1 **The use of jackknifing for the evaluation of geographic profiling reliability**

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3

4 **Abstract**

5 The use of geographic profiling (GP), based on "Rossmo's formula", a technique derived from criminology, has

6 proven to be effective in assessing the origin of invading species of *Caulerpa* in the Mediterranean. The application on

7 *Caulerpa taxifolia* and *C. racemosa* var. *cylindracea* showed the most probable center of spread of the algae. This

8 article discusses a method of assessing the degree of robustness of the results obtained with Rossmo's method using the

9 same species.

10 To provide an evaluation of the reliability of geographic profiling results we used the jackknife technique;

11 randomly eliminating part of the data set for a given number of replicates (500) in order to analyze the obtained result

12 for each replicate. The results are a series of images with geoprofiling prioritization, each produced with one of the

13 replicates. These images can be summarized in three different ways: (1) OR, depicting all the high probability pixels

14 from the series of replicates; (2) AND, depicting only those high probability pixels present in every replicate; and (3)

15 MEAN, depicting the mean color value for each pixel calculated from all the replicates. We show that jackknifing can

16 be a useful method to increase robustness of GP analysis, both in criminology, epidemiology and biological invasions.

17 Summarizing jackknifing results with the OR logical operator yields highest robustness and worst precision, while the

18 use of the AND operator increases precision but reduces robustness. Using the mean of the pixel values maintains the

19 visualization of the areas of highest priority, while also showing the surrounding area with varying colors, with a

20 meaning analogous to confidence limits.

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22 **Introduction**

23 Geographic profiling (GP) is an analytical technique used in criminology, with the aim of calculating the most

24 probable origin of linked crimes, which is usually the offender's home. GP is used by police forces around the world to

25 help focus investigations and prioritize suspects in cases of serial crimes (Rossmo 2012).

26 GP input consists of spatial data about the locations of linked crimes, which is used to create a probability surface

27 to overlay on the map of interest in the form of a geoprofile (Rossmo 2000). GP does not provide an exact origin

28 location, but, instead, provides a prioritization pattern for investigation based on a descending order of the probability

29 height on the geoprofile (Rossmo 2000).

30   The model is based on two components: a distance-decay function, such that the probability of a crime (or other

31   events with a localization on a map) decreases with increasing distance from the offender's residence; and a buffer

32   zone, within which the probability increases with distance (Rossmo 2000). The distance-decay function is due to travel

33   costs – both for human criminals and invasive species – (Stevenson *et al.* 2012), in economical or energy terms,

34   respectively. The buffer zone is linked to the avoidance by criminals of locations too close to their residence. In

35   biology, the existence and the extent of the buffer zone should be analyzed case by case. For example, Dramstad (1996),

36   Saville *et al.* (1997), Singh *et al.* (2001) and Stevenson *et al.* (2012) showed evidence of a buffer zone in trees and bees.

37   GP has been used in biology to analyze the origins of infectious diseases (Le Comber *et al.* 2011, Verity *et al.*

38   2014), to predict the locations of multiple nest locations of bumble bees (Suzuki-Ohno *et al.* 2010), and to study the

39   patterns of animal foraging (Le Comber *et al.* 2006; Raine *et al.* 2009) and shark hunting (Martin *et al.* 2009).

40   Stevenson *et al.* (2012) used GP to identify the origin of the invasion of a species, starting from the current known

41   locations of their populations. The places colonized by the invasive populations were considered analogous to crime

42   sites, while the source or sources of the invasion were considered analogous to the criminal's home. The same authors

43   tested GP in comparison to other spatial techniques, such as the center of minimum distance, the spatial mean, the

44   spatial median and a single parameter density model. GP gave better results compared to the other techniques in 52 of

45   the 53 data sets explored for invasive species in Great Britain. Stevenson *et al.* (2012) provided a list of values for the

46   buffer zone radius evaluated as the most appropriate in their analysis. The technique was applied with success on

47   biological invasions of algae (Papini *et al.* 2013) and insects (Cini *et al.* 2014).

48   Invasive species are considered to be one of the main causes of biodiversity loss (Vitousek *et al.* 1996; Wilcover *et*

49   *al.* 1998). Invasive species can damage native species through predation and competition, by modifying ecosystem

50   functions and by altering the abiotic environment and by spreading pathogens (Strayer *et al.* 2006; Ricciardi and Cohen

51   2007 Pimentel et al. 2005).

52   The invasion of macroalgae, such as some species belonging to genus *Caulerpa* (Caulerpales, Chlorophyta) is one

53   of the main threats to marine natural environments (Meinesz *et al.* 2001). Two species of *Caulerpa* J. V. Lamouroux,

54   *Caulerpa taxifolia* (Vahl) C. Agardh and *C. racemosa* (Forskål) J. Agardh var. *cylindracea* (Sonder) Verlaque,

55   Huisman and Boudouresque, caused severe biological pollution (Piazzi *et al.* 2005) in the Mediterranean. One

56   interesting feature of this invasion is that the origin is known - an accidental release from the aquarium of Monaco in

57   1984 (Meinesz and Hesse 1991; Meinesz *et al.* 2001; Turan *et al.* 2011). Geographic profiling of the invasive caulerpas

58   spread in the Mediterranean was already used with success by Papini *et al.* (2013), taking advantage of the fact that the

59   spreading origin of *Caulerpa taxifolia* is known, and the related data set is a good starting point for calibrating the

60   technique.

The GP analysis applied to biological invasions has certain limitations: the results obtained with Rossmo's formula are based on the postulate that all spreading events should come from one or a limited number of origins, which is not always true for biological invasions where secondary sites of invasion may frequently derive from the original primary or more independent introductions may occur (Santosuosso and Papini 2016). Furthermore, vegetative propagation and other "slow" ways of environmental spread may obscure the general pattern (Papini *et al.* 2013).

An alternative approach may be a series of geoprofiles using different time periods for the data (e.g., year 1, year 2, year 3, etc.), a technique already used with success in crime analysis (Rossmo and Velarde 2008). Such an approach allows for a better understanding of the spread from secondary sites, reducing the "noise" in the data. This was the approach taken by Stevenson *et al.* (2012), who fitted the parameters of the model using a maximum likelihood approach from a time series. Moreover, almost certainly some of the sites of the invading algae are unknown, making the final result approximate (Papini *et al.* 2013). This is also frequently true in criminology where the accuracy of data used for GP may affect the accuracy of the analysis (Snook *et al.* 2005 and Rossmo 2005).

A possible method to analyze the effect of the errors derived from the limitations linked to the geoprofile is the use of data resampling techniques such as jackknifing or bootstrapping (Miller 1974, Efron 1979, 1972, Efron and Tibshirani 1986, 1993). Both methods are commonly used in other biological analyses (Manly 2006); for example, bootstrapping is commonly used to assess the robustness of phylogenetic analysis (Felsenstein 1985). The two methods are very similar, consisting both in a random deletion of part of the data, with the jackknife using such a reduced data set, while the bootstrap substitutes the deleted data by duplicating some of the remaining data items (Meyer *et al.* 1986).

In this study, we used the jackknife technique (Miller 1974, Efron 1979) to test the robustness of a GP analysis. After van Belle *et al.* (2004), a statistical or an analytical procedure is robust if it performs well when the needed assumptions are not violated "too badly." After the same authors it is not a strictly mathematical definition, but robustness should provide a measure of the confidence limits of the obtained results. Even Umeton et al. (2011) defined robustness as "Robustness is the persistence of a system property respect to perturbations". In the case of the geographic profiling, the jackknife technique should provide an idea of the robustness of the analysis and of the confidence within which we can look for the point of origin of the sites of biological invasion by *C. racemosa* var. *cylindracea*. The assessment of the confidence limits of geographic profiling may be extended to other analyses, including those outside the field of biological invasions.

For assessing robustness, it is possible to create new data sets simply by resampling the observed data. Such an analysis requires to take a series of subsamples from data set a given number of times. Some observations appear once, others twice, others not at all (van Belle *et al.* 2004). In jackknifing, a part of the sample is systematically omitted, for

example by removing one data point at a time, and the analysis is then carried out for each newly constructed subset (Efron 1982; Efron and Tibshirani 1993).

Materials and methods

The model for geoprofiling analysis was described by Rossmo (2000), who compared the use of Manhattan and Euclidean distances, preferring the former to describe criminal movement in urban areas. However, Le Comber *et al.* (2006) and Stevenson *et al.* (2012) suggested that Euclidean distances are more appropriate for animal and plant movements in nature.

The geographic profiling function generates a surface where each pixel has a different priority score indicating the optimal search pattern for the sources of invasive species (Stevenson *et al.* 2012). For each pixel with coordinates (i, j) of the target area, the score function (p) is calculated as follows (Rossmo 2000):

$$p_{ij} = k \sum_{n=1}^{C} \left[\phi_* / (|x_i - x_n| + |y_j - y_n|)^f + (1 - \phi)(B^{g-f})/(2B - |x_i - x_n| - |y_j - y_n|)^g \right]$$

where

$$\phi_* \text{ is equal to 1 if } |x_i - x_n| + |y_j - y_n| > \text{B; 0 otherwise}$$

In this formula rapresentation it is used Manatthan metric: "$|x_i - x_n| + |y_j - y_n|$".

For point p with coordinates (i, j), the formula sums the probability across all the locations where the invading organism was found. After Rossmo (2000), Φ functions as a switch that is set to 0 for sites within the buffer zone, and 1 for sites outside the buffer zone. k is an empirically determined constant, which was set to 1 in our study. B is the radius of the buffer zone, and C is the number of events (in this case the reports about the presence in a given locality of the invader). f and g are parameters that control the shape of the distance-decay function on either side of the buffer zone radius. For our analysis we used the same parameters as in Papini *et al.* (2013). The parameters specify the increase in dispersal probability moving away from the source, reaching a maximum value at a distance equal to the radius of the buffer zone. This reflects the reduced probability of dispersal within the buffer zone and the fact that dispersal probability declines with distance (Stevenson *et al.* 2012).

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119   This function produces a search priority surface for the inputted locations on the user-provided map (Rossmo

120   2000). Rossmo described the equation as a curve, which, when plotted in three dimensions, resembles the shape of a

121   volcano with a caldera. The sum of these 'volcano' shaped decay functions produces a surface describing an optimal

122   search pattern for the location of the origin of the species invasions. To check the robustness of the results we

123   performed a jackknife (Miller 1974) analysis of the data set. We omitted 20% of the observations from the data sets for

124   each of 500 replicates. The number of necessary bootstrap replicates is a controversial issue. We followed the indication

125   by Pattengale *et al.* (2010) proposed for phylogenetic analysis (100-500 replicates). For each replicate, we performed a

126   geoprofiling analysis. The points in the map with highest priority were represented as red pixels (best 5%) and green

127   pixels (best 10%). The final result obtained after the jackknife procedure resulted in a final image where the position of

128   the red pixels and of the green pixels obtained in each replicate were combined with two logical operators (AND, OR)

129   and the mean value of the pixels (see below), using a Python script (jack.py) written by the authors. We used the known

130   invasion origin of *C. taxifolia* (Monaco) to calibrate our model, estimating the critical and map-dependent parameters B,

131   f, and g.

132   The distribution data for the invasive *Caulerpa* were obtained from Jousson *et al.* (1998) for *C. taxifolia* (since in

133   this case the spreading origin is known) and from Verlaque *et al.* (2003, 2004) and Piazzi *et al.* (2005) for *C. racemosa*

134   var. *cylindracea*.

135   Our programs were written in Python 2.6.4 (http://www.python.org/) and run on an Ubuntu 9.10 Karmic Koala

136   (http://www.ubuntu.com/) Operating System, Linux kernel 2.6.31. PIL (Python Imaging Library 1.1.6,

137   http://www.pythonware.com/products/pil/) was installed.

138   The results (Images) were blended with the original map with Python commands (see Software notes in

139   Supplementary material). The Python programs are released under GPL license and available at

140   www.unifi.it/caryologia/PapiniPrograms.html. The maps were downloaded from Open Street Map, available at

141   http://www.openstreetmap.org.

142   The images obtained with each jackknife replicate were summarized in three ways:

143   1. OR – the final image shows all the high probability pixels from any of the replicates, resulting in a

144   larger peak probability geoprofile area (corresponding in set theory to the union of the sets of high

145   probability pixels from each replicate).

146   2. AND – the final image shows only those high probability pixels that were present in every replicate,

147   resulting in a smaller peak probability geoprofile area (corresponding in set theory to the intersection

148   of the sets of high probability pixels from each replicate).

149   3. MEAN – the final image shows the mean color value for each pixel of coordinates (x, y), based on all

150   the replicates. This last method provides a zone with the RGB color corresponding to the AND zone

151   (the mean of the pixels found in the AND image are the same as they have the same high probability

152   value in every replicate), plus a zone with varying minor priority values obtained from the mean of

153   the different RGB values corresponding to the probability values in each replicate. This second

154   relaxed zone can be considered a fuzzy set (*sensu* Zadeh 1965) of varying priority pixels. This image

155   offers a general representation of the robustness of the analyzed data with respect to the AND or the

156   OR method

157   In Fig. 1 we show how 3 (example) images deriving from hyphotetical jackknife replicates can

158   be summarized with AND, OR and MEAN methods.

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161 **Results**

162   Figure 2 shows a summary of the jackknife images with the OR logical operator applied on the dataset of *C.*

163 *taxifolia*. As a result the number of red pixels (indicating maximum probability) is quite high, compared to the

164 following figures. Figure 2a is a higher magnification of this zone. Figures 3 and 3a show the result of the AND

165 technique, which showed no red pixels. That is the resampled data sets did not produce overlapping red areas. . Figures

166 4 and 4a show the results of the MEAN technique. The areas around the peak probability location show degrading RGB

167 values corresponding to varying probability values obtained by averaging the RGB values obtained from the whole

168 jackknifed data set. As a consequence, while there is an area of pure red pixels (RGB values 255,0,0), other shades of

169 red appear as a result of averaging various RGB values in a given point.

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172 **Discussion**

173   To provide an evaluation of the geographic profiling results we used the jackknife technique, which involves

174 randomly eliminating part of the data set for a given number of replicates followed by the reanalysis of the remaining

175 data. The results are a series of images with geoprofiling prioritization, each produced with one of the replicates. The

176 images can be summarized in three ways: (1) OR logical operator, showing all the high probability pixels from any of

177 the replicates (the set union); (2) AND logical operator, showing only those high probability pixels present in all the

178 replicates (the set intersection); and (3) MEAN, the mean probability value for each pixel calculated from all the

179 replicates.

180   The expansion of the red pixels with the OR logical operator is expected; as the robustness of the result increases,

181 the resolution decreases and the precision of the analysis is reduced. This is probably the most common way to integrate

182 the information from a series of bootstrap or jackknife replicates, as seen, for instance, in clinical investigations

183 (Steyerberg *et al.* 2006). The AND logical operator has the opposite effect as it takes into consideration only the red

184 pixels present in all the jackknife replicates. Consequently, the precision of the analysis increases, but not so the

185 robustness. The MEAN method stands somewhere in the middle of the two other methods. The highest priority pixels

186　found in the AND image are still red (if present), while other pixels prioritized in the OR image are shown in lighter

187　shades of red indicating their lower probability.

188　　All three methods provide useful information, with the OR maximizing robustness and the AND maximizing

189　precision. The MEAN method summarizes the information arising from both the AND and the OR logical operator and

190　provides a more synthetic summary of a jackknife analysis in this context.

191　　In conclusion, jackknifing can be a useful method to increase robustness of GP analysis in criminology,

192　epidemiology and biology. The concept of confidence limits is fundamental for assessing estimates of a parameter (Cox

193　and Hinkley 1973) or a series of parameters, for instance, the phylogenetic reconstruction of the relationships between

194　species (Felsenstein 1985). While in phylogenetic analysis the confidence limits of a phylogenetic reconstruction is

195　expressed as a percentage above branches of phylogenetic trees (for instance Fesenstein 1985 and Simeone et al. 2016),

196　as the results of geoprofiling are images, the confidence limits must be represented on the image itself. Summarizing

197　jackknife results with the OR logical operator yields the highest robustness and the worst precision, increasing the

198　number of highlighted pixels in the image, while the use of the AND operator increases precision but reduces the

199　number of highlighted pixels in the image and hence decreases robustness. Using the mean of the pixel values maintains

200　the visualization of the areas of highest priority, while also displaying the surrounding area using different colors,

201　providing information analogous to confidence limits.

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206　**References**

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310 **Figure Captions**

311   Figure 1 - Three (example) images deriving from hypothetical jackknife replicates can be summarized

312   with AND, OR, MEAN and even MODE methods. 1a, 1b, 1c represent three hypothetical different

313   areas of probability (only red pixels reported on figures) obtained from three GP analysis on three

314   datasets derived from Jackknife. 1d: OR summarization: all points that were red in just at least one of

315   the three starting figures are red also in the final figure. 1e: MEAN summarization: in each point of

316   the final figure, the color will correspond to the mean values found in each of the starting figures.

317   Only where the red pixels are present in a position (x, y) in all the jackknife-obtained figures (here

318   three of three), there will be plain red even in the final figure. 1f: AND summarization: Only where

319   the red pixels are present in a position (x, y) in all the jackknife-obtained figures (here three of three),

320   there will be plain red even in the final figure. In the rest of the final image, only white pixels can be

321   found.

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323 Figure 3 – OR image, showing all the high probability pixels from the replicates (corresponding to the union of the high

324 probability sets). Figure 3a – Higher magnification of the peak probability area.

325 Figure 4 – AND image, showing only those high probability pixels that were present in every replicate (corresponding

326 to the intersection of the high probability sets). Figure 4a – Higher magnification of the peak probability area. No red

327 pixel is present, that is the condtion of presence in all the images is not respected.

328 Figure 5 – Mean image, showing the mean color value for each pixel (corresponding to the AND image zone, plus a

329 varying RGB color zone corresponding to pixels found with high probability in only some replicates). Figure 5a –

330 Higher magnification of the peak probability area.

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