Area and Feature Guided Regularised Random Forest: a novel method for predictive modelling of binary phenomena. The case of illegal landfill in Canary Island

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ABSTRACT

This paper presents a novel method, Area and Feature Guided Regularised Random Forest (AFGRRF), applied for modelling binary geographic phenomenon (occurrence versus absence). AFGRRF is a wrapper feature-selection method based on a previous modification of Random Forest (RF), namely the Guided Regularised Random Forest (GRRF). AFGRRF produces maps that minimise the affected area without a significant difference in accuracy. For this, it tunes the GRRF hyper-parameters according to a trade of between True Positive Rate and the affected area (Success Rate). AFGRRF also addresses the ‘Rashomon effect’ or the multiplicity of good models. The proposed method was tested to model illegal landfills in Gran Canaria Island (Spain). AFGRRF performance was compared to that of other RF-based methods: (i) standard RF; (ii) Area Random Forest (ARF); (iii) Feature Random Forest (FRF); (iv) Area Feature Random Forest (AFRF) and (v) GRRF. AFGRRF predicted the smallest affected area, 19% of the island, at a similar True Positive Rate. This percentage is substantially smaller than the one predicted by RF (27.43%), ARF (26%), FRF (27.78%), AFRF (23%) and GRRF (29.67%).

1. Introduction

Predictive modelling algorithms identify and learn patterns between a target feature and other independent features from a given subset of training samples. Hence, predictive modelling enables estimation of said target feature’s behaviour using independent features, regardless of when it occurred (past, present or future), whereas forecasting makes projections into the future (Breiman 2001a, Quesada-Ruiz et al. 2019a). Predictive modelling has become an important tool for mapping the distribution of multiple geographical phenomena in Earth sciences (Soares and Pereira 2007, Dahal et al. 2008, Tehrany et al. 2013). These phenomena are often binary in nature.
i.e. occurrence: the absence or presence of the phenomenon (Breslow and Cain 1988, Schill et al. 1993, Carranza et al. 2008).

Following Rodriguez-Galiano et al. (2012), an occurrence map may be considered appropriate, in addition to being accurate, when: (a) the spatial distribution of the phenomenon is consistent with respect to the most important explanatory features; (b) it is replicable, achieving a certain stability in the predicted values and (c) the phenomenon is not over or underestimated. Ignoring this latter aspect may lead to cost overruns for many tasks, especially when we use GIS methods applied to binary mapping. Examples of this include: landslide prevention (Dahal et al. 2008, Harris and Grunsky 2015, Hong et al. 2017, Chen et al. 2019), where potentially affected areas must be defined to efficiently locate slope-stabilisation actions; flood prevention (Tehrany et al. 2013), requiring the construction of containment walls against possible floods; ecosystem conservation (Poulos et al. 2016, Huettmann et al. 2018, Zhang et al. 2019), where estimation of the presence and/or absence of the various habitats of an ecosystem helps to facilitate their respective management; and infectious disease (Cecchi et al. 2009, Bhunia et al. 2012, Iftimi et al. 2015) and agricultural pest control (Wittmann et al. 2001, Porretta et al. 2013, Kumar et al. 2016), which require locating the area that contributes to the spread of a given pathogen, as well as predicting the potential area that might be affected in future. In this sense, the concept of potentially affected area (hereafter affected area) is central to the predictive modelling of binary phenomena and refers to areas that may suffer or withstand potential damage or risk (i.e. areas with non-zero probability).

The accuracy of predictive modelling is largely grounded on the classification method and its optimisation using the training data (Foody 2004, Visser and Nijss 2006). Methods for predictive modelling have different abilities to learn patterns, sometimes needing a specific statistical distribution in the features (i.e. normality) (Rodriguez-Galiano et al. 2014, Leuenberger and Kanevski 2015, Arabameri et al. 2019). However, other aspects that have traditionally received less attention, such as the metrics for assessing performance or Feature Selection, are also important, and might have an impact on both the area and the spatial distribution (Rodriguez-Galiano et al. 2018). Predictive models are typically built using large sets of explanatory features (e.g. information about geology, biology or socioeconomic factors, etc.). However, even if the number of samples is notably larger than the number of features, high feature space dimensionality can overwhelm the method’s learning capacity (the curse of dimensionality; Chen 2009). Also, selecting a large number of features would lead to models that are difficult to both interpret and replicate. Thus, dimensionality reduction is often needed. Dimensionality reduction is primarily achieved by Feature Extraction or Feature Selection. Feature extraction methods reduce data down to a smaller representative set, projecting these into the most relevant directions of a lower feature space, as in the case of the Principal Component Analysis method (Lucas and Jauzein 2008, Menció and Mas-Pla 2008, Canela et al. 2011). Conversely, feature selection methods do not modify the features of the original data; rather, they select a reduced yet meaningful feature subset, improving both interpretability and the accuracy of the model (Blum and Langley 1997, Dash and Liu 1997, Guyon and Elisseeff 2003). Some negative effects could thus be averted using feature selection, such as (Rodriguez-Galiano et al. 2018): (i) model overfitting; (ii) limitation of the model’s interpretability due to high complexity; (iii) loss of generalisation capacity
and (iv) a significant increase in computational time. A controversial aspect of feature selection is the multiplicity of good models, which is also common in statistical algorithms, such as multiple regression or logistic regression. Different feature subsets might share good and similar accuracy, thus resulting in a non-unique solution or physical model explaining a phenomenon (Rashomon effect, Breiman 2001b).

Among the different approaches for feature selection, filters, embedded and wrapper methods stand out (Hall and Smith 1997, Tuv 2009). Filters select features regardless of the predictive model and accuracy of predictions (e.g. linear correlation) (Guyon and Elisseeff 2003, Dixon 2005). Current approaches include embedded methods, which are algorithms that include an internal estimate of a feature’s importance based on different metrics, such as gain or mean decrease in accuracy. Some examples of this algorithm type are decision trees or Random Forest (RF). However, embedded methods only provide a ranking of a feature’s importance and do not determine the optimal number of features (Bazi and Melgani 2006, Tuv 2009, Pal and Foody 2010, Rodriguez-Galiano et al. 2012). Finally, wrapper-based approaches select an optimal subset of features, repeatedly and automatically training the model with different subsets (Guyon and Elisseeff 2003). The design of the wrapper algorithm for feature selection requires three components: a predictive algorithm (i.e. RF, support vector machines or neural networks), a method for searching in the feature space (i.e. forward or backward deterministic search, exhaustive search, genetic algorithms etc.) and a metric for evaluating performance (i.e. RMSE in the case of regression, Receiver Operating Curve (ROC) or overall accuracy in the case of classification) (Rodriguez-Galiano et al. 2018). Wrappers are thus very computationally intense algorithms (Hall and Smith 1997, Navin Lal et al. 2006). RF-based algorithms are well-suited to building wrappers because of their low sensitivity to hyperparameter tuning and their robustness and speed from a computational standpoint (Breiman 2001a). Various RF-based wrapper methods have been proposed in Earth sciences, using either sequential search (Rodriguez-Galiano et al. 2018) or exhaustive grid search, such as Guided Regularised Random Forest (GRRF) (Deng and Runger 2013, Izquierdo-Verdiguier and Zurita-Milla 2020). This paper presents the Area and Feature Constrained Random Forest (AFGRRF) binary classification method. The proposed method is a new machine learning feature selection method that can also be used for predictive modelling. Other specific objectives include: (i) assessing the application of different Random Forest based algorithms to binary mapping; (ii) reducing the affected area and therefore the environmental management costs for binary phenomena.

2. Afgrrf classification method

2.1. Modelling background

AFGRRF is a modification of the GRRF algorithm that prevents an overestimation of the affected area by optimising both the True Positive Rate (TPR) and the affected area via Success Rate (SR) application (see Section 2.3). AFGRRF may be a novel way to address the Rashomon effect, by selecting the feature subset from among multiple good predictive models that leads to a smaller affected area. The proposed method is tested in a case study to predict the possible distribution of illegal landfills (ILs) on Gran Canaria island in Spain. Gran Canaria is an island within the Canary archipelago, which are an
outermost region of the European Union and a Spanish autonomous region. Gran Canaria has an area of 1560 km\(^2\) and is the second most populated among the islands (845,000 residents) after Tenerife (891,000 residents) (INE 2016a). The population of Gran Canaria is mainly located in coastal areas, while the interior is less populated. The Canary Islands rank eighth within the Spain’s gross domestic product. According to Cruz et al. (2011), the major driver of economic activity on Gran Canaria is the tourism, which has led to a strong boost in the construction sector. Tourism on Gran Canaria is fundamentally beach-related, being concentrated in the South of the island. Around 4.2 million people visited the island in 2016 (INE 2016b). The Canary Islands comprises a small and fragmented territory where space is a lack of resource, limiting and hampering territorial planning and land-use management. Hence, the creation of waste-management infrastructures (GOBCAN 2015, 2008) and the containment of ILs is an important challenge (GOBCAN 2015 2008, Quesada-Ruiz et al. 2019a, 2019b). IL are an environmental management problem for the Canary Islands as in many countries, harming the environment, human health and local economies (Quesada-Ruiz et al. 2019b).

The primary impacts of IL are local landscape deterioration, air pollution, aquifer pollution and increased risk to human health (Bridges et al. 2000, Monteiro Santos et al. 2006, Ichinose and Yamamoto 2011). The cost associated with locating and remediating IL has been estimated per year, for example by (i) the Environment Agency of the United Kingdom, at 120–175 million euros in the UK; (ii) The Queensland Government (Australia), at 4 million euros (EUR 420 per tonne) (Glanville and Chang 2015); (iii) The Pennsylvania Department of Transportation in the United States, with an annual tax cost for waste clean-up of approximately 8.6 million euros (EUR 710 per tonne) (PPRC 2016). Moreover, waste management on the Canary Islands is more challenging than in other places due to a lack of waste facilities (Quesada-Ruiz et al. 2018). Gran Canaria has experienced an increase of 317.7 ha in areas affected by IL between 2000 and 2012 due to urban sprawl and the housing bubble (Quesada-Ruiz et al. 2019a). Previous studies have identified ‘construction and demolition waste’ as the most abundant IL typology in Gran Canaria (Quesada-Ruiz et al. 2018). Additionally, the lack of dissuasive measures in more than 95% of IL cases reflects the urgent need for monitoring and prevention policies (Quesada-Ruiz et al. 2018). Hence, an accurate delimitation of IL-affected areas would reduce control and monitoring costs, supporting the implementation of deterrence measures such as environmental control patrols or installation of video cameras and posters, optimising and delimiting areas where prior intervention was implemented. On the other hand, it could help to local government to create citizen participation programs, encouraging the prevention of IL by the citizen participation and increasing their opportunities to utilise waste treatment infrastructures, with the objective of meliorate waste collection process and environmental education policies in those areas (Quesada-Ruiz et al. 2018).

This case study was selected because ILs are clearly binary in nature, i.e. they either exist or do not exist. Hence, they are suitable to test the applicability of the proposed method. Moreover, ILs represent a problem that requires significant economical resources and manpower from local authorities in order to control and manage them. Thus, further optimisation in modelling them helps to reduce the environmental management costs (Ichinose and Yamamoto 2011, Glanville and Chang 2015), which are mainly waste disposal and site remediation, and surveillance costs of landfilling (Tasaki et al. 2007).
2.2. Modelling principles

AFGRRF is a new algorithm that can be applied in the GIS framework for selecting feature subsets for mapping binary phenomena, applied in this case to predictive modelling of ILs. AFGRRF carries out a regularisation and an exhaustive grid search identical to the GRRF method (Deng and Runger 2013, Izquierdo-Verdiguier and Zurita-Milla 2018, 2020). AFGRRF generate multiple models based on different feature subsets spatially related with the occurrence of IL according to the 100 possible combinations of the gamma and lambda values (Figure 1), being their corresponding values between 0.1 and 1 by intervals of 0.1. AFGRRF trains multiple soft classification models with RF using the different feature subsets generated from the Guided Grid search regularisation. Each soft map built from different feature subsets is reclassified iteratively based on the SR. The results of SR can be shown in a graph where the TPR for different IL affected area percentages is represented (see Figure 7). The TPR (true positives/(true positives + false negatives)) is computed by finding the binary class probability membership threshold values that split the map in different affected areal quantiles. The TPR value is computed for each map reclassified as affected and unaffected by IL using an independent test. The model that is finally selected by AFGRRF is the one that is obtained from the feature subset that leads to the minimum IL affected area at a TPR equal to or greater than 90%. This TPR reference value can also be adjusted and modified according to the needs. Therefore, AFGRRF is based on optimising SR and minimising the IL potential affected area, serving as an alternative to traditional wrappers, which are based on overall accuracy. In that sense, the method proposed use a widely feature subset of possible features related to the ILs problem, such as distance to coast or distance to industrial areas, and selected the features or possible combinations of features according to their spatial distribution and relation with ILs occurrence. Hence, the method tries to map the minimal affected areas of ILs in a most accurate way, considering the ILs sample distribution, for reducing the cost of surveillance, recovery and restauration of the new possible potential affected areas. AFGRRF pseudocode could be summarised as follows:

1. Train a RF model.
2. Obtain the embedded RF importance.
3. Guided Grid search regularisation
   a. Initialise an empty subset of selected features and a threshold gain ($G^* = 0$)
   b. Fix the values of $\lambda$ and $\gamma$ to calculate $\alpha$.
   c. Computation of $G_{GRRF}$
   d. If, $G_{GRRF}(x_j, \nu) > G^*$ the feature $j$ is selected and the threshold gain is updated to the GRRF gain. Otherwise, the feature is not selected.
4. Multiple soft RF models are built from the various feature subsets.
5. Feature subset selection based on SR
   a. Each soft map is reclassified into multiple binary hard maps considering different percentages of affected area (pixel quantiles)
   b. TPR is computed for all binary maps at increasing areal percentages for each feature subset.
6. Model selection based on a trade-off between TPR and minimal area from SR.
2.3. Accuracy assessment metrics

Besides the wrapper's general performance metrics (overall accuracy or Kappa), other metrics are also used for binary classification, such as: the percentage of true positives.
and true negatives, and the percentage of false positives and false negatives (Fawcett 2006, Powers 2007). The true positives and true negatives represent the number of successes between the predicted values and real values for locations where a phenomenon is present and absent, respectively. The false positives and false negatives measure the percentage of errors between the predicted values and real values for locations where a phenomenon is present and absent, respectively. A good model will thus be one that contains a high percentage of true positives and true negatives and a low percentage of false positives and false negatives. Therefore, analysing false positives to avoid overestimations is just as important as analysing false negatives to avoid underestimations. However, none of these metrics take into consideration both the accuracy of the classifications and the extent of the area affected by a phenomenon. Binary maps, such as the occurrence of ILs, might be improved from the standpoint of economic cost of remediation and monitoring, if feature selection was optimised using metrics that consider both the accuracy and the extent of the affected area, such as the success rate (Chung and Fabbri 1999).

SR represents the TPR for binary predictive maps with increasing affected area (Chung and Fabbri 1999). The SR is represented in a graph with the TPR on the y axis and different affected area percentage on the x axis (see Figure 7). The maps for increasing areal percentages are computed by reclassifying taking into consideration the classification probability threshold values at different quantiles. The TPR is computed for each map using an independent test. This way, a map at a good accurate level (TPR) that minimises the affected area can be chosen when success rate function converges.

3. Experimental validation

3.1. Experimental data

An IL database for GC (Figure 2) was used for the experimental design. It was generated by interpreting digital orthophotos for the years 2012 and 2015 and through complementary field work in which 387 potential locations were visited (Quesada-Ruiz et al. 2018). 286 IL locations were obtained after filtering out IL that were less than two years old and with an area smaller than 2000 m² with a view to rejecting temporary and small dump sites (Quesada-Ruiz et al. 2018). Information on socioeconomic aspects obtained from the Spanish National Institute of Statistics (e.g. per capita income, population, industrial and tourism activity indices), as well as geomorphology was obtained for the study area from Spanish National Institute of Geography. After preliminary process, 117 features (see supplementary material: Table 1a and Table 1b) that could be linked to IL occurrence were derived from this information (Biotto et al. 2009, Alexakis and Sarris 2014, Quesada-Ruiz et al. 2019b), such as population size and density, per capita income, industrial and touristic activity indices, elevation and slope, etc. New features were extracted from this initial feature set using different GIS analysis procedures (Şener et al. 2011, Demesouka et al. 2014, Uyan 2014, Akbari and Rajabi 2017): interpolating socioeconomic information aggregated by population centres; considering the calculation of Euclidean distance between the IL location and elements of interest, such as infrastructure, equipment, population centres, coast, land use etc. (Biotto et al. 2009, Tasaki et al. 2007) computing kernel densities of elements of interest, such as
communication routes or buildings, and other distance-based search functions for different radio (250 m, 500 m, 1500 m) (Silverman 1986). Additionally, the Normalised Difference Vegetation Index (NDVI) (Silvestri and Omri 2008) was obtained from a SPOT-5 summer image for 31st August with 11% of cloud coverage and 10 m of spatial resolution. The primary features were rasterised, standardised and resampled at a spatial resolution of 10 m. Table 1 shows the main features used in the experimental design grouped by typology. Following Carranza et al. 2008, the database was completed by including no-IL locations (i.e. places free of IL) to distinguish areas of negative IL occurrence, carrying out a stratified random sampling (Quesada-Ruiz et al. 2018). The negative and positive IL occurrence locations were coded as 0 s and 1 s, respectively, with an overall result of 286 negative samples and 286 positive samples. All feature values were obtained for both negative and positive IL locations.

3.2. Experimental design

The performance of AFGRRF was compared to a baseline composed of five different RF methods: (i) Random Forest (RF); (ii) Area Random Forest (ARF); (iii) Feature Random Forest (FRF); (iv) Area Feature Random Forest (AFRF) and (v) GRRF. The hard classification methods (RF, FRF and GRRF) produce categorical maps, considering by default an arbitrary threshold value of 0.5 in the class conditional probability. The soft classification methods (ARF, AFRF and AFGRRF), which predict a class conditional probability, were assessed in terms of the smallest affected area at a TPR equal or higher than 90%. In this sense, the soft classification methods estimate the class conditional probabilities and after perform classification based on estimated probabilities. Each method used 500 trees and default mtry parametrisation (square root of the number
of features) to ensure the stability of the results. RF was an embedded method without feature selection to generate a hard classification model. FRF was a wrapper for feature selection that used RF embedded importance and a forward sequential search. Forward sequential search starts from the empty feature space and adds by steps the most important features until the value of a given performance metric decreases (Rodriguez-Galiano et al. 2018). Instead of a sequential search, GRRF was a wrapper that used a regularisation based on a grid search. In this sense, the GRRF model used different gamma and lambda values to obtain multiple feature subsets, enabling us to obtain multiple hard classification models and choose the one with the highest overall accuracy. On the other hand, ARF, AFR and AFGRRF used the same procedure as RF, FRF and GRRF, respectively, to obtain soft classification models. Nevertheless, ARF, AFR and AFGRRF maps are derived from the SR function, by reclassifying iteratively the class-conditional probabilities map for different affected area percentages (Figure 3) and choosing the best map for every method as that with the smallest affected area at a TPR higher than 90% threshold.

Three subsets were generated from the initial IL database to train and assess the method’s performance: training (60%), test 1 (20%) and test 2 (20%) (Ng 2018). We used this percentage in order to maintain a reasonable number of test samples. Test 1 was used as an internal validation for GRRF and AFGRRF, and test 2 to compare GRRF and AFGRRF with other RF-based methods. The McNemar test was applied between the best map generated by each method (ARF, AFRF and AFGRRF) (Foody 2004) to evaluate whether the differences between model accuracies were significant. It should

| Feature typology     | Units               |
|----------------------|---------------------|
| Socioeconomic        |                     |
| Population density   | km$^{-2}$           |
| Mining and extraction activity index | %     |
| Industrial activity index | %     |
| Distance             |                     |
| Distance to pit zones | m                  |
| Distance to transport infrastructure | m     |
| Distance to pit zones with different kernels | m     |
| Distance to transport infrastructures | m     |
| Distance to element of interest | m     |
| Distance to educational equipment | m     |
| Distance to coast     | m                  |
| Distance to protected areas | m     |
| Distance to cultural equipment | m     |
| Distance to agricultural areas | m     |
| Visibility           |                     |
| Visibility from the coastline | Unitless |
| Physiographic        |                     |
| Slope                | %                  |
| Altitude             | m                  |
| NDVI index           | Unitless           |
| Density              |                     |
| Buildings density    | km$^{-2}$          |
| Land use transitions density from 1990 to 2000 | km$^{-2}$ |
| Land use transition density from 1990 to 2012 | km$^{-2}$ |
| Impervious cover transitions density from 1990 to 2012 | km$^{-2}$ |
| Greenhouses density  | km$^{-2}$          |
| Communication routes density | km$^{-2}$ |
be noted that, in this case the interpretation of the McNemar test is backwards when compared to traditional studies on the evaluation of new classifiers, where it expected that the algorithm significantly outperforms a baseline. We therefore formulated two...
hypotheses: $H_0$) the models induced significant changes in the responses, i.e. the changes seen in the sampling were not due to chance; and $H_1$) the models did not induce significant changes in the responses, i.e. the changes observed in the sampling were due to chance. Results with statistical confidence above 95% were considered. Values lower than 1.96 in the McNemar test would imply that the maps are not significantly different (Foody, 2004), thus rejecting $H_0$.

4. Experimental results

The GRRF and AFGRRF methods (Table 2) were used to build 100 models (all possible combinations between lambda and gamma values). The most accurate GRRF model obtained lambda and gamma values of 1 and 0.3, respectively, with an overall accuracy of 94.59%. The best AFGRRF model obtained lambda and gamma values of 0.9 and 0.2, respectively, with an overall accuracy of 93.62%. Models with higher lambda values and lower gamma values outperformed the rest (Figures 4(B,C)). Nevertheless, exclusively considering overall accuracy did not minimise the affected area. In this sense, GRRF and AFGRRF estimated an affected area of 29.67% (462.80 km²) and 19.00% (296.40 km²), respectively. Thus, AFGRRF reduces the affected area by 166.4 km² while accuracy is only reduced by 3.52% when compared to the GRRF method. The RF, ARF, FRF and AFRF methods obtained 91.49%, 86.67%, 92.85% and 89.28% of overall accuracy, and affected areas of 27.43% (427.90 km²), 26.00% (405.60 km²), 27.78% (436.20 km²) and 23.00% (358.80 km²), respectively (Table 3). This means that the AFGRRF method reduced the affected area by 131.5 km², 109.2 km², 139.8 km² and 62.4 km² compared to the other methods (see Table 3). Therefore, considering a SR above 90%, AFGRRF reduced the affected area without drastically decreasing overall accuracy compared to GRRF. Furthermore, the differences between models were subtle according to the spatial distribution of values on the maps (Figure 5). Furthermore, as we can see in Figure 5, the spatial distribution of the misclassified sites are similar for the hard and soft models even when the threshold condition was a SR above 90%. Therefore, the results showed a significant reduction in affected areas for the AFGRRF method without a significant impact on performance, which may improve management and reduces the costs associated to environmental monitoring and protection activities.

The McNemar test revealed no significant differences between models (see supplementary material, Table 2). The map produced using the AFGGRF method was significantly similar to those methods at a higher accuracy level (RF, FRF and GRRF). In this sense, a subtle decrease in accuracy could lead to a reduction in the affected area. It should be noted that, McNemar is interpreted differently in this case study. This test is commonly used to know whether a proposed method outperforms a reference method. This is a statistically significant increase in accuracy. However, in this case, the objective was to test whether AFGRRF, a wrapper that selects a subset of features that minimise the affected area, has a similar performance. This is a non-statistically significant decrease in accuracy. ARF was the only statistically different method; it was less accurate than the rest and less capable in reducing the affected area without a significant decrease in the accuracy level (see Table 3).
For this study, where embedded and wrapper feature selection was applied, the selected features differed between methods in terms of number and typology (Table 4). The RF and AFR methods considered all features, while FRF and ARF

Figure 4. AFGRRF models for lambda and gamma: (a) Number of features selected; (b) Potential affected area for 90% success rate; (c) Overall accuracy.
Table 2. List of acronyms.

| Acronym    | Description                                  |
|------------|----------------------------------------------|
| AFGRRF     | Area Feature Guide Regularised Random Forest |
| AFRF       | Area Feature Random Forest                   |
| ARF        | Area Random Forest                           |
| FRF        | Feature Random Forest                        |
| GRRF       | Guide Regularised Random Forest              |
| IL         | Illegal Landfills                            |
| RF         | Random Forest                                |
| ROC        | Receiver Operating Curve                     |
| SR         | Success rate                                 |
| TPR        | True Positive Rate                           |

Table 3. Overall results.

| Method     | Minimum affected area (%) | Minimum affected area (km²) | Overall accuracy | Features selected |
|------------|---------------------------|----------------------------|------------------|-------------------|
| RF         | 27.43                     | 427.9                      | 91.49            | 113               |
| ARFa       | 26                        | 405.6                      | 86.67            | 113               |
| FRF        | 27.78                     | 436.2                      | 92.85            | 7                 |
| AFRFa      | 23                        | 358.8                      | 89.28            | 7                 |
| GRRF       | 29.67                     | 462.8                      | 94.59            | 11                |
| AFGRRFa    | 19                        | 296.4                      | 93.62            | 12                |

*Minimum affected area for success rate greater than 90%.

Figure 5. Map of illegal landfill potential occurrence for hard methods (RF: Random Forest; FRF: Feature Random Forest; GRRF: Guide Regularised Random Forest) and reclassified soft methods (ARF: Area Random Forest; AFRF: Area Feature Random Forest; AFGRRF: Area Feature Guide Regularised Random Forest).
methods selected seven features: mining and extraction activity index, distance to pit zones, distance to transport infrastructures, land use transitions density from 1990 to 2000, land use transition density from 1990 to 2012, impervious cover transitions density from 1990 to 2012 and greenhouses density (Quesada-Ruiz et al. 2018). The GRRF method selected eleven features: communication routes density, distance to pit zones with different kernels, distance to transport infrastructures, distance to element of interest, distance to educational equipment, distance to coast, visibility from the coastline (Gorr and Kurkand 2020) and population density. Finally, the AFGRRF method selected twelve features: buildings density, distance to transport infrastructures, distance to protected areas, distance to pit zones, distance to coast, distance to agricultural areas, distance to cultural equipment, slope, altitude, industrial activity index and population density. It should be noted that the affected area was larger for smaller feature subsets in AFGRRF (Figure 4).

Despite the selected features being different among methods, all of the methods considered proximity to the coast, agricultural areas, pit zones and transport infrastructures as important for IL occurrence, as in previous studies (Quesada-Ruiz et al. 2018, 2019b). Physiographic features were also particularly relevant, likely due to the rugged terrain of the island, especially for the proposed method, as shown by the Gini index values for the selected features (see supplementary material, Figure 1). This explains the visual similarities between the hard and soft maps (see Figures 6 and 7). The map in Figure 6(b) has a distinctive appearance because it takes into consideration the ‘population density’ feature. Feature selection-based methods obtained higher probability values for IL (Figures 6(b,c)). Figure 5 shows how the methods without feature selection (RF and ARF) produced coarser maps, distinguishing the general patterns in affected areas, but unable to identify finer patterns further inland. In contrast, when feature selection was carried out (FRF, AFRF, GRRF and AFGRRF) new affected areas were revealed, producing maps with finer spatial detail, especially in the case of GRRF and AFGRRF. Furthermore, methods that permit application of SR enabled spurious affected areas with lower probability to be filtered out (see Figures 6 and 7).

Table 4. Feature selected by Random Forest (RF), Area Random Forest (ARF), Feature Random Forest (FRF), Area Feature Random Forest (AFRF), Guide Regularised Random Forest (GRRF), Area Feature Guide Regularised Random Forest (AFGRRF).

| Method      | Selected Features                                                                 |
|-------------|----------------------------------------------------------------------------------|
| RF          | Mining and extraction activity index, Distance to pit zones, Distance to transport infrastructures |
| ARF         | Land use transitions density from 1990 to 2000, Land use transition density from 1990 to 2012, Impervious cover transitions density from 1990 to 2012, Greenhouses density |
| FRF         | Distance to coast, Distance to transport infrastructures, Distance to element of interest |
| AFRF        | Distance to educational equipment, Distance to transport infrastructures |
| GRRF        | Distance to element of interest, Distance to educational equipment, Distance to coast, Visibility from the coastline, Population density |
| AFGRRF      | Distance to transport infrastructures, Distance to protected areas, Distance to pit zones, Distance to coast, Distance to agricultural areas, Distance to cultural equipment, Slope, Altitude, Industrial activity index, Population density |
5. Discussion

A majority of the studies focused on IL modelling applying weighted methods without feature extraction or feature selection, despite the accuracy of predictive modelling depending on feature selection, among other factors (Rodriguez-Galiano et al. 2018). Furthermore, these weighted methods usually rely exclusively on expert knowledge (Biotto et al. 2009, Matos et al. 2012, Chu et al. 2013) or data-driven approaches, such as Logistic Regression (Keser et al. 2012, Lucendo-Monedero et al. 2015) or

Figure 6. Map of illegal landfill occurrence probability: (a) Random Forest; (b) Feature Random Forest; (c) Guide Regularised Random Forest.

Figure 7. Success rate. Solid line (AFGRRF), dash-dotted line (ARF), and dotted line (AFRF).
Discriminant Analysis (Quesada-Ruiz et al. 2019b). Other studies applied feature extraction, primarily Principal Component Analysis (Tasaki et al. 2007, Glanville and Chang 2015). In terms of GIS, expert knowledge methods are characterised by the combination and integration of multiple datasets. The intervention of an analyst with domain knowledge is thus indispensable to, for instance, determine the parameters of the method (Saaty 1980). In contrast, data-driven methods require less supervision to integrate multiple data layers to solve a geospatial problem.

While feature selection-based studies are scarce, there are a few examples of the application of embedded and wrapper algorithms using logistic regression with forward or backward search (Quesada-Ruiz et al. 2018, 2019b). Weighted methods build models that assign different importance to each feature of the feature space, considering subjective expert knowledge or filter-based, such as the Analytic Hierarchy Process of Saaty Method applied widely in GIS science (Saaty 1980). On the other hand, feature extraction and feature selection have less expert intervention than weighted methods, removing spurious or redundant features and reducing the feature space, either by combining the most relevant features or selecting them in an unbiased manner. Therefore, weighted methods consider the whole feature set, even when the statistical significance is low. Feature extraction allows removal of the least significant new features, but requires a subsequent selection process (selecting the most informative components based on the percentage of explained variance in Principal Component Analysis), with wrapper-based feature selection being the only fully automatable approach.

The definition of IL probability thresholds should be considered an important phase in the process of obtaining accurate binary/hard maps. Weighted methods (Biotto et al. 2009, Matos et al. 2012) and data-driven methods (Lucendo-Monedero et al. 2015, Quesada-Ruiz et al. 2019b) for mapping IL reclassified continuous values (i.e. between 0 and 1) consider a threshold value of 0.5. This threshold definition is arbitrary, as it relies on a symmetrical statistical distribution of probability values without considering spatial distribution or accuracy metrics. There are alternatives to arbitrarily choosing thresholds, such as analysis of ROC curves where a trade-off is sought between True Positive and False Negative rates to avoid overestimation and underestimation, respectively (Chu et al. 2013, Rodriguez-Galiano et al. 2014). The application of ROC is widely used in many scientific fields, such as bioinformatics, where a positive or negative diagnosis for certain diseases might be equally relevant (Beck and Shultz 1986). However, geoscience studies focusing on the spatial distribution of a binary phenomenon are different. Including negative cases for optimising threshold values could lead to underestimation of IL when negative occurrences are more frequent (i.e. there are more locations without IL than with IL). Therefore, our study or other spatially driven studies, such as landslides (Dahal et al. 2008, Hong et al. 2017, Chen et al. 2019) or mining (Carranza et al. 2008, Rodriguez-Galiano et al. 2015), focus on the positive cases. All of these studies are characterised by their interest in predicting a minimal area with the highest accuracy in positive cases, thus reducing costs associated with prospecting or monitoring. Hence, the method proposed not only could improve the delimitation of potentially affected areas by ILs but it could also facilitate the evaluation of the possible costs of recovery, or the implementation of dissuasive
and surveillance measures by minimizing the area (Quesada-Ruiz et al. 2019b). This paper proposes using SR as an alternative method to ROC for mapping binary problems, considering the TPR together with the area instead of the false positive rate. Figure 7 presents the results obtained from soft models, showing the percentage of cases correctly classified regarding affected area. SR allowed identifying AFGRRF as the model with smallest affected area for a TPR above 90%. SR also facilitated distinguishing affected areas, maximising the accuracy of positive occurrences while minimising the affected area (see Figure 5). The role of features to minimise the affected area was reinforced by using SR in a feature selection approach inside a wrapper. Modifying the GRRF algorithm to build a wrapper with SR as the accuracy metric may offer new methodological perspectives for feature selection when the phenomenon being studied has a binary behaviour, considering not just the overall accuracy metric but also the spatial criterion. Nevertheless, the application of AFGRRF has some limitations and requirements: (i) there must be a sufficiently large geospatial database with a large sampling size to assess and compare its application with respect to other feature selection methods; (ii) sampling must be separated into training, test 1 and test 2; (iii) an additional test (T1 in our case) is needed to optimise the affected area, that it is different from the test (T2 in our case) used to evaluate the overall accuracy of the models; (iv) a balanced sampling between negative and positive cases. In this sense, AFGRRF offers new perspectives for its application to other binary phenomenon such as: landslide prevention, flood prevention, ecosystem conservation, infectious disease or agricultural pest control. The sensitivity of the method to noise could also be studied, attending the errors in the positive or negative occurrences of the binary phenomenon, as well as its sensitivity to the reduction of the training data.

6. Conclusions

Predictive modelling of binary phenomena such as presence or absence focuses on the application of numerical methods to estimate the probability of occurrence of a phenomenon. This paper proposes a new method for feature selection that modifies the GRRF algorithm for use inside a wrapper, improving the mapping and modelling of binary phenomena and the accuracy of the affected area mapping to reduce environmental management costs of binary phenomena. AFGRRF addressed the ‘Rashomon effect’ or the multiplicity of good models. This new method, AFGRRF, uses a new metric for feature selection (SR), selecting the model built from a feature subset that minimises the affected area within multiple accurate models. This approach is an alternative to previously applied overall accuracy-based feature selection methods. Its novelty resides in selecting a feature subset that optimises both the True Positive Rate (TPR) and the potentially affected area using the SR. Hence, AFGRRF may offer new GIS methodological perspectives for feature selection in GISscience when the phenomenon being studied has a binary behaviour, considering not just the TPR metric but also the spatial criterion. In this sense, AFGRRF achieve to obtain a spatial distribution of the binary phenomenon without overestimation or underestimation consistent with respect to the most important explanatory features and allowing it replicability with certain stability. Probability maps are usually transformed into hard maps to facilitate
management actions. Hard maps are obtained using arbitrary thresholds that assume a symmetrical statistical distribution of probability values or other more sophisticated approaches, such as ROC. However, these approaches do not take into consideration the accuracy of the classifications with the extent of the affected or affected area. In this sense, geoscience studies are interested in predicting the minimal distribution area with the highest accuracy in positive cases in order to reduce the costs of prospecting or monitoring. Hence, our method proposed facilitated distinguishing affected areas, maximising the accuracy of positive occurrences while minimising the affected area and identifying the model with smallest affected area for a TPR above 90%. AFGRRF was tested on the predictive modelling of ILs in the Canary Islands. The performance of AFGRRF was compared to five different RF-based methods, showing the capability of AFGRRF to reduce the affected area without a drastic decrease in overall accuracy.

Author contributions

All authors contributed to the conceptualization of the work and devised the methods. Rodriguez-Galiano, V. together with Zurita-Milla, R. and Izquierdo-Verdiguier, E. supervised the work. All authors discussed the results. Quesada-Ruiz, L. and Rodriguez-Galiano, V. wrote most of the original draft. All authors reviewed and edited the manuscript.

Disclosure statement

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data and codes availability statement

The data and codes that support the findings of this study are available at https://github.com/AFGRRF/Area-Feature-Guide-Regularised-Random-Forest. The proposed AFGRRF code requires the following R libraries: RRF, Raster, Rgdal, and ROC written by others who are not affiliated with the research.

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