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# ENVIRONMENTAL SCIENCE





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### 土地利用回归模型在大气污染时空分异研究中的应用

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摘要:随着城市化、工业化、机动化进程的加快,大气污染已成为我国最严重的环境问题之一,对公众健康和生态环境造成了诸多负面影响. 土地利用回归,即 Land-use Regression(LUR)模型是目前模拟城市尺度大气污染时空分异的常用方法之一,其在欧洲和北美得到广泛的应用,而在国内,相关研究却不多. 本文在整理国内外文献的基础上,从构建 LUR 模型的主要步骤入手,包括监测数据获取、模型自变量生成、模型构建、模型检验和回归映射等方面,对 LUR 模型在大气污染时空分异研究中的进展进行归纳总结,进而展望了未来的研究重点与方向,即突出时空分异、扩展模型变量类别和改进模型构建方法. 本文旨在普及 LUR 模型在我国的应用,为人口暴露、流行病学研究和健康风险评价等提供方法论基础.

关键词:土地利用回归(LUR)模型; 大气污染; 时空分异; GIS; 研究进展

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# Application of Land-use Regression Models in Spatial-temporal Differentiation of Air Pollution

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Abstract: With the rapid development of urbanization, industrialization and motorization, air pollution has become one of the most serious environmental problems in our country, which has negative impacts on public health and ecological environment. LUR model is one of the common methods simulating spatial-temporal differentiation of air pollution at city scale. It has broad application in Europe and North America, but not really in China. Based on many studies at home and abroad, this study started with the main steps to develop LUR model, including obtaining the monitoring data, generating variables, developing models, model validation and regression mapping. Then a conclusion was drawn on the progress of LUR models in spatial-temporal differentiation of air pollution. Furthermore, the research focus and orientation in the future were prospected, including highlighting spatial-temporal differentiation, increasing classes of model variables and improving the methods of model development. This paper was aimed to popularize the application of LUR model in China, and provide a methodological basis for human exposure, epidemiologic study and health risk assessment.

Key words: land-use regression (LUR) model; air pollution; spatial-temporal differentiation; GIS; research progress

随着城市化进程的加快,城市面积、人口持续扩张,工业排放和能源消耗不断增加,我国面临着大气污染的严峻挑战<sup>[1]</sup>. 很多研究表明<sup>[2,3]</sup>,城市内大气污染物空间分异现象突出. 而国内大气污染暴露或流行病学研究<sup>[4]</sup>多忽略了大气污染物浓度的空间分异,导致了估计的误差<sup>[5]</sup>. 为了更好地模拟城市尺度大气污染物浓度的空间分布,国内外学者提出了许多方法,诸如污染物-气象逐步回归模型<sup>[6]</sup>、大气数值模拟技术<sup>[7]</sup>、扩散模型<sup>[8]</sup>和土地利用回归(Land-use Regression, LUR)模型<sup>[9]</sup>等. 而LUR 模型是目前最通用的方法之一,但其在我国应用较少.

本文在整理分析近年 LUR 模型研究案例的基础上,从构建模型的主要步骤入手,对模型在大气污染时空分异研究中的进展进行归纳,并展望未来的研究重点与方向. 本文旨在普及 LUR 模型在我国的应用,并为人口暴露、流行病学研究和健康风险评价等提供方法论基础.

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LUR 模型最早是由 Briggs 等[10]于 1997 年在小区域空气质量和健康分异研究中提出的. 它是一种模拟城市尺度大气污染物浓度空间分异的通用模型,通常利用数十个采样点的大气污染物浓度数据作为因变量,通过在地理信息系统(GIS)框架内获取站点周边的土地利用、交通、人口密度等数据作为自变量,建立回归模型来分析这些因素对大气污染物浓度空间分布的影响. 接着,利用模型对研究区内任意位置的污染物浓度进行估计. 模型考虑的自变量不仅有土地利用相关的变量,一般还有交通、工业排放、气候、地形、人口分布等要素. 但大多数研究中仍将之称为 LUR 模型[11].

自 Briggs 的研究后, LUR 模型的发展可大致分为两个阶段. 1997~2006 年为摸索阶段,模型尚未引起研究者的重视,仅在欧洲有一些尝试性的进展. 2007 年, Henderson 等[12] 完善了模型的构建方法, 2008 年, Hoek 等[13] 综述了模型的研究进展. 此后, LUR 模型的研究蓬勃发展,在欧洲和北美得到了广泛的应用,成为模拟城市尺度大气污染物浓度时空分异最主要、最体系化的方法之一. 图 1 采用文献计量的方法,统计了 1997~2014 年各洲发表的 LUR 模型研究案例的数量.

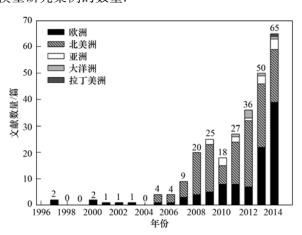


图 1 1997~2014 年各洲发表的 LUR 模型研究数量统计

Fig. 1 Number of studies published about land-use regression models in various continents between 1997 and 2014

传统的扩散模型需要高精度的污染源数据和气象数据,并需要初始化和参数化处理<sup>[14]</sup>,而空间插值法仅仅依据监测数据,难以获得小范围内污染物浓度的空间变化<sup>[13]</sup>.与这些方法相比,LUR模型具有明显的优势<sup>[15]</sup>,它对数据类别和精度需求较低,模型构建简便,并且能充分反映小尺度污染物浓度

的空间分异,模型具有优良的转移性.

#### 2 模型的主要构建步骤

学

本文在 PubMed 中搜索"air pollution"和"land-use regression"两个关键词, 收集和筛选了 2005 ~ 2015 年近 80 篇英文文献. 文章按照 LUR 模型的构建步骤,即监测数据获取、模型自变量生成、模型构建、模型检验和回归映射这 5 个方面来介绍模型.

#### 2.1 监测数据获取

污染物浓度监测数据作为 LUR 模型的因变量, 对于模型有着至关重要的作用. 数据的获取可分为 三类: 第一类是实验设计监测 (purpose-designed monitoring)<sup>[16]</sup>,即设计特定的监测方案来进行户外 污染物浓度的站点测量. 在国外已有研究中,大多 数研究均采用这种方法. 第二类是常规监测 (routine monitoring),即环保部门日常监测大气污染 所构建的监测网络. 国内多数研究的监测数据获取 均来源于该途径. 第三类是车载移动监测 (mobile monitoring),即搭载着污染物监测设备的车辆沿着 设定的路径行驶,每隔一定时间对污染物的浓度进 行一次采样,同时记录采样的地点. 此方法可视为 一种特殊的实验设计监测,多用于交通污染物的 LUR 模型构建以及与交通排放有关的人口暴露研 究[17]. 数据的获取途径不是唯一的,部分研究结合 了第一和第二种监测方法,以提高数据的精确度. 如 Rose 等[18] 在悉尼、Parenteau 等[19] 在渥太华、 Allen 等[20] 在乌兰巴托的研究中, 都采用了两种监 测手段获取污染物的数据. 表 1 总结了三类监测方 法的特点.

监测站点数目需要根据研究区的范围来确定.例如,Novotny等<sup>[21]</sup>针对美国全境的研究,选择的站点有 423 个<sup>[30]</sup>,而 de Hoogh 等<sup>[22]</sup> 在欧盟的 ESCAPE 项目中,每个城市选取了 20 个站点. 一般而言,常规监测途径的站点数目少于实验设计监测途径. Hoek 等<sup>[13]</sup>指出,40~80 个站点是城市尺度研究中合适的监测数目,当然也必须考虑城市人口和规模. 在污染源众多、景观格局复杂的城市环境中,Basagaña 等<sup>[23]</sup>建议应当选取至少 80 个监测站点来分析大气污染物的空间分异.

此外,监测时段也是 LUR 模型构建的重要因素. 各研究的监测时间不等,多则 8~9 a<sup>[24]</sup>,少则每次几小时<sup>[25]</sup>,一般根据监测方法和人力物力而定. 常规监测方法可以获取连续、长时间的监测数据,如 Estarlich 等<sup>[26]</sup>在西班牙的研究,监测的时间

近3年;而实验设计监测通常是由几个间断的1~2 周监测活动组成,这些间断的监测活动分散分布在 整个研究期内,所获得的浓度用来代替长期浓度[13]。

#### 表 1 不同监测方法特点对比

Table 1 Comparisons among different measurement methods

	1 0			
监测方法	站点类型和数目	成本	监测时间	主导单位
实验设计监测	依据研究区和监测污染物的特点,设定各种类型 的监测站点,类型齐全,数目一般较充足	高	依据实验设计,一般由几个1~2周的监测活动组成,总体监测时长较短,间断监测	研究团队
常规监测	根据已有的监测网络获取监测数据,监测站点类 型和数目得不到保证	低廉	监测时长不限,时间分辨率高,连续监测	政府机构
车载移动监测	监测站点类型为交通污染监测点,数目充足	较高	依据实验设计,一般由几个1~2周的监测活动组成,总体监测时长较短,间断监测	研究团队

#### 2.2 模型自变量生成

对浓度可能产生影响的因素均可用作 LUR 模型的自变量.就变量类别而言,使用较为广泛的主要有土地利用、交通排放、气象、人口密度、排放源分布、海拔等. 在构建时空 LUR 模型时,自变量还可能包含时间虚拟变量和动态变量<sup>[27]</sup>.

最常见的变量形式是以站点周边一定缓冲区内的影响因素分布情况来体现的[13].对于每个子类别,一般设置一组按照一定规律递增的缓冲区来定义.例如,对于主干道长度子类别,Majorroad\_i(i为100、200、300、500、1000)分别对应了站点周边半径100、200、300、500、1000 m内的主干道长度.缓冲区半径的设置对于模型结果有着重要影响,理论上,最小缓冲半径需要根据地理数据的空间精度来确定,而最大缓冲半径则与污染源和污染物的扩散模式有关[13].由于与交通排放相关的污染物(如NO<sub>x</sub>等)沿着离道路的距离呈指数递减<sup>[15]</sup>,交通变量的最大缓冲半径一般为1000 m,而土地利用、人口密度等变量的最大缓冲半径可达5000 m<sup>[28]</sup>.

数据的可获取性是影响自变量的重要因素. 以交通变量为例,其指示形式通常有两种,一是交通流量,二是道路长度. 交通流量能直接表征交通排放,然而其获取则较为困难,对于低等级道路的普及性也较差<sup>[13]</sup>. Henderson 等<sup>[12]</sup>运用道路长度变量与交通流量变量分别构建了 LUR 模型,两者的  $R^2$  并无显著差异. 随着信息技术的进步,开始有新变量加入到 LUR 模型中. 如 Wu 等<sup>[29]</sup>引入了饭店密度变量; Tang 等<sup>[30]</sup>考虑了建筑物高度和街道格局对污染物的影响. 近年来,国外也有一些研究尝试将卫星遥感数据作为 LUR 模型的自变量,以得到更大空间尺度的大气污染物浓度空间分异. 这类研究常用到的遥感产品有两类,第一类是气溶胶光学厚度数据(AOD),如 MODIS AOD 等,用来估计 PM<sub>2.5</sub>、PM<sub>10</sub>等大气污染物的空间分布<sup>[31]</sup>;另一类是对流层

 $NO_2$  柱丰度数据,由 Aura 卫星的臭氧监测仪(OMI) 提供,通常用于估计大尺度的  $NO_2$  浓度空间分 布[32].

#### 2.3 模型构建

在大多数的 LUR 模型中,污染物的浓度不做数学变换,即直接使用监测浓度作为因变量. 部分研究中,因变量是对数化的污染物浓度,不论哪种,均是为了得到较高的模型解释力[13].

LUR 模型采用一定的算法选取显著的变量得 到结果.模型的构建算法通常有两类,第一类是一 种后向算法(backward algorithm),其从有效性库 (available pool)中通过逐步回归的方法依次剔除变 量,该算法最早由 Henderson 等[12]提出,并在此后得 到了广泛的应用[33]. 具体的步骤如下:①将所有自 变量与因变量的相关程度按照其绝对值的大小依次 排序;②在每个子类别(记为 X)的自变量当中,确 定与因变量相关程度最高自变量,即排序最高的自 变量,记为 $X_i(i)$ 为对应的缓冲区半径);③在每个 子类别中,去除与 $X_i$ 相关性显著的变量(Pearson 检验中r>0.6),以消除变量之间的共线性; ④对剩 余自变量和因变量进行多元逐步线性回归; ⑤将如 下自变量在模型的有效性库中剔除:在显著水平下 不满足 T 检验或模型先验假定的; ⑥重复步骤 4 和 5.使得模型收敛,并剔除对于最终模型  $R^2$  贡献率不 足1%的自变量. 第二类算法是一种前向算法 (forward algorithm),其从一元线性回归入手,依据 一定规则逐步向回归方程中添加变量[34]. 该算法 也是欧盟 ESCAPE(European Study of Cohorts to Air Pollution Effects)项目所采用的算法. 具体地:首先, 构建因变量与所有自变量之间的一元线性回归模 型,从中挑选出修正  $R^2$  最高的模型,作为起始模型; 其次,依据一定规则向起始模型中添加其他变量. 这些规则有:①增加该变量对于模型修正  $R^2$  的贡献 超过1%;②增加该变量后,模型中所有变量系数的

符号均符合先验假定; ③增加该变量后,模型中所有变量在显著水平下满足 T 检验. 最后,算法遍历所有变量,直至无法向模型中继续添加变量. 不论如何,算法都需在显著水平下满足 T 检验,且选取的变量需符合先验假定和共线性诊断,最终使得模型收敛且获得足够大的 R<sup>2</sup>. 一些学者也选取了非线性回归<sup>[35]</sup>的方法来构建模型.

#### 2.4 模型检验

检验是 LUR 模型的重要环节,包含诊断检验和精度检验.由于 LUR 模型涉及到空间数据的回归,诊断检验除了 T 检验、共线性诊断和残差的正态分布检验外,还包括了残差的空间自相关检验[36].

以往研究主要采用交叉检验(cross validation)[13]来判断精度,交叉检验可分为三类. 第一类是留一检验(leave-one-out crossvalidation) [25],即用 n-1 个样本来建立回归方程, 计算出剩余一个样本的估计值,并与该样本的实际 大气污染物浓度进行比较. 这个过程被重复n次, 剩余样本的均方根误差(RMSE)被作为描述模型好 坏程度的结果. 第二种方法是 K 折交叉验证(K-fold cross-validation)<sup>[21]</sup>,文献[37]称之为分组交叉检验 (grouped cross-validation),即将初始采样平均分割 成 K 个子样本,一个单独的子样本被保留作为验证 模型的数据,其他 K-1 个样本用来训练. 交叉验证 重复K次,每个子样本验证一次,平均K次的结果 或者使用其它结合方式,最终得到一个单一估测. 其中,在 K 折交叉验证中,十折是最常用的[38]. 第3 种方法是 Holdout Validation [39], 随机从最初的样本 中选出部分,形成交叉验证数据,而剩余的样本被作 为训练数据. 一般来说,少于原样本 1/3 的数据被 选做验证数据. 3 种方法各有优缺点,运用最为广 泛的是留一检验. 留一检验避免了样本分割方式的 困扰,得到的结果是唯一的,但其工作量较大,Wang 等[40] 也指出了留一检验有可能会高估 LUR 模型的 预测能力. K 折交叉验证工作量较小,适合于样本 数量很大的研究,但其结果会受到样本分割方式的 影响[13]. 为了达到较好的检验效果,有些研究结合 了两种检验方法对 LUR 模型的精度进行验 证<sup>[30, 37]</sup>.

#### 2.5 回归映射

得到 LUR 模型后,利用回归方程对非监测点进行空间模拟,此过程称为回归映射(regression mapping)<sup>[10]</sup>,其精度取决于变量的最低空间分辨率.根据回归方程估计的污染物浓度通常存在异常

值,已有研究通常根据监测浓度的最大值和最小值限制浓度的范围<sup>[29,37]</sup>.

#### 3 模型结果

文献中,LUR 模型的修正  $R^2$  均值为 67.5%. 影响修正  $R^2$  的因素很多,Basagaña 等 $[^{23}]$  指出,监测站点和自变量个数均会对结果产生影响,而过少的监测样本和过多的模型变量则会导致  $R^2$  的虚高,Dons等 $[^{27}]$ 选取不同的变量估计黑碳浓度的时空分异,得到的修正  $R^2$  差别很大. Wu 等 $[^{29}]$ 则指出过大的污染物监测浓度的空间分异则会降低结果的修正  $R^2$ .

LUR 模型对于结果中所包含的解释变量个数并没有严格的规定,就整理的案例研究而言,通常包含3~5个变量. 就解释变量的类别而言,与交通排放有关的变量是模型中最常见的<sup>[41]</sup>,其次是土地利用、气象因素等. 污染物的种类不仅直接影响解释变量的类别,而且会关系到变量缓冲区的大小. Henderson等<sup>[12]</sup>指出,一次污染物 NO 对小缓冲区交通变量的响应比二次污染物 NO,更为强烈.

#### 4 模型应用

LUR 模型从 1997 年出现至今,已经应用于多种大气污染物,包括氮氧化物(NO、NO<sub>2</sub> 和 NO<sub>x</sub>)、颗粒物(PM<sub>10</sub>)、细颗粒物(PM<sub>2.5</sub>)、超细颗粒物(UFP)、二氧化硫(SO<sub>2</sub>)、黑碳(BC)、臭氧(O<sub>3</sub>)、挥发性有机物(VOC)等,这些研究都取得了较好的效果,且在流行病学领域中获得了广泛的应用. 如欧盟于 2008 年开展的 ESCAPE 项目<sup>[42]</sup>,比较系统地运用 LUR 模型估计了欧洲多个城市的大气污染长期人口暴露影响. 除了大气污染时空分异模拟和流行病学研究,LUR 模型还被用于城市热岛<sup>[43]</sup>、噪声污染<sup>[44,45]</sup>等领域的研究中,均体现出了巨大的潜力.

#### 5 模型展望

LUR 模型是模拟城市尺度大气污染物浓度空间分异的通用模型,其构建简便、耗费成本低、模拟精度高、且有着良好的可转移性,在欧洲和北美得到了广泛的应用. 以下就深化其研究进行简单展望.

#### 5.1 突出时空分异

虽然 LUR 模型有着很强的模拟空间分异的能力,但绝大多数的模型忽略了时间分异<sup>[27]</sup>. 近期有一些时空 LUR 模型的案例,主要通过三种方法来模

拟污染物的分异:一是根据区域背景监测站点浓度的时间变化来修正 LUR 模型的截距项<sup>[46]</sup>;二是借鉴面板数据的思想,在 LUR 模型中添加时间虚拟变量来表征不同时段<sup>[47]</sup>;三是针对不同时段利用动态变量,分别构建不同时段的模型<sup>[48]</sup>.也有研究综合了上述两种以上的途径来模拟污染物的时空分异<sup>[49,50]</sup>.构建时空 LUR 模型,可以更深入了解污染物浓度的变化规律及其影响因素,还能更精确地估计人群的污染物暴露水平,是研究的一个重要方向. **5.2** 扩展变量类别

目前解释变量常集中土地利用、交通、人口和海拔等,但由此得到的空间分异特征往往是有限的.因此,扩充变量类别,创新变量形式是当前研究的热点方向之一,这不仅能有效提高模型的解释力,而且可以突出特定因素对于污染物分布格局的影响. Tang 等[30] 将街道格局和建筑高度加入模型; Abernethy 等[16] 考虑风向的影响,这些都是对模型变量扩展的良好尝试. 在大气污染形势严峻的我国,污染源种类相对于国外更加复杂,其空间分布更为离散. 因此,利用新兴技术(3S、大数据等)获取这些排放源的分布情况对于 LUR 模型的构建有着重要的意义.

#### 5.3 改进构建方法

大多数 LUR 模型采用线性回归的方法,这有时并不能真实反映污染物浓度和解释变量之间的关系. 近年来也有研究采取了非线性回归的方法,Beckerman 等<sup>[35]</sup>和 Reyes 等<sup>[51]</sup>用贝叶斯最大熵值法对模型进行了改良;Olvera 等<sup>[52]</sup>用主成分分析法优化了模型,这些方法均对模型的解释 R<sup>2</sup> 有所贡献. 此外,还可以尝试广义加性模型、地理加权回归、人工神经网络等方法,以用于改进模型的构建方法,提升模型的解释能力.

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2015年10月21日,中国科技论文统计结果发布会在北京举行,会议公布了"百种中国杰出学术期刊" 获奖名单.《环境科学》连续14次荣获"百种中国杰出学术期刊"称号."百种中国杰出学术期刊"是根据中国科技学术期刊综合评价指标体系进行评定.该体系利用总被引频次、影响因子、基金论文比、他引总引比等多个文献计量学指标进行统计分析,对期刊分学科进行评比,其评价结果客观公正,为我国科技界公认,并具有广泛影响.

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