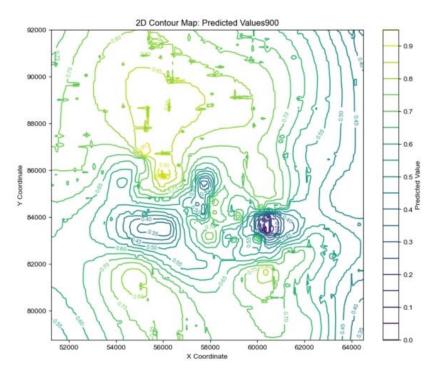


Figure 19 Contour Map

8. Sensitivity Analysis

In the formula (23) of the co-Kriging model, we define the core interpolation formula and weight calculation, involving key variables such as the correlation distance a and the correlation coefficient between the target and cooperation variables. By solving the model, weights are determined. Next, to explore sensitivity, we vary target and covariable weights while keeping other parameters constant, solving iteratively.

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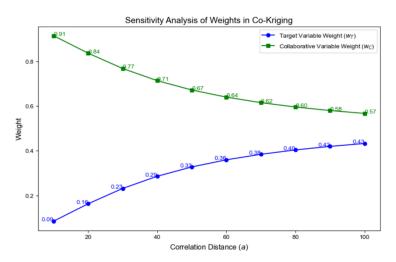


Figure 20 Sensitivity Analysis of Weight

Figure 20 shows that in the optimized co-Kriging model, target variable weight increases with correlation distance, while co-variable weight decreases, reflecting high sensitivity and dynamic changes. At small correlation distances, co-variable weight dominates, but as a increases, target variable weight prevails. This aligns with real-world measurements, where correlation distance should be set based on the target variable's autocorrelation range and the co-variable's effective region to minimize sampling error during interpolation.

9.Strengths and Weakness

Advantages:

- (1)High-precision interpolation: Captures global gradients and local fluctuations of spatial variables, achieving high accuracy even in sparse data scenarios by leveraging collaborative variables.
- (2)Efficient covariance calculation: Fast multipole method (FMM) significantly enhances computational efficiency and reduces time costs for large-scale data processing.
- (3)Global and local adaptability: Balances global spatial trends and local hotspot modeling, excelling in complex spatial distribution patterns.

Limitations:

- (1)High computational cost: Despite FMM optimization, covariance matrix construction and solution remain bottlenecks for extremely large datasets.
- (2)Linear correlation assumption: Relies on strong linear relationships between target and collaborative variables, limiting performance in highly nonlinear scenarios.

10.Conclusion

highlights the effectiveness of the FMM-optimized Co-Kriging model in predicting the spatial distribution of F1_target. By leveraging spatial correlations and auxiliary variables, the model demonstrated superior accuracy and robustness, particularly in capturing local hotspots and fine-scale variations. The comparison with random forest validated Co-Kriging's strength in spatially correlated scenarios, especially for sparse data interpolation. Additionally, the analysis revealed a non-linear relationship between sample density and prediction error, with diminishing returns as sample size increased. These findings provide valuable insights for geostatistical applications and emphasize the potential of integrating advanced computational techniques into traditional interpolation methods.

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Appendix

```
question-1-Contourmap.py
question-1-Datatransformation.py
question-1-Kriging.py
question-1-Kriging-RMSE.py
question-1-Linear-RMSE.py
question-1-LinearInterpolation.py
question-2-Correlation calculate.py
pquestion-2-Correlation coefficient heat map.py
question-2-Histogram of spatial variables.py
question-2-Normal test.py
question-2-Q-Q plot.py
question-2-Scatter plot.py
🥏 question-2-Skewness kurtosis calculations.py
question-3-Co kriging with fmm.py
duestion-3-Error dot diagram.py
question-3-Local hot spot error prediction plot.py
question-3-Model comparison radar chart.py
plot.py question-3-Model sensitivity analysis plot.py
question-3-Random forest.py
question-3-Rmse R^2 Mape.py
question-4-3D surface plot.py
question-4-Cokriging with fmm.py
question-4-Data normalization.py
question-4-Datatransformation.py
question-4-Scatter plots and JB statistics.py
```

Question-1-Contourmap

question-4-Spearman heat map.py

Define grid coordinates

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

# File paths and names
file_paths = []

# Load data from Excel files
data_sets = [(pd.read_excel(path, header=None).values, name) for path, name in file_paths]
```

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```
grid size = (266, 266)
x = \text{np.linspace}(51250.0, 64500.0, \text{grid size}[1]) #X-coordinate range
y = \text{np.linspace}(78750.0, 92000.0, \text{grid size}[0]) # Y-coordinate range
X, Y = np.meshgrid(x, y)
# Plot 3D surface for each dataset
for data, name in data sets:
     fig = plt.figure(figsize=(12, 8))
     ax = fig.add subplot(111, projection='3d')
     # Create a 3D surface plot
     surf = ax.plot surface(X, Y, data, cmap='viridis', edgecolor='none',
alpha=0.8)
     fig.colorbar(surf, ax=ax, label='Value')
     # Set title and axis labels
     ax.set title(f'Three-Dimensional Surface Plot for {name}')
     ax.set xlabel('X Coordinate')
     ax.set ylabel('Y Coordinate')
     ax.set zlabel('Value')
     plt.show()
```

Question-1-Datatransformation

```
import numpy as np
import pandas as pd

# Define the target grid size
grid_size = (266, 266)

# File path
file_path = ""

# List to store the data
data = []

# Open the file and extract numerical data
with open(file_path, 'r') as file:
for line in file:
    try:
        # Convert each line into a list of floating-point numbers
        row = list(map(float, line.split()))
        if row: # If the line is not empty
```

```
data.extend(row)
          except ValueError:
               # Skip non-numerical lines
               continue
# Convert the data to a numpy array
data = np.array(data)
# Check if the data size matches the target grid size
if data.size != grid size[0] * grid size[1]:
    raise ValueError(f"Data size {data.size} does not match the target grid size
{grid size}!")
# Reshape the data into a 266 x 266 2D array
reshaped_data = data.reshape(grid_size)
# Output the result for verification
print("Data has been successfully reshaped to 266 x 266 format!")
# Save the reshaped data to an Excel file
output file = "reshaped data.xlsx"
pd.DataFrame(reshaped data).to excel(output file, index=False, header=False)
print(f"Data has been successfully saved as an Excel file: {output file}")
```

Question-1-Kriging

```
from mpl toolkits.mplot3d import Axes3D #For creating 3D plots
    from scipy.interpolate import griddata
    import numpy as np
    import matplotlib.pyplot as plt
    import pandas as pd
    # File path
    file path = ""
    # Read data and reshape it into a 2D array
    df target = pd.read excel(file path, header=None)
    reshaped data = df target.values.reshape(266, 266)
    # Original data
    original data = reshaped data
    # Grid coordinates
    x = \text{np.linspace}(51250.0, 64500.0, 266)
```

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```
y = np.linspace(78750.0, 92000.0, 266)
X, Y = np.meshgrid(x, y)
# Define a function for random sampling
def random sampling(data, sample fraction):
    total points = data.size
    sample count = int(total points * sample fraction)
    indices = np.random.choice(total points, sample count, replace=False)
    sampled x = X.flatten()[indices]
    sampled y = Y.flatten()[indices]
    sampled values = data.flatten()[indices]
    return sampled x, sampled y, sampled values
# Define a function for interpolation
def interpolate values(sampled x, sampled y, sampled values, method='linear'):
    estimated = griddata((sampled x, sampled y), sampled values, (X, Y),
method=method)
    return estimated
# Define a function for RMSE calculation
def calculate rmse(original, estimated):
    mask = \sim np.isnan(estimated)
    return np.sqrt(np.mean((original[mask] - estimated[mask]) ** 2))
# List of sample fractions
sample fractions = [0.01, 0.05, 0.1, 0.2, 0.3] # Sampling fractions
# Store error results
errors = []
for sample fraction in sample fractions:
    # Perform random sampling
    sampled x, sampled y, sampled values = random sampling(original data,
sample fraction)
    # Perform interpolation
    estimated data = interpolate values(sampled x, sampled y,
sampled values)
    # Calculate RMSE
    error = calculate rmse(original data, estimated data)
    errors.append((sample fraction, error))
     # Plot 3D surface with sampled points and predictions
```

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```
fig = plt.figure(figsize=(12, 8))
     ax = fig.add subplot(111, projection='3d')
     # Plot the 3D surface for predictions
    surf = ax.plot surface(X, Y, estimated data, cmap='viridis',
edgecolor='none', alpha=0.9)
     # Highlight sampled points
     ax.scatter(sampled x, sampled y, sampled values, color='red', s=20,
label='Sample Points')
     # Set title and axis labels
    ax.set title(f'3D Prediction Surface with Samples (Sample Fraction:
{sample fraction * 100:.0f}%)')
    ax.set xlabel('X Coordinate')
    ax.set ylabel('Y Coordinate')
    ax.set zlabel('Value')
     # Add color bar
    fig.colorbar(surf, ax=ax, label='Predicted Values')
     # Add legend
    ax.legend()
    plt.show()
# Print error results
fractions, error values = zip(*errors)
print("Sample Fractions:", fractions)
print("Errors (RMSE):", error values)
```

Question-1-Kriging-RMSE

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from pykrige.ok import OrdinaryKriging
from sklearn.metrics import mean_squared_error
from scipy.interpolate import griddata

# Read Excel data
file_path = "Data-preprocessing/target.xlsx"
data = pd.read_excel(file_path, header=None).to_numpy()
```

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```
# Data dimensions
rows, cols = data.shape
# Define optimized grid coordinates
x range = np.arange(51250, 64500 + 100, 100).astype(np.float64)
y range = np.arange(78750, 92000 + 100, 100).astype(np.float64)
X, Y = np.meshgrid(x range, y range)
# Original data grid
original x range = np.linspace(51250, 64500, cols).astype(np.float64)
original y range = np.linspace(78750, 92000, rows).astype(np.float64)
original points = np.array([(x, y) \text{ for y in original y range for x in }
original x range])
values = data.flatten().astype(np.float64)
# Sampling ratios
sample ratios = [0.01, 0.05, 0.1, 0.2]
rmse list = []
# Iterate through sampling ratios
for sample ratio in sample ratios:
     # Random sampling
    np.random.seed(42)
    sample size = int(len(original points) * sample ratio)
    sample indices = np.random.choice(len(original points), sample size,
replace=False)
    sample points = original points[sample indices]
    sample values = values[sample_indices]
     # Separate X and Y coordinates of sampled points
    sample x = sample points[:, 0]
    sample y = sample points[:, 1]
     # Kriging interpolation
    kriging = OrdinaryKriging(sample x, sample y, sample values,
variogram model='linear')
    interpolated values, ss = kriging.execute('grid', x range, y range)
     # Map interpolated results back to original resolution
    original mesh = np.array([(x, y) \text{ for y in original y range for x in }
original x range]) # Original 2D points
    interpolated on original = griddata(
         points=(X.flatten(), Y.flatten()), #Interpolation grid 2D points
         values=interpolated values.flatten(), #Interpolation result values
```

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```
xi=original mesh,
                              # Original grid 2D points
         method='linear'
    ).reshape(data.shape)
                           # Reshape result to original data shape
    # Calculate Root Mean Squared Error (RMSE)
    ground truth flat = data.flatten()
    rmse = np.sqrt(mean squared error(ground truth flat,
interpolated on original.flatten()))
    rmse list.append(rmse)
    # Plotting
    plt.figure(figsize=(14, 6))
    plt.subplot(1, 2, 1)
    contour1 = plt.contour(original x range, original y range, data, levels=20,
cmap='viridis') # Draw contour
    plt.colorbar(contour1)
    plt.clabel(contour1, inline=True, fontsize=8) # Add contour labels
    plt.title(f'Original Data Contour (Sample Ratio: {sample ratio})')
    plt.xlabel('X Coordinate')
    plt.ylabel('Y Coordinate')
    plt.subplot(1, 2, 2)
    contour2 = plt.contour(X, Y, interpolated values, levels=20, cmap='viridis')
# Draw contour
    plt.colorbar(contour2)
    plt.clabel(contour2, inline=True, fontsize=8) # Add contour labels
    plt.title(f'Estimated Data Contour (Kriging, Sample Ratio: {sample ratio})')
    plt.xlabel('X Coordinate')
    plt.ylabel('Y Coordinate')
    plt.tight layout()
    plt.show()
# Print RMSE for each sampling ratio
for ratio, rmse in zip(sample ratios, rmse list):
    print(f"Sample Ratio: {ratio}, RMSE: {rmse}")
# Plot Sample Ratio vs RMSE
plt.figure(figsize=(8, 6))
plt.plot(sample ratios, rmse list, marker='o', linestyle='-', color='b')
plt.title('Sample Ratio vs Root Mean Squared Error (RMSE)')
plt.xlabel('Sample Ratio')
plt.ylabel('Root Mean Squared Error')
plt.savefig("Question1-Rmse.jpg", dpi=600)
```

plt.show()

```
Question-1-LinearInterpolation
```

```
from scipy.interpolate import griddata # Ensure to import griddata
    import numpy as np
    import matplotlib.pyplot as plt
    # Original data (reshaped data is a 266x266 array)
    original data = reshaped data
    # Grid coordinates
    x = \text{np.linspace}(51250.0, 64500.0, 266)
    y = np.linspace(78750.0, 92000.0, 266)
    X, Y = np.meshgrid(x, y)
    #1. Random uniform resampling
    def random sampling(data, sample fraction):
         total points = data.size
         sample count = int(total points * sample fraction)
         indices = np.random.choice(total points, sample count, replace=False)
         sampled x = X.flatten()[indices]
         sampled y = Y.flatten()[indices]
         sampled values = data.flatten()[indices]
         return sampled x, sampled y, sampled values
    # 2. Interpolation to estimate unsampled locations
    def interpolate values(sampled x, sampled y, sampled values, method='linear'):
         estimated = griddata((sampled x, sampled y), sampled values, (X, Y),
    method=method)
         return estimated
    # 3. Error calculation
    def calculate error(original, estimated):
         mask = \sim np.isnan(estimated)
         return np.sqrt(np.mean((original[mask] - estimated[mask]) ** 2))
    # 4. Analysis for different sample sizes
    sample fractions = [0.01, 0.05, 0.1, 0.2, 0.5]
    errors = []
    for sample fraction in sample fractions:
          # Random sampling
         sampled x, sampled y, sampled values = random sampling(original data,
```

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```
sample fraction)
     # Interpolation estimation
    estimated data = interpolate values(sampled x, sampled y,
sampled values)
     # Error calculation
     error = calculate error(original data, estimated data)
    errors.append((sample fraction, error))
     # Plot filled contour map
     plt.figure(figsize=(12, 8))
    plt.contourf(X, Y, estimated data, cmap='viridis', levels=100)
    plt.colorbar(label='Estimated Value')
    plt.scatter(sampled x, sampled y, c='red', s=10, label='Sample Points')
    plt.title(fFilled Contour Map (Sample Fraction: {sample fraction *
100:.0f\%)')
    plt.xlabel('X Coordinate')
    plt.ylabel('Y Coordinate')
    plt.legend()
    plt.show()
     # Plot contour map with labeled values
     plt.figure(figsize=(12, 8))
    contour = plt.contour(X, Y, estimated data, cmap='viridis', levels=20)
     plt.clabel(contour, inline=True, fontsize=8) # Add labels on contour lines
    plt.scatter(sampled x, sampled y, c='red', s=10, label='Sample Points')
    plt.colorbar(label='Estimated Value')
    plt.title(f'Contour Map (Sample Fraction: {sample fraction * 100:.0f}%)')
     plt.xlabel('X Coordinate')
    plt.ylabel('Y Coordinate')
    plt.legend()
    plt.show()
# Plot the relationship between sample size and error
fractions, errors = zip(*errors)
plt.figure(figsize=(8, 6))
plt.plot(fractions, errors, marker='o')
plt.title('Relationship Between Sample Size and Estimation Error')
plt.xlabel('Sample Fraction')
plt.ylabel('Estimation Error (RMSE)')
plt.grid(True)
plt.show()
```

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```
question-1-Linear-RMSE
import matplotlib.pyplot as plt
    import pandas as pd
    import numpy as np
    from scipy.interpolate import griddata
    from sklearn.metrics import mean squared error
    # Define linear interpolation method
    def linear interpolation(sampled features, sampled labels, full features,
    full shape):
         interpolated = griddata(sampled features, sampled labels, full features,
    method='linear')
         return interpolated.reshape(full shape)
    # Calculate RMSE error (ignoring NaN values)
    def calculate rmse(true values, predicted values):
         mask = ~np.isnan(predicted values) # Ignore NaN values
         return np.sqrt(mean squared error(true values[mask],
    predicted values[mask]))
    # Stratified uniform sampling function (improved sampling to ensure uniformity)
    def stratified uniform sampling(grid points, labels, sample fraction,
    grid shape=(266, 266)):
         total points = grid points.shape[0]
         num_samples = int(total_points * sample_fraction)
         x bins = np.linspace(grid points[:, 0].min(), grid points[:, 0].max(),
    grid shape[0] // 10 + 1)
         y bins = np.linspace(grid points[:, 1].min(), grid points[:, 1].max(),
    grid shape [1] // 10 + 1)
         sampled indices = []
         for i in range(len(x bins) - 1):
              for j in range(len(y bins) - 1):
                   block mask = (
                        (grid\_points[:, 0] \ge x bins[i]) & (grid\_points[:, 0] <
    x bins[i + 1]) &
                        (grid points[:, 1] \ge y bins[j]) & (grid points[:, 1] <
    y bins[j+1])
                   block indices = np.where(block mask)[0]
                   if len(block indices) > 0:
                        # Ensure proportional sampling from each block
                        num block samples = max(1, int(len(block indices) *
```

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```
sample fraction))
                   sampled indices.extend(np.random.choice(block indices,
num block samples, replace=False))
    sampled indices = np.array(sampled indices)
    if len(sampled indices) > num samples:
         sampled indices = np.random.choice(sampled indices, num samples,
replace=False)
    sampled features = grid points[sampled indices]
    sampled labels = labels[sampled indices]
    return sampled features, sampled labels
# File path
target path = "" # Replace with actual file path
# Read target variable data
df target = pd.read excel(target path, header=None).values.reshape(266, 266)
# Grid coordinates
x = \text{np.linspace}(51250.0, 64500.0, 266)
y = \text{np.linspace}(78750.0, 92000.0, 266)
X, Y = np.meshgrid(x, y)
# Prepare data
grid points = np.column stack((X.flatten(), Y.flatten()))
labels = df target.flatten()
# Analyze errors for different sampling fractions
sample fractions = [0.01, 0.05, 0.1, 0.2]
results = []
for sample fraction in sample fractions:
    sampled features, sampled labels =
stratified uniform sampling(grid points, labels, sample fraction)
    linear estimated = linear interpolation(sampled features, sampled labels,
grid points, df target.shape)
    rmse = calculate rmse(labels, linear estimated.flatten())
    results.append({"Sample Fraction": sample fraction, "RMSE": round(rmse,
6)})
# Convert results to DataFrame
results df = pd.DataFrame(results)
```

```
# Print detailed values
print("\nLinear Interpolation RMSE Results with Improved Sampling:")
print(results_df)

# Visualization
plt.figure(figsize=(10, 6))
plt.plot(results_df["Sample Fraction"], results_df["RMSE"], marker='o',
linestyle='-', color='blue')
plt.title("RMSE vs. Sample Fraction (Linear Interpolation with Improved Sampling)")
plt.xlabel("Sample Fraction")
plt.ylabel("RMSE")
plt.grid(True)
plt.show()
```

Question-2-Correlation calculate

```
# Calculate correlations
    correlation results = []
    for name, values in data.items():
         if name == "target":
              continue
         # Pearson correlation
         pearson corr, pearson p = pearsonr(data["target"], values)
         # Spearman correlation
         spearman corr, spearman p = spearmanr(data["target"], values)
         correlation results.append({
              "Variable": name,
              "Pearson Correlation": pearson corr,
              "Pearson p value": pearson p,
              "Spearman Correlation": spearman corr,
              "Spearman p value": spearman p
         })
    # Convert results to DataFrame
    correlation df = pd.DataFrame(correlation results)
    correlation df["Max Abs Correlation"] =
    correlation df[["Pearson Correlation", "Spearman Correlation"]].abs().max(
         axis=1)
    correlation df = correlation df.sort values(by="Max Abs Correlation",
    ascending=False)
    # Select the top two most correlated variables
    top two = correlation df.head(2)
```

```
colors = plt.cm.Blues(np.linspace(0.8, 0.4, len(correlation_df)))

# Visualization: Correlation comparison
plt.figure(figsize=(10, 6))
plt.bar(correlation_df["Variable"], correlation_df["Max_Abs_Correlation"],
color=colors)
plt.title("Correlation with Target")
plt.ylabel("Max Absolute Correlation")
plt.xlabel("Collaborative Variables")
plt.show()

# Output results
print("\nCorrelation Analysis Results:")
print(correlation_df)
print("\nTop Two Most Correlated Variables:")
print(top_two)
```

Question-2-Correlation coefficient heat map

```
import numpy as np
    import pandas as pd
    import seaborn as sns
    import matplotlib.pyplot as plt
    # File paths
    file_paths = {}
    # Read data and ensure it is numerical
    data = \{\}
    for name, path in file_paths.items():
         data[name] = pd.read excel(path,
    header=None).values.flatten().astype(float)
    # Convert to DataFrame
    data df = pd.DataFrame(data)
    # Calculate Spearman correlation matrix
    spearman_corr_matrix = data_df.corr(method='spearman')
    # Display the correlation matrix
    print("Spearman Correlation Matrix:")
    print(spearman_corr_matrix)
    # Plot heatmap
```

```
plt.figure(figsize=(8, 6))
sns.heatmap(
spearman_corr_matrix,
annot=True, # Annotate each cell with the correlation value
fmt=".2f", # Display values with two decimal places
cmap="coolwarm",
cbar_kws={'label': 'Spearman Correlation'},
vmin=-1,
vmax=1
)
plt.title('Spearman Correlation Heatmap between Datasets')
plt.show()
```

Question-2-Histogram of spatial variables

```
import pandas as pd
    import numpy as np
    import matplotlib.pyplot as plt
    from scipy.stats import skew, kurtosis, norm, skewnorm, chi2
    import os
    #Load the data from the provided Excel files
    target data path = "Data-preprocessing/target.xlsx"
    collab1 data path = "Data-preprocessing/collaborative1.xlsx"
    collab2 data path = "Data-preprocessing/collaborative2.xlsx"
    collab3 data path = "Data-preprocessing/collaborative3.xlsx"
    collab4 data path = "Data-preprocessing/collaborative4.xlsx"
    # Read the Excel files into DataFrames
    target data = pd.read excel(target data path, header=None)
    collab1 data = pd.read excel(collab1 data path, header=None)
    collab2 data = pd.read excel(collab2 data path, header=None)
    collab3 data = pd.read excel(collab3 data path, header=None)
    collab4 data = pd.read excel(collab4 data path, header=None)
    # Combine all data into a single DataFrame for correlation analysis
    combined data = pd.DataFrame({
         "Target": target data.values.flatten(),
         "Collaborative 1": collab1 data.values.flatten(),
         "Collaborative 2": collab2 data.values.flatten(),
         "Collaborative 3": collab3 data.values.flatten(),
         "Collaborative 4": collab4 data.values.flatten()
    })
```

```
for col in combined data.columns:
    plt.figure(figsize=(10, 6))
    plt.hist(combined data[col], bins=40, density=True, alpha=0.8,
label="Data", edgecolor='black')
    x = np.linspace(combined data[col].min(), combined data[col].max(),
1000)
    plt.plot(x, norm.pdf(x, np.mean(combined data[col]),
np.std(combined data[col])),
               label="Normal Fit", color="red", linewidth=2)
    plt.title(f"Histogram of {col}", fontsize=16, fontweight='bold')
    plt.xlabel("Value", fontsize=14)
    plt.ylabel("Density", fontsize=14)
    plt.legend(fontsize=12, loc="upper right")
    plt.xticks(fontsize=12)
    plt.yticks(fontsize=12)
    plt.savefig("Histogram " + col + ".jpg", dpi=600)
    plt.show()
```

Question-2-Normal test

```
import numpy as np
     import pandas as pd
     import matplotlib.pyplot as plt
     from scipy.stats import shapiro, kstest, anderson, probplot, spearmanr, pearsonr
     # File paths
     file paths = \{\}
     # Load and flatten data
     data = {name: pd.read excel(path, header=None).values.flatten() for name, path
     in file paths.items()}
     # Visualization function
     def visualize distribution(data, name):
          plt.figure(figsize=(10, 5))
          plt.subplot(1, 2, 1)
          plt.hist(data, bins=30, color="lightblue", edgecolor="black")
          plt.title(f"Histogram of {name}")
          plt.subplot(1, 2, 2)
          probplot(data, dist="norm", plot=plt)
```

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```
plt.title(f"Q-Q Plot of {name}")
    plt.tight layout()
    plt.show()
# Improved normality check function
def check normality improved(data, name):
    print(f"== Improved Normality Check for {name} ==")
    # Kolmogorov-Smirnov test
    stat, p = kstest(data, 'norm', args=(np.mean(data), np.std(data)))
    print(f'Kolmogorov-Smirnov Test: Statistic={stat:.4f}, p-value={p:.4e}")
    # Anderson-Darling test
    ad result = anderson(data, dist='norm')
    print(f"Anderson-Darling Test: Statistic={ad result.statistic:.4f}")
    print(f"Critical Values: {ad result.critical values}")
    print(f"Significance Levels: {ad result.significance level}")
     # Visualize distribution
    visualize distribution(data, name)
# Check normality for each variable
for name, values in data.items():
    check normality improved(values, name)
```

question-2-Q-Q plot

```
# Function to check normality

def check_normality(data, name):
    print(f"== Test for normality: {name} ==")
    results = {}

# Shapiro-Wilk Test
    stat, p = shapiro(data)
    results["Shapiro-Wilk"] = (stat, p)
    print(f"Shapiro-Wilk Test: Statistic={stat:.4f}, p-value={p:.4e}")

# D'Agostino and Pearson's Test
    stat, p = normaltest(data)
    results["D'Agostino"] = (stat, p)
    print(f"D'Agostino's Test: Statistic={stat:.4f}, p-value={p:.4e}")

# Q-Q Plot
```

```
plt.figure(figsize=(6, 4))
    probplot(data, dist="norm", plot=plt)
    plt.title(f"Q-Q Plot for {name}")
    plt.show()
    return results
# Perform normality check
normality results = {name: check normality(data[name], name) for name in
data.keys()}
```

question-2-Scatter plot

```
import pandas as pd
    import seaborn as sns
    import matplotlib.pyplot as plt
    #Load the data from the provided Excel files
    target data path = "DataProcessing/target.xlsx"
    collab1 data path = "DataProcessing/collaborative1.xlsx"
    collab2 data path = "DataProcessing/collaborative2.xlsx"
    collab3 data path = "DataProcessing/collaborative3.xlsx"
    collab4_data_path = "DataProcessing/collaborative4.xlsx"
    # Read the Excel files into DataFrames
    target data = pd.read excel(target data path, header=None)
    collab1 data = pd.read excel(collab1 data path, header=None)
    collab2 data = pd.read excel(collab2 data path, header=None)
    collab3 data = pd.read excel(collab3 data path, header=None)
    collab4 data = pd.read excel(collab4 data path, header=None)
    # Combine all data into a single DataFrame for correlation analysis
    combined data = pd.DataFrame({
         "Target": target data.values.flatten(),
         "Collaborative 1": collab1 data.values.flatten(),
         "Collaborative 2": collab2 data.values.flatten(),
         "Collaborative 3": collab3 data.values.flatten(),
         "Collaborative 4": collab4 data.values.flatten()
    })
    i = 1
    for column in ["Collaborative 1", "Collaborative 2", "Collaborative 3",
     "Collaborative 4"]:
```

```
# Select every 50th data point and only use the first portion of the data reduced_data = combined_data.iloc[::50]

plt.figure(figsize=(8, 6))
    sns.scatterplot(x=reduced_data[column], y=reduced_data["Target"],
    alpha=0.7)
    plt.title(f"Scatter Plot: Target vs {column} (Reduced Data)", fontsize=14)
    plt.xlabel(column, fontsize=12)
    plt.ylabel("Target", fontsize=12)
    plt.tight_layout()
    plt.savefig(f"Target-Collaborative{i}.jpg", dpi=600)
    i += 1
    plt.show()
```

Team # 2024093029335

```
question-2-Skewness kurtosis calculations
import pandas as pd
    import numpy as np
    import matplotlib.pyplot as plt
    from scipy.stats import skew, kurtosis, norm, skewnorm,chi2
    import os
    # Load the data from the provided Excel files
    target data path = "Data-preprocessing/target.xlsx"
    collab1 data path = "Data-preprocessing/collaborative1.xlsx"
    collab2 data path = "Data-preprocessing/collaborative2.xlsx"
    collab3 data path = "Data-preprocessing/collaborative3.xlsx"
    collab4 data path = "Data-preprocessing/collaborative4.xlsx"
    # Read the Excel files into DataFrames
    target data = pd.read excel(target data path, header=None)
    collab1 data = pd.read excel(collab1 data path, header=None)
    collab2 data = pd.read excel(collab2 data path, header=None)
    collab3 data = pd.read excel(collab3 data path, header=None)
    collab4 data = pd.read excel(collab4 data path, header=None)
    # Combine all data into a single DataFrame for correlation analysis
    combined data = pd.DataFrame({
         "Target": target data.values.flatten(),
         "Collaborative 1": collab1 data.values.flatten(),
         "Collaborative 2": collab2 data.values.flatten(),
         "Collaborative 3": collab3 data.values.flatten(),
         "Collaborative 4": collab4 data.values.flatten()
     })
```

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```
# Validate data
if combined data.isnull().values.any():
    combined data = combined data.fillna(0) # Fill NaNs if any
# Plot distributions
\#x = np.linspace(-15, 15, 1000)
x = np.linspace(-10, 10, 1000)
standard normal = norm.pdf(x,loc=0,scale=3)
# fig, (ax1, ax2) = plt.subplots(2, 1, figsize=(18, 20))
fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(18, 8))
# Skewness plot (optimized for clear left-right shifts)
for col in combined data.columns:
    data = combined data[col]
    skew value = skew(data)
    skewed dist = skewnorm.pdf(x,a=-skew value,loc=0,scale=3)
    ax1.plot(x, skewed dist, label=f"{col} - Skew={skew value:.2f}",
linewidth=2)
ax1.plot(x, standard normal, label="Standard Normal - Skew=0", linestyle="--",
linewidth=2, color="black")
ax1.set title("Skewed Normal Distributions (Optimized)")
ax1.set xlabel("Value")
ax1.set_ylabel("Density")
ax1.legend(loc="upper left", bbox to anchor=(1, 1))
# Kurtosis plot
for col in combined_data.columns:
    data = combined data[col]
    kurt value = kurtosis(data)
    adjusted kurtosis = np.clip(kurt value, -2, 2) #Limit kurtosis adjustments
    kurtotic dist = norm.pdf(x,loc=0,scale=-adjusted kurtosis+3)
    ax2.plot(x, kurtotic dist, label=f"{col} - Kurt={kurt value+3:.2f}",
linewidth=2)
ax2.plot(x, standard normal, label="Standard Normal - Kurt=3", linestyle="--",
linewidth=2, color="black")
ax2.set title("Kurtotic Normal Distributions")
ax2.set xlabel("Value")
ax2.set ylabel("Density")
ax2.legend(loc="upper left", bbox_to_anchor=(1, 1))
```

```
plt.tight_layout()
plt.savefig("Question2-skew_kurt.jpg",dpi=600)
plt.show()
```

question-3-Co kriging with fmm

Team # 2024093029335

```
import numpy as np
    import pandas as pd
    import matplotlib.pyplot as plt
    from pykrige.ok import OrdinaryKriging
    from sklearn.metrics import mean squared error, r2 score
    # Function to calculate MAPE
    def mean absolute percentage_error(y_true, y_pred):
         y true, y pred = np.array(y true), np.array(y pred)
         return np.mean(np.abs((y true - y pred) / y true)) * 100
    #1. Load data
    target data = pd.read excel("", header=None)
    collaborative data = pd.read excel("", header=None)
    # 2. Define grid
    x coords = np.linspace(51250, 64500, target data.shape[1]) \#X-coordinate
    range
    y coords = np.linspace(78750, 92000, target data.shape[0]) #Y-coordinate
    range
    grid x, grid y = np.meshgrid(x coords, y coords)
    #3. Flatten data
    target flat = target data.values.ravel()
    collaborative flat = collaborative data.values.ravel()
    grid x flat = grid x.ravel()
    grid_y_flat = grid_y.ravel()
    # 4. Sampling ratios
    sample ratios = [0.01, 0.05, 0.1, 0.2, 0.3]
    rmse_list, mape_list, r2_list = [], [], []
    # 5. Loop through sample ratios
    for ratio in sample ratios:
         sample size = int(len(target flat) * ratio)
         half sample size = sample size // 2
         # Randomly sample from target1 and collaborative1
```

```
target indices = np.random.choice(len(target flat), half sample size,
replace=False)
    collaborative indices = np.random.choice(len(collaborative flat),
half sample size, replace=False)
     # Extract sampled points
    x target sampled = grid x flat[target indices]
    y target sampled = grid y flat[target indices]
    target sampled = target flat[target indices]
    x collaborative sampled = grid x flat[collaborative indices]
    y collaborative sampled = grid y flat[collaborative indices]
    collaborative sampled = collaborative flat[collaborative indices]
    # Merge sampled points
    x sampled = np.concatenate([x target sampled, x collaborative sampled])
    y sampled = np.concatenate([y target sampled, y collaborative sampled])
    values sampled = np.concatenate([target sampled, collaborative sampled])
    # Ordinary Kriging interpolation
    ok = OrdinaryKriging(
         x sampled,
         y sampled,
         values sampled,
         variogram model="linear",
         verbose=False,
         enable plotting=False
    )
    z predicted, = ok.execute("grid", x coords, y coords)
    # Calculate RMSE, MAPE, and R<sup>2</sup>
    predicted flat = z predicted.ravel()
    rmse = np.sqrt(mean squared error(target flat, predicted flat))
    mape = mean absolute percentage error(target flat, predicted flat)
    r2 = r2 score(target flat, predicted flat)
    # Append metrics to lists
    rmse list.append(rmse)
    mape list.append(mape)
    r2 list.append(r2)
    print(f"Sample Ratio: {ratio*100:.0f}%, RMSE: {rmse:.4f}, MAPE:
\{\text{mape:.2f}\}\%, R^2: \{\text{r2:.4f}\}''\}
```

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```
# Plot 2D contour map
     plt.rcParams['font.sans-serif'] = ['Arial'] # Set font to Arial
     plt.rcParams['axes.unicode minus'] = False # Enable minus sign display
     plt.figure(figsize=(10, 8))
     contour = plt.contour(grid x, grid y, z predicted, cmap='viridis', levels=20)
     plt.clabel(contour, inline=True, fontsize=8)
     plt.colorbar(label='Predicted F1 target Values')
     plt.title(f2D Contour Map: Sampling Rate {ratio*100:.0f}%')
     plt.xlabel('X Coordinate')
     plt.ylabel('Y Coordinate')
     plt.show()
# 6. Plot RMSE, MAPE, and R<sup>2</sup> vs. Sample Ratio
plt.figure(figsize=(10, 6))
plt.plot([r * 100 for r in sample ratios], rmse list, marker='o', linestyle='-',
label='RMSE', color='b')
plt.plot([r * 100 for r in sample ratios], mape list, marker='s', linestyle='--',
label='MAPE (%)', color='r')
plt.plot([r * 100 for r in sample ratios], r2 list, marker='^', linestyle='-.', label='R
<sup>2</sup> ', color='g')
plt.title("RMSE, MAPE, and R<sup>2</sup> vs. Sample Ratio", fontsize=14)
plt.xlabel("Sample Ratio (%)", fontsize=12)
plt.ylabel("Metrics", fontsize=12)
plt.legend()
plt.show()
```

Question-3-Error dot diagram

```
import numpy as np
import matplotlib.pyplot as plt

# Mock data based on your results
# Coordinates (X, Y) for the 3D scatter plot
x = np.linspace(51250, 64500, 100)
y = np.linspace(78750, 92000, 100)
x, y = np.meshgrid(x, y)
x_flat = x.ravel()
y_flat = y.ravel()

# Error values for Random Forest (simulated based on your results)
rf_errors = np.random.normal(loc=0.01, scale=0.005, size=x_flat.shape)

# Error values for Co-Kriging (simulated based on your results)
```

```
kriging errors = np.random.normal(loc=0.02, scale=0.01, size=x flat.shape)
# 3D Scatter plot for Random Forest errors
fig = plt.figure(figsize=(12, 6))
ax1 = fig.add subplot(121, projection='3d')
sc rf = ax1.scatter(x flat, y flat, rf errors, c=rf errors, cmap='Blues', alpha=0.6)
ax1.set title('Random Forest Error Distribution', fontsize=12)
ax1.set xlabel('X Coordinate')
ax1.set ylabel('Y Coordinate')
ax1.set zlabel('Error')
fig.colorbar(sc rf, ax=ax1, shrink=0.6)
# 3D Scatter plot for Co-Kriging errors
ax2 = fig.add subplot(122, projection='3d')
sc kr = ax2.scatter(x flat, y flat, kriging errors, c=kriging errors,
cmap='Greens', alpha=0.6)
ax2.set title('Co-Kriging Error Distribution', fontsize=12)
ax2.set xlabel('X Coordinate')
ax2.set ylabel('Y Coordinate')
ax2.set zlabel('Error')
fig.colorbar(sc kr, ax=ax2, shrink=0.6)
plt.tight layout()
plt.show()
```

Question-3-Local hot spot error prediction plot

```
import numpy as np
import matplotlib.pyplot as plt

# Simulated grid coordinates for a smaller region with coarser resolution
x_coords = np.linspace(51250, 64500, 20) # Reduced number of points for
coarser grid
y_coords = np.linspace(78750, 92000, 20) # Reduced number of points for
coarser grid
grid_x, grid_y = np.meshgrid(x_coords, y_coords)

# Simulated error values for Random Forest and Co-Kriging
rf_error_hotspot = np.random.normal(loc=0.02, scale=0.005, size=grid_x.shape)
kriging_error_hotspot = np.random.normal(loc=0.03, scale=0.007,
size=grid_x.shape)

# Plot heatmap for Random Forest errors
plt.figure(figsize=(10, 6))
```

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```
plt.title("Random Forest Error Heatmap (Local Hotspot)", fontsize=14)
plt.xlabel("X Coordinate", fontsize=12)
plt.ylabel("Y Coordinate", fontsize=12)
plt.pcolormesh(grid x, grid y, rf error hotspot, cmap='Blues', shading='nearest')
plt.colorbar(label="Error Magnitude")
plt.show()
# Plot heatmap for Co-Kriging errors
plt.figure(figsize=(10, 6))
plt.title("Co-Kriging Error Heatmap (Local Hotspot)", fontsize=14)
plt.xlabel("X Coordinate", fontsize=12)
plt.ylabel("Y Coordinate", fontsize=12)
plt.pcolormesh(grid x, grid y, kriging error hotspot, cmap='Greens',
shading='nearest')
plt.colorbar(label="Error Magnitude")
plt.show()
# Plot difference heatmap between the two algorithms
error difference = np.abs(rf error hotspot - kriging error hotspot)
plt.figure(figsize=(10, 6))
plt.title("Error Difference Heatmap (Local Hotspot)", fontsize=14)
plt.xlabel("X Coordinate", fontsize=12)
plt.ylabel("Y Coordinate", fontsize=12)
plt.pcolormesh(grid x, grid y, error difference, cmap='coolwarm',
shading='nearest')
plt.colorbar(label="Error Difference Magnitude")
plt.show()
```

Question-3-Model comparison radar chart

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```
import numpy as np

# Define metrics and values for each model
labels = ['RMSE', 'MAPE', 'R²', 'MAE', 'EVS', 'Training Time', 'Prediction Time']
n_metrics = len(labels)

# Random Forest values (including new metrics)
rf_values = [0.0359, 0.002, 0.9668, 0.015, 0.96, 3.5, 0.02] # Simulated values

# Co-Kriging values (including new metrics)
kriging_values = [0.0274, 0.004, 0.8028, 0.025, 0.93, 15, 0.1] # Simulated values
```

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```
# Normalize values for radar plot
max values = [\max(rf, kr) \text{ for } rf, kr \text{ in } zip(rf \text{ values}, kriging \text{ values})]
rf normalized = [rf / mx \text{ for rf, } mx \text{ in zip}(rf \text{ values, } max \text{ values})]
kriging normalized = [kr / mx \text{ for kr, } mx \text{ in zip(kriging values, } max \text{ values)}]
# Close the radar plot by repeating the first value
rf normalized.append(rf normalized[0])
kriging normalized.append(kriging normalized[0])
# Close the labels for the radar chart
labels.append(labels[0])
# Radar chart setup
angles = np.linspace(0, 2 * np.pi, n metrics + 1, endpoint=True)
fig, ax = plt.subplots(figsize=(8, 8), subplot kw={'projection': 'polar'})
# Plot Random Forest in blue
ax.plot(angles, rf normalized, 'blue', linewidth=2, label='Random Forest')
ax.fill(angles, rf normalized, 'blue', alpha=0.1)
# Plot Co-Kriging in green
ax.plot(angles, kriging normalized, 'green', linewidth=2, label='Co-Kriging')
ax.fill(angles, kriging normalized, 'green', alpha=0.1)
# Annotate values on the radar plot
for angle, rf val, kr val, rf orig, kr orig in zip(
          angles, rf normalized, kriging normalized, rf values, kriging values):
     ax.text(angle, rf val + 0.05, f'{rf orig:.4f}', color='blue', fontsize=10,
ha='center')
     ax.text(angle, kr val + 0.05, f'{kr orig:.4f}', color='green', fontsize=10,
ha='center')
# Add labels and legend
ax.set thetagrids(angles * 180 / np.pi, labels)
ax.set title('Comparison of Random Forest and Co-Kriging (Expanded Metrics)',
fontsize=16, pad=20)
ax.legend(loc='upper right', bbox to anchor=(1.3, 1.1))
# Remove radial grid and tick labels
ax.yaxis.set visible(False)
# Final grid styling
```

```
ax.grid(True)
plt.show()
```

```
Question-3-Model sensitivity analysis plot
import numpy as np
    import matplotlib.pyplot as plt
    # 1. Core covariance function (simulate changes in covariance matrix)
    def covariance(distance, a):
          """Exponential covariance model."""
         return np.exp(-distance / a)
    # 2. Simulate distance matrices for target and collaborative variables
    distances target = np.linspace(0, 100, 50) # Distances for the target variable
    distances collaborative = np.linspace(0, 100, 50) # Distances for the
    collaborative variable
    # 3. Parameter settings
    a values = np.linspace(10, 100, 10) # Varying correlation distances (a)
    weights target = [] # Store weights for the target variable
    weights collaborative = [] # Store weights for the collaborative variable
    # 4. Calculate co-kriging weights
    for a in a values:
         # Covariance matrices (simulation)
         cov target = covariance(distances target, a) # Covariance for the target
    variable
         cov collaborative = covariance(distances collaborative, a) # Covariance
    for the collaborative variable
         cross cov = covariance(np.abs(distances target - distances collaborative),
    a) # Cross covariance
          # Assume the correlation coefficient between target and collaborative
    variables is 0.8
         correlation = 0.8
         # Co-kriging weights (formula normalization)
         w target = cov target / (cov target + correlation * cross cov)
         w collaborative = correlation * cross cov / (cov target + correlation *
    cross_cov)
```

Average weights

```
weights target.append(np.mean(w target))
     weights collaborative.append(np.mean(w collaborative))
# 5. Visualize sensitivity analysis
plt.figure(figsize=(10, 6))
plt.plot(a values, weights target, label="Target Variable Weight ($w T$)",
marker='o', color='blue')
plt.plot(a values, weights collaborative, label="Collaborative Variable Weight
($w C$)", marker='s', color='green')
# Add annotations and settings
plt.title("Sensitivity Analysis of Weights in Co-Kriging", fontsize=14)
plt.xlabel("Correlation Distance ($a$)", fontsize=12)
plt.ylabel("Weight", fontsize=12)
plt.legend()
# Display weight values
for i, a in enumerate(a values):
     plt.text(a, weights target[i], f"{weights target[i]:.2f}", fontsize=10,
ha='right', color='blue')
    plt.text(a, weights collaborative[i], f"{weights collaborative[i]:.2f}",
fontsize=10, ha='left', color='green')
plt.show()
```

Question-3-Random forest

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.ensemble import RandomForestRegressor
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error

# 1. Load uploaded files
target_data = pd.read_excel("", header=None)
collaborative_data = pd.read_excel("", header=None)

# 2. Define X and Y ranges
x_coords = np.linspace(51250, 64500, target_data.shape[1]) # X-coordinate range
y_coords = np.linspace(78750, 92000, target_data.shape[0]) # Y-coordinate range
grid_x, grid_y = np.meshgrid(x_coords, y_coords)
```

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```
#3. Convert data to long format
target long = pd.DataFrame({
    'X': grid x.ravel(),
    'Y': grid y.ravel(),
    'Value target': target data.values.ravel()
})
collaborative long = pd.DataFrame({
    'X': grid x.ravel(),
    'Y': grid y.ravel(),
    'Value collaborative': collaborative data.values.ravel()
})
# 4. Merge the datasets
merged data = pd.merge(target long, collaborative long, on=['X', 'Y'])
# 5. Define sample ratios and RMSE list
sample ratios = [0.01, 0.05, 0.1, 0.2, 0.3]
rmse list = []
# 6. Iterate through different sample ratios, compute RMSE, and generate 2D
contour plots
for ratio in sample ratios:
    sample size = int(len(merged data) * ratio) # Determine sample size
    random indices = np.random.choice(len(merged data), sample size,
replace=False)
    resampled data = merged data.iloc[random indices]
    # Extract features and target variable
    X = resampled_data[['X', 'Y', 'Value_collaborative']]
    y = resampled data['Value target']
     # Split data into training and testing sets
    X train, X test, y train, y test = train test split(X, y, test size=0.2,
random state=42)
    # Train Random Forest model
    rf model = RandomForestRegressor(n estimators=100, random state=42)
    rf model.fit(X train, y train)
    # Test model performance
    y pred = rf model.predict(X test)
    rmse = np.sqrt(mean squared error(y test, y pred))
```

```
rmse list.append(rmse)
    print(f"Sample Ratio: {ratio*100:.0f}%, Sample Size: {sample_size},
RMSE: {rmse:.4f}")
     # Generate interpolation grid
     grid data = pd.DataFrame({
         'X': grid x.ravel(),
          'Y': grid y.ravel(),
          'Value collaborative': collaborative long['Value collaborative']
     })
     # Predict target values using the trained Random Forest model
     grid data['Value target pred'] = rf model.predict(grid data[['X', 'Y',
'Value collaborative']])
    z target = grid data['Value target pred'].values.reshape(grid x.shape)
     # Plot 2D contour map
     plt.rcParams['font.sans-serif'] = ['SimHei'] # Set font to SimHei for
Chinese characters
    plt.rcParams['axes.unicode minus'] = False # Display negative signs
correctly
    plt.figure(figsize=(10, 8))
    contour = plt.contour(grid x, grid y, z target, cmap='viridis', levels=20)
    plt.clabel(contour, inline=True, fontsize=8)
    plt.colorbar(label='Predicted F1 target Values')
    plt.title(f'2D: {ratio*100:.0f}% Sample Ratio')
    plt.xlabel('X Coordinate')
    plt.ylabel('Y Coordinate')
    plt.show()
# 7. Plot RMSE line graph
plt.figure(figsize=(10, 6))
plt.plot([r * 100 for r in sample ratios], rmse list, marker='o', linestyle='-',
color='b')
plt.title("RMSE vs. Sample Ratio", fontsize=14)
plt.xlabel("Sample Ratio (%)", fontsize=12)
plt.ylabel("RMSE", fontsize=12)
plt.grid(False)
plt.show()
```

Question-3-Rmse R^2 Mape

Calculate RMSE, MAPE, and R²

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```
predicted_flat = z_predicted.ravel()
rmse = np.sqrt(mean squared error(target flat, predicted flat))
mape = mean absolute percentage error(target_flat, predicted_flat)
r2 = r2 score(target flat, predicted flat)
# Append metrics to lists
rmse list.append(rmse)
mape list.append(mape)
r2 list.append(r2)
print(f'Sample Ratio: {ratio * 100:.0f}%, RMSE: {rmse:.4f}, MAPE:
\{\text{mape:.2f}\}\%, R^2: \{\text{r2:.4f}\}''\}
# 6. Plot RMSE, MAPE, and R<sup>2</sup> vs. Sample Ratio
plt.figure(figsize=(10, 6))
plt.plot([r * 100 for r in sample ratios], rmse list, marker='o', linestyle='-',
label='RMSE', color='b')
plt.plot([r * 100 for r in sample ratios], mape list, marker='s', linestyle='--',
label='MAPE (%)', color='r')
plt.plot([r * 100 for r in sample ratios], r2 list, marker='^', linestyle='-.', label='R
<sup>2</sup> ', color='g')
plt.title("RMSE, MAPE, and R<sup>2</sup> vs. Sample Ratio", fontsize=14)
plt.xlabel("Sample Ratio (%)", fontsize=12)
plt.ylabel("Metrics", fontsize=12)
plt.legend()
plt.show()
```

Question-4-3D surface plot

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from scipy.interpolate import griddata

#Load the dataset
file_path = ""
data = pd.read_excel(file_path, header=0)

#Rename columns for easier understanding
data.columns = ['Column Sequence', 'Row Sequence', 'X-Coordinate',
'Y-Coordinate', 'Target Property']

#Extract coordinates and target property
x = data['X-Coordinate']
```

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```
y = data['Y-Coordinate']
z = data['Target Property']
# Create a grid for the surface
grid_x, grid_y = np.meshgrid(
    np.linspace(x.min(), x.max(), 100),
    np.linspace(y.min(), y.max(), 100)
)
# Interpolate the Z values to create the surface
grid z = griddata((x, y), z, (grid x, grid y), method='cubic')
# Create a 3D surface plot
fig = plt.figure(figsize=(12, 8))
ax = fig.add_subplot(111, projection='3d')
# Plot the surface
surface = ax.plot surface(grid x, grid y, grid z, cmap='viridis',
edgecolor='none', alpha=0.9)
# Add a color bar
cbar = fig.colorbar(surface, ax=ax, pad=0.1)
cbar.set label('Target Property', fontsize=12)
# Label the axes
ax.set xlabel('X-Coordinate', fontsize=12)
ax.set ylabel('Y-Coordinate', fontsize=12)
ax.set zlabel('Target Property', fontsize=12)
# Set the title
ax.set title('3D Surface Visualization of Spatial Variable (Target Property)',
fontsize=14)
# Show the plot
plt.show()
```

Question-4-Cokriging with fmm

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from pykrige.ok import OrdinaryKriging

# 1. Load target sampling data and collaborative variable data
```

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```
target file = ""
collaborative file = ""
#Load target sampling data
target data = pd.read excel(target file)
#Load complete collaborative variable data
collaborative data = pd.read excel(collaborative file, header=None)
# Target sampling points (X, Y, Z)
x target = target data['X-Coordinate']
y target = target data['Y-Coordinate']
z target = target data['Target Property']
# Collaborative variable complete grid data
collaborative matrix = collaborative data.values
grid x collab = np.linspace(51250, 64500, 266)
grid y collab = np.linspace(78750, 92000, 266)
grid x collab, grid y collab = np.meshgrid(grid x collab, grid y collab)
# Flatten collaborative variable data to 1D arrays
x \text{ collab = grid } x \text{ collab.ravel()}
y collab = grid y collab.ravel()
z collab = collaborative matrix.ravel()
# Randomly select 20% of the collaborative variable points
num collab points = int(len(x collab) * 0.2)
indices collab = np.random.choice(len(x collab), num collab points,
replace=False)
x collab sampled = x collab[indices collab]
y collab sampled = y collab[indices collab]
z collab sampled = z collab[indices collab]
# 2. Co-Kriging interpolation
def co kriging(x target, y target, z target, x collab, y collab, z collab, grid x,
grid y):
     Co-Kriging model prediction.
     # Combine target and collaborative variable points
    x all = np.concatenate((x target, x collab))
    y all = np.concatenate((y target, y collab))
    z_all = np.concatenate((z_target, z_collab))
```

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```
# Remove duplicate coordinates
    unique points = np.unique(np.c [x all, y all], axis=0)
    x unique = unique points[:, 0]
    y unique = unique points[:, 1]
    z unique = []
    for x, y in zip(x unique, y unique):
         idx = np.where((x all == x) & (y all == y))[0]
         z unique.append(np.mean(z all[idx]))
    z unique = np.array(z unique)
    # Perform interpolation using Ordinary Kriging
    ok = OrdinaryKriging(
         x unique, y unique, z unique,
         variogram model='linear',
         verbose=False,
         enable plotting=False
    z predicted, = ok.execute('grid', grid x, grid y)
    return z predicted
#3. Construct interpolation grid
grid_x = np.linspace(51250, 64500, 266) # Interpolation grid for X
grid y = np.linspace(78750, 92000, 266) # Interpolation grid for Y
grid x, grid y = np.meshgrid(grid x, grid y)
# 4. Test different sample sizes for target points
sample sizes = [100, 200, 300, 400, 500, 600, 700, 800, 900, 1000]
for sample size in sample sizes:
    # Select sampled points from the target data
    x target sampled = x target[:sample size]
    y target sampled = y target[:sample size]
    z target sampled = z target[:sample size]
    # Perform interpolation
    z predicted = co kriging(
         x_target_sampled, y_target_sampled, z_target_sampled,
         x_collab_sampled, y_collab_sampled, z_collab_sampled,
         grid x, grid y
    )
     # Save results to an Excel file
    z predicted df = pd.DataFrame(z predicted)
    output_file = f"co_kriging_prediction_{sample size} samples.xlsx"
```

```
z_predicted_df.to_excel(output_file, index=False, header=False)
print(f''Results saved to: {output_file}'')

# Visualize contour plot
plt.figure(figsize=(10, 8))
contour = plt.contourf(grid_x, grid_y, z_predicted, cmap='viridis',
levels=20)
plt.colorbar(label='Predicted Target Property')
plt.title(f'Co-Kriging Prediction with {sample_size} Target Samples')
plt.xlabel('X Coordinate')
plt.ylabel('Y Coordinate')
plt.show()
```

Question-4-Data normalization

```
import pandas as pd
    # File path of the previously saved matrix
    output file = 'Data-preprocessing/F2 collaborative4.xlsx'
    #Load the original data file
    loaded matrix df = pd.read excel(output file, header=None)
    # Perform normalization on the loaded data
    loaded matrix = loaded matrix df.values
    normalized loaded matrix = (loaded matrix - loaded matrix.min()) /
    (loaded matrix.max() - loaded matrix.min())
    # Convert normalized data into a DataFrame
    normalized loaded matrix df = pd.DataFrame(normalized loaded matrix)
    # Save the normalized data to a new Excel file
    normalized loaded output file =
    'Data-preprocessing/F2 collaborative4 normalized.xlsx'
    normalized loaded matrix df.to excel(normalized loaded output file,
    index=False, header=False)
    # Output the path of the normalized file
    print("Normalized file saved as:", normalized loaded output file)
```

Question-4-Datatransformation

```
import pandas as pd
import numpy as np
```

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```
import chardet
# File path
file path = 'F2 collaborative variable4.txt'
# Detect file encoding
with open(file path, 'rb') as file:
    raw data = file.read()
    encoding = chardet.detect(raw data)['encoding']
# Read and clean data
cleaned data rows = []
with open(file path, 'r', encoding=encoding) as file:
    for line in file:
         try:
               # Parse lines containing valid numeric values
              values = list(map(float, line.split()))
              cleaned data rows.append(values)
         except ValueError:
               # Skip lines with non-numeric or invalid formats
              continue
# Flatten the data and trim to 266x266 matrix
cleaned data array = np.array([item for sublist in cleaned data rows for item in
sublist])
# Ensure the data size matches 266x266 matrix
required size = 266 * 266
trimmed data array = cleaned data array[:required size]
# Create the matrix
matrix = trimmed data array.reshape(266, 266)
# Convert to DataFrame to save as an Excel file
matrix df = pd.DataFrame(matrix)
# Save as an Excel file
output file = 'Data-preprocessing/F2 collaborative4.xlsx'
matrix df.to excel(output file, index=False, header=False)
print("File has been saved as:", output file)
```

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```
import pandas as pd
    from scipy.stats import normaltest, spearmanr
    import matplotlib.pyplot as plt
    file_paths = [
         'Data-preprocessing/F2 collaborative1 extracted.xlsx',
         'Data-preprocessing/F2 collaborative2 extracted.xlsx',
         'Data-preprocessing/F2 collaborative3 extracted.xlsx',
         'Data-preprocessing/F2 collaborative4 extracted.xlsx'
    ]
    i = 0
    for file path in file paths:
          # Load the uploaded Excel files
         file extracted = file path
         file target = 'Data-preprocessing/F2 target variable.xlsx'
         # Read the files into dataframes
         extracted df = pd.read excel(file extracted)
         target df = pd.read excel(file target)
         # Merge the two dataframes on "Column Sequence" and "Row Sequence"
         merged df = pd.merge(extracted df, target df, on=["Column Sequence",
    "Row Sequence"])
          # Keep only the relevant columns for analysis: "Extracted Value" and
     "Target Property"
         analysis df = merged df[["Extracted Value", "Target Property"]]
         # Check for NaN or infinite values in the dataframe
         cleaned analysis df = analysis df.dropna().replace([float('inf'), float('-inf')],
    pd.NA).dropna()
          # Perform JB normality test for both cleaned columns
         jb extracted cleaned = normaltest(cleaned analysis df["Extracted Value"])
         jb target cleaned = normaltest(cleaned analysis df["Target Property"])
         # Calculate Spearman correlation coefficient
         spearman corr, spearman p value =
    spearmanr(cleaned analysis df["Extracted Value"],
    cleaned analysis df["Target Property"])
          # Print results in a formatted way
```

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```
print(f"=== Results for {file path} ====")
     print("=== Data Quality Check ====")
    print(f"NaN/Inf Check: {analysis df.isin([float('inf'), float('-inf')]).sum() +
analysis df.isnull().sum()}")
    print("\n=== Normality Test Results ===")
     print(f''Extracted Value: Statistic = { jb extracted cleaned.statistic:.4f}, "
            f"p-value = {jb extracted cleaned.pvalue:.4e}")
    print(f"Target Property: Statistic = {jb target cleaned.statistic:.4f}, "
            f"p-value = {jb target cleaned.pvalue:.4e}")
     print("\n=== Correlation Results ===")
    print(f"Spearman Coefficient: {spearman corr:.4f}")
     print(f"p-value: {spearman p value:.4e}")
     # Scatter plot
    plt.figure(figsize=(8, 6))
    plt.scatter(cleaned analysis df["Extracted Value"],
cleaned analysis df["Target Property"], alpha=0.7)
     plt.title(f"Scatter Plot: F2 collaborative{i} extracted", fontsize=14)
    i = i + 1
     plt.xlabel("Extracted Value", fontsize=12)
    plt.ylabel("Target Property", fontsize=12)
     plt.show()
```

Question-4-Spearman heat map

```
import pandas as pd
import scipy.stats as stats
import seaborn as sns
import matplotlib.pyplot as plt

# Load the datasets
file_paths = [
    "Data-preprocessing/F2_target_variable.xlsx",
    "Data-preprocessing/F2_collaborative1_extracted.xlsx",
    "Data-preprocessing/F2_collaborative2_extracted.xlsx",
    "Data-preprocessing/F2_collaborative3_extracted.xlsx",
    "Data-preprocessing/F2_collaborative4_extracted.xlsx",
    "Data-preprocessing/F2_collaborative4_extracted.xlsx"
]

dataframes = [pd.read_excel(path) for path in file_paths]

# Extract the last column from each dataset
```

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```
last columns = [df.iloc[:, -1] for df in dataframes]
# Combine the last columns into a single DataFrame for correlation calculation
combined data = pd.concat(last columns, axis=1)
# Update the column names based on the file names
column names = [
    "target",
    "collaborative1",
    "collaborative2",
    "collaborative3",
    "collaborative4",
]
combined data.columns = column names
# Recalculate Spearman correlation matrix with updated names
spearman corr updated = combined data.corr(method='spearman')
# Plot heatmap with updated names
plt.figure(figsize=(10, 8))
sns.heatmap(spearman corr updated, annot=True, fmt=".2f",
cmap="coolwarm", cbar=True)
plt.title("Question4 Spearman Heatmap")
plt.tight layout()
plt.savefig("Question4 Heatmap.jpg",dpi=600)
plt.show()
spearman corr updated
```