

Chapter 2

Spatial Prediction of Soil Antibiotics Based on High-Accuracy Surface Modeling

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Abstract The spatial prediction of soil antibiotic is more difficult than other normal soil properties due to the diverse sources of soil antibiotics. Few studies have attempted to predict soil antibiotic residues in intensive vegetable cultivation areas. High-accuracy surface modeling (HASM) is regarded as an important new technique in the pedometrics and digital soil mapping fields. A total of 100 surface soil samples were collected from the north-central part of the Shandong Province of China. The antibiotic concentrations, including ciprofloxacin (CF), enrofloxacin (EF), norfloxacin (NF), and fluoroquinolones (FQs), were analyzed using high-performance liquid chromatography–tandem mass spectrometry. We employed splines to compare its performance with that of HASM method. The errors of HASM for NF, CF, EF, and FQ were less compared to splines. HASM has less mean absolute error (MAE) and root mean square error (RMSE) than splines. The RMSEs of splines for FQ, CF, EF, and NF were 3.02, 2.34, 3.46, and 2.64 times larger than those of HASM, respectively. Therefore, HASM can be considered as an alternative and accurate method for interpolating soil antibiotics. It can also make the map more consistent with the true spatial distributions.

Keywords HASM · Soil antibiotics · Interpolation accuracy · Geostatistics

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2.1 Introduction

A large number of antibiotics are released into soils via animal manures applied to the soil (Bound and Voulvoulis 2004), because antibiotics are widely used in treating disease, protecting animal health, and improving the feeding efficiency of animals (Xie et al. 2012; Sarmah et al. 2006; Aust et al. 2008; Li et al. 2013, 2014). Accumulation of antibiotics in the soil can damage the structure of bacterial communities, be absorbed by vegetables or crops thereby threatening the safety of agricultural products, or be leached to groundwater thereby affecting environmental health (Xie et al. 2012; Martínez-Carballo et al. 2007). The apparent immobilization of soil antibiotics in the surface soils to a greater depth was attributed to the presence of higher percentages of clay and organic matter in the surface soils with residues of antibiotics bound strongly to soil particles (Sarmah et al. 2006).

In order to avoid the risk of soil antibiotics on vegetable quality and human health, it is vital to research the spatial patterns of soil antibiotics (Sarmah et al. 2006). So, it is necessary to explore an effective surface modeling methods for soil antibiotics. Low accuracy of interpolation results of soil antibiotics will result in incorrect risk assessment. There are several interpolators in spatial prediction for soil properties, such as kriging (Stein and Corsten 1991; Stein et al. 1988; Webster and Oliver 2001; Goovaerts 1999), inverse distance weighting (IDW) (Panagopoulos et al. 2006; Weber and Englund (1992, 1994); Gotway et al. 1996), and splines (Webster and Oliver 2001). However, the spatial predictions of soil antibiotics are more difficult than other normal soil properties due to the diverse sources of soil antibiotics. Few studies have focused on the interpolation of antibiotic residues in soils of the intensive vegetable cultivation areas.

High-accuracy surface modeling (HASM) is a spatial interpolation technique based on the fundamental theorem of surfaces (Yue 2011), which has been successfully used in soil property interpolation (Shi et al. 2011, 2009, 2012). The HASM method combined with some ancillary information can improve the interpolation of soil properties (Shi et al. 2011). Due to the specific characters of the spatial distributions of soil antibiotics, we added the distribution characters of soil antibiotics in different vegetable areas in HASM method to predict the spatial distributions of soil antibiotics. The aims of this study are (i) to explore the distribution characters of soil antibiotics in different vegetable areas, (ii) to assess the feasibility of HASM combined with the statistical characters of soil antibiotics in different vegetable types in spatial interpolation of soil antibiotics, and (iii) to evaluate the performance of HASM in improving the soil property interpolation compared with classical methods such as splines.

2.2 Data and Methods

2.2.1 Data

The study area of this study is an important vegetable area in the north-central part of Shandong Province, China, covering 160 km². There are several typical vegetables grown in this area, such as cucumber, tomatoes, peppers, melons, eggplant, and some leaf vegetables. Several types of animal manure such as chicken manure and cow dung as organic fertilizer were applied in this area. The map of manure applications has been shown in the previous reference (Li et al. 2013). The whole study area was with manure application. The study area was covered by 100 sampling sites. The average distance between soil sampling locations is approximately 1 km. The sampling sites were designed to cover evenly the whole area and to include different vegetable types, different manure types, and different application years. Three types of fluoroquinolone (FQ) concentrations, including ciprofloxacin (CF), enrofloxacin (EF), and norfloxacin (NF), were analyzed using high-performance liquid chromatography–tandem mass spectrometry. The regents and sample analysis methods were in detail in the former studies (Xie et al. 2012; Li et al. 2013, 2014).

2.2.2 Methods

A full discussion on the theoretical aspects of HASM applied for the interpolation of soil properties was given by Shi et al. (2009, 2011, 2012). We only introduced the main steps here. HASM uses samplings of soil antibiotics to globally fit a surface through several iterative simulation steps. This surface is then used to interpolate soil antibiotic values at unknown points. The iterative simulation steps are summarized as follows (Yue et al. 2010): (1) interpolate within the domain of the sample data $(x_i, y_j, \bar{u}_{i,j})$, from which we can get interpolated values $\{\tilde{u}_{i,j}\}$ at point (x_i, y_j) ; (2) $u_{i,j}^0 = \tilde{u}_{i,j}$ calculate the first fundamental coefficients $E_{i,j}^n$, $F_{i,j}^n$, and $G_{i,j}^n$ and the second fundamental coefficients $L_{i,j}^n$ and $N_{i,j}^n$ as well as coefficients in terms of $\{u_{i,j}^n\}$; (3) for $n \geq 0$, we can get $\{u_{i,j}^{n+1}\}$ by solving the HASM equations; and (4) the iterative process is repeated until simulation accuracy is satisfied.

Here, we calculated the mean values of antibiotic residues in the soils of different vegetable-type areas. Then, the mean values were grided as 100 m $\times$ 100 m over the whole study area. This layer was defined as $u_{i,j}^0$. So, the distribution characters of soil antibiotics in different vegetable-type areas were combined with HASM.

A total of 80 training points were randomly created as the interpolation data set, and the remaining 20 samples were used as the validation data set. We used the most common indices, the mean error (ME), the mean absolute error (MAE), and

the root mean square error (RMSE) as measures of interpolation quality (Shi et al. 2011, 2009, 2012).

As there are n sites belonging to the validation sample set, the ME, the MAE, and the RMSE are determined from the measured values $z(x_i)$ and the interpolated value $z^*(x_i)$. They are given by,

$$\text{ME} = \frac{1}{n} \sum_{i=1}^n [z^*(x_i) - z(x_i)] \quad (2.1)$$

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n [|z^*(x_i) - z(x_i)|] \quad (2.2)$$

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n [z^*(x_i) - z(x_i)]^2} \quad (2.3)$$

The ME is a measure of the bias of the interpolation, which should be close to zero for unbiased methods, and the MAE and RMSE are measures of the accuracy of interpolation which should be as small as possible for accurate interpolation.

2.3 Results and Analysis

2.3.1 Distributions of Soil Antibiotics in Different Types of Vegetable Areas

In the three soil FQ residues, soil CF has the highest mean concentration with 104.4 $\mu\text{g/kg}$, and the followings were the concentrations of soil NF and EF with 55.7 and 15.8 $\mu\text{g/kg}$, respectively (Table 2.1). The standard deviations (SDs) were high for FQ (151.07 $\mu\text{g/kg}$), indicating that the FQs varied largely with different vegetables planted and different inputs (Li et al. 2014). More than 25 % samples of soil FQs were over 222 $\mu\text{g/kg}$, and the maximum (Max) was 682.69 $\mu\text{g/kg}$. The concentrations of CF in the surface soil were much higher than the other two types of FQs; the mean, median, and Max were 104.4, 72.4, and 651.6 $\mu\text{g/kg}$, respectively. Soil NF followed, and the mean, median, and Max were 55.7, 33.3, and 288.3 $\mu\text{g/kg}$, respectively. The concentrations of soil EF were the lowest, and the mean and median were only 15.8 and 7.0 $\mu\text{g/kg}$, respectively. Soil EF in 25 % samples was less than 0.6 $\mu\text{g/kg}$.

There is a large variability of soil FQs in different soil samples, so we analyzed the distributions of soil FQs in different types of vegetables (Table 2.1). Tomato–tomato and cucumber–cucumber were the two main planted types in the north part of study area, accounting for more than 50 % area. There were 21 (72.4 % of all the samples (29 samples) more than 200 $\mu\text{g/kg}$) samples more than 200 $\mu\text{g/kg}$ for soil

Table 2.1 Descriptive statistics of antibiotics concentrations in surface soil (unit: $\mu\text{g/kg}$)

	Min	5 %	10 %	25 %	Median	75 %	90 %	95 %	Max	Mean	SD
FQ	9.1	20.5	31.2	63.8	132.2	222.3	413.8	509.9	682.7	175.2	151.1
NF	0.4	5.0	7.6	14.2	33.3	79.5	149.6	171.1	288.3	55.7	56.4
CF	2.4	8.7	13.0	29.3	72.4	141.0	221.2	302.1	651.6	104.4	117.5
EF	0.0	0.0	0.0	0.6	7.0	18.5	50.6	70.2	167.0	15.8	25.5

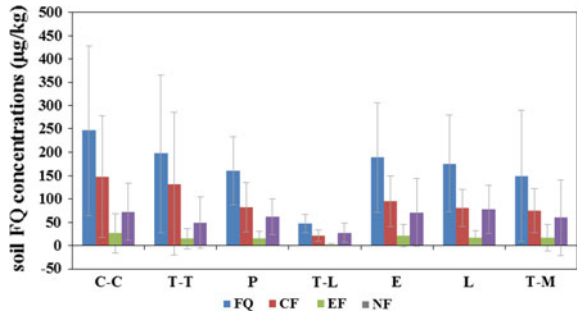


Fig. 2.1 Soil FQ concentrations in different vegetable planted areas. C–C cucumber–cucumber; T–T tomato–tomato; P pepper; T–L tomato–leaf; E eggplant; L leaf; T–M tomato–melon

FQs found in the two planted types. As shown in Table 2.1, higher FQ concentrations were mainly composed of higher CF residues, and a few higher NF samples located in the tomato–melon, eggplant, and leaf planted areas which were over 200 $\mu\text{g/kg}$.

The distributions of soil FQ residues in different planted vegetable types showed that FQ residues in the cucumber–cucumber-planted soil were the highest to 246.3 $\mu\text{g/kg}$ and followed by those in tomato–tomato, eggplant, leaf, pepper, and tomato–melon planted areas with 196.6, 187.9, 176.1, 160.5, and 149.3 $\mu\text{g/kg}$ (Fig. 2.1). The averages of soil CF in these two planted type area were also the highest, which were 147.5 and 132.4 $\mu\text{g/kg}$. The average of soil EF was fewer compared to the other two soil FQs, but the coefficients of variation were larger than 100 % only except for pepper and leaf planted areas.

2.3.2 Comparisons of the Performance of HASM and Splines

In order to compare the performance of HASM and splines, we computed ME, MAE, and RMSE (Table 2.2). HASM had higher accuracy in the two techniques, which performed better for the three indices than splines. The MEs of HASM for FQ, CF, EF, and NF were closer to zero than splines. Also, splines had larger

Table 2.2 The MEs, MAEs, and RMSEs of the validation set for HASM and splines (unit: $\mu\text{g/kg}$)

Soil antibiotics	Indices	HASM	Splines
FQ	ME	19.69	86.34
	MAE	46.66	168.13
	RMSE	68.73	207.23
CF	ME	-0.61	18.12
	MAE	44.03	109.88
	RMSE	58.97	137.72
EF	ME	6.54	21.62
	MAE	13.37	33.71
	RMSE	16.86	58.37
NF	ME	16.48	46.35
	MAE	33.69	75.98
	RMSE	39.16	103.28

MAEs and RMSEs for FQ, CF, EF, and NF. The MAE of HASM for FQ was $46.7 \mu\text{g/kg}$ and that of splines was $168.13 \mu\text{g/kg}$. For RMSE, HASM also performed better than splines. The RMSEs of splines for FQ, CF, EF, and NF were 3.02, 2.34, 3.46, and 2.64 times greater than those of HASM, respectively.

2.3.3 The Interpolated Maps by HASM Methods

We mapped the distributions of FQ, CF, EF, and NF by HASM (Fig. 2.2). The map based on HASM has more details in the interpolation maps and also has consistent maximum and minimum with those of soil samples. Although the spatial patterns of the two techniques had similar spatial distribution tendency of higher FQ residues in the north part of the study area, HASM showed lower values of FQs consistent with the concentration of soil samples. However, splines has not showed this character in the interpolation maps. The EF concentrations in the soil of the study area were the lowest in the three types of the FQs, which had lower values less than $100 \mu\text{g/kg}$ except a small part of the north. Although a few higher values over than $200 \mu\text{g/kg}$ of NF were in the southeast of the study area, most of the NF concentrations in the soil were less than $100 \mu\text{g/kg}$. In these three types of soil FQs, CF values were the highest. For example, there were about half areas of the study area more than $150 \mu\text{g/kg}$, and 10 to 20 % areas of the study area were more than $200 \mu\text{g/kg}$.

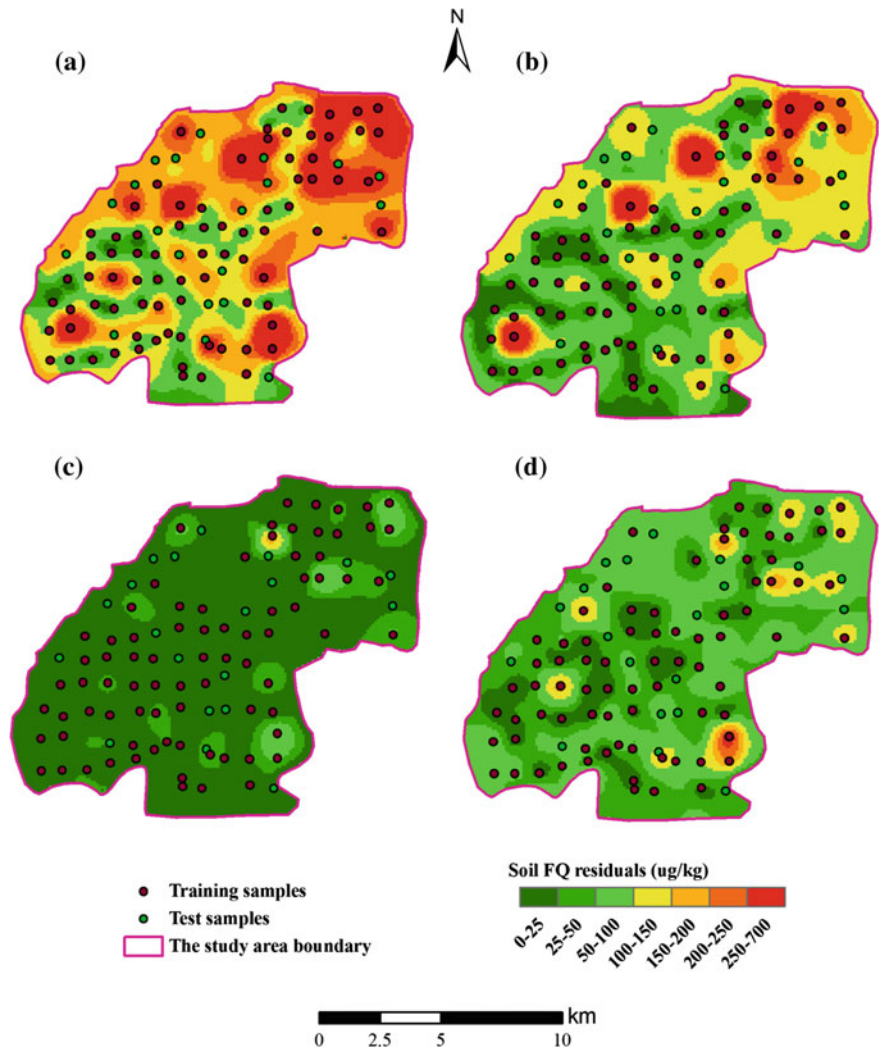


Fig. 2.2 The spatial patterns of soil FQ, CF, EF, and NF residues obtained by HASM. **a** FQ, **b** CF, **c** EF, **d** NF

2.4 Conclusions

China is the country which is the largest producer and consumer of antibiotics compared to the other countries in the world, and antibiotics can be easily added to soil particles with fertilizers of livestock and poultry feces. Fluoroquinolones (FQs) are the most frequently detected antibiotics in the feces of farm livestock and poultry in China. However, relatively few studies focus on the interpolation of soil

antibiotic residues in the intensive vegetable cultivation area. High-accuracy surface modeling (HASM) is regarded as an important new technique in the pedometrics and “digital soil” fields. The HASM method is a spatial interpolation technique based on the fundamental theorem of surfaces. In this study, a total of 100 surface soil samples were collected from the north-central part of the Shandong Province of China to test the performance of HASM with that of classical method. We found that the errors of HASM for NF, CF, EF, and FQ were less compared to splines. HASM has less MAE and RMSE than splines. The RMSEs of splines for FQ, CF, EF, and NF were 3.02, 2.34, 3.46, and 2.64 times larger than those of HASM, respectively. Therefore, HASM can be considered as an alternative and accurate method for interpolating soil antibiotics. HASM is not only as an alternative and accurate method for interpolating soil antibiotics, but also can make the map more consistent with the true spatial distributions.

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