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基于多源辅助变量和随机森林模型的耕地土壤重金属含量空间分布预测

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摘要: 农田土壤重金属含量的空间预测对于监测耕地污染和确保生态农业可持续发展至关重要。从地形、气候、土壤属性、遥感信息、植被指数和人为活动这6个方面选取了32个环境变量作为辅助变量,并构建随机森林(RF)、回归克里格(RK)、普通克里格(OK)和多元线性回归(MLR)模型来预测耕地土壤中As、Cd、Cr、Cu、Hg、Ni、Pb和Zn的含量。结果表明,与RK、OK和MLR相比,RF模型对As、Cd、Cr、Hg、Pb和Zn的预测性能更高,而OK和RK模型分别对Cu和Ni含量的预测精度更高,表现为预测拟合优度(R^2)最高而平均绝对误差(MAE)和均方根误差(RMSE)最低。不同预测方法对同种土壤重金属元素预测结果的空间分布趋势基本一致,8种重金属含量的高值区均分布在南部的平原地区,但RF模型对空间预测的细节刻画得更为突出。随机森林影响因子重要性排序表明,兰溪市土壤重金属含量空间分异主要受Se、TN、pH、海拔、年均温、年均降雨量、距河流距离和距工厂距离的共同影响。因此,随机森林可以作为土壤重金属空间预测的一种有效方法,为区域土壤污染调查、评价和管控提供科学参考。

关键词: 土壤重金属; 环境变量; 随机森林; 空间预测; 影响因子

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Prediction of Spatial Distribution of Heavy Metals in Cultivated Soil Based on Multi-source Auxiliary Variables and Random Forest Model

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Abstract: Spatial prediction of the concentrations of soil heavy metals (HMs) in cultivated land is critical for monitoring cultivated land contamination and ensuring sustainable agriculture. In this study, 32 environmental variables from terrain, climate, soil attributes, remote-sensing information, vegetation indices, and anthropogenic activities were used as auxiliary variables, and random forest (RF), regression Kriging (RK), ordinary Kriging (OK), and multiple linear regression (MLR) models were proposed to predict the concentrations of As, Cd, Cr, Cu, Hg, Ni, Pb, and Zn in cultivated soils. In comparison to those of RK, OK, and MLR, the RF model had the best prediction performance for As, Cd, Cr, Hg, Pb, and Zn, whereas the OK and RK models had highest prediction performance for Cu and Ni, respectively, showing that R^2 was the highest, and mean absolute error (MAE) and root mean square error (RMSE) were the lowest. The prediction performance of the spatial distribution of soil HMs under different prediction methods was basically consistent. The high value areas of eight HMs concentrations were all distributed in the southern plain area. However, the RF model depicted the details of spatial prediction more prominently. Moreover, the importance ranking of influencing factors derived from the RF model indicated that the spatial variation in concentrations of the eight HMs in Lanxi City were mainly affected by the combined effects of Se, TN, pH, elevation, annual average temperature, annual average rainfall, distance from rivers, and distance from factories. Given the above, random forest models could be used as an effective method for the spatial prediction of soil heavy metals, providing scientific reference for regional soil pollution investigation, assessment, and management.

Key words: soil heavy metals; environmental variables; random forest; spatial prediction; influencing factors

土壤是人类生存发展不可或缺的自然资源,也是各种污染物的源和汇^[1,2]。重金属不能被土壤微生物降解,易在土壤中富集,是影响土壤环境质量的主要污染物之一^[3,4]。随着工业化和城市化的快速发展以及对粮食的需求增加,人类活动向土壤中输入的重金属也不断增加^[5,6]。耕地土壤中重金属富集不仅会导致农作物减产和农产品重金属含量超标,而且会通过食物链给人体健康造成威胁^[7-9]。因此,开展耕地土壤重金属空间预测,揭示影响其空间分异

的主要因素,对耕地土壤污染管控和生态农业可持续发展具有重要意义。

土壤中重金属原始含量主要受自然因素如成土

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母质、气候、生物活动及地形的影响^[1,3,10]。然而,随着工业化和城市化的快速发展,人类活动(工农业污染、交通污染和生活垃圾污染)已成为影响土壤重金属含量的重要因素^[11,12],使得土壤重金属呈现复杂的空间异质性特征,导致土壤重金属含量的空间分布预测更加困难^[9]。经典统计学方法只能描述土壤重金属含量的总体变化特征,无法刻画土壤重金属含量的空间分布特征^[13]。地统计模型通过借助变异函数研究具有一定随机性和结构性的各种变量的空间分布及变异规律,在土壤重金属空间预测中得到了广泛应用^[14,15]。然而,地统计方法是对土壤重金属数据进行直接插值,存在平滑效应,难以识别土壤重金属的局部异常值;同时也无法描述环境变量对土壤重金属空间分异的影响^[16]。随着3S技术的发展,地形、气候、遥感、土地利用和社会经济等环境变量变得易于获取,多元线性回归、回归克里格和地理加权回归等方法被广泛用于区域土壤重金属空间分布预测^[17-19]。然而,此类方法难以揭示土壤重金属与环境变量之间复杂的非线性关系。因此,人工神经网络、支持向量机、分类与回归树和随机森林等机器学习模型逐渐被用于土壤重金属空间预测中^[20-22]。其中,随机森林模型结构简单,避免了其他算法中常遇到的过度拟合和多重共线性等问题,对土壤重金属含量具有较高的预测精度^[2,9]。

兰溪市是浙江省传统商品粮基地。改革开放以

来,兰溪市社会经济取得了快速发展,成为浙江中西部的工业基地,纺织、水泥、电镀、生物制药及采矿等行业在生产活动中排放的重金属元素在局部地区引起了耕地土壤重金属富集。本研究通过对兰溪市777个耕地表层土壤样品中As、Cd、Cr、Cu、Hg、Pb、Ni及Zn含量进行分析,结合地形、气候、土壤属性、遥感数据、植被指数和人为活动等环境辅助变量,构建了MLR、OK、RK及RF模型,开展耕地土壤重金属的空间预测,探讨各类模型的精确性与适用性;揭示影响研究区土壤重金属空间分布的主要因素,以期为区域土壤污染调查、评价和管控提供科学参考。

1 材料与方法

1.1 研究区概况

兰溪市(29°05'20"~29°27'30"N, 119°13'30"~119°53'50"E)位于浙江省中部,金衢盆地北缘,总面积约1 313 km²。兰溪市属亚热带季风气候,四季分明,年平均气温17.6℃,年平均降水1 200~1 400 mm。地势东北高、西南低、中部相对平坦,土壤主要为红壤、黄壤、岩性土、潮土和水稻土等。耕地主要分布在盆地中心地带及河谷两侧阶地,面积约占全市总面积的40%,主要农作物为水稻、油菜、棉花、茶叶和果蔬等。兰溪市产业集聚特征明显,主要为纺织、化工、水泥、机械、电力、有色金属冶炼、压延加工和医药制造等。

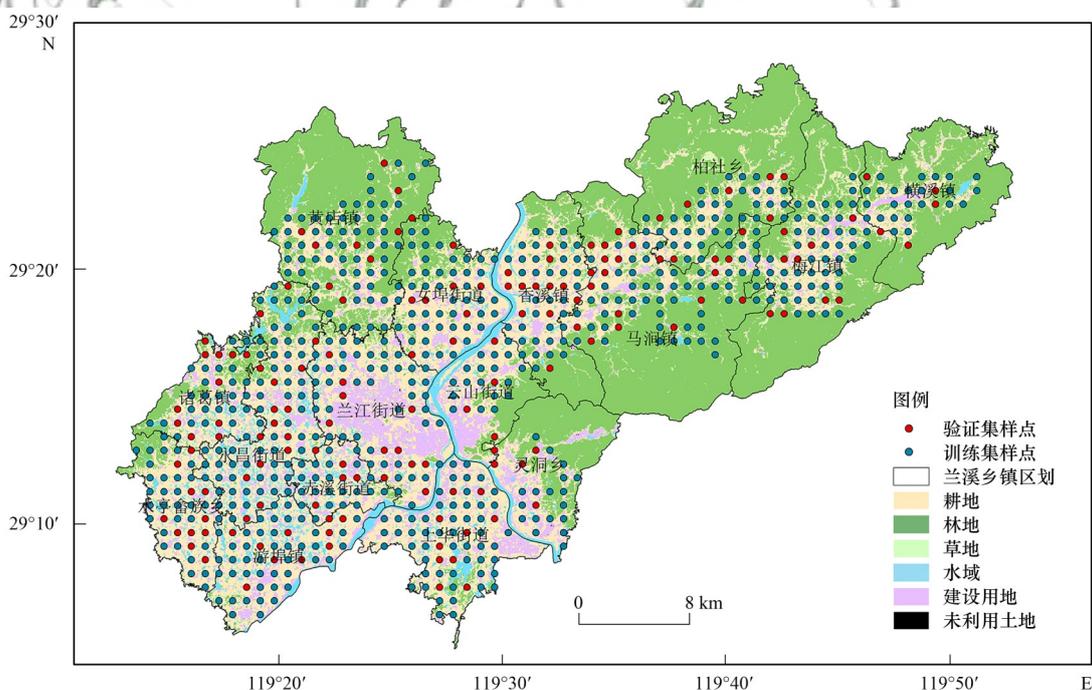


图1 研究区概况及采样点示意

Fig. 1 Location of the study area and soil sampling sites

1.2 样品采集与分析

利用网格布点法(1 km × 1 km)在研究区内进行

耕地表层(0~20 cm)土壤样品采集,共采集样品777个。在每个采样点半径1 m范围内采集5个土壤表层

样品,5个样品混合后作为该点样本,并用GPS记录地理坐标.土壤样品置于无尘实验室中风干、磨碎,过2 mm筛去除石头、动植物残体等杂物,然后过0.149 mm筛子待测. Cr、Cd、Cu、Pb、Ni、Zn采用硝酸、高氯酸、氢氟酸消解,用电感耦合等离子体质谱仪(ICP-MS)测定;As和Hg采用王水-水浴消解,Se采用硝酸、硫酸、盐酸消解,用电感耦合等离子体发射光谱仪(ICP-AES)测定.土壤pH利用pH计测定,土壤全氮(TN)采用凯氏定氮法测定.分析过程中使用试剂均为优级纯,用水均为超纯水.采用国家土壤标准参照物(GSS-24)和20%平行样进行质量控制,误差保持在5%以内.

1.3 环境辅助变量及数据来源

本研究从地形、气候、土壤属性、遥感信息、植

被指数和人为活动这6个方面选取了32个环境变量作为辅助变量(表1).其中,地形因子从DEM数字高程模型中提取,遥感信息从Landsat 8影像中提取,植被指数通过计算各波段获得^[23].土壤属性因子通过普通克里格法进行空间插值后,提取30 m分辨率的栅格数据. DEM数据、Landsat 8影像和气候因子栅格数据均来源于地理数据空间云(<http://www.gscloud.cn>);人口密度数据来源于中国科学院资源环境科学与数据中心(<https://www.resdc.cn>).到工厂距离、到道路距离、到河流距离和到建设用地距离通过卫星影像数据及实地调查,利用ArcGIS 10.2的欧式距离工具进行提取.人口密度、年平均温度和年平均降水量通过最近邻域法将尺度降至30 m的栅格.

表1 土壤重金属预测环境辅助变量

Table 1 Environmental auxiliary variables for heavy metal prediction in soil

辅助变量		分辨率	文献
地形	海拔、坡向、坡度、剖面曲率、平面曲率和粗糙度	30 m	[19]
气候	年平均温度和年平均降水量	1 km	[19]
土壤属性	Se、pH和TN	30 m	[24]
遥感信息	Band2、Band3、Band4、Band5、Band6和Band7	30 m	[24]
植被指数	差值植被指数、比值植被指数、红绿比值指数、归一化植被指数、改进土壤调节植被指数、绿度植被指数、大气抗阻植被指数、黏土矿物比值和水分胁迫指数	30 m	[24, 25]
人为活动	人口密度、到工厂距离、到道路距离、到河流距离和到建设用地距离	1 km	[26]

1.4 模型构建

1.4.1 多元线性回归

多元线性回归(MLR)通过构建土壤重金属含量与多个辅助变量之间的近似表达式从而进行预测^[27].逐步多元回归是将变量逐个引入,每引入一个新变量会对已引入的变量逐个进行显著性检验,剔除不显著的辅助变量,利用最终保留的变量与土壤重金属含量构建线性回归方程^[20].逐步多元回归计算公式如下:

$$y = a_0 + a_1x_1 + a_2x_2 + \dots + a_nx_n \quad (1)$$

式中, y 为耕地土壤重金属含量, a_0, \dots, a_n 为常数项, x_1, \dots, x_n 为通过筛选得出的对于研究区耕地土壤重金属含量影响最为显著的变量.

1.4.2 普通克里格

普通克里格法(OK)是基于已知样点与半变异函数的结构性,对未采样点土壤重金属含量进行线性无偏估值,被广泛应用于土壤重金属含量的空间分布研究^[5, 15].半变异函数计算公式为:

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

式中, $\gamma(h)$ 为半变异函数; h 为两个样点间的空间距离; $Z(x_i)$ 为 $Z(x)$ 在 x_i 地理位置上的土壤重金属含量;

$Z(x_i+h)$ 为 $Z(x)$ 在 x_i+h 地理位置上的重金属含量; $N(h)$ 为样本点对的数量.

1.4.3 回归克里格

回归克里格(RK)是一种混合插值方法,由MLR和OK法结合而成,即通过建立辅助变量与土壤重金属含量之间的多元线性回归方程,分离趋势项,并对残差进行OK插值,最后将回归预测的趋势项和残差的普通克里格估计值进行空间叠加,从而得到未采样点土壤重金属含量预测值^[17].因此,RK法中趋势项表达了辅助变量对土壤重金属空间变异的影响,残差估值反映了去除辅助变量影响后的土壤重金属空间变异^[18].

1.4.4 随机森林

随机森林(RF)是一种利用多棵决策树对样本训练并预测的机器学习模型^[22].随机森林回归通过重复且有放回地从原始样本中随机选取 n 个样本形成 n 棵回归树(ntree),每次未被抽取的样本则组成袋外数据(OOB);然后从变量中选取最能有效分割数据的 m 个变量(mtry),根据袋外误差最小原则确定mtry值;最后将形成的多棵回归树集合为随机森林,并求取平均值输出^[24, 27].

1.5 精度检验方法

在进行空间预测时,随机提取土壤重金属样点的70%作为训练集,余下30%作为验证集,首先利用训练集与辅助变量进行建模,然后验证集样点的预测值和实测值比较,并通过计算验证集的平均绝对误差(MAE)、均方根误差(RMSE)和拟合优度(R^2)评价预测精度.MAE、RMSE以及 R^2 的计算公式如下:

$$MAE = \frac{1}{n} \sum_{i=1}^n |P_i - O_i| \quad (3)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (O_i - P_i)^2} \quad (4)$$

$$R^2 = \frac{\sum_{i=1}^n (P_i - \bar{O}_i)^2}{\sum_{i=1}^n (O_i - \bar{O}_i)^2} \quad (5)$$

式中, P_i 和 O_i 分别为样本*i*的预测值和实测值; \bar{O}_i 为实测值的平均值; n 为验证集样本数量.

2 结果与分析

2.1 兰溪市耕地土壤重金属含量特征

研究区8种土壤重金属含量的描述性统计值见

表2 兰溪市耕地土壤重金属含量描述性统计分析¹⁾

Table 2 Statistical description of cultivated soil heavy metals in Lanxi City

项目	pH	As	Cd	Cr	Cu	Hg	Ni	Pb	Zn
均值/ $\text{mg} \cdot \text{kg}^{-1}$	5.58	7.53	0.22	41.83	20.80	0.12	15.44	31.89	74.69
变异系数/%	11.99	66.08	59.47	33.63	27.67	57.53	38.40	24.43	32.49
偏度	0.67	8.37	5.71	1.05	1.31	2.32	1.91	3.01	6.10
峰度	1.42	103.94	57.21	1.68	3.72	10.20	6.01	19.85	74.08
浙江省土壤元素背景值/ $\text{mg} \cdot \text{kg}^{-1}$	—	9.20	0.07	52.90	17.60	0.09	7.06	23.70	70.60
金衢盆地土壤元素背景值/ $\text{mg} \cdot \text{kg}^{-1}$	—	6.49	0.19	39.07	18.08	0.10	12.45	35.12	72.13
中国农田土壤污染风险筛选值/ $\text{mg} \cdot \text{kg}^{-1}$	—	30.00	0.40	250.00	50.00	0.50	70.00	100.00	200.00

1) $n=777$,“—”表明无数据,pH值无量纲,农田土壤污染风险筛选值选择 $5.5 < \text{pH} \leq 6.5$ 时的筛选值为参考标准

算环境辅助变量对各重金属影响的重要性.结果表明所选择的环境辅助变量对8种土壤重金属的解释度在24.98%~55.87%之间(表3).如图2所示,土壤Se含量、到工厂距离和年平均温度是影响土壤As含量的重要影响因素.土壤Cd含量受土壤pH、土壤Se含量和土壤TN含量影响较大.土壤Se含量、到河流距离和年平均温度是土壤Cr含量的重要影响因子.耕地土壤Cu含量分布主要受土壤TN含量、土壤Se含量和年平均温度等因素的影响;Hg含量分布主要受土壤TN含量、土壤Se含量和到工厂距离的影响;而土壤pH、土壤Se含量和平均温度是土壤Ni含量的重要影响因子;Pb含量分布主要受到河流距离、Se含量和TN含量等因素的影响;Zn主要受到河流距离、土壤Se含量和土壤pH的影响.

表2. $\omega(\text{As})$ 、 $\omega(\text{Cd})$ 、 $\omega(\text{Cr})$ 、 $\omega(\text{Cu})$ 、 $\omega(\text{Hg})$ 、 $\omega(\text{Ni})$ 、 $\omega(\text{Pb})$ 和 $\omega(\text{Zn})$ 的均值分别为7.53、0.22、41.83、20.80、0.12、15.44、31.89和74.69 $\text{mg} \cdot \text{kg}^{-1}$,均未超过中国农田土壤污染风险筛选值^[28].与浙江省土壤背景值相比^[29],Cd、Cu、Hg、Ni、Pb和Zn的含量均值高于浙江省相应土壤元素背景值,尤其Cd和Ni的含量均值分别是浙江省背景值的3.14倍和2.21倍.与金衢盆地土壤元素背景值相比^[30],除了Pb之外,As、Cd、Cr、Cu、Hg、Ni和Zn的含量均值均略高于金衢盆地相应土壤元素背景值,表明兰溪市耕地土壤重金属含量已经存在不同程度的积累.变异系数可以反映人类活动对土壤重金属富集的影响程度.研究区8种土壤重金属的变异系数介于24.43%~66.08%,其中Cr、Cu、Pb和Zn属于中等变异,As、Cd、Hg和Ni属于强变异^[31],表明研究区土壤重金属一定程度上受到人类活动的干扰.偏度和峰度表明土壤重金属数据呈现出正偏态分布.

2.2 环境辅助变量筛选

为了避免预测变量之间的多重共线性影响模型预测效果,将环境辅助变量的方差膨胀因子>10的变量剔除后利用随机森林模型中的importance函数计

表3 随机森林模型参数和结果¹⁾

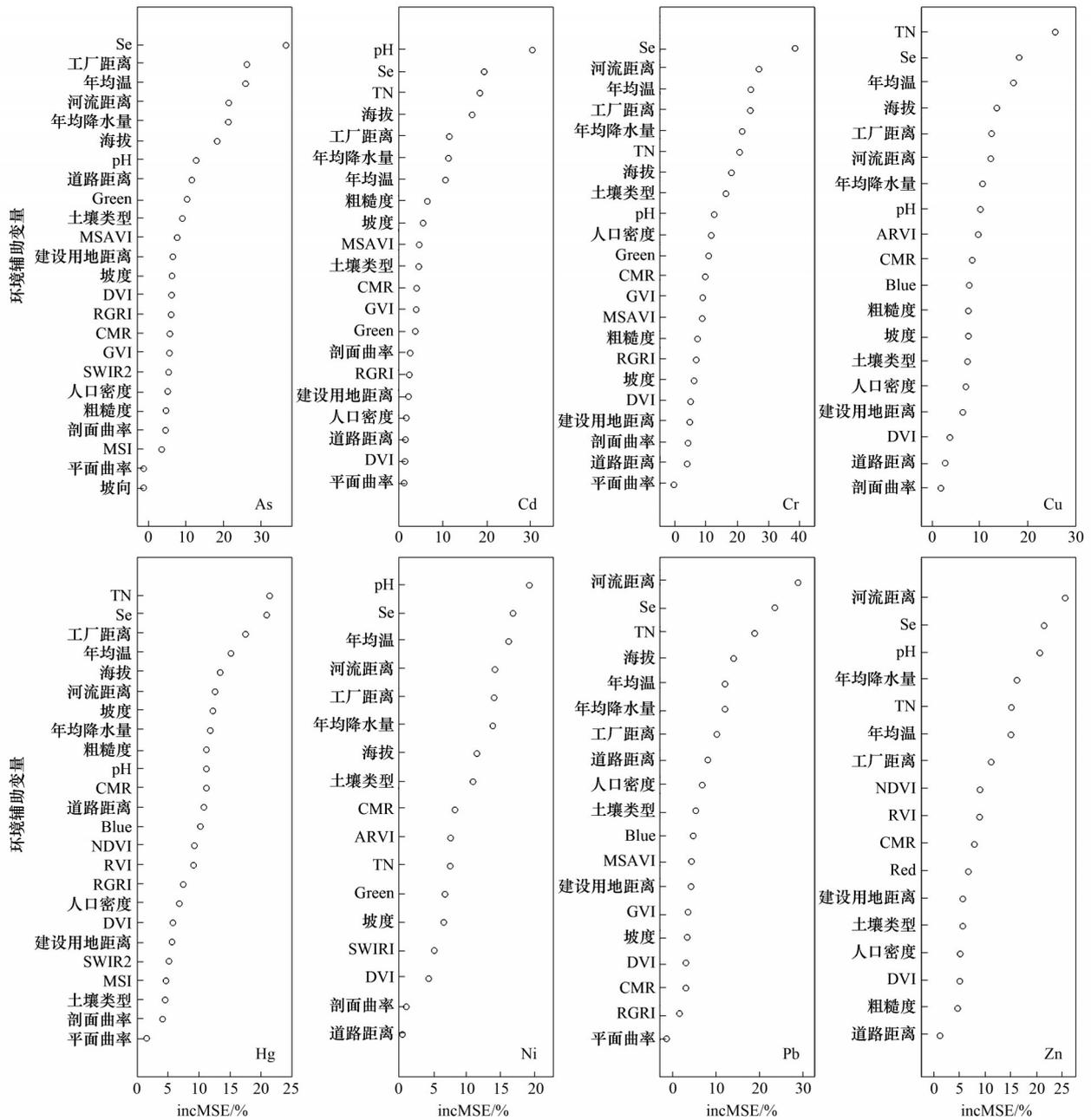
Table 3 Model parameters and explained variations by random forest model

元素	mtry	ntree	nodesize	OOB	Var/%
As	3	800	5	2.316	51.37
Cd	3	300	5	0.002	55.87
Cr	3	300	5	68.068	52.74
Cu	3	600	5	15.309	24.98
Hg	4	800	5	0.001	36.41
Ni	3	600	5	10.830	35.33
Pb	4	500	5	10.515	53.17
Zn	3	400	5	155.108	43.02

1)Var为环境变量对目标变量的解释度

2.3 不同模型预测精度对比

通过验证集数据对MLR、OK、RK及RF模型计算后得到各模型对8种土壤重金属预测的 R^2 、MAE



Blue 为蓝波段, Green 为绿波段, Red 为红波段, SWIR1 为短波红 1, SWIR2 为短波红外 2, MSI 为水分胁迫指数, CMR 为黏土矿物比值, MSAVI 为改进土壤调节植被指数, RVI 为比值植被指数, RGRI 为红绿比值指数, NDVI 为归一化植被指数, GVI 为绿色植被指数, DVI 为差值植被指数, ARVI 为大气抗阻植被指数, incMSE 为变量重要性程度

图 2 环境辅助变量对土壤重金属空间预测的相对重要性

Fig. 2 Relative importance of environmental auxiliary variables to spatial prediction of soil heavy metals

和 RMSE(表 4). 4 种模型预测结果表明, RF 模型对 As 含量的预测 R^2 最高, 为 0.589; 而 MLR 模型对 Cu 含量的预测 R^2 最低, 为 0.155. MAE 和 RMSE 的变化范围分别为 0.029 ~ 10.057 $\text{mg}\cdot\text{kg}^{-1}$ 和 0.038 ~ 13.099 $\text{mg}\cdot\text{kg}^{-1}$, 最小值和最大值分别来自于 RF 模型对 Hg 含量的预测和 MLR 模型对 Zn 含量的预测. 在 4 种模型中, RF 模型对 As、Cd、Cr、Hg、Pb 和 Zn 含量的预测精度最高, OK 模型对 Cu 含量的预测精度最高, 而 RK 模型对 Ni 含量的预测精度最高, 表现为预测 R^2 最高而 MAE 和 RMSE 最低.

2.4 不同模型空间预测

由图 3 可知, 不同预测方法对同种土壤重金属元素预测结果的空间分布趋势基本一致. As 的高值主要分布在兰溪市的中部和西部. MLR 与 OK 预测的高值区和低值区呈大片块状分布, 难以反映土壤 As 含量局部变异情况, 预测效果较差; 而 RK 和 RF 的预测结果显著优于 MLR 与 OK, 其中 RF 在研究区中西部的预测效果更精细. Cd 的高值主要分布在研究区的南部, 低值主要分布在研究区的西北部. MLR 预测结果仅能反映区域耕地土壤 Cd 分布的大体趋势, 与其

表 4 4 种模型土壤重金属预测精度评价¹⁾
Table 4 Validation of prediction of soil heavy metals by four models

模型	参数	As	Cd	Cr	Cu	Hg	Ni	Pb	Zn
MLR	R^2	0.422	0.418	0.299	0.155	0.379	0.185	0.209	0.185
	MAE	1.406	0.037	8.580	3.314	0.029	3.255	3.623	10.057
	RMSE	1.787	0.048	10.585	4.247	0.038	4.079	4.468	13.099
OK	R^2	0.530	0.262	0.551	0.372	0.285	0.455	0.435	0.401
	MAE	1.239	0.041	6.452	2.711	0.031	2.547	3.088	8.505
	RMSE	1.625	0.054	8.451	3.627	0.041	3.357	3.850	11.114
RK	R^2	0.578	0.279	0.524	0.339	0.310	0.478	0.436	0.383
	MAE	1.189	0.041	6.830	2.782	0.031	2.497	3.085	8.704
	RMSE	1.530	0.053	8.707	3.717	0.040	3.264	3.823	11.271
RF	R^2	0.589	0.516	0.575	0.316	0.467	0.433	0.477	0.408
	MAE	1.171	0.032	6.451	3.007	0.028	2.812	2.820	8.440
	RMSE	1.520	0.044	8.400	3.815	0.035	3.530	3.647	11.111

1) 黑体字表示每种重金属的最优预测模型

他模型相比,对高值与低值的预测偏差较大,而OK的空间预测结果存在明显的平滑效应,RF和RK空间预测结果更能反映局部的变异特征,尤其以RF在空间预测细节更突出。Cr、Cu和Ni高值主要分布在研究区西部以及南部的小范围区域内。OK和MLR预测分布图的高值区和低值区呈大片块状分布,很难反映局部空间变异情况,预测精度较低,RK和RF的预测结果均较好地反映了局部小范围的空间变异情况。Hg含量呈现西部高东部低的分布趋势。OK预测的高值区和低值区呈大片块状分布,难以反映局部空间变异情况,而RK存在一定的平滑效应,预测精度不高;MLR与RF预测结果更加精细,但RF比MLR更能模拟局部小范围的非线性关系,制图效果更优。Pb和Zn含量的空间预测结果相似,高值主要分布在研究区的南部,并沿着金华江、衢江和兰江分布,但不同模型对研究区东北部的含量预测存在明显差异。此外,MLR对研究区西部含量预测值比其他模型明显偏低,RF的预测效果更为精密。

3 讨论

3.1 耕地土壤重金属空间分布影响因素

耕地土壤重金属空间分布受自然条件(地形、气候、母质等)和人类活动(工业生产、农业活动等)的共同影响。研究区As、Cr和Ni的高值区主要分布在研究区的中西部,该区域纺织厂较多,耕种面积广,受农业以及工业活动影响较大。因子重要性排序表明,土壤Se含量、年平均温度和到河流距离、到工厂距离是影响As、Cr和Ni的最主要因子(图2)。已有研究表明,Se能够与重金属形成复合物或产生拮抗效应从而降低农作物的吸收量^[32]。温度和降水则通过影响土壤中As和Cr的迁移转化从而影响其含

量^[19,33]。到河流距离、到工厂距离反映了农业灌溉以及工厂排放等人类活动对土壤重金属含量产生的影响。有研究表明,农药和化肥的生产与使用,化工和纺织等工业活动均能导致土壤环境中的As、Cr和Ni含量增加^[34]。

研究区Cd和Cu含量的分布受土壤理化性质的影响较大(图2)。农业活动引起的土壤理化性质变化会影响土壤重金属的迁移、活性和吸持能力^[24,35]。研究区农业耕作过程中有机肥(家禽粪肥等)及无机肥(尿素、磷肥和复合肥)的施用是当地Cd积累的重要原因^[34]。此外,农业生产过程中喷洒的除草剂、杀菌剂和杀虫剂中均含有大量的Cu,而家禽饲养中常在饲料中添加硫酸铜或氨基酸螯合铜以补充Cu元素,最终通过粪便进入土壤中^[36,37]。

研究区Hg含量的高值区主要分布在研究区的中部与西部,而TN含量、Se含量和离工厂距离是影响Hg元素空间分布的重要因素(图2)。已有研究表明,自然界中Hg元素的自然来源含量较少,Hg的富集主要受农用化肥的施用、冶炼工业的废气排放和城区生活垃圾焚烧的排放影响^[2,10]。

Pb和Zn的高值区空间分布范围较小,集中分布在金华江、衢江和兰江交汇地带。距河流距离是影响Pb和Zn的最重要因素,其次为pH和TN含量(图2)。一方面,河流沿岸区域工业较为发达,是重要的水泥、食品和建材生产基地,生产过程中会排放含Pb和Zn等重金属元素的粉尘、废气和废水^[13],导致土壤中的Pb和Zn逐渐富集。另一方面,上游地区农业播种面积较广,交通流量较大,因此排放的Pb和Zn通过大气沉降或者直接排放进入河流,随河流输送到中下游^[14]。

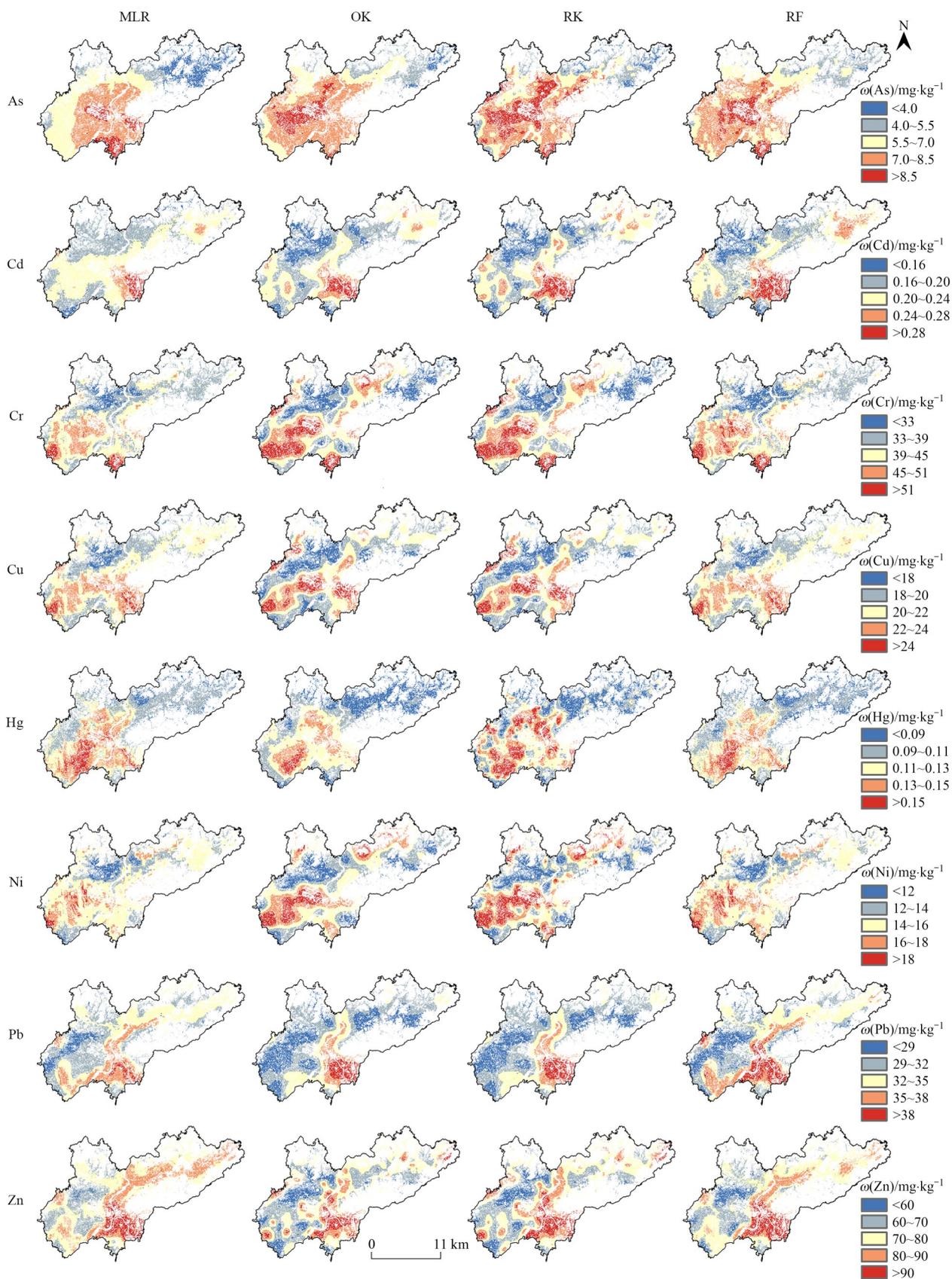


图3 4种模型对土壤重金属空间预测对比

Fig. 3 Comparison of spatial prediction of soil heavy metals by four models

3.2 不同模型预测性能对比

对于研究区土壤重金属的空间预测,不同模型

的性能存在差异. 在本研究中,OK和MLR仅能反映区域耕地土壤重金属含量分布的总体趋势,难以反

映局部变异情况,预测精度相对较低(表4);RK与RF则能较好地反映局部空间变异情况,尤其RF预测空间分布图呈现出“低值区缩小连片、中值区扩大平稳、高值区缩小集中”的特征,制图效果也更为精密(图3)。MLR、OK和RK均是对变量的线性估计,然而土壤重金属含量的空间分布与环境因子之间存在复杂的非线性关系^[17,38,39]。有研究表明RF、支持向量机、人工神经网络等非线性模型的预测能力显著高于线性模型^[40-42]。OK忽视了影响土壤中重金属含量分布的过程性因素,不能充分反映各种环境因素对土壤重金属的影响^[14]。RK既利用了多源辅助变量如土壤理化性质、地形以及遥感光谱信息等,又利用了空间信息,弥补了OK无法模拟环境因子影响的不足^[17,43]。本研究表明,RK对As、Ni和Pb等重金属元素的预测效果优于OK和MLR模型。部分研究表明了RK预测精度高于MLR和OK模型。例如,高中原等^[18]对南方某市冶炼厂周边区域土壤重金属含量进行空间分布模拟时,发现融合自然和人为因素的RK方法明显提高了土壤Cd含量的空间预测精度。在本研究中,RF对8种重金属空间预测的决定系数(R^2)介于0.316~0.589之间,MAE和RMSE分别小于8.44和11.111(表4),能够较为准确地揭示重金属元素含量与多源辅助变量间的非线性关系,是研究区土壤重金属空间预测的最优模型。金昭等^[16]对比了9种机器学习模型对土壤重金属空间预测精度,发现RF的预测 R^2 介于0.263~0.488之间,高于其余模型。相似的,Azizi等^[24]结合机器学习模型和环境变量对伊朗西部地区土壤重金属进行空间预测,发现RF结合环境变量能显著提高土壤重金属的预测能力,Cu和Ni的预测 R^2 分别能达到0.60和0.67。这主要是因为RF结合了Bagging集成学习理论和随机子集空间方法,具有较强的非线性挖掘能力,在计算过程中不需要数据分布符合任何假设,可以定量描述变量的贡献程度,并弥补了ANN和CART等模型的不稳定、过度拟合和对多重共线性不敏感等不足^[44,45]。在环境变量与土壤重金属含量空间分布关系相对复杂的区域,随机森林的预测优势更加显著,因而预测精度相对较高^[16]。

4 结论

(1)除了Pb之外,As、Cd、Cu、Cr、Hg、Ni和Zn的含量均值均略高于金衢盆地相应土壤元素背景值,变异系数介于24.43%~66.08%,表明兰溪市耕地土壤重金属含量存在不同程度积累并受到一定程度人类活动的干扰。

(2)RF对兰溪市耕地土壤As、Cd、Cr、Hg、Pb和

Zn含量的预测精度更高,而OK和RK分别对Cu和Ni含量的预测精度更高,表现为预测 R^2 最高而MAE和RMSE最低。

(3)不同预测方法对同种土壤重金属预测的空间分布趋势基本一致,8种重金属含量的高值区均分布在南部的平原地区。MLR、OK和RK能反映区域耕地土壤重金属含量分布的总体趋势,但RF对空间预测的细节刻画得更为突出。

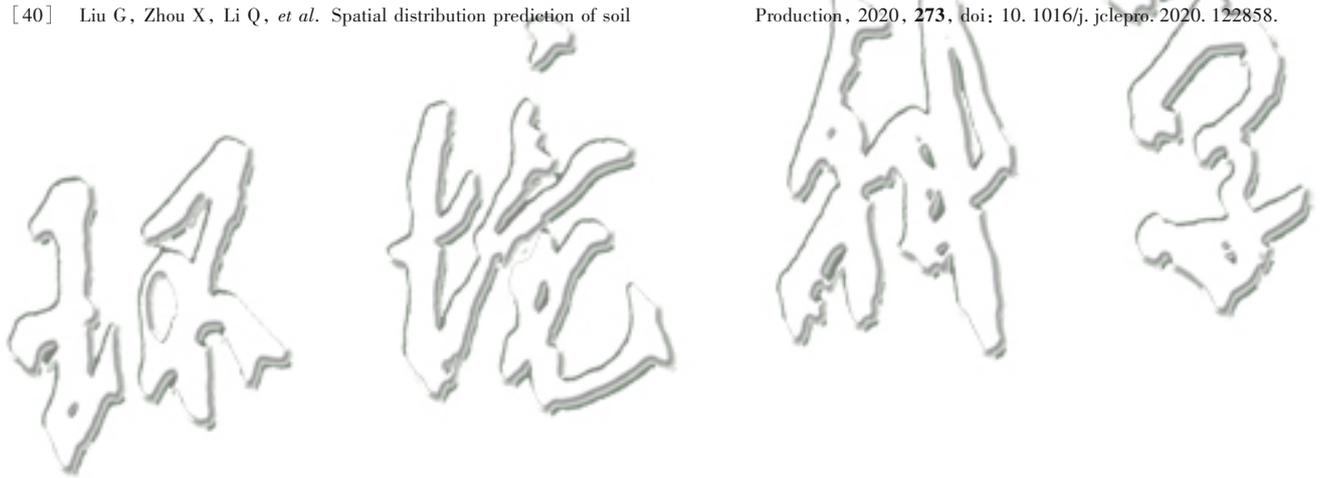
(4)环境辅助变量相对重要性表明,兰溪市土壤重金属含量空间分异主要受:自然因子(海拔、年均温、年均降雨量)、土壤性质(Se含量、TN含量、pH)和人类活动(距河流距离、距工厂距离)的共同影响。

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