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Causal inference between bioavailability of heavy metals and environmental factors in a large-scale region☆

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ABSTRACT

The causation between bioavailability of heavy metals and environmental factors are generally obtained from field experiments at local scales at present, and lack sufficient evidence from large scales. However, inferring causation between bioavailability of heavy metals and environmental factors across large-scale regions is challenging. Because the conventional correlation-based approaches used for causation assessments across large-scale regions, at the expense of actual causation, can result in spurious insights. In this study, a general approach framework, Intervention calculus when the directed acyclic graph (DAG) is absent (IDA) combined with the backdoor criterion (BC), was introduced to identify causation between the bioavailability of heavy metals and the potential environmental factors across large-scale regions. We take the Pearl River Delta (PRD) in China as a case study. The causal structures and effects were identified based on the concentrations of heavy metals (Zn, As, Cu, Hg, Pb, Cr, Ni and Cd) in soil (0–20 cm depth) and vegetable (lettuce) and 40 environmental factors (soil properties, extractable heavy metals and weathering indices) in 94 samples across the PRD. Results show that the bioavailability of heavy metals (Cd, Zn, Cr, Ni and As) was causally influenced by soil properties and soil weathering factors, whereas no causal factor impacted the bioavailability of Cu, Hg and Pb. No latent factor was found between the bioavailability of heavy metals and environmental factors. The causation between the bioavailability of heavy metals and environmental factors at field experiments is consistent with that on a large scale. The IDA combined with the BC provides a powerful tool to identify causation between the bioavailability of heavy metals and environmental factors across large-scale regions. Causal inference in a large system with the dynamic changes has great implications for system-based risk management.
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1. Introduction

Heavy metals in soil originate from various anthropogenic activities, such as industry, agriculture, mining, processing of ores and transportation. They pose a serious threat to the livelihoods and health of mankind and ecosystems (Baker et al., 2014; Singh and Kalamdhad, 2011). Due to transfer of heavy metals from soil to plants, the uptake of nutrient elements in plants is affected, for instance, the uptake of silicon could be suppressed by Arsenic (Guo et al., 2007); the metabolism of plants is disturbed; growth and proliferation are retarded or curbed; and the health of animals and human beings is influenced via the food chains (Kumar et al., 1995). The toxicity of heavy metals not only depends on the total concentrations of heavy metals but most importantly, toxicity depends on the bioavailability of heavy metals (Leita et al., 1999). Assessing

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the bioavailability of heavy metals is important in evaluating human and environmental risks, and defining mitigation strategies. However, the cause-effect relationships between the bioavailability of heavy metals and environmental factors are generally obtained from field experiments at local scales at present, and lack sufficient evidence from large scales. Causal inference between bioavailability of heavy metals and environmental factors across large-scale regions is challenging because of the changing biophysical and biogeochemical in the real world. The conventional correlation-based approaches used for causation assessments across large-scale regions, at the expense of actual causation, can result in spurious insights. Thus, we need to consider new ways to identify causality between bioavailability of heavy metals and environmental factors across large-scale regions, which will enhance the discovery of true causal effects in evaluation of human and environmental risk.

Many researchers explored the cause-effect relationships between the bioavailability of heavy metals and environmental properties using randomized controlled perturbation experiments. For instance, causation between the variables can be identified by controlling environmental properties (e.g., Fe, soil organic matter (SOM) and total organic carbon (TOC) contents) in field experiments of heavy metals (Yu et al., 2016b). In many settings, however, such experiments are time consuming and often specific to a specific set of conditions or experimental treatments, and most field experiments do not combine a wide range of realistic interacting causal factors, making it difficult to extrapolate experimental to larger-scale real world. Across large-scale regions, conventional statistical approaches are commonly used to determine correlations between the bioavailability of heavy metals and environmental factors, but these conventional methods suffer from the inability to resolve causal relationships (Arshad et al., 2008; Hu et al., 2013; Khan et al., 2015). Two state-of the-art high-dimensional regression approaches (i. e., Lasso and Elastic-net) were adopted to determine the relative importance of impacting factors across large-scale regions based on correlation, but these methods were not designed for causal inference (Maathuis et al., 2010). Correlation does not imply causation. Causation is often confused with correlation, which indicates the extent to which the two factors tend to increase or decrease in parallel. There may be a third factor or a group of factors that are responsible for the fluctuations in both factors. For example, when soil properties and bioavailability of heavy metals are measured, a statistically significant negative correlation has been shown between CEC and the bioavailability of Pb (Pietrzykowski et al., 2014). This correlation does not indicate that low CEC causes the high bioavailability of Pb, but that CEC decreases while the bioavailability of Pb increases in parallel. A third factor or a group of factors, such as soil pH or clay minerals, are more likely to be responsible for this observed correlation (Harter, 1983). To identify causality from large-scale observational data, causal models serve as important tools when the possible causal relationships between the variables are known. There are two competing causal models: the Rubin Causal Model (RCM) and the Causal Diagram Model (CDM). The RCM is an approach to identify causality with high accuracy; however, this approach suffers from a major shortcoming: it is impossible to observe the causal effect on a single unit (Rubin, 2005). One must seek comparable homogeneity units, which often cannot be achieved in the regions without historical monitoring records. The RCM is also difficult to interpret. CDM enables the visualization of causal relationships between variables in a causal diagram based on nonparametric structural equations (Pearl, 1995). A newly proposed CDM method, Intervention calculus when the directed acyclic graph (DAG) is absent (IDA) combined with the backdoor criterion (BC) (Maathuis et al., 2010), provides a well-established statistical framework for causal inference. This approach has been successfully applied in genetics and bioinformatics (Taruttis et al., 2015; Zhang et al., 2014c). The IDA combined with the BC can be used to simulate an intervention process and predict the causal effects of the intervention (Pearl, 1995), and this method has enabled the cost-effective capture of causal relationship for large-scale observations (Maathuis et al., 2010). The IDA combined with the BC approach, based on mathematically justified statistics, can obtain bounds on total causal effects and identify latent variables in causal relationships under some assumptions (Maathuis et al., 2009). Hence, the IDA combined with the BC has great potential to infer causation and estimate causal effects between the bioavailability of heavy metals and environmental factors from observational data across large-scale regions.

In this study, we aim to identify causal relationships and estimate causal effects between the bioavailability of heavy metals and environmental factors in a large-scale region using the IDA combined with the BC approach. Transfer factor (TF) of metal is an index for quantifying the relative differences in bioavailability of metals to plants, indicating their mobility in the soil. TF is regarded as a function of both soil and plant properties (Kachenko and Singh, 2006a). In this study, TF was used to denote the bioavailability of metals to plants. The Pearl River Delta (PRD) in China was considered in a case study. We collected 94 pairs of soil (0–20 cm depth) and vegetable (lettuce) samples from agricultural land across the PRD. The concentrations of heavy metals (Zn, As, Cu, Hg, Pb, Cr, Ni and Cd) in the soil and lettuce, the biogeochemical factors and soil weathering indices were measured in 94 samples. Lettuce was chosen because it is one of the most common leafy vegetables grown and consumed in the PRD (Zhang et al., 2014a). The estimated bioavailability of the heavy metals across large-scale regions plays a critical role in developing regulatory strategies and managing regional risk.

2. Materials and methods

2.1. Study site

The PRD is located in the southern region of Guangdong province in south China, and homes a population of 42 million and comprises a total area of 25,000 km^2. It includes nine cities (Guangzhou (GZ), Shenzhen (SZ), Zhuhai (ZH), Foshan (FS), Jiangmen (JM), Dongguan (DG), Zhongshan (ZS)), Huizhou (HZ) and Zhaoqing (ZQ)). Dominated by a humid subtropical climate, the average annual air temperature in the PRD ranges from 14.65 to 22.22 °C and the average annual precipitation ranges from 1566 to 2133 mm (Statistics Bureau of Guangdong Province, 2011). The main soil types are Udic Ferralsols, Stagnic Anthrosols, and Orthic Halosols (IUSS Working Group WRB, 2006). In the past three decades, the PRD has experienced a rapid transition from an intensively cultivated region to one of the world's largest manufacturing bases and one of the world's most densely urbanized regions (Jinmei and Xueping, 2015). Lettuce is one of the most common leafy vegetables grown and consumed in the PRD. Lettuce accumulates metals at relatively high internal level due to its high root uptake efficiency and subsequent translocation from the roots to the tissues above ground (Malandrino et al., 2011; Peijnenburg et al., 2000).

2.2. Data sources

A total of 94 pairs of soil (0–20 cm depth) and lettuce samples (leaf) were collected from agricultural land across the PRD in 2011 (Fig. 1). We used the same data published in Chang Chunying's doctoral thesis (Chang, 2014). Samples were sealed in polyethylene

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