CAN COMPLEX NETWORKS DESCRIBE THE URBAN AND RURAL TROPOSPHERIC 0₃ DYNAMICS?

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1 <u>ABSTRACT</u>

2	Tropospheric ozone (O_3) time series have been converted into complex networks
3	through the recent so-called visibility graph (VG), using the data from air quality stations
4	located in the western part of Andalusia (Spain). The aim is to differentiate the behavior
5	between rural and urban regions when it comes to the ozone dynamics. To do so, some
6	centrality parameters of the resulting complex networks have been investigated: the
7	degree, betweenness and shortest path.
8	Results from these parameters coincide when describing the difference that
9	tropospheric ozone exhibits seasonally and geographically. It is seen that ozone behavior
10	is multifractal, in accordance to previous works. Also, it has been demonstrated that this
11	methodology is able to characterize the divergence encountered between
12	measurements in urban environments and countryside.
13	Additionally, the promising outcomes of this technique support the use of complex
14	networks for the study of air pollutants dynamics, adding nuances to those reported by
15	descriptive statistics or multifractal analysis.
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22 <u>KEYWORDS</u>

23	-	Tropospheric ozone
24	-	Visibility graphs
25	-	Centrality measures
26	-	Complex networks
27	-	Time series

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29 1. INTRODUCTION

In the last few decades, tropospheric ozone has been the focus of many studies performed in different areas and scales around the world. This interest on ozone dynamics analysis and characterization has been awaken because it is one of the main photochemical oxidants on account of its abundance. When this irritant gas is found in high concentrations, severe impacts affect human health and harvest (Doherty et al., 2009). Those mentioned harms have a severe impact for economy, leading to losses of several billions of dollars annually (Miao et al., 2017).

37 The gas object of the presented work is a secondary pollutant and it is known that its 38 creation and destruction mechanisms are related to photochemical and nonlinear 39 processes (Graedel and Crutzen, 1993; Trainer et al., 2000). The mentioned processes 40 depend on meteorological features such as wind direction, temperature, and principally 41 solar radiation (Graedel and Crutzen, 1993; Guicherit and van Dop, 1977). They have 42 been analyzed for the Mediterranean basin by some authors previously (Cieslik and 43 Labatut, 1997; Güsten et al., 1994; Kouvarakis et al., 2000; Ribas and Peñuelas, 2004). Besides, tropospheric ozone concentration levels depends also on the presence of other 44

45 gases, such as nitrogen oxides and volatile organic compounds (called precursors) that 46 are produced in the urban and industrial areas (Sillman, 1999). Because of all these 47 considerations the analysis of the temporal dynamics of ozone becomes a very complex 48 task. As a consequence, traditional statistical analysis of ozone may offer a limited view 49 of more complex dynamics of signals where the level of variability is high (Pavón-50 Domínguez et al., 2015).

51 One of the focuses on this topic is the difference encountered between rural and urban areas (García-Gómez et al., 2016; Jirik et al., 2017; Kumar et al., 2015). Despite the fact 52 that ozone is created mainly in urban nuclei, it is proven that higher concentrations of 53 54 this contaminant are measured within rural regions, leading to reduction of crop yields among other environmental problems (Tai and Val Martin, 2017). One reason attributed 55 56 to this phenomenon is the transport of ozone by the wind to the less industrialized 57 regions. In those areas the destruction rate of ozone is less significative than in urban 58 ones.

In the last few years, a new technique to analyze temporal series has been developed 59 60 (Lacasa et al., 2008). This technique relies in the use of complex networks obtained from 61 the transformation of those signals (ground-level ozone concentration time series in this case). It was given the name of Visibility Graph (VG). These complex networks have 62 63 proven to have several advantages such as: i) they inherit the features of the associated 64 time series, which ends up resulting on additional feedback through the degree distribution (that will be defined later). ii) In addition, they can be used for analyzing 65 series of several variables simultaneously, which could be very helpful for finding 66 67 correlations between tropospheric ozone and its precursors; iii) and lastly, this recent

bridge between complex networks and temporal series opens a wide range of newopportunities within the study of complex signals.

In the presented work, the complex networks obtained from ozone time series through the VG are used to retrieve the centrality parameters. These parameters give information about the most important nodes in a system and will be further explained in subsection 2.3. Finally, the main purpose is to check the ability of this methodology to analyze the differences in the behavior of the tropospheric ozone between urban and rural environments.

76 2. MATERIALS AND METHODS

77 2.1. <u>Data</u>

The region that is the object of this analysis corresponds to the Guadalquivir Valley (South-western part of Spain) since the area has the proper orography, weather and anthropic conditions to be vulnerable to pollution by tropospheric ozone (Domínguez-López et al., 2014).

The data used here correspond to 1-hour monthly ozone concentration values collected from 2013 to 2017. The measurements were performed at four different stations located in the province of Cadiz (see Figure 1). Two of them are located in the southeastern part of the region (Algeciras and Alcornocales) and the others in the northwestern one (Cadiz and Prado del Rey). Algeciras and Cadiz correspond to urban areas, whereas the other two are situated within the natural reservoir named "Parque natural de Los Alcornocales", and so they have been labelled as rural.

These stations are part of the network that monitors the air pollution levels in the region
of Andalusia, co-funded by the European Union and the Consejería de Medio Ambiente

91 y Ordenación del Territorio (Regional Environmental and Territory Management
92 Department). The data was collected and provided lastly by the EEA (European
93 Environmental Agency).

Figure 2 shows ozone concentration time series for four months from 2015 for two different locations: Alcornocales (rural) and Algeciras (urban). One clear difference between the two of them is that in the urban station, the lowest values measured are in many occasions close to zero. On the other hand, in the rural one that is not indeed the case: the ozone concentration does not vanish in the whole month or barely does it. This behaviour can be extended to all the rest of the years included in the presented study.

As it was clearly seen in Figure 2, the ozone concentrations reach especially high values in summer, where the case in winter is the exact opposite. Those differences were observed for this area (Adame et al., 2008; Jiménez-Hornero et al., 2010), and the reason is that the most suitable conditions for the ozone creation are found around summer. The temperature and solar radiation progressively raise and reach their peak in July, which allows higher creation rates and therefore concentration. One of the reactions that governs this mechanism is the following (Graedel and Crutzen, 1993).

$$NO_2 + O_2 \leftrightarrow O_3 + NO \tag{1}$$

This photochemical reaction is reversible and tends to the ozone creation (rightwards direction) when there is energy (light) available and vice versa when there is not. For that reason, the highest and lowest values of ozone are always measured during the day and night, respectively. The same happens summer and winter, as discussed previously.

113 2.2. Visibility graphs

One possible definition for a graph is a set of points vertices or nodes that are connected through lines called *edges*. As commented above, a tool that makes possible the transformation of a time series into a graph was introduced by Lacasa et al. (2008) and called Visibility Graph (VG). One of the main features that rises the interest of researchers relies on the fact that it inherits many properties of the original series.

The first thing that must be done for constructing the visibility adjacency matrix (which contains all the information of the new network), is to stablish a method to decide which points (or nodes) in the system are connected to each other or have visibility. The criterion is the following: two arbitrary points from the time series (t_a, y_a) and (t_b, y_b) will have visibility (and will be connected in the graph) if any given point (t_c, y_c) that is located in between $(t_a < t_c < t_b)$ fulfills the following condition:

$$y_c < y_a + (y_b - y_a) \frac{t_c - t_a}{t_b - t_a}$$
 (2)

One example of how this method works can be seen in Figure 3, where it is applied to a sample time series as an illustration. It can be observed that the original temporal series has been transformed into a complex network, where some of the points are connected by edges. This new graph will inherit the complexity of the original series (Lacasa et al., 2008; Lacasa and Toral, 2010), meaning that a regular graph would be created from a periodic time series, for instance.

After applying this visibility method, the result is a NxN adjacency binary matrix, with N the total number of points in the system. The information of the nodes is given by each row of the matrix, so that $a_{ij} = 1$ means that the node *i* and *j* have visibility; whereas 134 $a_{ij} = 0$ means the opposite case (no edge connects those two nodes). The algorithm 135 can be substantially simplified (reducing the computational cost of the process) if some 136 considerations are considered. These can be done thanks to the properties that the 137 adjacency matrix holds. The properties are listed below:

- Hollow matrix: Since there are no intermediate nodes to fulfill the condition, in the case of the diagonal, all the elements are zero ($a_{ii} = 0$). Hence a node does not have visibility with itself.
- Symmetric matrix: Due to the reciprocity of the visibility between two nodes, all the nodes in system fulfill $a_{ii} = a_{ii}$. This is a property of all undirected graphs.

• Nearest neighbors: The elements that surround the diagonal are always 1 ($a_{ij} =$ 144 1 for $j = i \pm 1$). This is because each point always sees the closest previous and 145 next node (there are no points in between to prevent the visibility).

146 With all these considerations, every visibility adjacency matrix has a general form as147 follows:

$$A = \begin{pmatrix} 0 & 1 & \dots & a_{1,N} \\ 1 & 0 & 1 & \vdots \\ \vdots & 1 & \ddots & 1 \\ a_{N,1} & \dots & 1 & 0 \end{pmatrix}$$
(3)

148 2.3. <u>Centrality measures</u>

When trying to retrieve information from a given complex network, one of the most commonly used approaches is discerning which of them are the most important nodes in the system. To this purpose, centrality measures comes usually in handy. This concept was initially applied to the study of social networks and later transferred to other fields of knowledge (Agryzkov et al., 2019; Joyce et al., 2010; Liu et al., 2015). This work has
been focused on two of them: the degree and betweenness centrality measures, which
will be explained afterwards.

156 2.3.1. Degree centrality

A possible definition for the degree of a node (k_i) is the number of other nodes that have visibility with it $(k_i = \sum_j a_{ij})$. For instance, in Figure 3, the degree of the three first nodes are k = 3, k = 2 and k = 3, respectively. On the whole, it is possible to obtain the probability that corresponds to each degree, by simply counting how many times each value is repeated. From there, the degree distribution of the sample P(k) can be retrieved.

163 By analyzing the degree distribution that is built from the VG it is possible to describe 164 the nature of the time series, as previous works have shown (Lacasa et al., 2008; Mali et 165 al., 2018). It has been probed its capability to distinguish between fractal, random or periodic signals, for instance. Thus, by studying the degree distribution, a first insight of 166 167 the behaviour of the ozone concentration time series can be yielded as first step before 168 getting into a more complex analysis. As some previous works explain (Lacasa et al., 169 2009; Lacasa and Toral, 2010), time series which have VGs whose degree distributions can be fitted to a power law $P(k) \propto k^{-\gamma}$ correspond to scale free due to the effect of 170 171 hub repulsion (Song et al., 2006). The term hub refers to the nodes with unlikely highest 172 number of links (highest degrees, see Figure 4). The right tail of each degree distribution, 173 governed by those hubs, can be represented in a log-log plot and fitted by a simple linear 174 regression. The slope obtained by this regression provides an interesting parameter, the 175 so-called γ exponent, which has already been used in some works (Lacasa and Toral,

2010; Mali et al., 2018). In Figure 4a, thanks to the v-k plots (Pierini et al., 2012), it is
possible to appreciate how *hubs* from the VG are related to the largest values of ozone
concentration.

179 2.3.2. <u>Betweenness centrality</u>

Before presenting this quantity, it is necessary to introduce a definition for the shortest path (SP). It can be understood easily that the SP for a pair of nodes (i, j) in a VG is the minimum number of edges between both. Consequently, the SP between two consecutive nodes will be the unit.

The betweenness of a node (b_i) for an undirected graph is defined as the total number of SPs which passes through this node and mathematically:

$$b_{i} = \sum_{\substack{j=1\\j\neq i}}^{N} \sum_{\substack{k=1\\k\neq i,j}}^{N} \frac{n_{jk}(i)}{2N_{jk}}$$
(4)

where N_{jk} is the total number of SPs from node j to node k and $n_{jk}(i)$ is the number of SPs from node j to k, that contains the node i. It is divided by two in order not to repeat the same pair of nodes twice in an undirected graph (the path from j to k and vice versa give the same information).

The mentioned parameter estimates the centrality of a node by considering whether it is between many of the nodes (Latora et al., 2017). In an equivalent way to the degree *hubs*, some points with a remarkably higher betweenness exist. For the seek of clarity, authors propose the term *skyline hubs* to refer to those with unlikely high betweenness. This name has been chosen because of its similarity to the skyline drawn by the skyscrapers in a city. Those temporal nodes are characterized by being the points which the SPs of many other nodes will pass necessarily through. In Figure 4b it is possible to see how they are related to *hubs* and therefore to some peaks of the time series. They are a more selective way to identify key nodes in the signal.

199 3. <u>RESULTS AND DISCUSSION</u>

The first step was to transform the ozone concentration time series from all the locations for all the months (from 2013 to 2017) into complex networks with the VG algorithm. In this section, the results that are shown and discussed were obtained from the direct analysis of these networks.

204 3.1. <u>Degree centrality</u>

205 Following the definition of degree (k) given previously (subsection 2.3.1), the 206 number of edges connected to each node in the different VGs was computed. From 207 these values, it has been possible to construct the degree distribution of the networks, 208 as shown in Figure 5. In this plot, the degree distribution of the whole year (2015 shown 209 as reference) was computed; with the final aim of discerning whether this distribution 210 could give some insight on the difference between ozone dynamics in rural and urbanized areas. This first guess was motivated by previous works that use it in order to 211 212 analyze the nature of the time series for several quantities (Lacasa and Toral, 2010; Mali 213 et al., 2018).

The results for all the years and months are quite similar indeed, in accordance with previous studies (Carmona-Cabezas et al., 2019); and for that reason, only one year (2015) is used for the sake of clarity in Figure 5. As can be seen in the cited plot, the tail of the distributions follows a power law of the form $P(k) \propto k^{-\gamma}$, that leads to a linear part of the curve when plotted in logarithmic scale both k and P(k). This behaviour

219 points to the fractal nature of the signal, which was expected looking at some prior 220 analyses (Jiménez-Hornero et al., 2010; Pavon-Dominguez et al., 2013). The slope of the 221 linear portion in absolute value leads to the computation of this γ parameter. It is clear 222 that the trend is negative, since the nodes with biggest degrees and known as hubs 223 correspond usually to the high values of the distribution (see Figure 4), whose likeliness 224 is very low. In all the cases studied here, the distributions are almost overlapped and finally the exponent $\gamma \sim 3.4$ roughly for all of them (see Table 1), as depicted in Figure 5. 225 226 For that reason, this parameter alone is not able to distinguish the dynamics of the 227 tropospheric ozone in the different regions on which this study focuses (urban - rural). Nevertheless, it does give useful information about the nature of the time series as 228 229 discussed and validates the data, since equivalent studies for different years and geographical area gave similar values of γ (Carmona-Cabezas et al., 2019). 230

Looking at the average degree (\overline{k}) of all the nodes from the VGs of each month, some 231 232 information can be drawn. In Figure 6a), this averaged value is plotted for each month 233 and the first thing that can be commented is that the shape of the curves changes along 234 the year. For all the studied locations, there is an increasing tendency towards summer that then decays typically after August. This behaviour was expected as \overline{k} would mean 235 236 a higher number of hubs in the signal and those are related to the greatest 237 concentrations of ozone as shown in Figure 4. That is in the end due to the more suitable 238 conditions for ozone formation that exist in summer with respect to the other season (specially winter). One interesting thing that was as well observed by the authors in a 239 recent study (Carmona-Cabezas et al., 2019) is the fact that this quantity drops around 240 241 April and November. One possible explanation is the weather of spring and autumn,

unstable by nature, that favors the dispersion of gases and particles in the air
(tropospheric ozone amongst them), as discussed in other studies (Dueñas et al., 2002).

244 Also, looking at Figure 6a), a clear difference between the curves of the rural (blue) and 245 urban (red) areas is found. Having all the same behaviour mentioned before, the values 246 of Prado del Rey and Alcornocales (both rural) are sensibly higher than those of Algeciras and Cadiz (urban). The difference between summer and winter is as well more 247 248 pronounced in the rural locations. Authors attribute this fact to the transport of ozone 249 with the wind (Dueñas et al., 2004), added to the process of destruction of that secondary contaminant, rather than its formation. This effect would correspond to the 250 251 leftwards direction of the photochemical reaction described before (Equation 1). After 252 the ozone is created, it starts to react with the Nitrogen Oxide during night conditions 253 (absence of light and lower temperatures). As could be observed in Figure 2 and Figure 254 4, the ozone values reach minima of zero quite often in the urban area of Algeciras for 255 instance, which is not the case for the rural location of Alcornocales. That is directly 256 related to the higher concentrations of NO from factories and vehicle emissions that can 257 be found in an industrial area such as Algeciras; in contraposition to the natural reservoir 258 of Parque natural de los Alcornocales. Therefore, the ozone that is created and 259 transported to the rural areas studied here cannot be transformed to other gases at the 260 same rate as in the city, leading to higher concentrations values on average. This can be 261 observed as well in Table 1.

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264 Another parameter from the computed degrees that can be seen (Figure 6b) is the standard deviation of k (σ_k). As it was discussed in a previous work on this topic 265 266 (Carmona-Cabezas et al., 2019), it is related with the differences encountered between daily and night values of ozone concentration. As expected, maxima are found again for 267 268 summer, seemingly due to the fact that the biggest differences in UV radiation and 269 temperature in this area are found in that season between day and night. Again, drops of this quantity σ_k are observed in both spring and autumn, which authors attribute to 270 the same reason as in the case of \overline{k} . 271

Now the curves of σ_k in rural and urban areas are more similar than in the case \overline{k} , but still a difference can be observed. This lower difference with respect to the curves of \overline{k} can be explained using the same effect discussed before: the destruction of ozone is lower in the rural areas.

276 3.2. <u>Betweenness centrality</u>

277 After the mentioned analysis of the degree, authors checked the suitability of the 278 next centrality parameter: betweenness (b). Moreover, the average SP quantity was 279 obtained in order to get more information about the time series, since it is directly 280 related to b (see Equation 4). Both of them were computed for every node in the VGs (from each month). After the information of each node was retrieved, the average was 281 282 taken for SP, whereas in the case of the betweenness centrality, the median has been 283 chosen. This decision was motivated by the fact that the distribution of the betweenness 284 is much more skewed than those of the degree centrality and SP. In addition to that, the 285 vast majority of values of b are zero or very close to it (see Figure 4). For those reasons, 286 authors consider median as a more representative measure of the overall behaviour

rather than the mean. Results for *b* and SP can be observed in Figure 7, where thedifferent locations studied can be seen.

289 On the one hand, in Figure 7a) the betweenness centrality shows a seasonal pattern as 290 well as the degree, being this one more pronounced in the rural areas than in the urban 291 ones. As can be easily seen, the minimum values are reached for late spring, summer and early autumn (from May to October), in contrast to the degree centrality, which was 292 293 maximum for this period. The reason of these minima is that the higher are the 294 concentrations of ozone, the greater will be the amount of degree hubs and skyline hubs, as it was shown in Figure 4a). Since skyline hubs allow faster connections between 295 nodes, less edges will be necessary to link them through the SP. And so, the average of 296 297 this amount will be reduced over this period and vice versa for the rest of the year. This 298 reduction in the average SP is seen in Figure 7b). By definition, the shorter is the SP 299 between two points, the less nodes will be necessary for them to pass through, resulting on a lower betweenness in general (what is indeed happening in summer). 300

301 When it comes to the differences encountered in b between rural and urban 302 environments, which is not shown in the SP, authors attribute this effect to the degeneracy of the SP. In the computation of the average of this quantity, degeneracy is 303 304 not taken into account because only the length is used and not the number of possible 305 SP between two given nodes. That is not the case for the betweenness, whose definition is based on this degeneracy N_{ik} (see Equation 4). The larger N_{ik} , the lower will be the 306 resulting value of betweenness for each node, leading to a final lower median for all 307 308 months and vice versa. Authors consider that the difference in the degeneracy among 309 areas can be related to the dynamics of tropospheric ozone for diurnal values. That is

because SPs always use mainly the highest values (*skyline hubs*) to cover most of the
distance between two nodes. As a result, a higher degeneracy can be interpreted as a
signal with a smoother envelope, because more options will be available to construct SP
with same lengths. The opposite for the case of irregular envelope can be argued using
the same reasoning.

315 4. <u>CONCLUSIONS</u>

316 On the whole, results show that the use of complex networks for analyzing temporal 317 series of tropospheric ozone is suitable to distinguish the dynamics in rural and urban areas. The probability distribution of the degree centrality P(k) identifies the nature of 318 the signals, being fractal for all the cases, as it was previously known (Jiménez-Hornero 319 320 et al., 2010; Pavon-Dominguez et al., 2013). Moreover, by looking at the values of \overline{k} and σ_k a seasonal behaviour has been observed. Besides, clear differences between rural 321 322 and urban locations can be appreciated from those values, specially in the case of the 323 average degree. Betweenness centrality has turned out to be a supplementary source of information for diurnal behaviour (envelope of the signals) and differences among 324 325 the studied locations. All these outcomes support the capability of complex network 326 analysis to describe ozone dynamics and transport from the urban to the rural environments. 327

To conclude, the advantages of using VGs for the analysis of time series and particularly from tropospheric ozone must be emphasized. In the last years, advances in the field of complex networks have made them a very convenient tool for several reasons: their computation efficiency, suitability for big data series and wide range of application, among others. In addition to that, since VG is a state-of-the-art methodology, it opens

multiple possibilities for future works. Authors consider appropriate to focus on the use of *multiplex visibility graphs* (Lacasa et al., 2015) to study multivariate time series. Furthermore, the concept of *skyline hubs* could be employed to identify relevant points in a time series, leading to different ways of understanding the betweenness centrality parameter applied to time series, similarly to degree *hubs*.

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Figure 1: Location of the air quality control stations from which the data was retrieved.
The image in the left-bottom corner shows the position of the studied area in the
Iberian Peninsula. Green area indicates the natural reservoir "Parque natural de Los
Alcornocales".

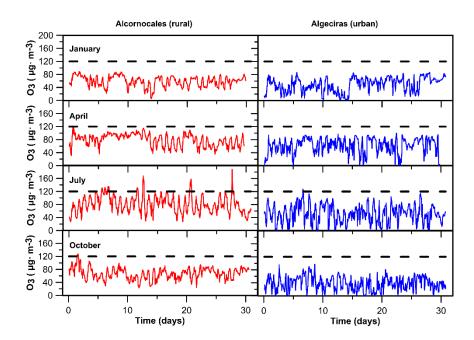


Figure 2: Examples of ozone concentration time series for four months and a given
year (2015) in two locations, one rural (red) and the other urban (blue). The dashed
line indicates the value 120 μg/m³ stablished as a reference (World Health
Organization, 2005).

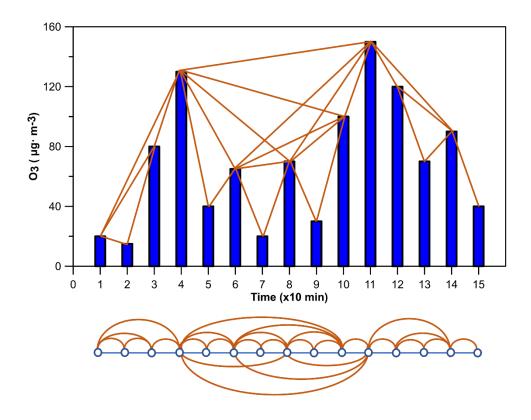


Figure 3: Sample time series transformed into a complex network through the
visibility graph algorithm. Below, all the connections are shown in a more visual
way.

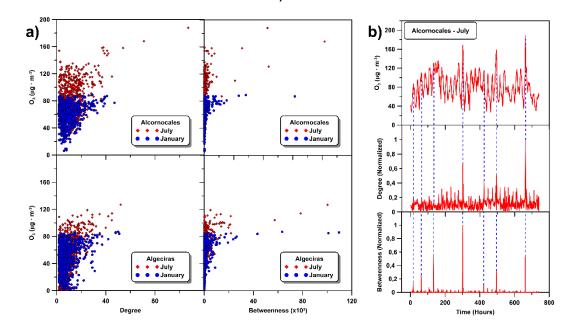


Figure 4: a) Plots of the values of tropospheric ozone concentration against the degree
and betweenness of each point. b) Temporal distribution of these two quantities and
the ozone concentration for a given month and location. Blue dashed lines in b) are
used to associate several peaks.

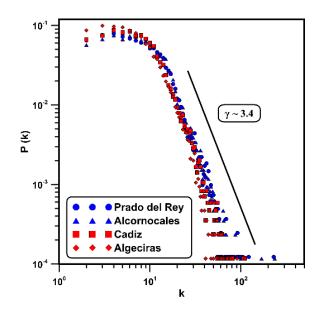


Figure 5: Annually degree distribution for the four places studied. The shown year
corresponds to 2015 as an example, since all the other years have been checked to
give equivalent information. The red and blue colors refer to urban and rural
environments, respectively.

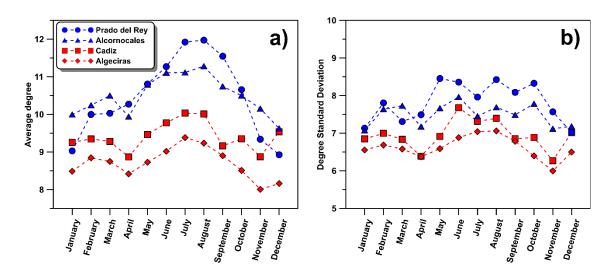


Figure 6: Computed average degree and standard deviation from the degree
distribution of each month in the four locations considered. Each monthly value is the
average of the computed ones from all the years available.

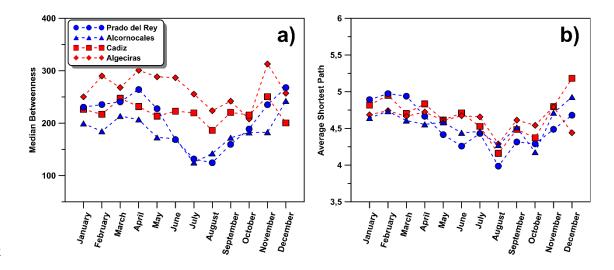


Figure 7: a) Median betweenness and b) average SP computed from the VG of each
month in the four locations. Blue values indicate rural area, while the red ones are
urban. Each monthly value is the average of the computed ones from all the years
available.

	Location	$\overline{O_3}(\mu g \cdot m^{-3})$	$\bar{\gamma}$
Northwestern	Prado del Rey	81 <u>+</u> 4	3.50 <u>+</u> 0.13
coast	Cadiz	69 <u>+</u> 3	3.37 <u>+</u> 0.25
Southeastern	Alcornocales	72 <u>+</u> 3	3.39 <u>+</u> 0.15
coast	Algeciras	54 <u>+</u> 5	3.40 <u>+</u> 0.12

509Table 1: Mean concentration and gamma exponent for each location (averaged for all510the years).

1 HIGHLIGHTS

- Ozone time series are converted to complex networks through the visibility
 graph.
- 4 Centrality measures are used to acquire information from the complex networks.
- 5 *Skyline hubs* are introduced as a tool to identify relevant points in a signal.
- 6 Urban-rural differences are exposed looking at degree and betweenness values.

