Form and Function in Spatial Interaction: A New Approach to Spatial Structure

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Summary

Gravity Spatial Interaction Models have been used consistently to model migration, commuting, and trade. However, classic gravity models were developed and have mainly been used to predict among networks where origins can serve as destinations, and vice versa. Without this *unipartite* structure, gravity model performance is not as clear. Additionally, spatial interaction models are usually assessed using their predictive performance alone, which does not allow evaluate how well the models capture the overall *pattern* of flows. Both of these problems result from one common source: the concept of "spatial structure" is still not clearly or consistently conceptualized or used appropriately in models. In this work, we explore the concept of spatial structure and analyze its representation in current modelling frameworks. We then explore the potential of a graph structure measure, Page Rank, to provide a general measure of spatial structure. We examine Page Rank by comparing how classical spatial interaction model accessibility terms and Page Rank respond to changes in the interaction network with unipartite and bipartite structure. Lastly, we compare models built with these measures using standard predictive performance methods, as well as comparing their fidelity to the overall spatial structure of observed networks. We find that Page Rank is sensitive to network structure in both unipartite and bipartite graphs, and it accounts for changes in structure in both a local and a global sense. We also find that Page Rank improves upon classic measures of accessibility in spatial interaction modelling, since it does not depend on unipartite structure and it yields better estimates in terms of both predictive performance and pattern replication. Overall, this work encourages us to think more critically about measures of spatial structure in spatial interaction models and widen our ideas of what constitutes "good performance" from a spatial interaction model.

KEYWORDS: spatial interaction, spatial structure, urban flow, origin-destination, network structure.

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1 Introduction

Spatial Interaction models (SIMs) are a body of methods used for analysis and prediction of Spatial Interactions, which is a broad term encompassing any movement over space that results from a human process (Heynes and Fotheringham, 1984; Wilson, 1971). They have been extensively used social sciences (Fischer and Reggiani, 2004), economics (Batten and Boyce, 1987), and medicine (Barrios et al., 2012). With new data sources, there are new applications (Zhang et al., 2019; Cao et al., 2020), theories created (Simini et al., 2012) and new discussions convened (Hilton et al., 2020) about the long-standing "Gravity" family of SIMs.

However, there remain unresolved problems at the foundation of spatial interaction modelling. The most prominent debate in SIM literature is about spatial structure, which regards how spatial structure is represented in SIMs (Griffith, 2007). This debate has been around since 1970s Curry (1972) and remains active today. The spatial structure debate is comprehensively discussed by (Oshan, 2020), who highlights the need to (1) integrate appropriate measures of spatial structure into SIMs and to (2) shift our focus towards modelling the human behaviour element of spatial interaction. Going further, we believe that what *exactly* is meant by "spatial structure" and how it relates to the human behaviour remains vague and under-theorized. This has had a significant impact on our understanding of spatial structure and subsequently SIMs. Moreover, this vagueness limits our progress towards more appropriate methods.

Fortunately, network science can provide useful ways to formally define spatial structure. It provides advanced tools for investigation, measurement, and evaluation of spatial interaction networks.

In this paper, we provide a more explicit definition of what "spatial structure" means in terms of networks and their structures, and investigate the spatial structure of networks that are distinctly different from each other in terms of their geographical scale, aggregation level and their structural properties. We examine the potential of graph theory, specifically graph structure measures, to provide a more flexible representation of spatial structure. To do this, we first elaborate on the spatial structure debate and define "spatial structure" in spatial interaction using concepts from network science. Second, we compare this new definition with a common measure of "structure" developed in spatial interaction research. Specifically, we compare the sensitivity of Page Rank (**?**) with the "Accessibility" term from a Competing Destination model (Fotheringham, 1983) to network changes for different spatial interaction topologies. Lastly, we compare the predictive accuracy and spatial pattern accuracy of models built with traditional approaches or with Machine Learning techniques (XGBoost).

We apply this framework to two structurally different interaction networks; a unipartite one, and a bipartite one. We also broaden our definition of "performance", considering both predictive accuracy in terms of individual flows as well as properties of the entire predicted spatial interaction graph. Through this example, we hope to push spatial interaction modelling in a new direction: towards more explicit ideas about spatial structure and in both model design and model validation.

We show that comparing the spatial patterns of spatial interaction should be an essential step in evaluating model performance, as traditional goodness-of-fit measures are insensitive to global and local spatial patterns. We also provide an overview of the effectiveness of spatial interaction models for topologically different networks, which is both novel and should be part of any spatial interaction study. It is important to note: we are not trying to show that network science tools are the most effective way to incorporate spatial structure in SIM, but that different spatial interactions with different properties require new, more appropriate approaches for representing and validating spatial structure.

We proceed as follows. Section two expands the typical spatial interaction frame of analysis in two ways: (1) models are applied to two very different interactions topologies, and (2) are compared with richer ideas about what "accuracy" means. Section three then clarifies the unclear definition of the concept of spatial structure and model construction. It investigates what spatial structure is from both geographical and network science perspectives, how models incorporate it in both fields, and where human behavioural sits within the frameworks. We then give a brief guide for model construction. Section four provides a description of methods for (1) investigation of Page Rank potential as a interaction structure measure, (2) comparison of Page Rank with accessibility from Competing Destination model, and (3) model building and models performance evaluation. Section five then interprets the results, and section six discusses them in the wider context of spatial interaction and network science, and concludes.

2 Two core concerns of spatial interaction models application

Spatial interaction, spatial networks, and spatial structure have very long histories in geography (Haggett and Chorley, 1969; Haggett et al., 1977). In fact, geographers have long developed network structure measures specifically to quantify the structural properties of interactions and compare them to each other. Recent work has begun to incorporate methods from graph theory and network science for the geographical analysis of flows (Batty, 2003; Zhong et al., 2014a; Batty, 2017, 2018). Furthermore, quite a few studies use graph theory as a feature engineering tool to inform spatial interaction model selection (Hoang et al., 2016; Chai et al., 2018; Yang et al., 2020b; Yao et al., 2020), and more use graphs to describe the structure of spatial interaction (Austwick et al., 2013; Zhong et al., 2014b; Tranos et al., 2015; Batty, 2017; Yang et al., 2020b). Thus, we see a renaissance occurring at the cutting edge of spatial interaction modelling, informed by network science.

However, two major limitations of this new wave of spatial interaction research are that (1) it considers a narrow range of typical structures of networks of interaction and (2) it adopts very simple prediction-oriented tests for model validation.

2.1 Building models on "standard" networks

A vast majority of the methodological papers developing SIMs analyse spatial interaction systems that are very similar in their nature and structure. For example Fotheringham (1983) considers movements across the US, Griffith and Jones (1980) looks at movements across Canada, and Griffith (2007) at Germany. LeSage and Llano (2013) test the models on goods distribution data across Spain and Wei et al. (2016) uses good distribution data across China. Here all origins are also destinations, as in *unipartite* graph, and the graphs are fully connected. Despite this fundamental similarity, the fact that the same model specification can be used to make predictions across trade, travel, migration and beyond should be seen as a significant success.

Nevertheless, in each of these cases, the spatial interaction network has "origins" that can also serve as "destinations" in the process. Although these are all real-world networks, not all real-world networks have these properties. In fact, many do not. The spatial structure of an interaction network can change drastically depending on geographical scale, the properties of interacting places, or properties of the actors in spatial interaction network. Moreover, given the actors are humans, there are several types of randomness that can affect our analysis of the system (García-Callejas et al., 2018).

The hunt for generality in the SIM literature suggests that not only we try to build models for 'all scales', 'all people' and 'all interactions', we also seek models for 'all networks', which is a known issue to geographers (Jones, 2010). For example, we find only one study concerning *bipartite* networks (Peña and Rochat, 2012), which are spatial interaction systems where origins cannot act as destinations and vice versa. This is despite the common occurrence of bipartite interaction networks in biology and medicine Pavlopoulos et al. (2018), epidemiology Ergun (2002), and in geography Neal et al. (2020). In order to fully understand the generality of SIMs, it is necessary to understand how they work for interaction networks with fundamentally different structures. This is not just important for the validity of our methods: it can also open up new opportunities for the knowledge and expertise of spatial interaction modelers to contribute to the wider scientific community.

2.2 Validation of complex model outputs

In addition to this concern about graph structure, the ability of SIMs to reproduce *spatial patterns* of interaction is similarly poorly studied. Most work defines very simple "goodness-of-fit" measures using traditional predictive measures such as R-squared, root mean square error or other measures more specific to spatial interaction such as the Common Part of Commuters (Robinson and Dilkina, 2017). These measures evaluate the models' outputs in terms of their predictive performance for each flow in isolation, *without* any indication of spatial context or relationship between that flows. In other words, when we evaluate how well a model predicts individual flows, we still do not know how well the model reproduces the overall pattern of flows. This can result in misinterpretation of model performance. For example, two models may have comparable predictive accuracy, but one may miss-characterize the system of interaction overall by, for example, systematically over-predicting in-flows to hub nodes. Current model comparison and validation methods can not account for this.

We can find studies concerning similar issue in different fields. For example Chérel et al. establishes a Pattern Space Exploration (PSE) method for comparing spatial patterns of simulation from models of urban movement. Indeed, concern with the correspondence between predicted and observed (or two observed) *patterns* is long-standing (Tobler; Cliff, 1970), but has not been generally applied in spatial interaction modelling [1].

3 Concepts and constructs in spatial interaction modelling and network science

Network science is an important aligned field of study for geographers. However, geographers have their own definitions, naming conventions and strategies for constructing models and incorporating spatial structure in their models.

[1] Long and Robertson (2017) provides a comprehensive overview on existing research on spatial pattern comparison.

[2] Ducruet and Beauguitte (2014) summarizes the differences between geographers and network scientists and discusses the reasons why geographers paid rather limited attention to complex networks research in the past.

[2].

In this section, we elaborate on how this divide affects the concept of 'spatial structure' in spatial interaction. First, we explore how networks are studied in both fields. Second, we closely investigate the concept of spatial structure and its role in representing these concepts. Third, we conclude by combining this information into one conceptual framework which can build more useful spatial interaction models.

3.1 Studying complex networks and their dimensions

Although 'networks' exist in both geography and network science, there is a major difference in how they are studied. First, network scientists study networks as objects, often investigating their static structural properties, or focusing on how the connections evolve dynamically. Geographers, on the other hand, focus on the social processes that generate the network or the specific drivers of specific movement choices through the network. This affects the methods applied in the research in each of those disciplines.

Second, network science analyses networks of any shape, size or structure. This means that methods in network science are tested on a wide variety of networks. There are simple networks (those with a single kind of weight on edges), spatial networks (those with edges that represent spatial relationships) and even multilayered networks (those with many differently-weighted parallel edges). An example of network with one type of edge is the network of journal article citations, where the edge represents a citation to another article. Spatial networks in network science are specifically those networks that include spatial relationships between nodes in one layer, and then also contain some information about the functional relationship between nodes in another layer (Barthelemy, 2011) . For example, in human migration networks, we consider the volume of the people migrating between places and the space between them (usually represented by distance). Multilayered networks could also model human migration, if we think of distance as one kind of weight on the edge, and different demographic flows (e.g. children and adults, or split by gender) provide the other weights on the edge. [3] Geographers don't often use this "multigraph" terminology, but their interest is usually spatial or multilayered networks: all geographical processes happen in some space (geographical or geometrical). Thus, geographical networks usually have at least two weights on edges, one weighted by distance, and the other weighted by the strengths of the interaction itself.

Thinking about *complex networks* in this manner can help provide clarity about the structure of a given process. For example, Bullmore and Sporns (2009) divides the network system of brain function into *structural* and *functional* systems. The *structural* layer represents the "locational" network of brain, and uses distances as the edge weights, so that spatially "close" regions of the brain are near one another in the structural brain network. In contrast, the *functional* layer uses neural connections that work together to facilitate different brain functions as the edge weights. Thus, *functionally* close regions of the brain are those that activate together. This makes it clear that the brain network has both a "locational" and "functional" layer, each with their own structures. This kind of abstraction and improved conceptualization can also make sense of networks in geography.

[3]Kivela et al. (2014) provides a comprehensive discussion on the components and models of multi-layered networks in network science.

3.2 What is a spatial structure?

This distinction between location and function made by Bullmore and Sporns (2009) maps easily onto networks of human interaction. Each link in a spatial interaction network always has a locational weight (often distance) and a functional weight (the interaction). This is reminiscent of some of the earliest thinking about spatial interaction models, and the original distinction between a form and function of geographical phenomena (Goethe, 1817). In the early geographical literature, we can find descriptions of spatial structure focused on notions of "gravity" in SIMs (Griffith and Jones, 1980). Later, work exposing the interconnection between the relative and the absolute arrangement of spatially-interacting places uses the term *geographical location* to describe spatial structure more generally (Bennett and Haining, 1985; Lo, 1991). Indeed, Bennett and Haining (1985) divided spatial interaction models into (a) *Models of spatial structure*, that are concerned with the locational properties of the interaction network, (b) *Models of spatial interaction*, that look at the function generated by the actors, and (c) *Models of structure-interaction*, that combine both of these aspects. Building on this division, a contemporary definition from (Oshan, 2020):

> Spatial structure characterizes the organization, distribution, or relative arrangement of entities embedded within a spatial system

tells us that spatial structure and interaction structure combine to represent all the possible elements, effects and relations existing in the spatial interaction network.

Further, the definition of spatial network structure from network science perspective is very similar to the one above. It is generally described as the combination of locational aspects of the network and functional aspects of the network (Gastner and Newman, 2006; Barthelemy, 2011). We then can separately define the locational aspects as those belonging to some geographical embedding (Barthelemy, 2011), and the topological aspects as the description of the network arrangement based on the functional relationship between the network entities (Barabási, 2016). Thus, topology is a broader term that consists of one or more functional relationships such as weigted edges, their directions, network sparsity, bipartity or connectedness.

Current spatial interaction literature does not describe interaction networks and their elements as done in network science, and has largely focused on using locational weights to predict functional weights. However, the two are deeply intertwined, as the definitions of spatial structure from both Bennett and Haining (1985) and Oshan (2020) suggest. The assumption that locational structure unambiguously governs functional structure indicates this confusion about the concept of spatial structure: since "interaction" is not thought of separately from "structure" in geography, spatial interaction function is mainly form plus error. However, with a better conceptual definition of spatial structure (Figure 1) we can not only think more critically about building SIMs, but also develop a richer notion of 'validity' for SIMs.

3.3 Building better models

The previous section suggests that spatial structure in spatial interaction has two major components, the functional part and the locational part. Admittedly, this is not an entirely new thought to geographers. While debate around the proper specification of locational structure is well documented (Oshan, 2020), the functional part of the network has not received the same critical attention. Nevertheless, there is a work that discusses the missing functional element as

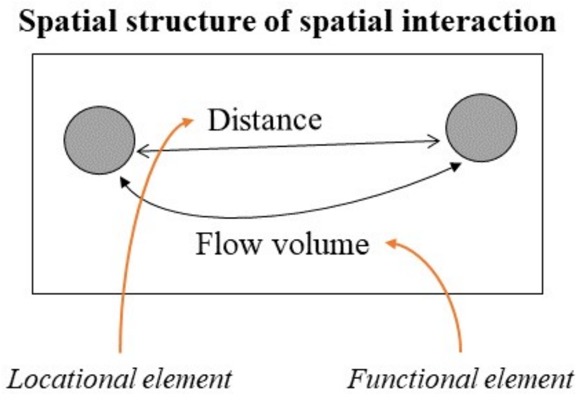

Figure 1: The spatial structure of a network can be also defined as the combination of locational and functional structure. We then talk about spatial structure when we study network locational and functional space together as a spatial network/interaction network.

a behavioural aspect of SIMs, and even develops methods to account for it. For example, Smith (1975) introduced probability theory describing the small random influences on people's choices of destination that should be incorporated within spatial interaction framework. Further, Fotheringham (1983) introduced an *Accessibility* term that weights destinations according to how accessible they are to a certain origin. Justifying this choice, Fotheringham (1986) argues that people make a hierarchical set of decisions about the destinations: people first consider clusters of destinations and second individual destinations within that cluster. This agrees with studies that discuss the gender difference of decision-making in spatial interaction (Stillwell, 1978; Hanson and Pratt, 1995), the importance of cognitive space (Cadwallader, 1975), and even the socio-economic factors for movement (Hanson and Hanson, 1981; Golledge and Stimson, 1996). Thus, our understanding of the decision-making process underlying the functional structure of spatial interaction is fairly sophisticated.

All of these models aim to represent some behavioural elements of interaction but consider only a few known properties of the interacting elements, such as their age, gender, status or the locational connection of places or people. Only one, Fotheringham (1983), considers function in a way; it considers a binary output of if flow is even possible between two places. However, flow volume represents a kind of revealed preference which directly informs us about peoples' behaviour, and should be used for effective prediction. Thus, current work focuses well on what generates flows, but often does not examine what flows themselves can show us about the decisions people may make.

Thus, we focus on Fotheringham (1983)'s "Competing Destinations" (CD) model, which uses a behavioural argument to justify the use of observed flows to represent accessibility. In this model, *accessibility* represents the ease with which a destination is reachable from one or many origins. In subsequent work, it has also been defined as the potential of opportunities for interaction (Bruinsma and Rietveld, 1998; Long, 2017). It is measured by the interaction of two main variables; distance and destination choice, which are heavily dependent on selection of origins and destinations, demarcation of the area under research, choice of infrastructure and the process of interaction initiation (Bruinsma and Rietveld, 1998). In terms of its specification, the "Competing Destinations" model is a standard gravity model (as we will discuss in next section) with an additional term representing the accessibility of each destination to an origin. As such it is a measure that mixes functional structure of the flow network with the locational structure of the distances between origins and destinations.

Improving on this, we see the potential for graph structure measures to capture the functional structure of interaction network directly. Using graph structure information to enhance the flow prediction is not very common practice, in fact we find only one example of this application. Yang et al. (2020b) uses degree centrality, betweenness centrality and Page Rank to enhance models of bike-sharing flow. From those, the first simply counts the number of links into and out of the nodes and the second measures how many paths across the network lead to each node. Page Rank, however, is much more conceptually related to Fotheringham's notion of accessibility, given that it measures the importance of the nodes based on the number of links connected to it, the number of links connected to its neighbours as well as the volumes of all those links. In order to investigate the potential of Page Rank to represent functional structure of information, we incorporate Page Rank into a spatial interaction model and compare it to the typical gravity model and a CD specification.

4 Exploring locational and functional structure in spatial interaction

To explore this new measure of the functional structure of spatial interaction networks, we have two empirical exhibits shown in Figure 2. First, we illustrate how Page Rank measures the structure of the spatial interaction network in quite a different fashion than the CD accessibility term (Figure 2: Left). We do this by examining changes to Page Rank/accessibility for controlled changes in network structure. Second, we compare the predictive and pattern performance of models with no measure of structure, with CD accessibility, and with Page Rank. We define three SIMs (4.3) using two estimators (GLM and XGBoost) and compare those models using traditional predictive performance measures as well as comparison between the overall *pattern* of flows in the predicted and observed networks. (Figure 2: Right).

4.1 Data

In order to demonstrate the importance of data variety and showcase the difference in models performance for different types of networks, we used two different real-world spatial interaction network. First, we consider migration flows in England and Wales, which is an aggregated interaction that can be represented as a unipartite graphs. Second, we use prescription fulfillment data in the southwest of England. This is individual (or household-level) interaction between patients (at doctors offices) and pharmacies (where prescriptions are filled), yielding a bipartite graph (Fig. 4) [4].

4.2 Investigating the response to change

To investigate how CD and Page Rank measure spatial structure, we show how each measure responds to changes in network (Figure 2: Left). Conceptually, there are 5 types of changes that can happen in interaction network.

1. A node can change its mass. For example, a city could increase its mass if many chil-

[4] Detailed information on the data and replication information can be found in appendix (8.1)

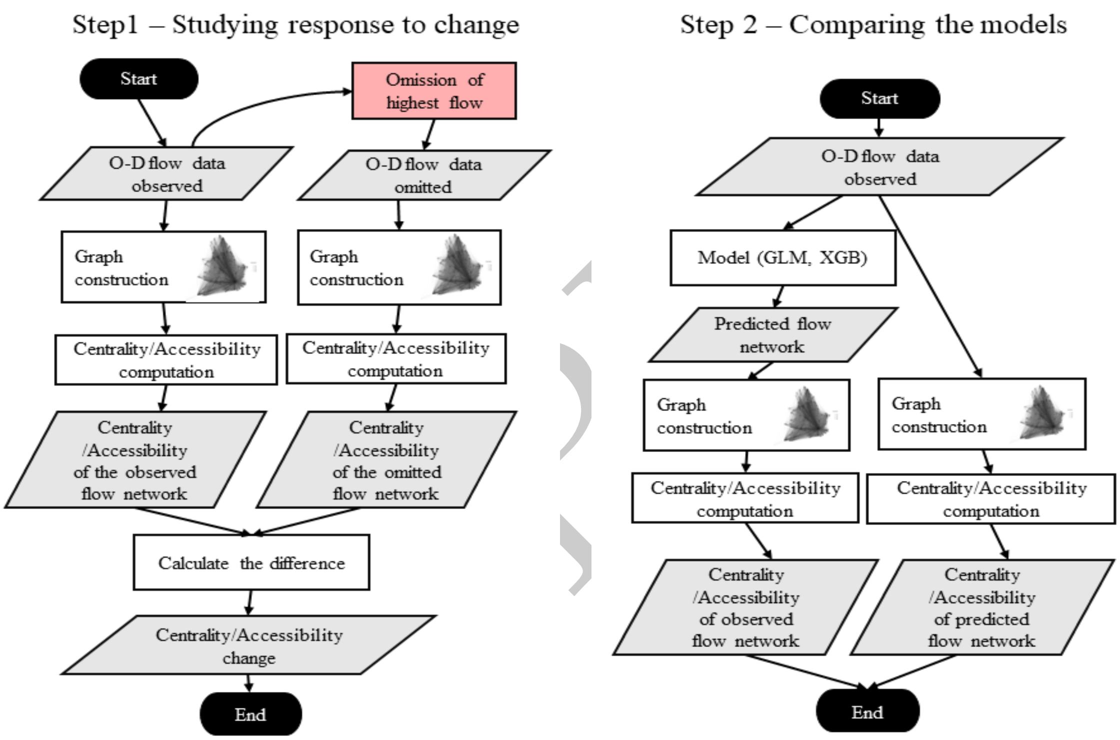

Figure 2: Flow diagram of the two exhibits in this paper.

dren are born in the city.

2. A node can change its position. This could happen if a pharmacy relocates to a different building.

3. A node can be added or removed. For example, a pharmacy can close down or open.

4. An edge can change its weight. Here, migration rates to a city could increase or decrease.

5. An edge can be removed, such as if a country closes its borders to another country.

However, not all of these are possible for the networks used in this study. Local authorities cannot simply change their positions or be taken off the map. Similarly, pharmacies and general practitioners hardly change a positions, yet they can close their premisses or open a new ones. Thus, to illustrate spatial structure measures, we modify the network to induce changes 1,4 and 5, exemplified in Figure 3:

1. Halve the mass the biggest node

4. Halve the volume of the highest flow edge

5. Remove the highest flow edge

For each data and each change scenario we then estimate centrality and CD accessibility for each changed graph, and compare it to the values from the original, unmodified graph.

In this study, we use the Page Rank and CD accessibility terms to measure structure. Starting with Page Rank, designed **?** to rank webpages in a search engine, the iterative algorithm (Formula 1) assigns proportions of importance to each node depending on how well it is connected to its neighbours and rest of the nodes

$$PR_i = \frac{1-d}{N} d \sum_i \frac{PR(k)}{NumLinks(k)} \tag{1}$$

In this formula, d is the damping factor, N is the total number of nodes in the network, k ranges over all pages that link to page i, and $NumLinks(k)$ is the number of links present on every possible node k linked to node i. Page Rank can be easily applied in open source software for both Unipartite (NetworkX package (Hagberg et al., 2008)) an Bipartite networks (Birankpy package (Yang et al., 2020a)).

In contrast, the accessibility term from a CD model is defined using the flow and distance between destinations. Let our origin i be connected to a destination j. Then, the flow from i to j is denoted F_{ij}, and the distance separating i and j is d_{ij}. And, let the "mass" of location i (often understood to be the total population) be denoted m_i. Then, the CD accessibility of destination j to origin i is:

$$A_{ij} = \sum_{\substack{k=1 \\ (k \neq i,j)}}^{n} m_k d_{jk} \tag{2}$$

Where A_{ij} is the destination accessibility, defined as the sum of the mass m, at each destination k weighted by the distance d to each destination.[5] We then calculate the difference between the Page Rank and CD accessibility for the observed and modified network.

4.3 Models

After illustrating how these measures of accessibility work, we also include them into *models of* spatial interaction. Thus, we define three spatial interaction models here. The first is the

[5]In the CD model, there is an additional estimated parameter, σ, that that measures the importance of distance in determining the perception of the accessibility. But, for our illustration here, we set $\sigma = 1$ arbitrarily. We acknowledge that changing σ will change the magnitude of accessibility. However, as we will discuss, we are use *changes to the network* in order to illustrate the sensitivity of the two measures. Thus, as long as σ stays constant for the set of changes considered, its exact value is neutral.

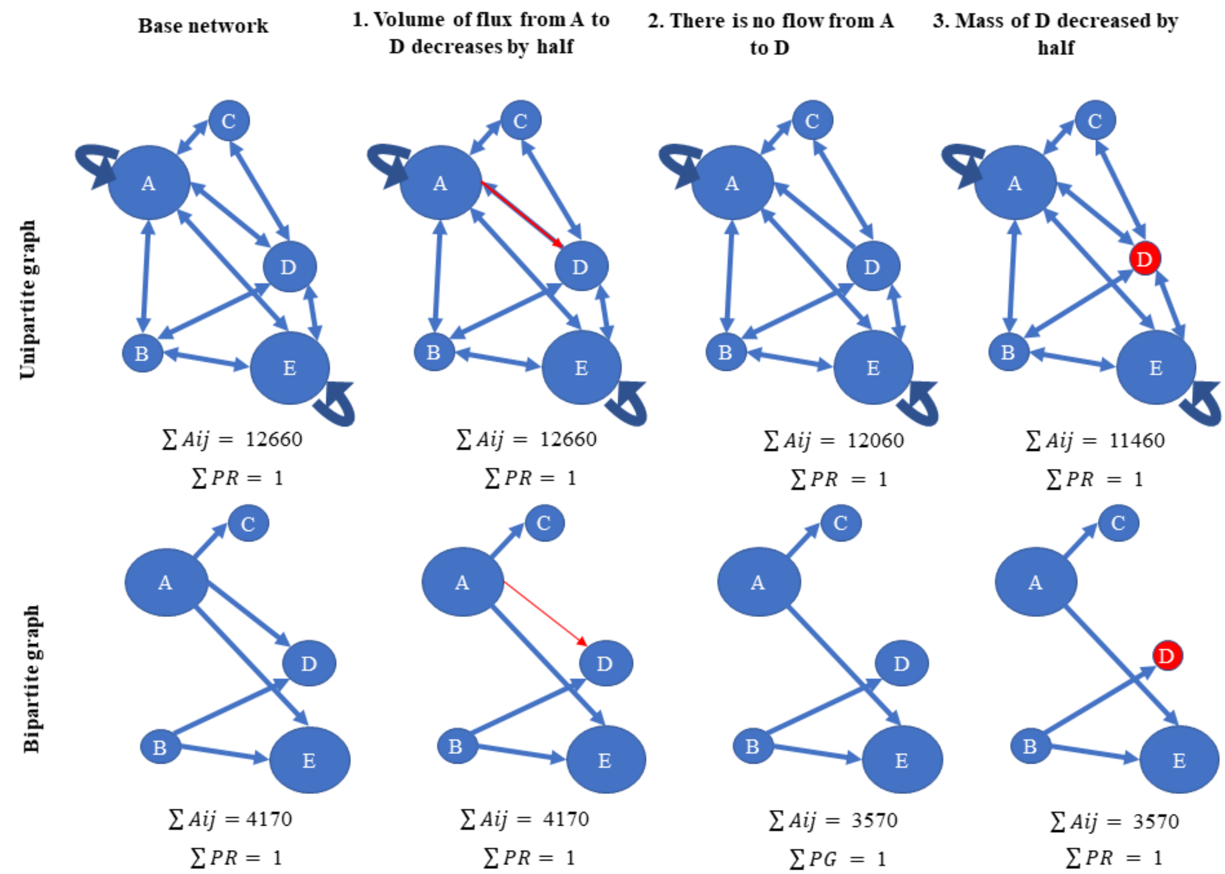

Figure 3: By investigating three simple scenarios, we can observe how both, CD accessibility and Page Rank, changes in the network. This figure is only a visual example of the scenarios.

Unconstrained Spatial Interaction Model Equation 3, also known as the standard "Gravity model:"

$$F_{ij} = km_i^{\phi} m_j^{\alpha} f(d_{ij}, \beta) \tag{3}$$

This is our baseline model. Here, F_{ij} is the total flow between origin i and j, ϕ is the estimated "productiveness" of origins, α is the estimated "attractiveness" of destination j, and a friction parameter β, and k is a constant. For this paper, we seek to keep the model simple by using a negative exponential distance decay function, $f(d_{ij}, \beta) = e^{d_{ij}/\beta}$ using the great circle distance between locations.

Our second model is the Unconstrained Competing Destination Model Equation 4 (CD-SIM):

$$F_{ij} = km_i^{\phi} m_j^{\alpha} f(d_{ij}, \beta) A_{ij}^{\delta} \tag{4}$$

where now A_{ij} is used as an additional predictor, with δ as the "strength" of accessibility. The third model incorporates Page Rank as an additional term into first model (5) intending to

Figure 4: Both interactions, prescription flow and migration flow, can be translated into a graph theory as an bipartite and unipartite graph.

capture functional structure:

$$F_{ij} = km_i^{\phi} m_j^{\alpha} f(d_{ij}, \beta) PR_i^{\kappa^1} PR_j^{\kappa^2} \tag{5}$$

Where PR_i and PR_j represents the Page Rank of origins (i) and destinations (j) and its parameters κ^1 and κ^2.

Throughout, we use a log-normal version of to model the migration network and Poisson one to model the prescriptions. This is because the dependent variable in prescription flows is a count of prescriptions (integer), while in the migration data, the movement factor is a factor (decimal number). Furthermore we consider two different estimators: **General Linear regression** and **Extreme Gradient Boosting regression** (XGBoost). We adopted XGBoost because it is a powerful machine learning technique with past success in modelling interactions (Robinson and Dilkina, 2017; Yang et al., 2020b).

4.4 Variables

While both of the flow networks define human interaction, each of them has a unique representation. So, our control variables are different in the two examples. By the definition, the masses of the baseline gravity model are expected to be volumes of the same property that creates the flow between the places. In both of our cases, this is a population volume at each place. If it was not possible to retrieve the number of people related to the place, we looked at its immediate surrounding instead.

4.5 Model evaluation

To test the models, we opted to divide the data temporally, using data from 2017 as a training (in sample) data set and 2018 as a testing (out of sample) data set. This 'hold-out' re-sampling strategy is often used in forecasting problems. To evaluate the predictive performance of the models, we used four measures commonly used across the literature. We compare the ground truth flow volume values F_{ij} with the predicted flow volume values $\hat{F}_{ij}$ using two generic statistical methods (R-squared, Root mean squared error) and two methods specific to interaction models evaluation that are used in the recent literature (Sorensen Similarity Index, Common Part of Commuters (Lenormand et al., 2012, 2016; Robinson and

[6] A detailed description of each measure and exact definition can be found in appendix of this paper 8.2.

Dilkina, 2017)). [6] We then compare the spatial structure of the observed and predicted network using the correlation between the Page Rank in the observed and predicted data set.

5 Results

Here, we first explore how sensitive the two measures of structure are to network change. We then move into assessment of the models performance.

5.1 Investigating response to change

By estimating CD Accessibility and Page Rank for each of the scenarios, we can observe their sensitivity to network change. However, before considering the empirical evidence, we can identify one important difference directly from their equations. CD accessibility is a 'local' measure of *flow importance* which relies on distance between all accessible destinations to each origin. In contrast, Page Rank is a "global" measure of *node importance* which relies on connections within all nodes in the network. The first is additive, while the second is fractional.

This means that, empirically, CD accessibility is less responsive to changes in the network (5). Whilst no change is observed in accessibility when flow volume decreases by half, removing a whole edge or changing the mass on destinations changes accessibility. On the other hand, Page Rank changes for all network nodes, except when we manipulate the destination masses. More importantly, the change in Page Rank is generally bigger for the bipartite network then for the unipartite one. This is perhaps because each connection carries more weight, as there are fewer possible connections in a bipartite network. It is hard to say if the same is true for the CD accessibility as there are very few cases where we observe change.

The major difference here is in the number of nodes each measure considers and how. CD accessibility considers only those nodes, that are directly connected to nodes that experienced change (Figure 6 and 7, left). Because there is no consideration of the flow volume between the nodes, there is no notion of how strong the relations between them are. Instead, the relation is considered binary: nodes either are or are not related. On the other hand, Page Rank allocates fractions to each network node based on the strength and number of connections, as well as how many and how strong their neighbours' connections are (Figure 6 and 7, right). This means that the Page Rank of an node within a network is based not only on direct connections, but also on the rest of connections within a network.

Moreover, the more volume there is between nodes, the more Page Rank sees them as important to each other. Thus, we can observe the response to change is much higher for those nodes that are functionally related to affected nodes and for those nodes that are more important for the network in general. Due *indirectly* to distance decay, these tend to be nearer to the affected origin/destination pair. In contrast, CD accessibility explicitly accounts for distance.

From observing the response to change in CD accessibility and Page Rank, we can make two main conclusions. Firstly, Page Rank measures both local and global relationships in the network, whilst CD accessibility measures mainly the local ones. Second, by considering the number and strengths of connections in the network, Page Rank is sensitive to both direct and indirect aspects of spatial structure, whilst CD accessibility measures one very local part of spatial structure in an interaction network.

		Accessibility from Competing Destination			Page Rank				
Mean change	**Type**	**Flux volume decreases by half**	**Flux volume is zero**	**Mass of destination decreases by half**	**Flux volume decreases by half**	**Flux volume is zero**	**Mass of destination decreases by half**	**Type**	*Mean change*
Affected flux	Unipirtite	0%	0%	0%	1.3%	2.9%	0%	Unipirtite	**Affected nodes**
	Bipirtite	0%	0%	0%	25.5%	57.1%	0%	Bipirtite	
Other fluxes	Unipirtite	0%	18.7%	0.2%	0.01%	0.2%	0%	Unipirtite	**Other nodes**
	Bipirtite	0%	0%	0.2%	0.5%	1.1%	0%	Bipirtite	

Figure 5: Mean percentage change in accessibility and Page Rank for all nodes in tested networks. Accessibility changes only if whole flux is removed, whilst Page Rank changes in both occasions.

5.2 Modelling with Spatial Structure

Here, we use two different estimators (GLM, XGBoost) to estimate Spatial Interaction models of both real networks (Migration flows, Prescription flows) and compare their performance with and without spatial structure terms (CD accessibility, Page Rank). Here we compare the predictive performance of the models by measures traditionally used in spatial interaction literature (R^2, RMSE, SSI, CPC). We also compare the spatial structure patterns to asses the models ability to replicate the spatial structure of the observed interaction network.

Comparing the models with traditional predictive performance measures clearly shows that XGBoost is a more efficient estimator in all cases. It increases the models R^2 approximately by 15% for the unipartite network and by 47% for the bipartite network, as well as CPC score which increased by 3% points for the unipartite network and 20% for the bipartite network. The same holds when analysing the models' performance or spatial pattern. The Page Rank between observed and predicted network, R^2 increased on average by about 5% for the unipartite graph and by 52% for the bipartite graph. Nevertheless, comparing the models separately shows very different patterns. To our surprise the CD model performed either the same or worse than the baseline SIM, and in the rest of the cases, the CD model only performed marginally better. On the other hand, including Page Rank results in either the same or better accuracy for the models. The R^2 of the model with Page Rank as an additional term increased by approximately 3% for the unipartite network and by 15% for the bipartite network. Thus, Page Rank is very useful to describe the spatial structure of any spatial interaction network, especially the bipartite network.

Comparing the spatial pattern of the observed and predicted networks from each model also supports these findings. We find that the XGBoost estimator is generally better in capturing general spatial pattern than GLM in both types of network. Nevertheless, we also observe differences in which models best replicate the spatial pattern. The CD model has similar pattern replication to base line mode, which is approximately 95% for the unipartite network and 63% for the bipartite network,. The model that includes Page Rank as additional term improves the pattern replication on average by 1% to the

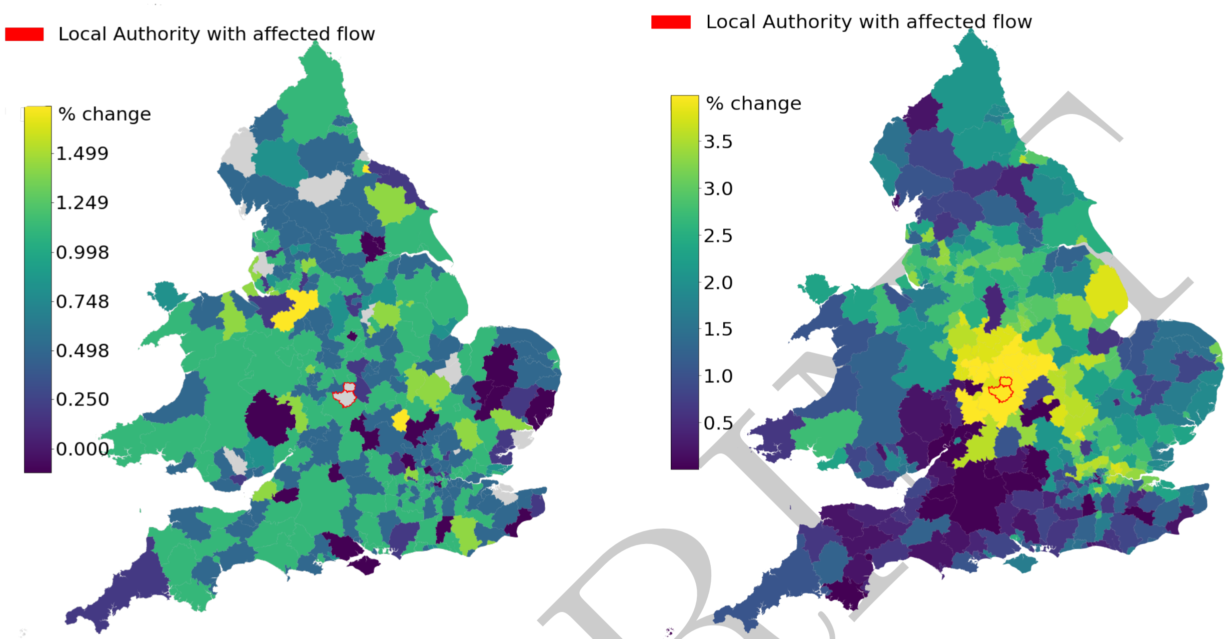

Figure 6: Left: Local Authorities, those connected to affected origin, in which Accessibility changed after flow omission, Right: Local Authorities in which Page Rank changed after flow omission. Based on Intra-migration flows

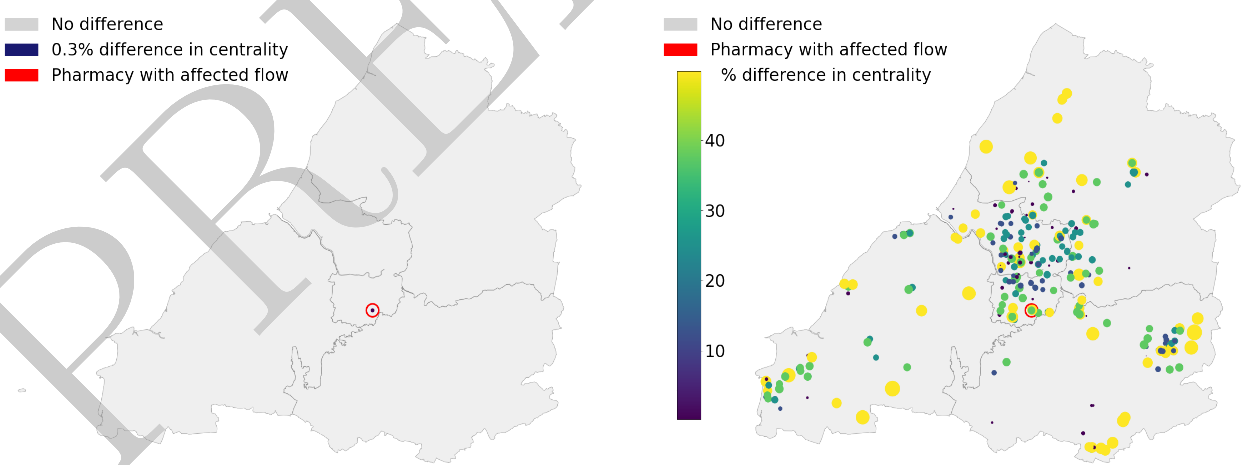

Figure 7: Left: Pharmacies in which Accessibility changed after flow omission, Right: Pharmacies in which Page Rank changed after flow omission. Based on Intra-migration flows

baseline model in the unipartite network and by approximately 10% in bipartite network. Thus, Page Rank helps models capture the spatial pattern of spatial interaction network better than traditional approaches, bipartite networks, but this depends on the topology of the interaction network, and the model estimator.

Unipirtite network - migration flow

Log-normal regression

	In sample			Out of sample		
	SIM	CD-SIM	PR-SIM	SIM	CD-SIM	PR-SIM
R2	0.14	0.15	**0.17**	0.13	0.14	**0.16**
RMSE	3.81	3.79	**3.77**	4.09	4.07	**3.73**
CPC	0.7	0.7	0.7	0.69	0.69	**0.73**
SSI	0.8	0.8	0.8	0.8	0.8	**0.82**
Page Rank Pattern R2	0.92	0.93	**0.94**	0.92	0.93	**0.94**

Log-normal XGBoost regression

	In sample			Out of sample		
	SIM	CD-SIM	PR-SIM	SIM	CD-SIM	PR-SIM
R2	0.32	0.32	0.32	**0.29**	0.28	0.28
RMSE	3.44	3.43	**3.42**	3.73	3.77	3.73
CPC	0.74	0.74	0.74	0.73	0.73	0.73
SSI	0.83	0.83	0.83	0.83	0.83	0.82
Page Rank Pattern R2	0.98	0.98	**0.99**	0.98	0.98	0.98

Figure 8: Migration models results: Comparison between baseline model (Log-normal SIM), Competing destination and SIM with a Page Rank as an additional term. The bold values represent the best values for per row.

Bipartite network - prescription flow

Poisson regression

	In sample			Out of sample		
	SIM	CD-SIM	PR-SIM	SIM	CD-SIM	PR-SIM
R2	0.32	0.32	**0.37**	0.32	0.32	**0.37**
RMSE	1003	1003	**984**	1003	1003	**984**
CPC	0.32	0.32	**0.33**	0.32	0.32	**0.33**
SSI	0.47	0.47	**0.52**	0.47	0.47	**0.52**
Page Rank Pattern R2 origin|destination	0.32|0.38	0.32|0.38	0.2|0.66	0.32|0.38	0.32|0.38	0.2|0.66

Poisson XGBoost regression

	In sample			Out of sample		
	SIM	CD-SIM	PR-SIM	SIM	CD-SIM	PR-SIM
R2	0.73	0.73	**0.97**	0.73	0.73	**0.97**
RMSE	627	627	**204**	627	626	**204**
CPC	0.51	0.51	**0.56**	0.51	0.51	**0.56**
SSI	0.74	0.74	**0.88**	0.74	0.74	**0.88**
Page Rank Pattern R2 origin|destination	0.91|0.79	0.91|0.79	**0.97|0.98**	0.91|0.79	0.91|0.79	**0.97|0.98**

Figure 9: Prescription models results: Comparison between baseline model (Poisson SIM), Competing destination and SIM with a Page Rank as an additional term. The bold values represent the best values for per row. PSE in bipartite network is estimated separately for origin and destination, hence *origin*|*destination*.

6 Discussion and Conclusion

In this paper, we re-examine an important aspect of spaital interaction networks: spatial structure. We use Page Rank to characterize the *functional* structure of spatial interaction networks with two different topologies (unipartite and bipartite structures) and compare models effectiveness in terms of both predictive accuracy and how well the overall *pattern* of flows is reproduced. By using two data sources with very different structure and at very different spatial scales, we show that model performance does depend on the measure of spatial structure, but that this is moderated by the topological structure of the network. Specifically, it is much harder to model interaction in a bipartite network than in a unipartite network. In general, it could be said that bipartite networks, where the flow structure is restricted, are more difficult to predict in terms of both individual flow and the patterns of flows. This suggest that an inclusion of prior information about the structure or network typology would be beneficial for the models performance.

Second, we tested if network structure measure such as Page Rank could provide such information to our models. And although Page Rank has a potential in this direction, our future work should explore more explicit incorporation of such important information, as well as exploration of other interaction networks with different properties to those used in this paper.

Third, we make the argument that SIMs need to be validated both on predictive accuracy and a more holistic measure of *pattern accuracy*. We show that validating a model's ability to replicate the patterns of flow can play crucial role in model comparison, especially in cases where there is a big variation in the flow distribution. It also helps us understand the structure of the flow (mis)predictions, which is usually lost with aggregate measures of goodness-of-fit. This was traditionally accounted to the varying spatial structure in the literature.

We show that Page Rank is a very useful measure of flow pattern, as it captures both local and global structures. In particular, it improves upon existing ideas of accessibility in SIMs, such as competing destination accessibility, which only measures the local structure of the interaction network. It is also more sensitive to structure in bipartite networks, which are generally understudied in the spatial interaction literature. Although we provide a practical justification of Page Rank and believe it has a potential in pattern validation methods for interaction networks, better theory would be useful in guiding the search for more this is an area of spatial interaction research yet to be explored by the scientific community. Additionally, this exercise reinforces that flow patterns are much harder to replicate for bipartite interactions and suggests that machine learning estimators are better in capturing the overall nature of the network, in addition to predicting specific flows well.

The literature suggests that the theory and the application of how we capture spatial structure in SIMs is disconnected. Spatial structure is defined very broadly without an indication of how it relates to model building or commonly used concepts of network. By reviewing past and current literature, we find inspiration from network science in neuroscience. Specifically, the spatial structure of interaction has two major components: one related to the locational relationships between interacting entities and one related to functional relationships. These describe the form and the function of the interaction, retrospectively. Thus, models of spatial interaction and its structure should include terms describing both elements. The locational element is included in all models by default as a distance, however, the functional element is often missing or is misrepresented. Spatial Interaction models need to be extended to include the *functional* properties of the network and provide its broader theoretical reasoning.

We would also like to note that we see the distinction between locational and functional element of spatial structure as moving on a scale rather than two separated properties. Some structures are predominantly locational, and the rest is the mix of both in varying proportions. We observed this in the two datasets used in this paper, where base gravity model (including only the locational element of distance) is better in capturing the structure of migration flows than the prescription flows, which suggests that the locational element of spatial structure is much more prominent in migration flows then in prescription flows. This could be a result of level of aggregation, scale, or how much is the interaction related to social, economic, or other aspects affecting human decisions. Further research could focus on investigating this process in detail and identifying its source. Overall, we argue that both better theory, measures, and validation methods are needed for spatial interaction science.

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8 Appendix

8.1 Data described

Migration flows. Migration is one of the most common types of flow data on which SIMs are used and are simply records of where individuals lived and where they moved. This paper uses the UK migration (ONS) dataset, which is published every year by the Office for National Statistics (ONS). These are based primarily on records from the NHS central patient register, since people usually change their doctor or update their information soon after moving. To provide more accurate estimates, the ONS combines the data from NHS register with two other sources: the Personal Demographic Service (PDS) and the Higher Education Statistics Agency (HESA). In the migration flows, both origin and destination locations are Local Authorities (LA).

The volume of the individuals on flow is then represented by a modeled movement factor. We have limited our study to England and Wales in order to keep the expostition simple.

Prescription flows. Prescription flows are records of prescriptions that are prescribed by a General Practitioner (GP) to a patient, who then takes the prescription and visits a pharmacy where the drug is dispensed. This flow represents a move from GP to the pharmacy. All prescription items are recorded by the National Health Service, together with the identification numbers and address of the origin (GP) and the destination (pharmacy). These records are then published each month (NHSBSA, 2020), aggregated to number of items per each pair of GP and pharmacy, and go back as far as March 2012.

The locations of all the origins and destinations were constructed by geo-locating the postcodes from the GP and pharmacy register (NHSDigital, 2020). Although the data itself, as well as the GP and pharmacy register, includes the complete addresses, those were not used for geolocation because approximately 53% of the prescription flow records have inconsistencies in the address or combination of address and the unique identification numbers. Furthermore, we limited the records for only those within an Avon area (City of Bristol, South Gloucestershire, North Somerset and Bath and North East Somerset) in order to make analysis tractable. From the original 665,000 flow records within the county of Avon, the working subset accounts for 510,000 flow records, 77% of all flows in Avon.

The number of prescribed items between each pair of origin and destination is a direct representation of the volume of patients flowing from GP to pharmacy.

8.2 Predictive performance measures

R-squared (R2) is a score measure that explains to what extent the variance of one variable explains the variance of the second variable. This score, given by formula 6, ranges from 0 to 1, where 0 represents no similarity of the observed and predicted values and 1 represents perfect fit.

$$R^2 = 1 - \frac{\sum_{i,j=1}^{n}(F_{ij} - \hat{F}_{ij})}{\sum_{i,j=1}^{n}(F_{ij} - \bar{F}_{ij})} \tag{6}$$

Where $\bar{F}_{ij}$ is the mean observed flow volume.

Root Mean Square Error (RMSE) is a standard deviation of the prediction errors (residuals) (equation 7. In other words, it measures how much error there is between the observed and predicted values. The RMSE of 0 represents perfect fit, and the higher it's arbitrary value is, the worst the prediction is.

$$RMSE = \sqrt{\frac{1}{n}\sum_{i,j=1}^{n}(F_{ij} - \hat{F}_{ij})^2} \qquad (7)$$

Sorensen Similarity Index (SSI), originally introduced by Sorensen (1948) in ecology studies, is a measure of similarity between two samples. The SSI became popular across many fields and it's modified version has been used for evaluation of flow models increasingly in past 3 decades (Lenormand et al., 2012; Masucci et al., 2013; Yan and Zhou, 2019). We have replicated the modified version of the SSI from Oshan (2016), given by 8, which has been incorporated in the SpInt Python package. The index ranges from 0 to 1, where 0 represents no similarity of the observed and predicted values and 1 represents perfect fit.

$$SSI = \frac{1}{(n)}\sum_{i,j=1}^{n}\frac{2 * \min F_{ij}, \hat{F}_{ij}}{F_{ij} + \hat{F}_{ij}} \qquad (8)$$

Common Part of Commuters (CPC) is given by equation 9, is based on the Sorensen index and is almost identical to the Bray-Curtis similarity score, also used in ecological studies (Legendre and Legendre, 2012; Robinson and Dilkina, 2017). It is the most commonly used measure for evaluation of the flow model in today's literature (Lenormand et al., 2016; Robinson and Dilkina, 2017; Yan and Zhou, 2019). This score evaluates how much of the observed flows are correctly reproduced by the model. In other words, it represents the percentage of the flows that are correctly located within the origin and destination pairs. It ranges between 0 and 1, where 0 represents no similarity and 1 represents complete fit.

$$CPC = \frac{2(\sum_{i,j=1}^{n} \min F_{ij}, \hat{F}_{ij})}{\sum_{i,j=1}^{n} F_{ij} + \sum_{i,j=1}^{n} \hat{F}_{ij}} \qquad (9)$$

It is a similarity measure based on Sorensen Index, computing which part of the commuting flows is correctly reproduced, on average, by the simulated network. It varies between 0, when no agreement is found, and 1, when to two networks are identical.

8.3 Comparing spatial pattern figures

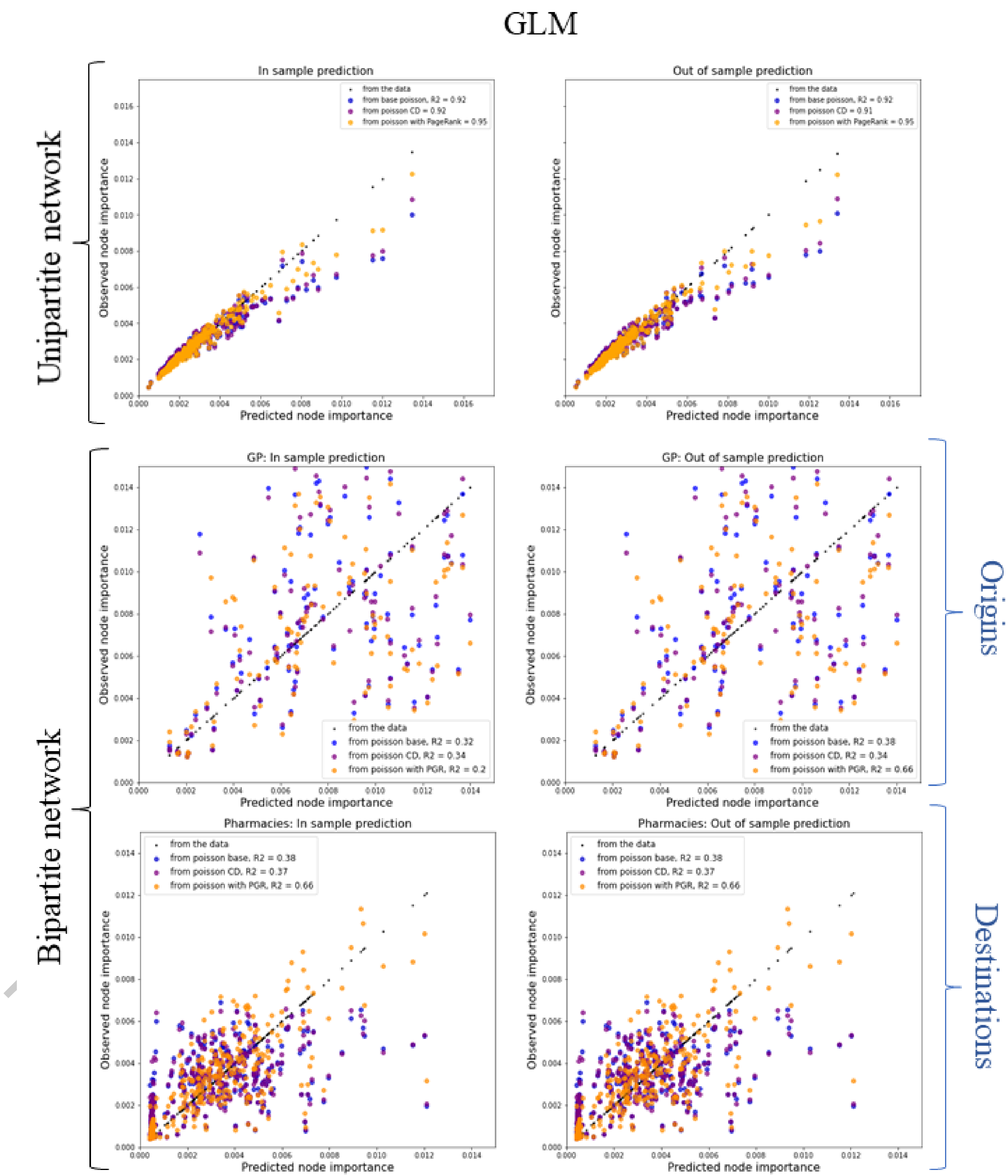

Figure 10: Pattern validation: Graphs of observed node/place importance against node importance predicted from GLM models.

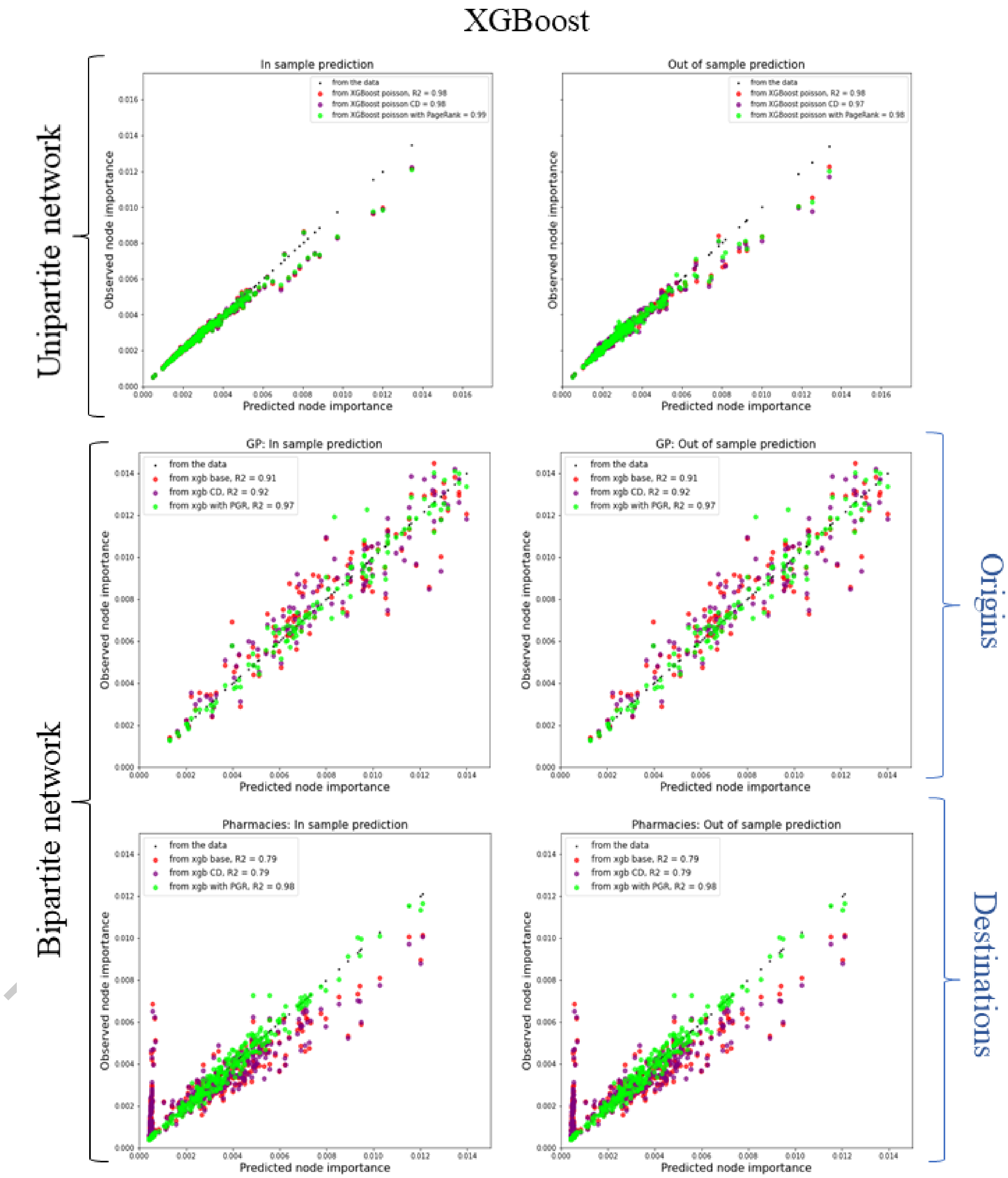

Figure 11: Pattern validation: Graphs of observed node/place importance against node importance predicted from XGBoost models.