



1 **Dynamic Complex Network Analysis of PM_{2.5} Concentrations in the UK**
2 **using Hierarchical Directed Graphs (V1.0.0)**

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25 *Abstract*

26 Worldwide exposure to fine atmospheric particles can exasperate the risk of a wide range of
27 heart and respiratory diseases, due to their ability to penetrate deep into the lungs and blood
28 streams. Epidemiological studies in Europe and elsewhere have established the evidence base
29 pointing to the important role of PM_{2.5} (fine particles with a diameter of 2.5 microns or less) in
30 causing over 4 million deaths per year. Traditional approaches to model atmospheric
31 transportation of particles suffer from high dimensionality from both transport and chemical
32 reaction processes, making multi-scale causal inference challenging. We apply alternative
33 model reduction methods – a data-driven directed graph representation to infer spatial
34 embeddedness and causal directionality. Using PM_{2.5} concentrations in 14 UK cities over a 12-
35 month period, we construct an undirected correlation and a directed Granger causality network.
36 We show for both reduced-order cases, the UK is divided into two a northern and southern
37 connected city communities, with greater spatial embedding in spring and summer. We go on
38 to infer stability to disturbances via the network trophic coherence parameter, whereby we
39 found that winter had the greatest vulnerability. As a result of our novel graph-based reduced
40 modeling, we are able to represent high-dimensional knowledge into a causal inference and
41 stability framework.

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43 Key words: complex network; atmospheric pollution; PM_{2.5}

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58 **1. Introduction:**

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60 1.1 Background and rationale

61 Atmospheric particulate matter can be attributed to both local emissions (by both stationary
62 and mobile sources) and regional transport processes. Causal inference between primary
63 (emitted directly by the emission sources) and secondary (produced in the atmosphere by the
64 transformation of gaseous pollutants) is challenging. For example, whilst combustion sources
65 such as road traffic account for the bulk of anthropogenic PM emissions and cause PM_{2.5}
66 formation (Munir, 2017; AQEG, 2012), meteorological conditions can also influence PM_{2.5}
67 concentrations through dispersion, and deposition. Due to the high data complexity and
68 dimensionality caused by the contribution of atmospheric chemistry transport processes and a
69 range of emission sources in ambient PM_{2.5} concentrations, we need to overcome the high
70 dimensionality challenge and compress the concentration data into 2-dimensional (2D)
71 network. European legislation sets current and future caps on anthropogenic emissions of
72 primary and secondary-precursor components of PM_{2.5} at national level and from individual
73 sources (Vieno et al., 2016). In addition, it is well-known that ambient PM derives from both
74 transboundary emissions and transport (Vieno et al., 2016), creating challenges to develop
75 effective mitigation scenarios at the local level (Vieno et al., 2016; Zhang et al., 2008; van
76 Donkelaar et al., 2010).

77 1.2 Importance & Impact

78 Atmospheric particulate matters impact human health (WHO, 2006, 2013) and climate change
79 through radiative forcing (IPCC, 2013). The global health burden from exposure to ground
80 level PM_{2.5} is substantial. According to the Global Burden of Disease project, exposure to
81 ambient PM_{2.5} concentrations prevailing in 2005 was responsible for 3.2 million premature
82 deaths and 76 million disability-adjusted life years (Vieno et al., 2016; Lim et al., 2012). In
83 Europe, exposure to ambient PM_{2.5} is still a major health issue. For the period 2010–2012, it
84 was reported by the European Environment Agency report that 10–14 % of the urban
85 population in the EU28 countries were exposed to PM_{2.5} exceeding the EU annual-mean PM_{2.5}
86 reference value (25 µg m⁻³), while 91–93 % were exposed to concentrations exceeding the
87 WHO annual-mean PM_{2.5} (10 µg m⁻³) (Gehrig et al., 2003; EEA, 2014). Meeting the standards
88 focused on PM_{2.5} is complicated by the considerable chemical heterogeneity. PM long-term
89 exposure has been identified to be more serious than the daily (short-term) exposure to higher
90 PM concentrations that was first linked to impacts on human health (Pope and Dockery, 2006;
91 Harrison et al., 2012). Long-term impact studies have provided the foundation for calculation



92 of health impacts from PM exposure in the UK and Europe, which are significant
93 (COMEAP,2010). Changes in the direction of studies towards PM_{2.5}, associated with the
94 evidence that long-term PM levels play important role alongside short-term peaks, in terms of
95 health outcomes, has caused changes in legislation (Defra, 2007, Official Journal, 2008).

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97 1.3 Modeling Challenges

98 Challenges associated with traditional modelling of PM evolution to infer regional and local
99 influences include the need to embed a chemical complexity, range of emission sources and
100 transformative processes in Eulerian models. In this study, for the first time, we explore the
101 potential for compressing ambient PM_{2.5} network data into 2-dimensional (2D) network,
102 establishing a simple graph to infer causality and stability. This is a timely study as strategic
103 investments in national and local air quality monitoring networks require an evaluation on the
104 usefulness, or not, of network design. Whilst this study focuses on a sparse distributed network,
105 we discuss future applications for local networks across cities, for example. In a graph, each
106 node in the graph is a city, which exhibits a temporal signal (PM_{2.5}) and is connected to other
107 cities if they exhibit a close association in terms of either correlation (undirected) or Granger
108 causality (directed).

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110 2. Materials and Methods:

111 2.1 Ground-level PM_{2.5} data



112 Hourly $PM_{2.5}$ concentrations were observed at 15 monitoring stations in different cities (from
113 UK-air defra dataset website¹) shown in Figure 1 and coordinates given in SI – List S1. The
114 study period was divided into four seasons (meteorological seasons) Spring: 1st March 2017-
115 31st May 2017, Summer: 1st June 2017- 31st August 2017, Autumn: 1st September 2017- 30th
116 November 2017, and Winter: 1st December 2017- 28th February 2018. Also, $PM_{2.5}$ emissions
117 sources data were downloaded from the UK National Atmospheric Emission Inventory (NAEI)
118 website.



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131 Figure 1. Studied stations in the UK.

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133 2.2 Cross correlation calculation for spatial distribution of $PM_{2.5}$ in the UK

134 To measure the similarity of $PM_{2.5}$ concentration time series among each pair of cities in the
135 current study, the hourly based cross-correlation (XCROSS) was calculated using PAST
136 (PAleontological Statistics) version 3.25, for all site pairs (106 pair of cities) in four seasonal
137 windows (spring, summer, autumn, and winter). These periods were selected to try and capture
138 the effect of seasonal changes on the measured similarity between $PM_{2.5}$ concentration time

¹ <https://uk-air.defra.gov.uk/data/openair>



139 series. A flexible threshold (above 70%) was applied to decide which pairs were strongly
140 correlated (Gehrig et al., 2003).

141 2.3 Granger Causality calculation in PM_{2.5} network in the UK

142 The Granger causality test as a statistical hypothesis test for determining whether one time
143 series is useful in forecasting another, thus for measuring the ability to predict the future values
144 of a time series using prior values of another time series, was applied (using Eviews, version
145 11) to each pair of cities in the network during different seasons. When the p-value was less
146 than alpha level (5%), the null hypothesis was rejected, and we could decide which time series
147 can forecast another one. The Granger Causality test assumes that both the x and y time series
148 (x and y represent PM_{2.5} concentration series for different stations in our network) are
149 stationary, which was not the case in current study. As a result, de-trending was first employed
150 before using the Granger Causality test. To retain the same degrees of freedom (Statistical
151 parameter estimation is based on different amounts of data or information. The number of
152 independent pieces of data that go into the estimation of a parameter are called the degrees of
153 freedom (DF). Mathematically, DF represents the number of dimensions of the domain of
154 a random vector, or how many components should be known before the vector is fully
155 determined.), with annual data, the lag number is typically small (1 or 2 lags). For quarterly
156 data (which was our case), the appropriate lag number is 1 to 8. If monthly data is available, 6,
157 12, or 24 lags can be used given enough data points. The number of lags is critical since a
158 different number of lags can lead to different test results. As a result, optimal lags were chosen
159 based on Akaike Information Criterion (AIC). The optimal lag number that ensures the model
160 will be stable is thus 7 in our study. It is possible that causation is only in one direction, or in
161 both directions (x Granger-causes y and y Granger causes x). We chose the direction based on
162 the lowest p-value. For example in spring, according to our analysis, results suggest that
163 ‘activity’ in Manchester is statistically influencing Preston with a p-value= 5×10^{-29} , while
164 Preston is statistically affecting Manchester with a p-value= 3×10^{-8} . Therefore we infer that the
165 first statement (pollution from Manchester is influencing Preston’s concentrations) is the
166 correct one to select due to its lower p-value. Please note the language chosen reflects the
167 statistical inference for the network analysis; However, the mapping of inference to
168 atmospheric behavior and known challenges around PM_{2.5} source apportionment is important
169 and discussed.

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171 2.4 Trophic coherence



172 Trophic coherence is a way of hierarchically restructuring a directed network and labelling the
173 hierarchical levels (trophic levels – as derived from food webs and predation levels). Trophic
174 levels have been shown to be an effective compressed metric to infer stability on large directed
175 networks with no clear input output definition. The bottom (basal) nodes are those where all
176 energy comes from (e.g. major source of pollution), and the coherence of the whole network is
177 a proxy for stability against disturbances. The trophic level (s_i) of a node i , is the mean trophic
178 level of its in-neighbours:

$$179 \quad s_i = 1 + \frac{1}{k_i^{in}} \sum_j a_{ij} s_j$$

180 where $k_i^{in} = \sum_j a_{ij}$ is the number of in-neighbours of the node i and a_{ij} is the adjacency matrix
181 of the graph. Basal nodes k_i^{in} have trophic level $s_i = 1$ by convention (Pagani et al., 2019). In
182 our study, to interpret trophic coherence in a directed causal network, the initial stage was
183 introducing basal nodes.

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185 Stations with a low trophic level are $PM_{2.5}$ sources while stations with a high trophic level are
186 receptors according to this definition. The trophic level of a station is the average level of all
187 the stations from which it receives $PM_{2.5}$ pollutant plus 1. $x_{ij} = s_i - s_j$ is the associated trophic
188 difference of each edge. As always, $p(x)$ (the distribution of trophic differences) has a mean
189 value of 1, and when the network is more trophically coherent, the variance of this distribution
190 is smaller. The incoherence parameter q is the measurement of the trophic coherence of
191 network, which is the standard deviation of $p(x)$:

$$192 \quad q = \sqrt{\frac{1}{L} \sum_{ij} a_{ij} x_{ij}^2 - 1},$$

193 where $L = \sum_{ij} a_{ij}$ is the edges (the number of connections) between the nodes (stations) in the
194 network. When $q = 0$, the network is perfectly coherent however q with the values of greater
195 than 0 shows less coherent networks.

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197 **3. Result and Discussion:**

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199 3.1 Spatial distribution of $PM_{2.5}$ over the UK

200 Interesting information about the spatial distribution of the $PM_{2.5}$ concentrations over the UK
201 can be obtained when analysing the cross correlation of the hourly values between the different



202 sites. Results suggest that two groups of cities were connected to each other with XCROSS
203 value above 70%. The first group (Northern Group A) includes Preston (Pre), Manchester
204 (Man), Chesterfield (Chest), Leeds, Nottingham (Not), Newcastle (New), Birmingham (Bir),
205 and Liverpool (Liv), while the second one (Southern Group B) includes Bristol (Bri), Oxford
206 (Oxf), Southampton (South), Plymouth (Ply), Norwich (Nor), and London (two stations named
207 LonB and LonR). For the seasons of spring, summer, and autumn, the combination of groups
208 does not change, but the value of XCROSS does (Figure 2). In wintertime the combination of
209 cities in and out of clusters changes (Figure 2-D). The connected cities, generating a directed
210 dynamic network, are seasonally visualized in Figure 2.

211 As the networks are very spatial (i.e., distance is a significant impedance factor), a general
212 measure of how spatially embedded it is, was studied. The pair of stations were divided into
213 groups based on the distance (Table 1). To quantify the level of spatial embeddedness, a
214 relationship between Cross correlation and distance between each pair of cities was studied
215 (Table 1). A very high spatially embedded part of the network for all seasons was formed below
216 100 Km, while less spatial embeddedness of network was witnessed when the distance
217 increased to above 200Km (for all seasons). A main part of the network (100 Km) was formed
218 in cluster A with percentage of 67%, 54%, 60%, and 89% during spring, summer, autumn, and
219 winter, respectively. This value in cluster A reduced (for all seasons) when increasing the
220 distance between pair of cities reaching the value of zero during autumn and winter. Since the
221 distance between cities in cluster was dominantly above 100Km, the dominant part of the
222 network in cluster B was formed below 200 Km (100-200Km), with percentage of 38%, 52%,
223 46%, and 23% during spring, summer, autumn, and winter, respectively. This value in cluster
224 B had a reduction (for all seasons) by increasing the distance between pair of cities reaching
225 the value of zero during autumn, while during wintertime it was 19% for distance above
226 200Km. The number of outliers (pair of connected cities out of group A &B) had its highest
227 values of 40%, 100%, and 81% during spring, autumn, and winter, respectively when the
228 distance between cities was above 200Km. During autumn, for distances above 200Km, the
229 original network was not formed, while during winter, group B was formed. The number of
230 paired cities in the network had a reduction by 50% between spring and winter, when the
231 distance was below 100Km (the same reducing trend was witnessed in both groups). For
232 distances below 200Km, the network was weakened by %50. Interestingly, when the distance
233 between cities increased above 200 Km, during winter the network was strengthened by 17%
234 comparing to spring.

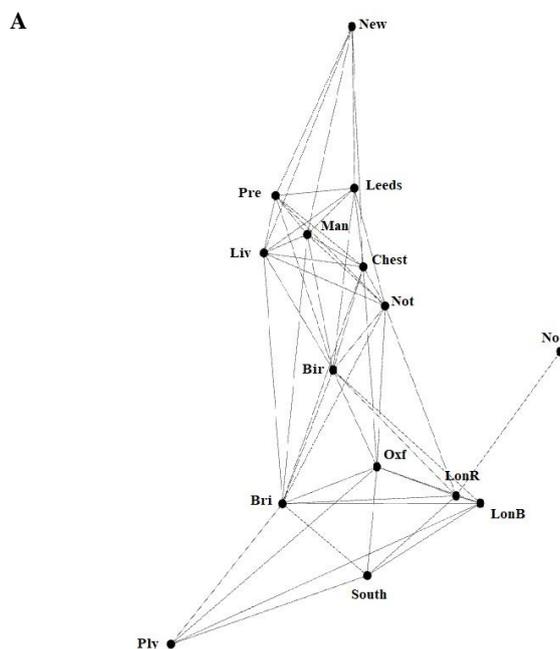
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236 Table 1. The relationship between Cross-Correlation (XCROSS) of the daily values of PM_{2.5} and
 237 distance of the cities in UK.

Distance	Pair of connected cities in network	Pair of connected cities in group A	Pair of connected cities in group B	Outliers (pair of connected cities out of groups)
Spring				
<100Km	18 (43%)	12 (67%)	6 (33%)	0
<200Km	42 (81%)	24 (57%)	16 (38%)	2 (5%)
>200Km	10 (19%)	3 (30%)	3 (3%)	4 (40%)
Summer				
<100Km	13 (52%)	7 (54%)	6 (46%)	0
<200Km	25 (90%)	12 (48%)	13 (52%)	0
>200Km	3 (10%)	2 (67%)	1 (33%)	0
Autumn				
<100Km	15 (54%)	9 (60%)	6 (40%)	0
<200Km	28 (93%)	9 (27%)	13 (46%)	9 (27%)
>200Km	2 (7%)	0	0	2 (100%)
Winter				
<100Km	9 (35%)	8 (89%)	1 (11%)	0
<200Km	26 (41%)	14 (54%)	6 (23%)	6 (23%)
>200Km	37 (59%)	0	7 (19%)	30 (81%)

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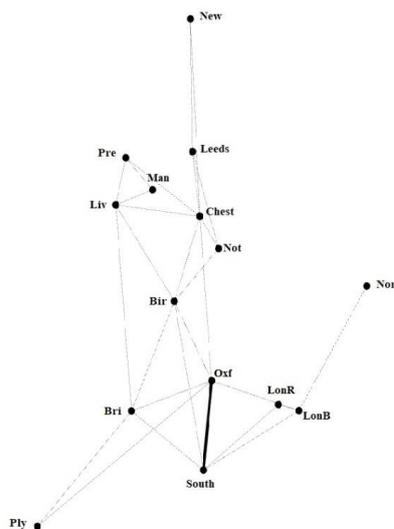
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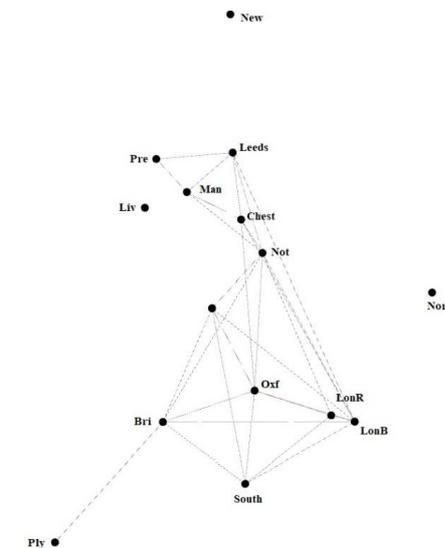
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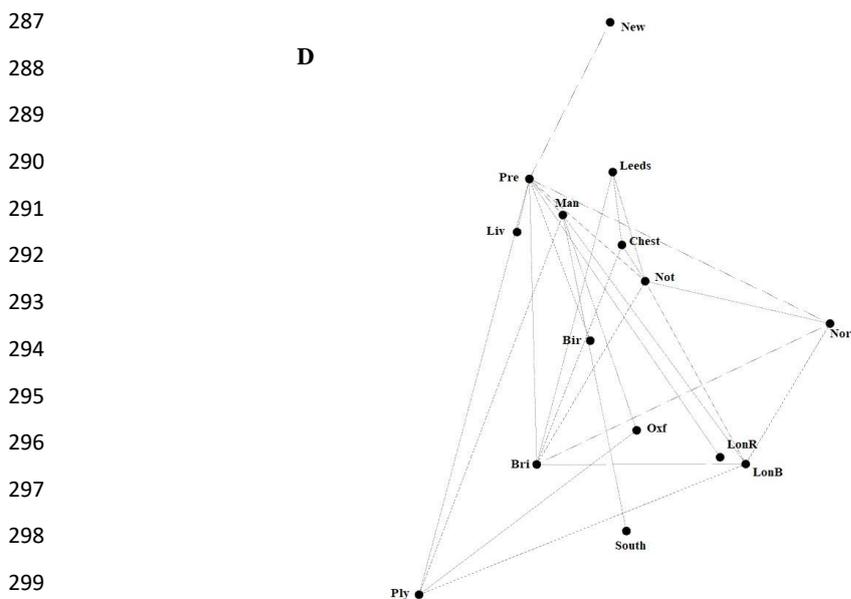
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300 Figure 2. Cross correlation based dynamic network including; A) spring window, B) summer window,
301 C) autumn window, and D) winter window in 2017-2018, UK.

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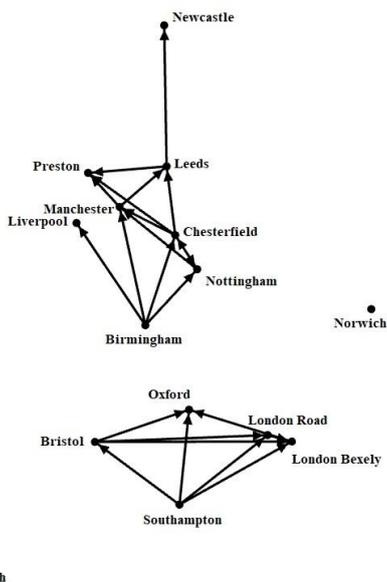
304 3.2 Granger causality test

305 The main result from this study is that cities with the strongest Cross correlation have the lowest
306 p-value (below 5%) (Figure 3). In spring, as already noted, results suggest that, statistically,
307 activity in Manchester is causing concentrations to change in Preston with $p\text{-value} = 5 \times 10^{-29}$
308 (i.e. Manchester $PM_{2.5}$ data can be used to predict the future $PM_{2.5}$ values of Preston) and
309 Bristol is causing Oxford with a p-value of 9×10^{-28} . In summer, Liverpool is causing Preston
310 with a p-value of 7×10^{-17} . Manchester is causing Preston with $p\text{-value} = 6 \times 10^{-23}$ in autumn,
311 while Chesterfield is causing Nottingham with a p-value of 1×10^{-7} in wintertime. The results
312 look very spatial and the distance is a significant impedance factor. The distance between all
313 paired cities was below 50Km. Based on Table 2, when the distance between pair of cities
314 increases the order of p-value increases too.

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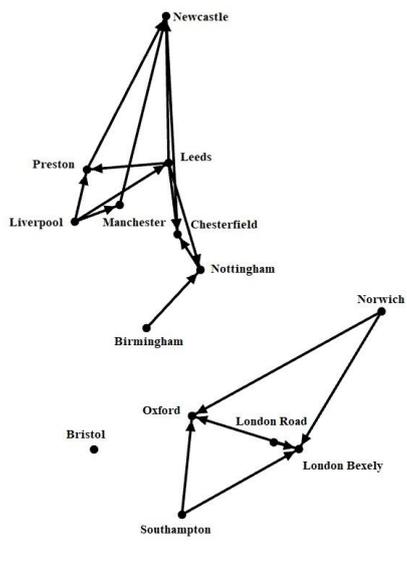
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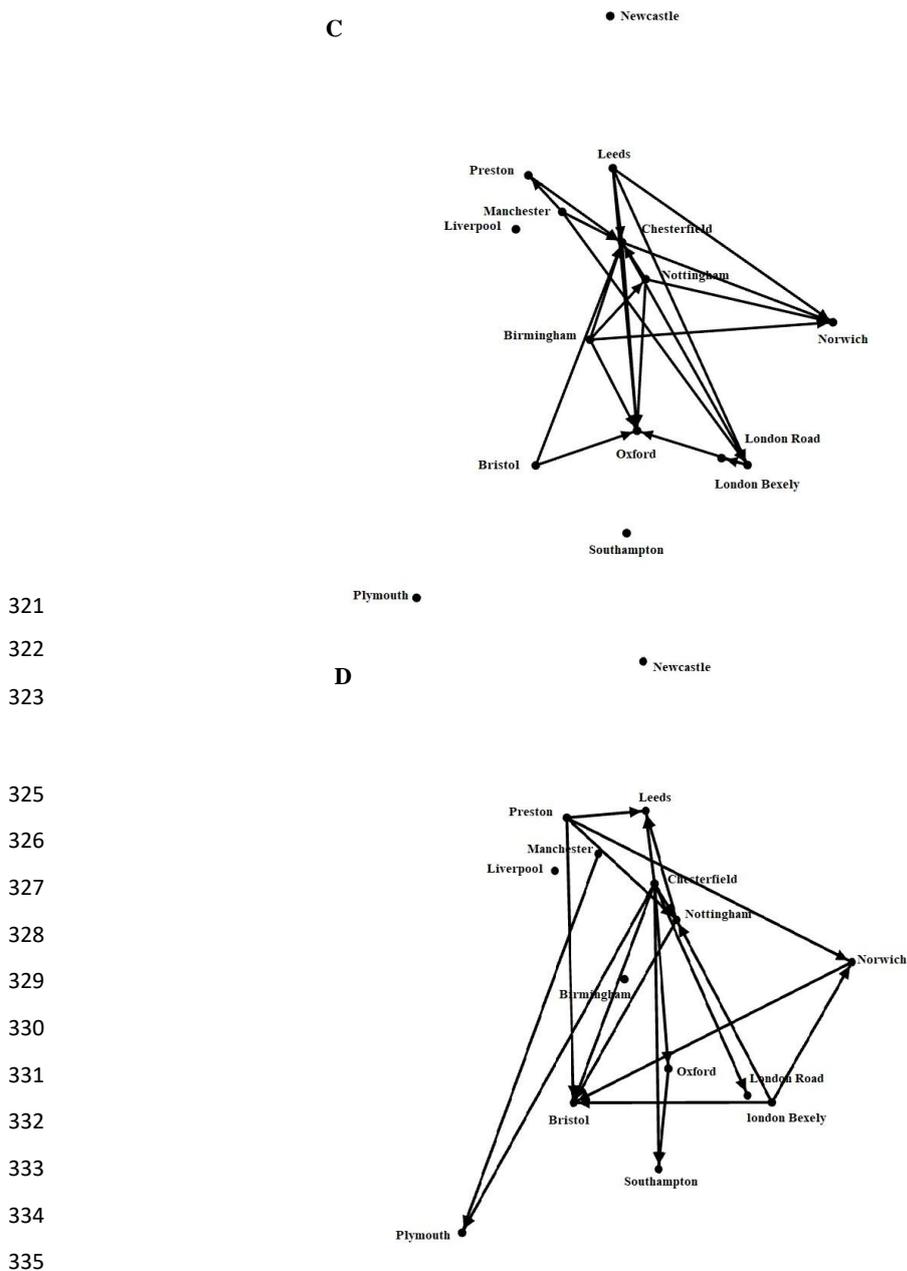
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336 Figure 3. Granger based dynamic network including; A) Spring window, B) Summer window, C)
337 Autumn window, and D) Winter window in 2017-2018, UK.

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341 Table 2. Comparison among Granger causality results (p-values) in different seasons.
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Source	Target	Distance (Km)	p-value
Spring			
Manchester	Preston	43.66	5×10^{-29}
Bristol	Oxford	91.78	9×10^{-28}
Summer			
Liverpool	Preston	42.62	7×10^{-17}
Leeds	Newcastle	131	5×10^{-11}
Autumn			
Manchester	Preston	43.66	6×10^{-23}
Chesterfield	Oxford	165.11	3×10^{-20}
Winter			
Chesterfield	Nottingham	36.17	1×10^{-7}
Chesterfield	Bristol	213.74	7×10^{-6}

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345 A directed graph is defined (Bang-Jensen and Gutin, 2008) as an ordered pair $G = (N, E)$,
 346 where N is a set of nodes (i.e. stations) and E is a set of ordered pairs of nodes, called edges
 347 (i.e the probability values for F statistics). The hierarchical structure of a directed graph can be
 348 presented by its trophic coherence property. The whole idea is that hierarchical systems have
 349 fewer feedback loops and experience less cascade effects. The incoherence parameter (q) was
 350 used to measure the coherence of the seasonal causal network to show how trophic distance is
 351 tightly associated with edges concentrated around its mean value (which is always 1) (Johnson,
 352 et al., 2014). We observed incoherent network in our seasonal datasets (Table 3).

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354 Table 3. Incoherence factor of seasonal directed networks in current study.

Directed network	Incoherence factor (q)
Spring	0.69
Summer	0.37
Autumn	0.49
Winter	0.35

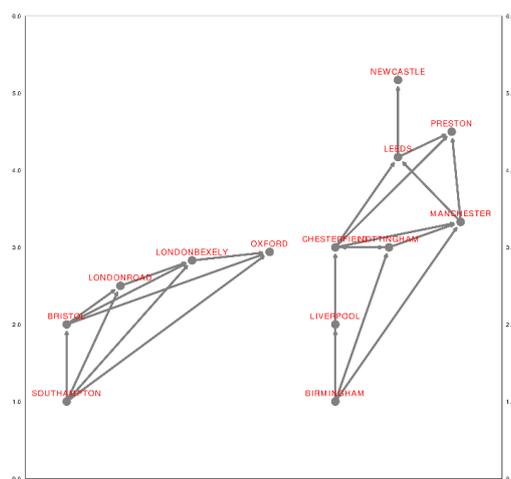
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356 The highly incoherent season was spring with $q = 0.69$, whilst a less incoherent network was
 357 found to be winter ($q = 0.35$). In figure 3, according to the parameter definition, the basal nodes
 358 with the low trophic level represent the major pollution source nodes, while stations with high
 359 trophic levels are ones who act as receptors in the causal network. During springtime, due to
 360 well mixing of the lower atmospheric layer, the network was well formed. In group A,



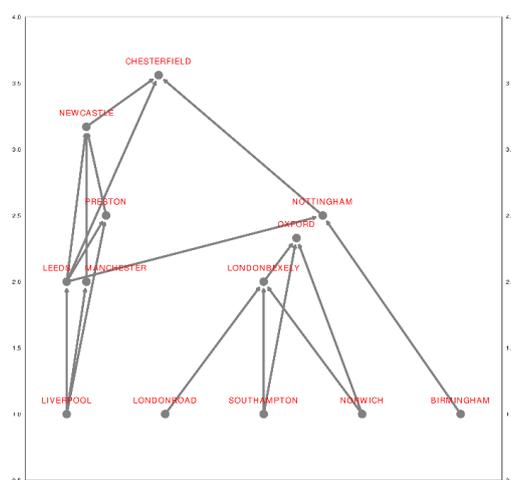
- 361 Birmingham with low trophic level was classified as a pollution source, while in group B
- 362 Southampton was pollution source with low trophic level.

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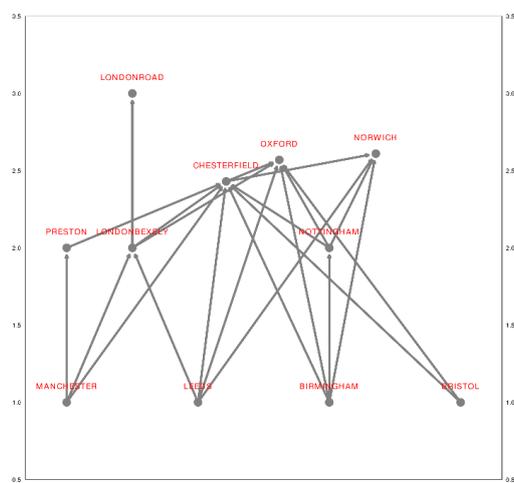
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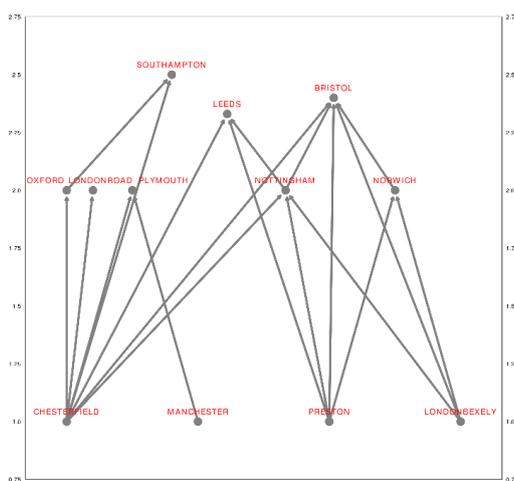
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372 Figure 3. The hierarchical structure and basal nodes of causal network including; A) Spring window,
373 B) Summer window, C) Autumn window, and D) Winter window in 2017-2018, UK.

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376 **4. Discussion:**

377 *4.1 The effect of meteorological parameters on network structure*

378 Based on the previous analysis, this connection (network) indicates that meteorological
379 conditions and diurnal emissions from a wide range of common sources (such as traffic), rather
380 than locally specific sources and events, dominate the relative variations of the concentrations
381 of fine particles over long periods (Gehrig et al., 2003). During wintertime, the meteorology is
382 characterized by frequent inversions, forming an efficient obstacle for the distribution and
383 homogenization of PM. As a result, only tight spatially embedded parts of network (below
384 100Km with the highest percentage of restored network) could ‘withstand’ meteorological
385 influences and further parts (above 100Km) started to collapse from a network perspective. In
386 winter time, the plausible reason of connecting the cities out of the initial network (81% of
387 connected cities were out of the initial network with distance above 200 Km) might be higher
388 average seasonal wind speeds (in all studied stations), probably due to the balance among
389 greater dilution and shorter transport times at higher wind speeds, which allows less time for
390 PM dispersion and deposition over further distances (Harrison et al., 2012).

391 Indeed, it is well known that changes in meteorological parameters (e.g., wind speed and
392 direction, temperature, and rainfall) can significantly affect PM_{2.5} concentrations and formation
393 mechanisms (AQEG, 2012; Vieno, et al., 2016). In addition to primary sources, secondary
394 sources are dependent on meteorological conditions and the abundance of precursors.
395 Secondary aerosols have a significant contribution in PM_{2.5} concentrations in the UK, where a
396 large proportion transboundary secondary PM_{2.5} transferred from Europe is made of nitrate
397 particles in the form of ammonium nitrate (AQEG, 2012; Vieno, et al., 2016). One plausible
398 reason of connection within a network can be common transboundary sources.

399 The association among wind direction and PM_{2.5} can provide a better picture of the origins of
400 the measured PM_{2.5} concentrations. With this in mind, there is an outstanding coherence
401 throughout the patterns across the Group A and Group B in the UK. Hence, there is, a minor
402 variation between cities in the south (Group B) and those in the north or close to northern part
403 (Group A) of the UK (Harrison et al., 2012). High PM_{2.5} concentrations in Group B (southern
404 sites) are more attributed to winds from the east through to southeast, which are often attributed
405 to a blocking high pressure over the Nordic countries, giving rise to a south-easterly or easterly
406 air flow that cause transportation of emissions from eastern Europe, northern Germany, and
407 the Belgium and Netherlands to the southern cities in the UK (Harrison et al., 2012; Barry and



408 Chorley, 2010). Nonetheless, the arriving air flow in the northern parts of the UK from the east
409 to southeast sector will not have passed through these same emission origins.

410 On the other hand, High $PM_{2.5}$ concentrations in Group A (northern cities or close to northern
411 part) are more important attributed to the winds blowing from the northeast through to east,
412 drawing air flow (likely to start blowing when a low pressure runs up the English Channel)
413 northward across European emission sources (to mainly be emission sources of precursors of
414 secondary PM), out into the North Sea, then reaching northern parts of the UK from a north-
415 easterly direction (Barry and Chorley, 2010).

416

417 **5. Conclusion:**

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419 In current study, we use $PM_{2.5}$ concentrations in 14 cities in the UK over 52 weeks to infer an
420 undirected correlation and a directed Granger causality network. We show for both network
421 cases (group A & B), two robust spatial communities divide the UK into the northern and
422 southern city clusters, with greater spatial embedding in spring and summer.

423 Based on the granger causality test, we infer that $PM_{2.5}$ data of cities with the strongest Cross
424 correlation (having the lowest p-value) can be helpful to predict the future $PM_{2.5}$ values in the
425 network. However, there are of course multiple caveats with this statement, some of which are
426 reflected in our discussions around known influences from meteorological and source
427 variability. We leverage on the directed network to infer stability to disturbances via the trophic
428 coherence parameter, whereby we found that winter had the greatest vulnerability.

429 As already noted, this connection (network) suggests that meteorological conditions and
430 emissions from regional origins rather than specific local origins and events dominate the
431 relative variations of the urban background $PM_{2.5}$ concentrations (Gehrig et al., 2003) using
432 this sparse network data. We know that PM with emission sources from continental Europe,
433 probably as secondary PM, can play an important role in affecting $PM_{2.5}$ levels in different
434 parts of the UK (Harrison et al., 2012). However, our study has some limitations including a
435 short period of time over which the network was analysed. Also, to have a better understanding
436 of network, evaluating a predictive network based $PM_{2.5}$ model using meteorological
437 parameters, and contributions from identified clusters in the UK, would be helpful. This work
438 acts as a demonstrator for the information that can be extracted from an undirected correlation
439 and a directed Granger causality network. Further work is needed, alongside ancillary data that
440 might support the extracted relationships such as source apportionment data and transport



441 activity, for example. The approach might also be better suited to more local networks, such as
442 monitoring stations across a city.

443 *Code availability.* The code for computing the trophic level of each node in the network, the
444 trophic difference and finally trophic coherence (q) of the network with all scripts needed to
445 reproduce the results in this study is available at [https://github.com/kohyar88/PM2.5--Trophic-](https://github.com/kohyar88/PM2.5--Trophic-Coherence-/tree/v1.0.0)
446 [-Coherence-/tree/v1.0.0](https://github.com/kohyar88/PM2.5--Trophic-Coherence-/tree/v1.0.0) with DOI number of 10.5281/zenodo.3661483.

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