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Integration of clustering and principal component analyses in MCDA to identify feasible regions for managed aquifer recharge

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ABSTRACT

Managed aquifer recharge (MAR) provides a nature-based solution to water scarcity issues, contributing to the design of effective water management policies. The novelty of this study lies in the integration of multivariate statistical methods within the framework of multicriteria decision analysis to provide nonsubjective, semi-automatic estimations of MAR feasibility based on three thematic layers, particularly intrinsic (hydro-geological, topographical, meteorological) features, water availability and demand for MAR. The concept of MAR typology is used to define the MAR problem and select a set of criteria for each thematic layer that are relevant for the Sado River Basin (southern Portugal). The hierarchical clustering algorithm (HCA) is used to partition the study area into distinct subregions based on selected criteria. For each subregion and thematic layer, a set of weight coefficients for the criteria is generated via products of the cumulative variance of the principal scores with the corresponding eigenvector matrix, which are then used to generate multiple realizations of the thematic maps. The results reveal that the majority of the study area (60%) has mean feasibility scores less than 0.54, whereas the remaining 40% (highest values) vary within a smaller interval (0.54–0.67). The present results are consistent with the previous study, with both identifying the same high-suitability regions. Additionally, it allows exploration of the variability in criteria weights across multiple realizations, providing a preliminary indication of how this variability can influence the results. This approach can easily be implemented in software and ultimately automated, supporting the unsupervised streamlining of the decision-making process.

1. Introduction

The optimal management of water quality and availability is arguably one of the most significant current and future challenges at the global level (Wheeler et al., 2021), and is directly linked to UN Sustainable Development Goals (SDGs), particularly "Zero hunger" (SDG.2), "Clean water and sanitation" (SDG.6), "Responsible consumption and production" (SDG.12), "Climate action" (SDG.13), "Life below water" (SDG.14) and "Life on land" (SDG.15) (UN, 2022). The intensification of climate change during recent decades has led to the emergence of more frequent and severe droughts at a global scale, causing a plethora of negative consequences, such as a reduction in the land area covered by surface water bodies (Liu et al., 2022), increased occurrence of fires (Xiang et al., 2023), and soil erosion (Borrelli et al., 2017). The adverse impacts of extreme droughts add to the water stresses imposed on freshwater resources due to human activities, which further exacerbate water scarcity issues.

Managed aquifer recharge (MAR) is a nature-based solution to water-scarcity issues that is widely used at a global scale (Sallwey et al., 2019) and refers to the intentional recharge of aquifers for later recovery and/or environmental benefits. Compared with surface water storage techniques, MAR suffers from lower evaporation losses, is not prone to algae blooms, and, owing to slower groundwater dynamics, is less responsive to contamination episodes (Ross and Hasnain, 2018; Vanderzalm et al., 2022). MAR can also contribute to wetland restoration, the restoration of overused or brackish aquifers, the mitigation of seawater intrusion, the enhancement of carbon sequestration in soil systems, the enhancement of water supplies and water supply security, etc (Dillon, 2005; Dillon et al., 2022). Furthermore, this technique is highly adaptable to climate variations, with the potential to provide cheaper and more economic solutions in the longer term (Casanova et al., 2016; Halytsia et al., 2022). At the European level, the European Commission has

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devoted significant efforts and funding resources for the optimal implementation of these solutions across different contexts to support EU strategies, such as the "EU Biodiversity strategy for 2030″ and "EU Adaptation Strategy", enhancing the resilience of the European territory to climatic conditions (Wolf et al., 2021).

However, there is a lack of sufficient long-term scientific evidence on the cost efficiency of these technologies, as well as their optimal implementation with respect to the sustainability of water resources at the catchment level (Alam et al., 2021; Gonzalez et al., 2024; Maliva, 2014). A major issue is the lack of a holistic, broadly accepted framework for MAR success, especially when multiple recharge objectives are needed (Seidl et al., 2024). A plethora of studies have focused on providing a mechanistic understanding of successful MAR projects (Abarca et al., 2006; Bekele et al., 2013; Perzan et al., 2023; Wallis et al., 2011), aiming at identifying the primary factors responsible for MAR success, mostly at river basin, regional or national scale.

Multicriteria decision analysis (MCDA) is often used to balance the relative importance of multiple factors with respect to a specific objective, assisting decision makers in identifying the optimal choice among alternatives (dos Santos Amorim et al., 2020; Hajkowicz and Collins, 2007); however, traditional MCDA approaches can be sensitive to correlated input factors, subjective weighting schemes, and increasing dimensionality, which may limit their ability to objectively represent complex relationships and spatial variability in multivariate datasets.

In the presence of spatially distributed attributes, MCDA is often incorporated into geographical information systems (GISs) to enable the assessment of the available alternatives at each location (Sallwey et al., 2019). Many existing studies have attempted to identify suitable locations for MAR with the use of MCDA based only on intrinsic characteristics of the candidate regions (Fuentes and Vervoort, 2020; Jadav and Yadav, 2023; Rahman et al., 2013; Yosef et al., 2024), such as topography, soil and aquifer properties, land-use and land-cover, and meteorological conditions, since these factors affect groundwater recharge processes, scarcity phenomena and the use of alternative water storage methods such as MAR. Sallwey et al. (2019) collected information from 63 case studies to analyze the methodologies and datasets that were used to derive MAR suitability maps, focusing on the MAR schemes, criteria, weights, and decision rules used. The review article concluded that a large variety of criteria and recharge methods are adopted to identify suitable MAR sites, although a strong bias toward the adoption of topographical criteria in addition to the common use and characterization of hydrogeological features was identified.

Apart from the intrinsic hydrogeological properties, which reflect the capacity to store and recover water in aquifers, additional thematic layers should be considered prior to selecting appropriate MAR sites. In particular, the water availability for infiltration/injection and the water demand for such methods should be analyzed and incorporated into the decision-making process. These two factors are closely related to socioeconomic and regulatory factors that strongly affect the long-term sustainability and success of MAR projects. Aloui et al. (2022) attempted to incorporate three thematic layers (i.e., intrinsic suitability, water availability for MAR, and water demand) for the identification of feasibility regions for MAR within the Enfidha plain (NE of Tunisia). The authors selected a number of relevant criteria to map each thematic layer independently, whereas the resulting thematic maps were subsequently combined in a simplistic way (i.e., assigned equal weights) to map the MAR feasibility levels. Additionally, more recent studies have proposed an integrated, stakeholder-adapted framework for finding feasible regions for MAR (Ebrahim et al., 2024; Martins et al., 2024a; Panagiotou et al., 2024a), focusing on engaging key stakeholders at different stages of the MCDA (i.e., problem formulation, criteria selection, ranking and weighting processes, discussion and validation of the results). The concept of MAR typology was recently introduced (Chekirbane et al., 2025; Martins et al., 2024a; Panagiotou et al., 2024a) to characterize the driver for MAR implementation on the basis of the recharge objective (e.g., mitigation of seawater intrusion, water storage), adequate MAR technique (e.g., infiltration basins, injection wells), and available water sources for MAR (e.g., tertiary treated wastewater, surface water surpluses, rainwater, damwater). Consequently, each recharge problem was strongly dependent on site-specific characteristics and the opinions of local stakeholders, enhancing the wide acceptance of MCDA outcomes by water users and water managers. As a result, the identification of feasible locations for MAR is a nontrivial task prior to the implementation stage of a MAR project, depending on the balance among several intrinsic, socioeconomic and regulatory factors, and on the biased, often conflicting, perspectives of multiple stakeholders.

However, the assignment of weights for each criterion and thematic layer is a challenging and often subjective task due to the different viewpoints among decision makers, potentially leading to compromises that are not optimal with respect to a specific objective. This subjectivity motivates the need to explicitly assess the variability of the MCDA outcomes associated with alternative weighting scenarios. Furthermore, the resulting weights are associated with significant uncertainties due to the large discrepancies among the different perspectives. This fact is particularly true for complex decisions such as the identification of feasible regions for MAR due to the plethora of factors that can affect the successful implementation of such solutions, including topographical, meteorological, hydrological, and socioeconomic factors, among others. There are several popular methods that use inputs from each decision maker to rank and determine the criteria weights, such as the analytical hierarchical process (AHP) (Saaty, 1977), frequency ratio (Boughariou et al., 2021), PROMETHEE (He et al., 2020), and TOPSIS (Mohamed Mouhoumed et al., 2023). Nevertheless, traditional MCDA methods exhibit inherent limitations that become profound in complex applications, such as in natural resource management. As quoted by Rosenhead and Mingers (2001), some of the major shortcomings of these methods are: "(1) *comprehensive rationality*, which unrealistically presumes or aspires to substitute analytical results and computations for judgement; (2) the creative generation of alternatives is de-emphasised in favor of presumably objective feasible and optimal alternatives; (3) misunderstanding and misrepresenting the reasons and motivations for public involvement; (4) a lack of value framework beyond the typical *utilitarian precepts*". Therefore, alternative methods must be used that mitigate these limitations, such as searching for solutions that are less subjective to the personal perspectives of decision-makers while taking into account the statistical properties of the available, often large multidimensional datasets.

Principal component analysis (PCA) is a statistical method that is often used for the identification of linear associations in multivariate correlated data, enabling the reduction of dimensionality while preserving as much information as possible along the principal directions of the original dataset (de Costa et al., 2024). This method allows the generation of simplified, more comprehensive patterns of complex datasets, providing robust input for ranking processes and facilitating the evaluation of alternatives during complex decision-making analysis, such as MAR feasibility. Consequently, numerous studies have incorporated PCA into decision-making processes to rank the criteria without the requirement of consulting multiple decision-makers (Dugger et al., 2022; Navane and Sahoo, 2021; Rahmani et al., 2021; Zhu, 1998). For example, Zhu (1998) compared the performance of data environment analysis (DEA) and PCA to rank the performance of decision-making units by assigning weights to a set of preselected criteria to evaluate the economic status of Chinese cities. The results revealed that PCA and DEA produced consistent and mutually complementary predictions, whereas tau-correlation tests were used to validate the consistency between the rankings of the criteria for both methods. Dugger et al. (2022) evaluated the efficiency of PCA in ranking a number of pilot candidates for the United States Army on the basis of emotional intelligence and safety attributes. The authors followed the methodology proposed by Zhu (1998) to develop a simplified expression for determining the criteria weights by multiplying the proportion of the variance along each

principal direction with the elements of the eigenvector matrix. The computations were repeated for all possible combinations of the 29 candidates to validate the consistency of the rankings, identifying the computational complexity as the main limitation of their study. In addition, the authors emphasized the need to evaluate the general applicability of the proposed methodology using other datasets. The above limitation becomes more apparent for large high-dimensional datasets, such as those used to conduct MAR suitability assessment. Recently, de Costa et al. (2024) comprehensively reviewed the extent to which principal component analysis is integrated into machine learning models to conduct a multicriteria decision-making process. This study analyzed 16 studies, published between 2000 and 2023, that employed PCA-based decision-support techniques to determine criteria weights and evaluate the performance of alternatives in a wide range of disciplines, such as logistics, market adaptability, weapons system selection, building evaluation, healthcare, water resource sustainability, etc. Most (69%) of the studies adopted the preferences of the decision makers to determine the criteria weights, resulting in subjective evaluations of the alternatives. Furthermore, the authors emphasized the necessity of using innovative machine-learning methods to handle complex datasets, enabling the automatic determination of weighting coefficients for the criteria which will be used to evaluate the alternatives.

Clustering analysis (CA) is a category of unsupervised machine learning that is often used to explore the statistical associations among several attributes, assisting in the interpretation of the available datasets (Rahbar et al., 2026). These algorithms are widely used in groundwater management to group samples into distinct populations (clusters), and even to divide geographical areas into subregions that exhibit similar characteristics, assisting in a better understanding of the connection between the status of aquifer systems and potential causes (Güler et al., 2012; Panagiotou et al., 2024b; Tewari et al., 2024). Unlike other traditional classification schemes, such as graphical tools (Güler et al., 2002), clustering methods can handle large high-dimensional datasets, for example those that combine chemical and physical parameters, although additional postprocessing is needed to identify trends and/or processes associated with the problem of interest. These resulting clusters are constructed concerning the distributions of the criteria, which can be used to rank or select optimal alternatives. In a very recent review article, Rahbar et al. (2026) highlighted the capacity of hierarchical clustering analysis (HCA) to group samples based on attribute similarity, without the necessity of predefining the number of clusters, in contrast to other clustering methods, such as K-means and K-medoids.

Numerous studies have reported the integration of clustering algorithms into multicriteria decision-making processes across various domains, including entrepreneurship (Crum et al., 2022), medical (Hendricks and Khasawneh, 2021; Sarría-Santamera et al., 2020), and marketing (Punj and Stewart, 1983). Interestingly, only one study that integrates CA and MCDA to delineate the optimal regions for MAR installation has been reported (Tewari et al., 2024). Moreover, a search of Web of Science and Google Scholar using the keywords "principal component analysis", "multicriteria decision analysis" and "managed aquifer recharge" revealed no previous studies that incorporate PCA into MCDA frameworks for MAR suitability assessment. In addition to the potential novelty of integrating both PCA and CA into MCDA for MAR site selection, this approach offers data-driven estimations of MAR suitability, reducing the subjectivity and biases often associated with characterizing the relative importance of criteria on the basis of their perceived attributes, as in traditional methods. It also provides realizations of the criteria weights that reflect the spatial characteristics of distinct subregions within the study area, which can be also used to assess the impact of these weights to the MCDA outcomes in a physical manner.

Therefore, the present study primarily aims to: 1) integrate multivariate statistical methods (i.e., PCA and CA) into the multicriteria decision-making process to identify feasible regions for MAR in a nonsubjective manner, 2) assess MAR feasibility as a function of intrinsic suitability, water availability and water demand for MAR, and 3) present a practical methodology for quantifying the variability of alternative weight realizations that reflect the spatial zoning of MAR-related factors into regions with similar criteria characteristics. The presented process can be easily programmed and ultimately automated to calculate thematic maps, supporting the unsupervised streamlining of the decision-making process. To ensure the acceptance of the MCDA outcomes by the authorities and policy-makers, key governmental stakeholders from the water sector are engaged in criteria selection, and weighting of the thematic layers to compile the MAR feasibility map. The resulting maps, together with discussions with key stakeholders during the implementation stages of the MCDA, aimed at contributing to the general objective of this study, which is the further adoption of MAR by the community and policy-makers.

The applicability of the proposed methodology is tested in the southern Portuguese Sado River Basin and the Ribeiras do Alentejo River Basin. This region, selected as representative of the southern region of Portugal, is hydrologically characterized by medium to high interannual variability in water availability and extremely high water-stress (Kuzma et al., 2023), and often faces water-related challenges. These hydrological conditions, particularly after prolonged and recurrent drought periods, led to a situation in which surface water reservoirs are unable to store sufficient water (see yearly Drought Monitoring reports conducted by the Environmental Agency[1]). According to projected climate change scenarios, this area is highly likely to experience increased water scarcity due to decreasing rainfall (Martins et al., 2024b), requiring the implementation of alternative integrated water resource management strategies to not only rely on surface water storage.

Furthermore, the proposed methodology can be applied to other geographical contexts and spatiotemporal scales, provided that sufficient and comparable spatial datasets are available. However, regional transferability may be constrained by factors such as data resolution and coverage, as well as the need to adapt criteria and weighting schemes to local hydrogeological, climatic, and land-use conditions. To test this methodology, several criteria that are commonly used to conduct MCDA-based MAR suitability analysis were collected from an extensive database compiled by Panagiotou et al. (2022), which was further modified on the basis of the feedback of relevant stakeholders and data availability. The final set of criteria describes major aquifer, soil and geomorphological characteristics, which are often considered the main MAR implementation constraints.

2. Materials and methods

2.1. Description of the study area

The study area is located in the Alentejo administrative region (southern region of mainland Portugal) and refers to two main river basins: the Sado River Basin, which accounts for 92% of the studied area, and the Ribeiras do Alentejo River Basin (Fig. 1). While the former is a fully developed watershed composed of several subwatersheds and surface water reservoirs, the latter is composed of small extension coastal streams.

It is limited to the west by the Atlantic Ocean, to the north and east by the transboundary Tagus and Guadiana River basins, respectively, and to the south by the Mira River basin. The area experiences a Mediterranean climate, with hot, dry summers and mild, wet winters. The average annual rainfall is 586 mm/y for the Sado River Basin and 640 mm/y for Ribeiras do Alentejo (APA, 2023b) (see Fig. SM1 in the Supplementary material). Agricultural lands cover 61% of the study area, whereas forests and seminatural areas account for 33%. In contrast, artificial surfaces—including urban fabrics (i.e., urban structures and

[1] https://apambiente.pt/agua/relatorios-de-monitorizacao-agrometeorologica-e-hidrologica#.

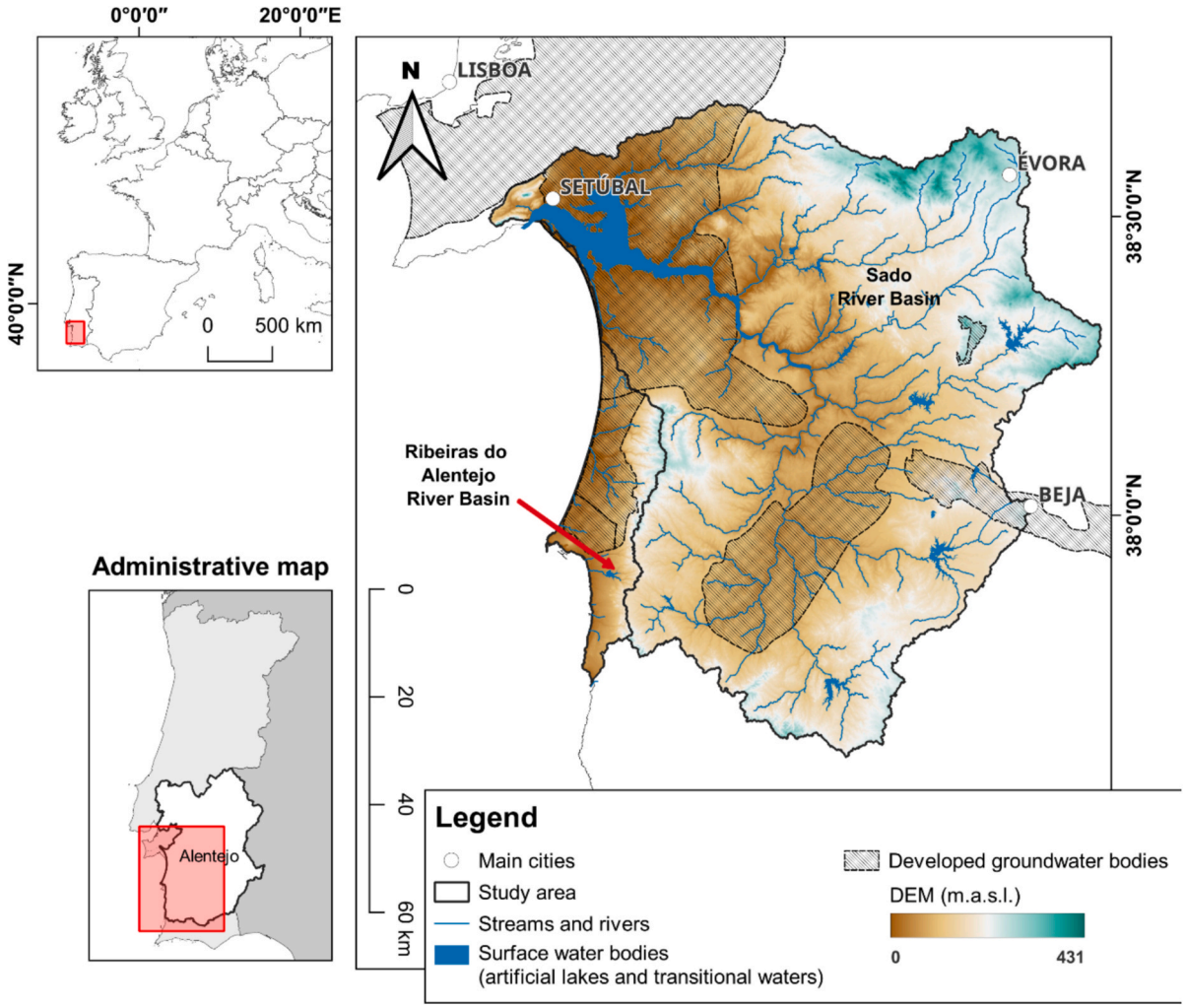


Fig. 1. Geographical location and basic topographical and hydrological information of the demonstration site.

transport networks)—occupy less than 2% of the total area.

Despite having less than 7% of Portugal's total population (Instituto Nacional de Estatística, 2022), this region faces considerable water demand pressures, primarily from the agricultural sector, which accounts for 85% of total water consumption (APA, 2023a). Agriculture, particularly irrigated crops, is a relevant sector of the regional economy (Silveira et al., 2018), with a 74% sector increase in gross value added, 53% evolution in the farming of companies' turnover and 43% in the number of workers for the period of 2014–2018 (APA, 2023a). However, intensive water use poses challenges for sustainable water management, especially given the region's susceptibility to droughts and climate variability (Ferreira et al., 2018). The region comprises or intersects six fully developed groundwater bodies, mainly multilayer sedimentary aquifer systems (Almeida et al., 2000), that represent an important source of water, not only for agricultural uses but also for urban supply. The competition between different water uses under a water-stressed scenario highlights the challenges in water management, which require integrated solutions for the sustainable use of this resource at the regional level. Although several surface water reservoirs and coupled irrigation structures, mainly composed of water distribution channels, exist in the study area, the National Water Resources System (https://snirh.apambiente.pt/) reported that the percentage of stored volume in surface reservoirs per hydrological year showed a decreasing trend, with September 2017 representing the most historically stressful situation in the period between 2000 and 2024, when storage fell below 20% of capacity (see "Supplementary Material" file, Fig. SM1). Currently, no water transfer systems from neighboring river basins are in place. Moreover, these surface storage limitations may be further exacerbated under future conditions, as Martins et al. (2024b) assessed water availability scenarios and identified a high likelihood of reduced natural groundwater recharge and surface runoff in the region, primarily due to projected decreases in rainfall and increases in evapotranspiration (Espinosa and Portela, 2022; IPCC, 2023; Portela et al., 2020). Consequently, the selected demonstration site serves as a prime example of these challenges, underscoring the need for innovative water resource management strategies.

2.2. Methodology

Fig. 2 shows an overview of the proposed methodology, which comprises five distinct steps. The first step involves the collection of data from multiple sources (i.e., Earth observation repositories, in-situ measurements, literature surveys, lab analyses, and model outputs) that contain information about MAR-related factors, hereafter called criteria. After summarizing the main statistical properties of the dataset, the Box-Cox transformed criteria are used as inputs to the K-means clustering algorithm to partition the study area into subregions, with the number of clusters determined based on the silhouette coefficient (Step 2). Step 3 involves calculating the criteria weights for each subregion (cluster) using the PCA-based approach proposed by Dugger et al. (2022), resulting in multiple realizations of the weight dataset. The criteria maps are also normalized to a common scale [0.1, 1] based on literature

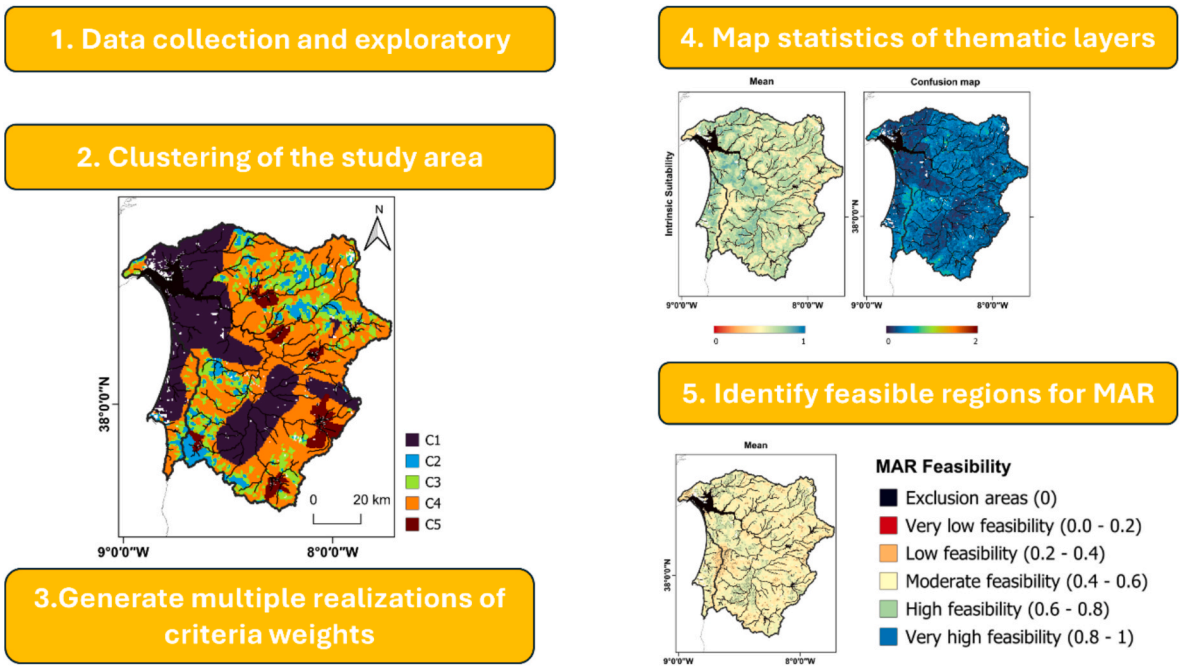


Fig. 2. Overview of the proposed methodology.

values, the opinions of MAR experts, and the statistical characteristics of the datasets. The lower bound of 0.1 reflects the assumption that no area outside the defined exclusion zones is completely unsuitable for MAR implementation. Setting the lower bound above zero allows these areas to be included in the aggregation process, acknowledging that, although MAR may be technically feasible, implementation could entail increased risk of long-term failure. Then, the criteria weights and the normalized criteria maps are combined to generate multiple realizations of the MAR thematic maps, which are then aggregated to estimate the spatial distribution of basic statistical moments of the thematic layers (Step 4). In Step 5, the mean thematic maps are used to identify regions of high MAR feasibility. The results are then compared with MAR thematic and feasibility maps produced by Martins et al. (2024a) using the analytical hierarchical process.

2.2.1. *Factors affecting the feasibility of MAR projects*

As noted in the introductory section, the selection and weighting of criteria and thematic layers should reflect site-specific characteristics, the typology and features of the MAR feasibility problem being addressed, and the input of key stakeholders to provide meaningful outcomes for policy-makers.

From the established MAR typology, a set of criteria has been selected for each thematic layer – intrinsic suitability (IS), water availability (WA) and water demand (WD) – based on the previous discussion conducted by Martins et al. (2024a), including inputs from major stakeholders from the water sector. Table 1 briefly describes the base information and sources of the selected criteria. As expected, the IS criteria are closely related to the hydrogeological (e.g., aquifer geometry, lithology, productivity, and water quality), topological (e.g., slope and soil occupation/use) and soil features (e.g., texture and layer thickness) of the study area. These factors are selected and normalized to represent the relative capacity of a site to receive, infiltrate, store, and potentially recover water through the MAR surface spreading method. With respect to the WA criteria, the selection process was driven mainly by the availability level of the potential surpluses, not only naturally generated runoff but also nonconventional anthropogenic sources such as treated wastewater. The criteria associated with the WD are strongly related to farming activities, representing crop irrigation needs and the potential depletion of groundwater resources, since these factors can drive the adoption of such MAR practices. The base criteria information is sourced from public validated databases and maps, such as the Portuguese Water Resources Database (SNIRH), the Environmental Protection Agency (APA) and the National Laboratory of Energy and Geology (LNEG), in both vector and raster formats, with varying scales and resolution (see Table 1). Both raster and vector datasets were reprojected to a common coordinate reference system, namely ETRS89 TM06 Portugal (EPSG:3763). Subsequently, all vector datasets were rasterized and, together with the existing raster datasets, resampled into a common 500 m resolution grid, which was deemed acceptable given the regional scale of the analysis. For example, the geological mapping used for the Aquifer Lithology is at a scale of 1:500,000 (Table 1); converting this vector dataset into a raster with 500 m spatial resolution resulted in minimal information loss, with the main geological boundaries remaining clearly identifiable.

Importantly, the number of selected criteria associated with each thematic layer is reduced compared to Martins et al. (2024a), in line with the findings of Miller (1956), who suggested that the number of criteria considered in the analytical hierarchy process should not exceed nine to ensure consistent pairwise comparisons. Although the proposed data-driven methodology is not subject to this limitation, the reduction was adopted here to enable a meaningful comparison between the outcomes of the proposed approach and AHP-based predictions. Particularly, nine criteria are used to calculate the intrinsic suitability map, whereas four and three criteria are considered in the MCDA analysis for the water availability and water demand maps, respectively. Table 1 presents an explanation of the processes applied in the base information to determine the necessary criteria, along with a brief reasoning behind the standardization process of converting all original criteria maps into a common scale ranging from 0.1 to 1. A value of 1 represents the maximum MAR score for intrinsic suitability, water availability, and water demand, respectively. The aggregation of these three thematic layers through a weighted linear combination produces the MAR feasibility layer, with values ranging from 0.1 to 1.

The full details of the corresponding standardized values for both numerical and categorical criteria are provided in the Supplementary Information of Martins et al. (2024a). As an example of the standardization process that is adopted to map the Aquifer lithology (LT) criterion, each lithological formation description in existing geological maps

Table 1
Details of the criteria used to conduct the decision-making process.

Criteria	Base data description	[Data Type] Normalization reasoning
Intrinsic Suitability		
Aquifer geochemistry (AGC)	Spatial distribution of Chloride (mg/L), Electric conductivity (μS/cm) and Nitrates (mg/L) parameters. 100 m resolution IDW-based geostatistical surfaces were generated from the point measurements of the selected parameters, distributed throughout the study area. Sourced from SNIRH, using data from 2021 to 2022 hydrological year.	[Continuous variable] Lower groundwater quality (e.g., areas with concentrations above the established qualitative thresholds for groundwater) represents higher suitability.
Aquifer geometry (AGM)	Based on the aquifer dynamics and structure characterizations (e.g., Multilayer, phreatic to confined, high thickness). Categorical characterization conducted by the Portuguese Environmental Agency (APA) for all Groundwater Bodies. This varied from limited, insignificant aquifers (low thickness, low permeability) to porous phreatic aquifers.	[Discrete variable] Phreatic aquifers represent higher suitability when compared to confined aquifers. Multilayer aquifers show lower suitability when compared to homogeneous aquifers, high thickness aquifer (higher storage capabilities).
Aquifer lithology (LT)	Lithological description from the existing geological maps (1:100 000, LNEG) clustered into main lithological groups (e.g., sedimentary, volcanic, etc.) (vectorial dataset).	[Discrete variable] E.g., homogeneous sedimentary lithologies show higher suitability vs compact metamorphic rocks.
Aquifer storage capacity (SC)	Computed difference between topographic surface (digital terrain model with 30 m resolution based on SRTM dataset) and the groundwater levels (GW) for year 2022), providing the total thickness of the unsatured zone; the GW level surface was computed with IDW 100 m resolution based on point measurements, sourced form SNIRH; corrections to the computed GW level were made by assuming all streams as discharge areas.	[Continuous variable] Very surficial GW levels represent lower suitability for infiltration (easily contaminated).
Land slope (LS)	Slope computed from surface SRTM 30 m resolution digital terrain model.	[Continuous variable] High slope areas show low suitability vs plains.
Soil occupation (SO)	Evaluation of the occupation based on the CORINE Land Cover 2018 (Copernicus, 2018) map and classification (vector dataset).	[Discrete variable] Unused areas have higher potential for implementation, hence higher suitability vs dense urban areas that may lack free space.
Specific yield (SYS)	Aquifer productivity classification presented by the Portuguese Environmental Agency (APA) in the River Basin Management Plans (vector dataset).	[Discrete variable] Capacity of recovering infiltrating water. Low specific yield corresponds to lower suitability.
Topsoil texture (TST)	Soil texture classes map, based on soil maps of 1:25 000 to 1:50 000 scale.	[Discrete variable] Clayey texture (low infiltration capacity) represents low suitability vs sandy texture (high infiltration capacity).
Vadose zone thickness (VZT)	Soil thickness map, grouped into interval classes (e.g., <10 cm, 10 to 50 cm, etc.), based on soil maps of 1:25 000 to 1:50 000 scale.	[Discrete variable] The higher the thickness of the vadose zone the higher the suitability (the vadose zone has the depuration capacity which may protect the groundwater quality).
Water Availability		
Direct runoff [DR]	Spatial distribution of average direct run-off (mm/yr) computed with daily sequential soil–water budget model (BALSEQ) [1941–2019] (Martins et al., 2024b). The model provided, for small watersheds, the average yearly aggregated direct run-off (vector dataset).	[Continuous variable] Areas whose characteristics can generate higher amounts of direct runoff represent higher water availability areas.
Distance to source (nonconventional) [DSNC]* Distance to source (dams) [DSD]** Distance to source (dams) [DSR]***	Based on the classification conducted under the current RBMPs, we selected the following three criteria. See Martins et al. 2024a for more details. (vector dataset): * Distance buffer weighted by quality status and discharged volume ** Distance buffer score weighted by quality status and reservoir volume *** distance buffer score weighted by quality status	[Discrete variable] Lower the proximity and lower the quality of the source represent low water availability, evolving to maximum water availability in buffers with high proximity and high source quality.
Water Demand		
Crop Pattern [CP]	Evaluation of crop types based on the CORINE land cover 2018 (Copernicus, 2018) for agricultural areas (vector dataset).	[Discrete variable] Based on water needed for irrigation for each crop type. The presence of highly water dependent (irrigated) crops indicates higher water demand. On the other hand, non-irrigated or rainfed crops represent lower water demand.
Consumption per unit area for agriculture supply [CAS]	Computed based on abstracted volumes for agriculture sector (hm^3/yr). This data was provided by the Portuguese Environmental Agency (APA), for the reference year of 2018, in m^3/yr, aggregated for river basin area (vector dataset).	[Continuous variable] Higher abstracted volumes are related to higher water demand.
Decrease of groundwater levels [DGWL]	Based on the characterization of the GW quantity status conducted under the current RBMPs for all the GWB in the	[Discrete variable] Decreasing groundwater levels point to a higher need for water, hence avoiding depletion.

(continued on next page)

Table 1 (*continued*)

Criteria	Base data description	[Data Type] Normalization reasoning
	study area (APA, 2023a). These are classified based on decreasing, stable, or increasing GW level trends.	Decreasing status highlight high demand for MAR and water.

(adapted from Martins et al., 2024a).

(1:100 000 scale) was analysed based on available information regarding the type (sedimentary, compact) permeability, heterogeneity, fractures, or deterioration. The lithologies were aggregated into main lithological groups and classified on a scale ranging from 0.1 (lowest capacity for water infiltration, storage, and recovery) to 1 (highest capacity for water infiltration, storage, and recovery). Low-fractured crystalline rocks (metamorphic or plutonic) were assigned low suitability, whereas homogeneous sands were considered highly suitable for MAR. Other nuances were also considered, often described in Explanatory Notes of Geological Maps, such as hydrogeological capabilities, existing aquifers, etc. In the case of numerical (continuous) variables, a standardization function was adopted given the maximum and minimum intervals (e.g., land slope computed from a digital terrain model or the direct run-off distribution).

Next, a multicollinearity analysis is applied to the non-transformed dataset to identify the set of criteria to be used in the MCDA. Multicollinearity is an issue that often occurs in problems involving the processing of high-dimensional datasets. In particular, it involves the presence of high correlations among linear expressions of variables that can lead to significant variance (errors) of the regression coefficients, making challenging the identification of the impact of these variables to the model outcomes (Alin, 2010; Chan et al., 2022). The variance inflation factor (VIF) and tolerance index (TOL) are extensively used to quantify the impact of the multicollinearity effects, expressed as:

$$VIF_j = \frac{1}{1-R_j^2}, TOL_j = \frac{1}{VIF_j} = 1 - R_j^2, \tag{1}$$

where R_j^2 denotes the coefficient of determination of the j-th variable as a regression function of the remaining variables. As a rule of thumb, VIF values larger than 5 and TOL values lower than 0.1 indicate the presence of strong multicollinearity effects (Tsangaratos et al., 2023). Consequently, the criteria dataset is constructed by including only the variables which do no exhibit strong multicollinearity.

2.2.2. Clustering of the study area and calculation of criteria weights

The Shapiro-Wilk normality test was applied to randomly selected representative subsets of the data (500 entries per criterion). This approach was adopted to mitigate the well-known sensitivity of formal normality tests to large sample sizes and spatial dependence. The test was repeated for several subsets to ensure that the results were not sensitive to the particular sample, yielding consistent outcomes. The results showed that suitable transformations should be applied to reduce the skewness of the criteria prior performing the clustering analysis. Consequently, the Box-Cox transformation function (Box and Cox, 1964; Panagiotou et al., 2024a) is applied to the sampling dataset:

$$x_{\alpha,i} = \begin{cases} \dfrac{y_{\alpha,i}^{\lambda} - 1}{\lambda}, \ if \lambda \neq 0 \\ \ln\left(y_{\alpha,i}\right), \ if \lambda = 0 \end{cases}, \text{for } \alpha = 1, \cdots., n, \ i = 1, \cdots., n_{cr}, \tag{2}$$

where $y_{\alpha,i}$ and $x_{\alpha,i}$ denote the values of the original and Box-Cox transformed sampling dataset, respectively, n denotes the total number of samples (spatial locations in this case), and λ is the optimal value of the transformation parameter that better approximates the normal distribution, estimated through maximum likelihood. This transformation is often used to reduce the skewness of the initial dataset so that it is more suitable for use in classification (e.g., clustering) and regression tasks.

Next, the classification of the transformed dataset is performed using the agglomerative hierarchical clustering algorithm (HCA) (Rahbar et al., 2026; Ebrahimi et al., 2022; Madrigal-Solís et al., 2024). Compared to other traditional clustering methods (Hartigan and Wong, 1979; Nourani et al., 2022; Panagiotou et al., 2024a), HCA is often used in classification problems because a) it does not require random initializations of the clusters (i.e., each sample initially corresponds to a single cluster), b) does not require a priori specification of a number of clusters (e.g., as in K-means), c) provides a dendrogram-based representation of cluster relationships, and d) is well suited for exploratory regionalization of multivariate spatial data. Therefore, HCA provides a conservative and interpretable framework for regionalization, well suited for identifying robust large-scale spatial subzones, rather than explicitly optimizing cluster compactness as in methods such as K-means or K-medoids.

This algorithm adopts a bottom-up approach to assign each sample into a group (cluster). Each input datapoint is initially assigned as individual cluster. The next step focuses on progressively merging clusters according to a linkage criterion. In this study, Wards' criterion (Murtagh and Legendre, 2014; Ward, 1963) was adopted because it minimizes the increase in within-cluster variance at each merging step, yielding compact and internally homogeneous clusters that are particularly appropriate for multivariate datasets. Compared to alternative linkage methods (e.g., single, complete, or average linkage), Ward's criterion is less sensitive to chaining effects and tends to produce more balanced and stable clusters, which is desirable for spatial regionalization and subsequent zonal analyses. Consequently, the pairs of clusters with the smallest dissimilarity value are merged into a single cluster. This process is repeated until all data points are merged into a single cluster. The total number of clusters (K_{opt}) was selected through visual inspection of the dendrogram, focusing on major linkage height increases that indicate dominant separations in the hierarchical structure. This approach aims to balance parsimony and interpretability rather than to identify a formally optimal cluster number. Therefore, the dendrogram was used as an exploratory tool to guide the selection of a reasonable number of clusters representing dominant spatial groupings.

Consequently, the study area was first partitioned into spatially coherent zones based on the HCA results to account for spatial heterogeneity and ensure robustness across different subregions. PCA was then applied independently within each zone, and zone-specific weight sets were constructed using the cumulative explained variance and the corresponding loading matrices following the approach of Dugger et al. (2022). This procedure resulted in K_{opt} distinct weight sets, one for each spatial zone, allowing the weighting scheme to adapt to regional differences in multivariate structure.

A step-by-step calculation of the weighting coefficients, as well as the MAR thematic and feasibility indicators, is presented in the remainder of this section. For each of the K_{opt} spatial zones, the Box-Cox-transformed dataset ($x_{\alpha,i}$) is subjected to z score transformation:

$$z_{\alpha,i} = \frac{(x_{\alpha,i} - \mu_i)}{\sigma_i}, \text{ for } \alpha = 1, \cdots., n, \ i = 1, \cdots., n_{cr}, \tag{3}$$

where n_{cr} denotes the total number of criteria, and μ_i, σ_i denote the mean and standard deviation of Box-Cox transformed criterion i, respectively. As discussed in Section 2.2.1, a 500 m spatial resolution is selected in this study, resulting in 31,600 locations within the area of interest. By construction, each z-score-transformed variable has a mean of zero and a variance of one, and its covariance matrix is calculated as:

$$C_{i,j} = \frac{1}{n}\sum_{\alpha=1}^{n} z_{\alpha,i}.z_{\alpha,j}, \text{ for } i,j = 1, \cdots, n_{cr}, \tag{4}$$

where the diagonal elements denote the variance of each criterion, and the off-diagonal elements denote the covariance between pairs of variables. Note that the covariance matrix coincides with the correlation matrix for z scores. Next, the covariance matrix is decomposed into an orthogonal matrix (V) that contains the eigenvectors (columns) of C and the diagonal eigenvalue matrix *D,* whose diagonal elements are the eigenvalues of *C*:

$$C_{ij} = V_{i,k} D_{kq} V_{j,q}, i, j = 1, \cdots, n_{cr.} \tag{5}$$

The PCA-transformed, uncorrelated, variable P_i is then calculated via the following matrix multiplication:

$$P_i = z_{k,i} V_{k,i}, \text{for } i, = 1, \cdots, n_{cr,} \tag{6}$$

where k is a summation index. Consequently, the weighting coefficient of the i-th criterion (w_i) is obtained through the following equation (Dugger et al., 2022):

$$w_i = \left\{ \left| \sum_{k=1}^{n_{pc}} \widetilde{P}_k V_{i,k} \right| \right\}_i, i = 1, \cdots, n_{cr}, \tag{7}$$

where $\widetilde{P}_k$ denotes the variance proportion of the k-th principal component (in descending order), and where n_{pc} denotes the number of principal components that have been considered in the MCDA (always less than or equal to n_{cr}). The above process is repeated for the K_{opt} subregions, resulting in K_{opt} realizations of weighting coefficients. The thematic index (*TI*) is then calculated to evaluate the MAR suitability of each location (l_a) via weighted linear combination (WLC):

$$TI_j(l_a) = \left\{ \sum_{k=1}^{n_{cr}} w_k SS_k(l_a) \right\}_j, j = 1, \cdots K_{opt}, \tag{8}$$

where $SS_i(l_a)$ is the score of the i-th criterion at geographical location l_α. The above equation is applied across all three thematic layers (i.e., intrinsic suitability, water availability and water demand). Details on the generation of the criteria score maps can be found in Section 2.2.1 of this study, as well as in de Costa et al. (2024). The K_{opt} realizations for each thematic layer are then aggregated to estimate the spatial variation of the statistical moments (e.g., mean and variance) of the thematic indicators. These moments quantify the methodological variability associated with the weighting scheme and spatial stratification, reflecting the sensitivity of the expected outputs to model configurations. In this study, the following moments are considered:

$$\overline{TI}_j(l_a) = \frac{1}{K_{opt}} \left\{ \sum_{k=1}^{K_{opt}} TI_j(l_a) \right\}_j, TI_j^{con}(l_a) = \frac{\max\left(TI_j(l_a)\right) - \min\left(TI_j(l_a)\right)}{\overline{TI}_j(l_a)}, \tag{9}$$

where the $\overline{(.)}$ and $(.)^{conf}$ symbols denote the mean and confusion index (i.e., ratio of the difference between maximum and minimum over the mean) of a thematic layer, respectively. Low confusion levels indicate low ambiguity of the expected results, strengthening the confidence of the policymakers when incorporating these outcomes in their strategies.

Consequently, the feasibility index (*FI*) is derived from the mean *TI* maps through the following equation:

$$FI(l_a) = \sum_{k=1}^{3} \widetilde{w}_k \overline{TI}_k(l_a), \tag{10}$$

where $\widetilde{w}_k$ denotes the weight coefficient of the k-th thematic layer, which is jointly determined with key stakeholders via an analytical hierarchical process (AHP). For comparison purposes, the feasibility index is calculated by combining the thematic weights $\widetilde{w}_k$ with the corresponding thematic indicators. In particular, a single AHP-based MAR feasibility map is generated by computing, at each location, the weighted sum of the mean TI scores using the corresponding thematic weights, as calculated in Martins et al. (2024a). Additionally, the realizations of the thematic layers are compared with the AHP-derived MAR thematic indicators by computing the root mean square error (RMSE) at each location, given by:

$$RMSE_j = \sqrt{\frac{\sum_{a=1}^{n} \left(TI_j(l_\alpha) - TI_j^{AHP}(l_\alpha) \right)^2}{n}}, j = 1, 2, 3, \tag{11}$$

where $TI_j^{AHP}(l_\alpha)$ denotes the value of the thematic index at location (l_α) for the j-th thematic layer. In this context, RMSE is used as a measure of overall deviation between two alternative MCDA-based scoring approaches, rather than as a validation against observed reference data. As the normalized Euclidean (L2) distance between score vectors, it provides a scale-consistent measure of global disagreement across all spatial units and is particularly suitable for detecting substantial differences in the spatial distribution of suitability scores.

The entire statistical analysis was conducted in Rstudio environment (Posit team, 2024) with the use of **R4.4.1** (R Core Team, 2024). The **stats::prcomp** library is used to perform PCA, **stats::hclus** for HCA, **caret::BoxCoxTrans** for Box-Cox transformation, and **olsrr::ols_coll_diag** is used to conduct multicollinearity analysis. Moreover, the QGIS software is used to compile the spatial maps of the MAR-related factors.

3. Results and discussion

3.1. Data exploratory analysis

The boxplots in Fig. 3 show the distribution of the criteria scores, which were obtained by normalizing the criteria values of the original dataset (Table 1). This information is complemented by Table SM1 (see the "Supplementary Material"), which summarizes the basic statistical moments of the normalized criteria dataset. Inevitably, the normalization process of the criteria is inherently prone to subjectivity, as the determination of minimum and maximum cutoff suitability values, together with normalization reasoning, depends on expert interpretation. In this study, these normalization parameters are treated as fixed inputs and are not explicitly varied; therefore, the variability metrics reported later primarily reflect methodological variability associated with weighting, spatial stratification, and aggregation, rather than variability in the normalization bounds themselves.

With respect to intrinsic suitability, the aquifer lithology (ALT) has the highest mean score (0.806), reflecting consistently moderate-to-high suitability across all locations (pixels). In particular, the interquartile interval ranges from 0.6 (25th percentile) to 1.0 (75th percentile and beyond), attributed mainly to the presence of porous lithologies with acceptable characteristics to receive and store water in the vast majority of the study area. In contrast, the large interquartile ranges observed for ASC (i.e., aquifer storage capacity) and TST (i.e., topsoil texture) demonstrate significant spatial variability in suitability across different sites. The AGM (i.e., aquifer geometry) mean (0.204) is also the lowest among all criteria in the dataset, meaning that the normalization process resulted in a large portion of the study area where the MAR suitability scores were below 0.5. Although the ALT criterion consistently exhibits high scores, the presence of other high-scoring criteria and the use of a weighted-average aggregation prevent any single criterion from dominating the MAR intrinsic suitability outcomes, ensuring robustness of the composite scores.

The DSR has the highest median value among the water availability criteria (0.71) because of the dense drainage that is present in the entire domain of the study area, together with a weak skewness of the distributions toward the lower part of the interquantile range. The opposite is true for direct runoff (DR), which has very low suitability for a large portion of the study area. Additionally, small-scale regions are associated with intermediate DR scores (Fig. SM2) because of the occurrence

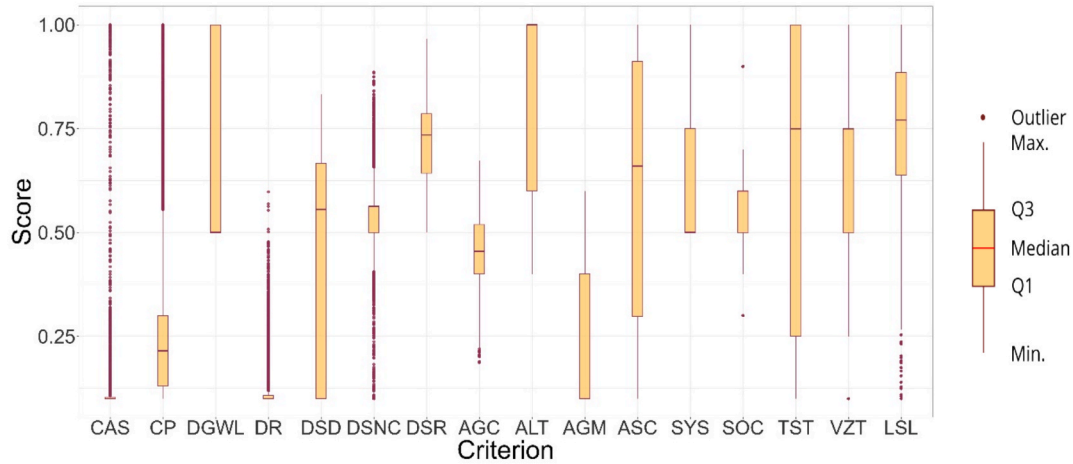


Fig. 3. Boxplots of the criteria scores for the three thematics: (a) water demand (Consumption per unit area for agricultural supply (CAS); Crop Pattern, (CP); Decrease of groundwater levels (DGWL)), (b) water availability for MAR (Direct runoff (DR); Distance to source (dams) (DSD); Distance to source (non-conventional) (DSNC); Distance to source (rivers) (DSR)), and (c) intrinsic suitability (Aquifer geochemistry (AGC); Aquifer Geometry (AGM); Aquifer Lithology (ALT); Aquifer Storage Capacity (ASC); Land Slope (LSL); Soil Occupation (SOC); Specific Yield Storativity (SYS); Top Soil Texture (TST); Vadose Zone Thickness (VZT)). Basic descriptive statistics of the criteria are provided in Table SM1 ("Supplementary Material").

of extreme local precipitation events. The criterion representing the decrease in groundwater level (DGWL) has the highest mean score (0.663) among the water demand criteria, mainly attributed to the presence of a decreasing trend in the northeastern part of the Sado River basin (Fig. SM2). This situation leads to a high demand for MAR, whereas in the remaining area GW levels are stable but show no increasing trend; consequently, standardized scores higher than 0.5 are assigned for this criterion. The criterion associated with agricultural supply (CAS) exhibits the lowest mean score (0.112) and the highest skewness (6.87) among all criteria across the thematic layers, reflecting the fact that most water abstraction for agricultural purposes is concentrated in a small portion of the study area.

SYS and AGM exhibit the highest VIF values and lowest TOL values respectively, indicating the presence of non-trivial regression relationship with the remaining variables. CAS and DSR exhibit the lowest associations with the other variables due to low values of the coefficient of determination ($R^2 \approx 0.07$). Nevertheless, all criteria exhibited Variance Inflation Factor (VIF) values below 2, which is substantially lower than the widely adopted thresholds of 5 or 10 for indicating problematic multicollinearity. As a result, no criteria were near any exclusion threshold (Table 2), and the selection of criteria was therefore insensitive to the exact choice of VIF or tolerance cutoffs.

Consequently, all criteria (16 in total) are used as input to the clustering and decision-making analyses. The criteria dataset is Box-Cox transformed prior to performing the clustering analysis, resulting in a significant reduction of the skewness levels (Table SM2). The optimal values of the Box–Cox transformation parameter (λ) for each criterion are also reported for reproducibility purposes.

3.2. Determination of the weighting coefficients for each subregion of the study area

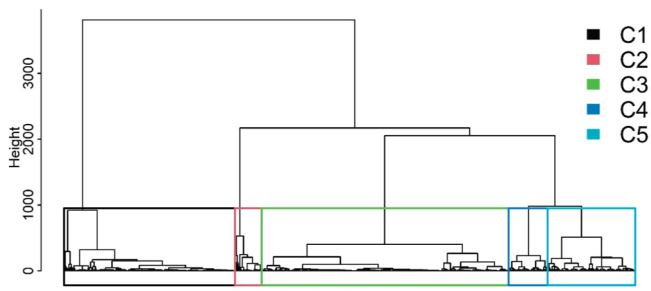
The study area is partitioned into 5 distinct clusters according to the dendrogram which is obtained from the agglomerative HCA (Fig. 4a), whereas the spatial distribution of the clusters is shown in Fig. 4b. Clusters 4 and 1 contain the largest number of data points, 13,666 and 9,452, respectively, followed by Clusters 3 (4,849), Cluster 2 (2,149) and Cluster 5 (1,477). The results highlight the relevance of geological and hydrogeological features in the analysis. This is particularly evident for Cluster 1 (C1) when overlapped with the map presented in Fig. 1, whose area corresponds to the area of occurrence of the regional developed groundwater bodies, Tejo – Sado Basin Left Margin Aquifer System (NW), Alvalade Basin (central area) and Gabros de Beja (E), respectively. This observation shows a strong association between this cluster and increased MAR suitability with respect to aquifer storage capabilities, aquifer lithology and aquifer geometry.

The distribution of Cluster 2 (C2) and Cluster 3 (C3) closely correspond to areas with relatively high direct runoff (DR) - see standardized map in SM2. The spatial extent of Cluster 5 (C5) is strongly associated with regions exhibiting high scores for the criterion representing agricultural water consumption per unit area (CAS) (Fig. SM2). Cluster 4 (C4) essentially represents the areas where no developed groundwater bodies exist.

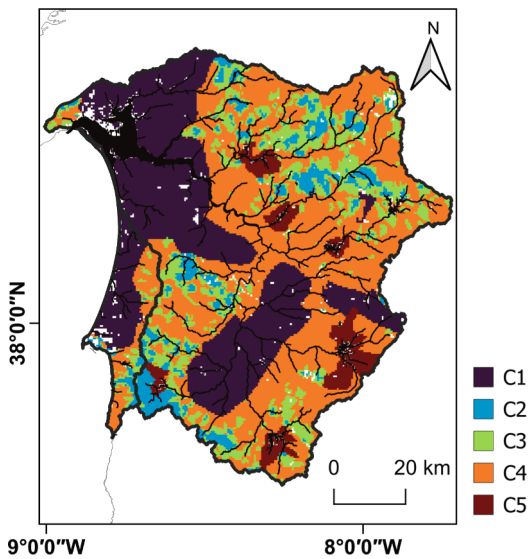
For each subregion, principal component analysis is again applied to the Box-Cox values of the criteria separately for each thematic layer, whereas the outcomes of the PCA are used to calculate the criteria weights via Eq. (7). For comprehensive purposes, a step-by-step calculation of the weighting coefficient for a single criterion is shown in the Supplementary material (O1). Moreover, the percentage of cumulative variance for each cluster and thematic layer, together with the number of PCs which are used to calculate the weights, are displayed in

Table 2
VIF and TOL values for each criterion.

MAR Criteria	CAS	CP	DGWL	DR	DSD	DSNC	DSR	AGC
VIF	1.076	1.169	2.32	1.105	1.186	1.084	1.045	1.887
TOL	0.929	0.855	0.434	0.905	0.843	0.923	0.957	0.537
MAR Criteria	**ALT**	**AGM**	**ASC**	**SYS**	**SOC**	**TST**	**VZT**	**LSL**
VIF	1.793	3.491	1.044	4.698	1.064	1.246	1.314	1.135
TOL	0.559	0.300	0.958	0.224	0.940	0.802	0.761	0.881



(a)



(b)

Fig. 4. (a) Dendrogram of the hierarchical clustering analysis based on the Box-Cox transformed criteria dataset. (b) Geographical distribution of the five subregions obtained from the clustering analysis.

Table SM3. Table 3 shows the criteria weights for each subregion and thematic layer, revealing major discrepancies among the different clusters. For comparison purposes, an AHP-based estimation of the weight coefficients is also shown, extracted from the expert-based analysis of the criteria pairwise comparison (PC) conducted by Martins et al. (2024a). The pairwise comparison matrix from which the AHP-based weights were extracted is shown in Table SM4. As also shown in Table 3, the AHP-PC reconfiguration for the selected criteria in this study exhibited a consistency ratio (CR) below the maximum recommended value (0.1 according to Saaty, 1980).

The PCA-based weights exhibit strong zonal variability across the five spatial zones identified by the clustering analysis, with separate criteria-weights sets estimated for each zone. In contrast, such geographical contrasts are not captured by the AHP-based analysis, which relies on a single, spatially uniform weighting scheme. Consequently, the mean weights derived from the PCA-based realizations exhibit notable differences compared to those obtained using the AHP-PC approach. For example, the weight for aquifer geochemistry (AGC) varies from 0.001 (C2) to 0.160 (C1), with a mean value of 0.041, which less than half of the weight obtained using the AHP-PC. The aquifer storage capacity (ASC) has the highest mean value among all the intrinsic criteria (0.2798), followed by the soil occupation (SOC) (0.2428), and topsoil texture (TST) (0.1204). On the other hand, the ALT, AGC, AGM, VZT and LSL scores exhibit small-scale variations across the entire study area. In general, the computed intrinsic weights are comparable with the AHP-based values of the criteria weights (readjusted from Martins et al., 2024a), with a minimum of 0.01 difference (VZT) and a maximum of 0.19 (SOC), with less smoothness between values of the PCA-based criteria weights. Similar observations are obtained for the criteria weights of the WA thematic layer, in which the maximum difference between AHP-PC and PCA-based methods is 0.08 (DSD). DR and DSNC both show mean weights above 0.3 for the PCA-based method, whereas AHP-PC-based weights do not surpass 0.3 in all the considered criteria.

For WD thematic layer, the AHP-PC-based method identifies DGWL as the most important criterion (0.62), whereas for PCA-based method the most relevant is CAS followed closely by CP (0.42 and 0.39, respectively). The highest discrepancy between the estimations of the two methods occurs for DGWL criterion, probably attributed to the

Table 3
Details of the PCA-based weights of the selected criteria for each cluster, together with the AHP-based weights readjusted from Martins et al. (2024a). C1 refers to Cluster 1, C2 refers to Cluster 2, etc. CR refers to the AHP consistency ratio of the pairwise comparison matrix.

Criteria*	C1	C2	C3	C4	C5	Mean	AHP	CR
Intrinsic Suitability (IS)						Weight = 0.579		
AGC	0.16	0.001	0.007	0.007	0.03	0.041	0.109	0.096
ALT	0.016	0.067	0.06	0.02	0.009	0.0344	0.177	
AGM	0.051	0	0	0	0.243	0.0588	0.216	
ASC	0.19	0.309	0.51	0.148	0.242	0.2798	0.116	
SYS	0.177	0	0.004	0.005	0.243	0.0858	0.133	
SOC	0.193	0.405	0.142	0.457	0.017	0.2428	0.052	
TST	0.099	0.145	0.186	0.15	0.022	0.1204	0.078	
VZT	0.02	0.036	0.071	0.207	0.023	0.0714	0.083	
LSL	0.095	0.038	0.019	0.006	0.171	0.0658	0.037	
Water Availability (WA)						Weight = 0.234		
DR	0.532	0.13	0.315	0.311	0.523	0.3622	0.298	0.092
DSD	0.113	0.161	0.015	0.342	0.003	0.1268	0.203	
DSNC	0.166	0.542	0.55	0.239	0.151	0.3296	0.296	
DSR	0.189	0.168	0.121	0.108	0.323	0.1818	0.203	
Water Demand (WD)						Weight = 0.187		
CAS	0.718	0.188	0.591	0.537	0.062	0.4192	0.239	0.016
CP	0.088	0.685	0.27	0.401	0.528	0.3944	0.137	
DGWL	0.194	0.126	0.139	0.062	0.41	0.1862	0.623	

*Aquifer geochemistry (AGC); Aquifer geometry (AGM); Aquifer lithology (ALT); Aquifer storage capacity (ASC); Land slope (LSL); Soil occupation (SOC); Specific yield (SYS); Topsoil texture (TST); Vadose zone thickness (VZT); Direct runoff (DR); Distance to source, nonconventional (DSNC); Distance to source, dams (DSD); Distance to source, rivers (DSR); Consumption per unit area for agriculture supply (CAS); Crop pattern (CP); Decrease in groundwater levels (DGWL).

inefficiency of PCA in handling highly skewed distributions (Koch et al., 2022) such as those occurring for this criterion.

3.3. Compilation of suitability and feasibility maps and validation with AHP-based results

The multiple realizations of the criteria weights were combined with the score maps of the criteria (Fig. SM2) through weighted linear combination (Eq. (8)) to generate five spatial realizations of each thematic layer. Table 4 shows the suitability values at different percentiles, together with the AHP predictions. With respect to intrinsic suitability, the minimum values vary from 0.229 (C5) to 0.311 (C1), where a smaller (relative) spread is observed (standard deviation equal to 0.04). The biggest dispersion is observed for the 80th percentile values, ranging between 0.660 and 0.834 (0.07 standard deviation). The mean PCA-based results reveal that the majority of the study area (at least 60%) has suitability values less than 0.654 in all regions, whereas the remaining 40% (highest values) vary within a similar interval (0.654–0.891). In addition, the quantiles of the mean intrinsic suitability scores exhibit small discrepancies compared with the AHP-based ones, being in general less than 0.08 for all percentiles. With respect to RMSE, C1 and C5 show the best agreement between the PCA-based and AHP predictions, whereas C3 shows almost three times higher deviations than the former clusters. These results are associated with the discrepancies among the realizations of the weighting dataset.

Regarding water availability (WA), the discrepancies do not exceed 0.04 in the entire range of percentiles, being less than 0.02 below the 60th percentile. The dispersion of the WA criteria weights across different realizations is the lowest among the thematic layers. Moreover, RMSE values across all realizations are less than 0.1, highlighting the good agreement between the two approaches for all clusters.

Larger discrepancies between the two methods are observed for WD across all percentiles, with the maximum difference (0.34) occurring at the 80th percentile. This observation is partly attributed to the fact that the WD indicator is calculated from the fewest number of criteria among the thematic layers, which also exhibit strong spatial variability across the study area (Fig. SM2), both at small scales (CP, CAS) and at larger scales (DGWL). Moreover, WD exhibits the largest deviations between the AHP and the PCA-based predictions among all thematic layers, reaching RMSE values close to 0.3 for C4, whereas C5 displays the smallest discrepancies (0.1).

Nevertheless, with some exceptions, the predictions of the two methods are closely comparable over the entire range of percentiles, indicating that the proposed methodology can provide realizations of the thematic scores with mean values similar to those provided by the AHP-based methodology (Fig. SM3) without requiring the nonsubjective opinions of multiple stakeholders. The qualitative agreement between MAR indicators derived from the PCA-based approach and those obtained through AHP demonstrates convergence between independent analytical methods. However, in the absence of independent ground-truth data, this convergence cannot be interpreted as external validation or evidence of predictive accuracy. Rather, the comparison serves as an assessment of internal robustness across weighting frameworks, highlighting structural coherence between approaches without implying empirical confirmation. This agreement provides additional confidence to the plausibility of the predictions.

Next, the thematic maps were aggregated to estimate basic statistical moments at each geographical location. Fig. 5 shows the spatial variation in the mean thematic indicator values ($\overline{TI}$), together with their confusion levels. The mean intrinsic suitability resulting from the PCA-based weighting method has a median value of 0.62, with a minimum value of 0.28 and a maximum value of 0.89. The most suitable regions for MAR spreading methods are concentrated in the eastern part of the study area, as well as in the southcentral part. According to Fig. SM2, these regions are characterized by favorable lithological conditions (i.e., sedimentary rocks and karstic formations) and topsoil content due to the presence of medium-to-coarse textures, whereas large scores of specific yields are also observed in the northeastern part of the study area. With respect to aquifer geometry, high suitability levels are observed in the southcentral part because of the presence of porous, phreatic aquifers with thicknesses between 10 m and 50 m, which favor infiltration, storage, and eased recovery. More information regarding the raw data for the criteria can be found in Martins et al., (2024a). In contrast, regions with lower suitability values (<0.4) correspond to areas that not only lack suitable aquifers but also exhibit steep morphologic slopes, hence MAR implementation is considered less favorable (Meles et al., 2024). The largest discrepancies between the predictions of the two methods are observed in the northern part of the study area. However, the percentage difference (PD), defined as $100\% \times \frac{\overline{TS_j} - TS_j^{AHP}}{TS^{AHP}}$, rarely exceeds 25% across the entire study area, with the highest values occurring in regions where geological conditions are less suitable for MAR implementation. Overall, PD values less than 5% are observed in most parts of the study area. Low confusion is observed in the regions with high mean suitability scores, which indicates low ambiguity and high robustness of the results. Higher confusion levels are observed in the regions of low-to-moderate mean intrinsic suitability values ($\overline{IS}$), indicating strong spatial variability that follows the partitioning of the study area into subregions.

With respect to water availability, the lowest thematic indicators are observed in areas far from the source buffers (rings), where no water sources for MAR are expected to be found. The confusion map shows greater ambiguity in these areas, which are also associated with greater percentual differences from the AHP method. These differences are mostly controlled by the DSNC since this criterion is assigned the highest weighting coefficient, where the rings around this type of source are visible. For this thematic, the maximum obtained value is 0.68, the minimum is 0.28, and the mean is 0.5.

The maximum value of the WD indicator is 0.79, the mean is 0.39, and the minimum is 0.27, with lower values concentrated in the southern and western parts of the study area, which are characterized by low DGWL scores. Additionally, these areas coincide with the areas with the highest confusion values and percentage differences.

Table 4
Percentiles of the suitability indicators for each set of weights derived from each cluster.

Percentiles (%)	C1	C2	C3	C4	C5	Mean	AHP
Intrinsic Suitability (IS)							
0	0.311	0.297	0.207	0.265	0.229	0.282	0.289
20	0.511	0.538	0.493	0.561	0.418	0.512	0.471
40	0.570	0.624	0.614	0.616	0.501	0.589	0.521
60	0.620	0.693	0.729	0.662	0.562	0.654	0.575
80	0.676	0.767	0.834	0.719	0.660	0.720	0.669
100	0.852	0.953	0.976	0.947	0.826	0.891	0.816
RMSE	0.066	0.136	0.167	0.134	0.072	0.115	
Water Availability (WA)							
0	0.224	0.216	0.176	0.175	0.251	0.226	0.240
20	0.302	0.436	0.383	0.285	0.338	0.362	0.372
40	0.327	0.489	0.414	0.399	0.363	0.396	0.415
60	0.349	0.523	0.438	0.446	0.384	0.421	0.456
80	0.366	0.549	0.460	0.476	0.402	0.444	0.482
100	0.574	0.701	0.636	0.574	0.624	0.576	0.588
RMSE	0.098	0.075	0.055	0.052	0.079	0.072	
Water Demand (WD)							
0	0.178	0.150	0.156	0.125	0.264	0.174	0.349
20	0.181	0.167	0.163	0.135	0.277	0.185	0.353
40	0.191	0.230	0.194	0.172	0.335	0.229	0.369
60	0.218	0.286	0.237	0.204	0.440	0.288	0.404
80	0.289	0.350	0.275	0.238	0.546	0.340	0.679
100	0.903	0.936	0.931	0.969	0.945	0.907	0.827
RMSE	0.266	0.242	0.274	0.304	0.101	0.237	

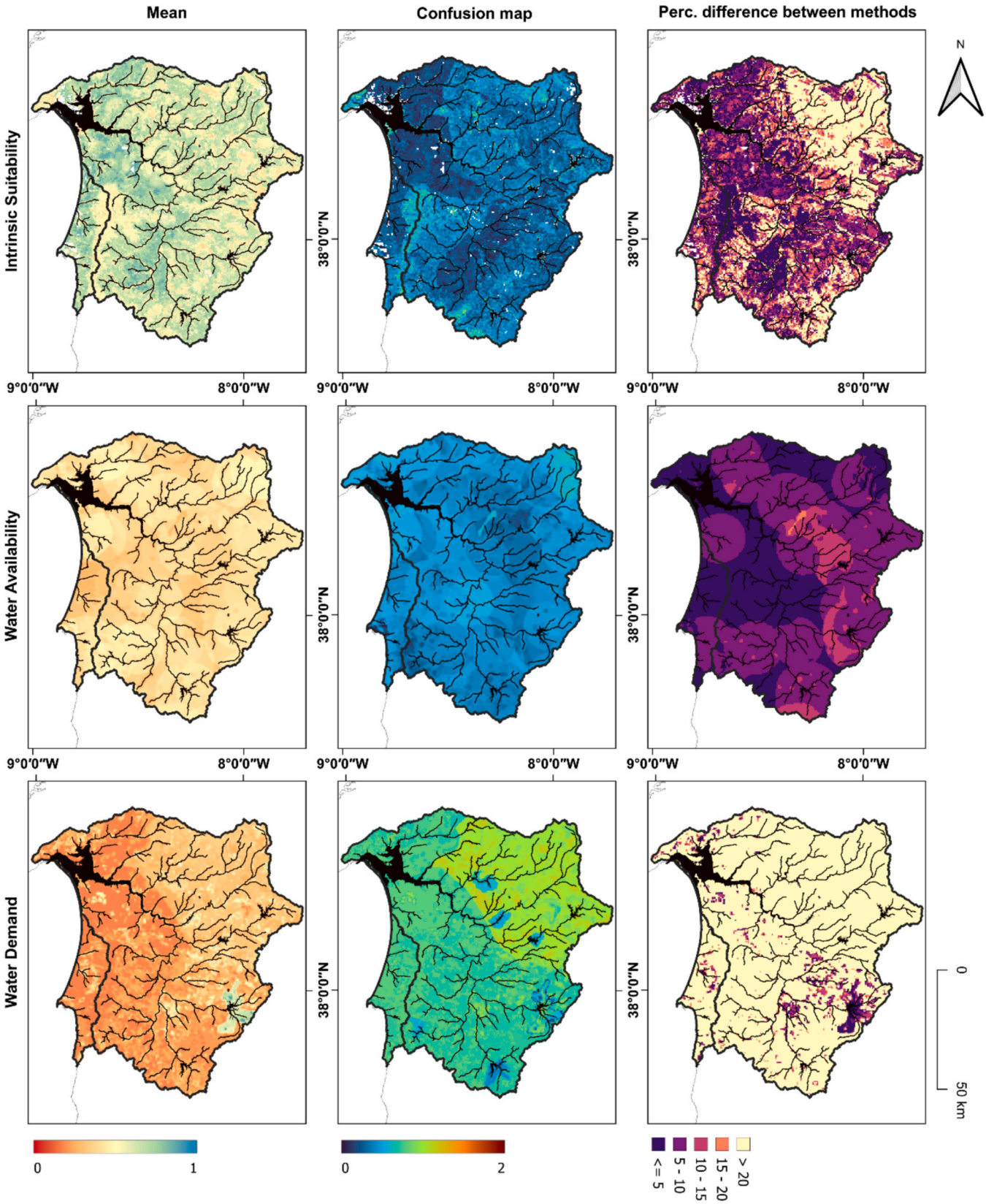


Fig. 5. Geographical distribution of the basic statistical moments (i.e., mean and confusion index) of the intrinsic suitability, water availability, and water demand. The mean thematic maps are compared with the analogous AHP predictions (TS^{AHP}) by predicting the percentage difference (PD) indicator at each location (l_a), defined as $100\% \times \frac{\overline{TS_j} - TS_j^{AHP}}{TS^{AHP}}$.

The spatial patterns of the feasibility index (FI), together with the AHP-based predictions for this indicator, are presented in Fig. 6. The maximum, minimum and median FI values are 0.67, 0.34 and 0.52, respectively, which are similar to the corresponding values for the AHP predictions (see Table SM5). As shown in Fig. 6, most of the study area (90%) is classified as "moderately feasible" for MAR, with values ranging between 0.4 and 0.6 (5th-95th percentiles). In contrast, only a small portion of the study area (5%) exhibits high feasibility levels (0.6–0.8) for both methods (Fig. SM4). The results indicate strong smoothing of the spatial variation in the feasibility levels, attributed mainly to (1) the relatively high number of criteria included in the analysis (16 in total) and (2) the normalization principles adopted to generate the scores of the criteria. In both methods, higher MAR feasibility values are strongly related to the presence of developed groundwater bodies consisting of permeable lithologies. This observation reflects the crucial role of fulfilling the main MAR implementation requirements: the capacity to store water and the capacity to recover it when needed. Similar to the results observed for the thematic maps, the percentage difference of the FI is small, indicating that both methods produce largely consistent results. Although relatively noticeable differences exist (up to 0.1), these discrepancies are confined to small-scale regions, particularly in the central and northern parts of the study area.

4. Discussion and limitations

The outcomes of this study provide a systematic screening framework to identify regions with high MAR feasibility based on three thematic factors: intrinsic suitability (topography, soil, hydrogeology), water availability (proximity, quantity, quality), and water demand (criteria reflecting the region's primary groundwater use, namely irrigation; see APA, 2023a). While additional non-physical, economic, and regulatory factors are important for final decision-making, the present results offer a reproducible and scalable first step for highlighting promising regions where MAR interventions are most likely to be feasible. Therefore, further elaboration is needed to provide a complete feasibility assessment of an area of interest that can promote the adoption, implementation, and successful operation of MAR by policymakers and water managers.

4.1. Nonphysical factors that affect MAR feasibility

This study focused on assessing the MAR feasibility based solely on

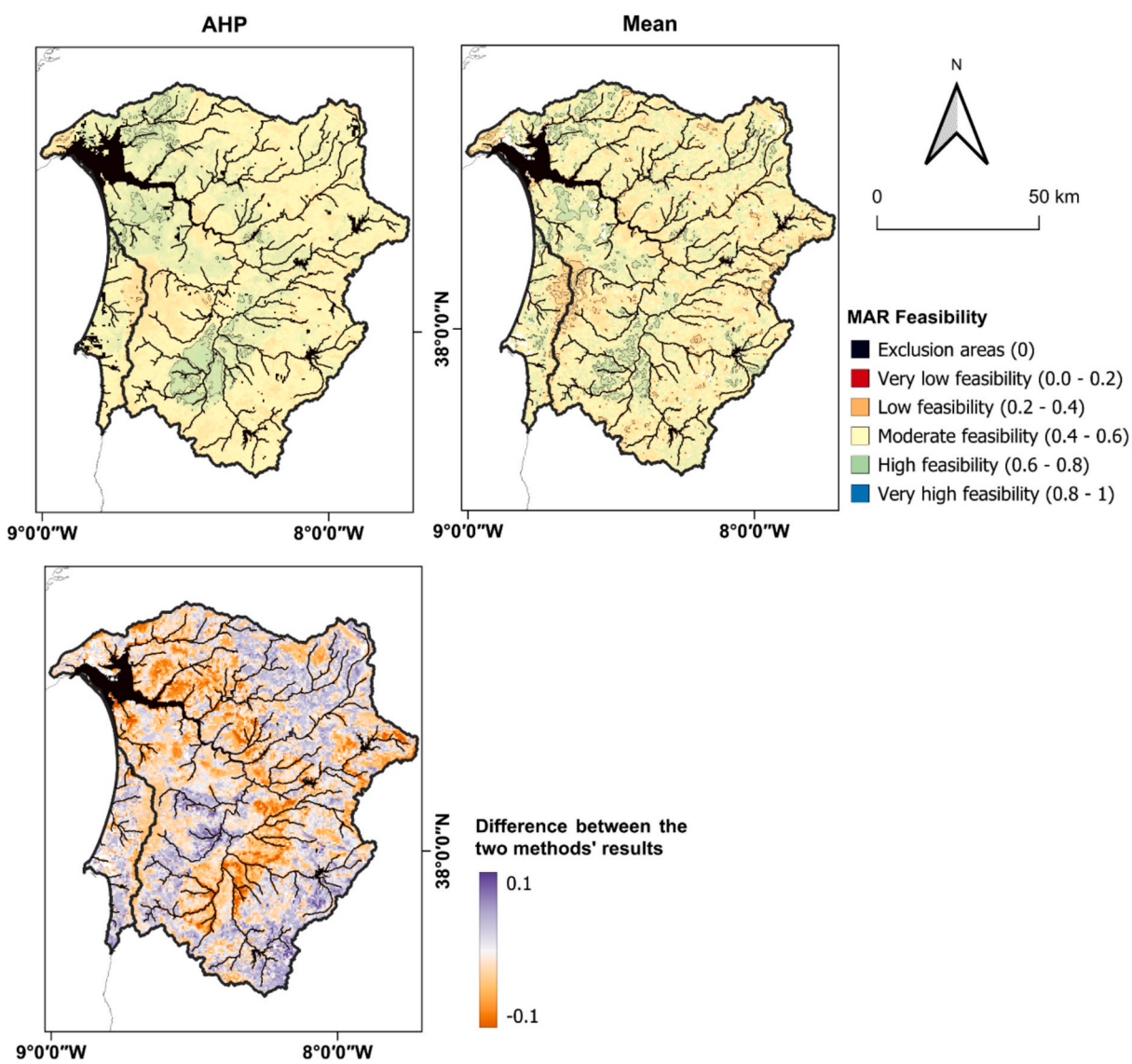


Fig. 6. Geographical distribution of the feasibility indicator (*FI*). A comparison is conducted with the FI predictions using an analytical hierarchical process (FI^{AHP}). The difference between the predictions of the two methods at each location (l_a) is defined as $FI(l_a) - FI^{AHP}(l_a)$.

physical factors. However, additional factors should be considered that are not related to technical aspects but instead pertain to policy and economic constraints. The costs of MAR configurations are affected by a range of intrinsic, socioeconomic, institutional and legal factors. For example, the geological characteristics of the vadose zone and the aquifer strongly affect the water recovery and infiltration rates, regulatory conditions influence project setup expenses, whereas socioeconomic factors affect labour and capital costs (Dillon et al., 2009). With respect to spatial MCDA for MAR, economic factors (e.g., infrastructure and operation costs) can be incorporated into spatial MCDA for MAR as cost-based criteria or penalty layers, institutional factors (e.g., governance capacity and stakeholder acceptance) can be represented through zonal or expert-derived indicators, and legal or regulatory constraints can be introduced as binary exclusion masks or suitability modifiers within the mapping framework. Integrating these dimensions would enable a more comprehensive assessment of MAR feasibility beyond technical considerations (Scanlon et al., 2016; Maliva, 2014).

In Portugal, the implementation of low economic stress-prone spreading methods, such as infiltration basins or ditches, particularly in or close to agricultural and *peri*-urban areas, can contribute to the adoption of sustainable water management practices at the local and regional scales. These practices become more relevant given the outlook of changing rainfall patterns in the study area that are likely to result in more stress on surface water resources, together with the national objective of valuing and maximizing the use of treated wastewater (non-conventional source) from the perspective of storing every source possible. Therefore, these types of MAR methods can be easily promoted within farmers and farming associations at both local and regional scales as easy-to-replicate local-scale interventions, with low complexity in terms of design and less robust maintenance practices. The promotion of simple MAR methods among farmers and farming associations is supported by real-world pilot studies and policy initiatives that demonstrate their technical and operational accessibility. For example, the AgriMAR project reports the use of low-tech infiltration ponds and locally available materials in the coastal plains of Bangladesh to store freshwater underground for dry-season irrigation, yielding positive benefit-cost ratios and demonstrating feasibility and farmer buy-in under resource-limited conditions (AgriMAR, 2019). Similarly, on-farm flood recharge trials in the Kings River Basin (California) have shown that intentional infiltration of excess surface water across agricultural fields can enhance groundwater levels with minimal disruption to normal farming operations (Bachand et al., 2016). Such examples illustrate that, where regulatory support and basic infrastructure are present, low-complexity MAR approaches can be integrated into agricultural water management frameworks.

These approaches can be coupled with other methods to retain peak flows and store them in wet periods which may result in reconverting current existing surface storage infrastructure (see the examples presented in Ferencz et al., 2024; Goharian et al., 2020). This is an important factor for policy-makers since agriculture is, as already stated, not only the main water consumer but also a significant economic actor that relies heavily on infrastructure adaptation and modernization to face the climatic challenges ahead. The development of reliable and potentially updatable feasibility maps can thus represent a first step toward promoting such solutions among stakeholders.

In addition to cost analysis, appropriate incentives for favorable MAR schemes, the legal framework of rights for water recharge, storage and recovery (RSR), and the yearly allocation rules that apply for extracting groundwater need to be clearly defined and put in practice in a transparent manner. With respect to the Portuguese legal framework, MAR is considered a complementary measure for achieving good chemical and quantitative status, provided that it does not result in adverse impacts (Ghannem et al., 2024). There is currently no market in Portugal, whereas any entity (e.g., a single citizen or farmer) can extract groundwater as long as it is collected from a low-powered pump. Higher abstraction volumes require a permit from the water authority (APA, Portuguese Environmental Agency), which ensures that the requested volumes are sustainable within the overall budget of the water body (both surface and groundwater; for the latter, abstractions must not exceed 80% of natural recharge). In accordance with Portuguese law 226-A/2007, MAR systems that enhance natural recharge without compromising compliance with the environmental objectives established for the groundwater body are permitted (e.g., basins or small dams in streams, typically built to increase infiltration and decrease flood impacts). On the other hand, the lack of specific regulations for MAR can create legal uncertainty regarding its implementation, monitoring requirements, and long-term management, potentially hindering broader adoption and investment in such systems. This is particularly relevant when non-conventional sources, such as treated wastewater, are used, as they can pose a risk of aquifer pollution if not properly monitored or managed.

4.2. Main advantages and limitations of the proposed weighting process

Although the proposed methodology can be directly applied to other geographical contexts and scales, the criteria normalization and weighting processes are case-site sensitive. The incorporation of a clustering technique allows the PCA-based MCDA to elaborate the case-site datasets to generate multiple realizations of the criteria weights driven by the characteristics of the available data for each subregion, enabling the quantification of variabilities associated with these weights.

However, it does not consider other sources of uncertainty, such as those related to input data quality, spatial resolution (e.g., a limited number of sampling locations or three-dimensional variability in aquifer properties such as spatially interpolated hydraulic conductivity and specific yield), or temporal variations in MAR suitability (e.g., seasonal differences between wet and dry time periods). Consequently, the reported confidence and confusion indicators should be interpreted as conditional on the available data and current spatial assumptions. Excluding these additional sources may underestimate total uncertainty, particularly in regions with sparse or highly heterogeneous information. Nevertheless, the current analysis provides a systematic and reproducible screening framework for identifying the most robust MAR-feasible regions based on the available information.

Depending on the characteristics of the available data, different spatial resolutions should be considered when assessing the impact of this factor on the results, enabling the selection of a resolution that best suits the needs of practitioners for the specific problem of interest. With respect to the temporal aspect, it is important to select a specific seasonal period (wet or dry) prior to performing the MCDA, as this choice significantly affects the criteria values (e.g., groundwater levels and aquifer geochemistry) and, consequently, the normalization of the criteria maps. In contrast, traditional methods, such as the AHP, often rely on either the standard deviation of the stakeholders' opinions (Martins et al., 2024a) or the consistency ratio index (de Brito and Evers, 2016) to conduct sensitivity analysis, without addressing the quantification of neither uncertainty nor variability.

Another limitation of the proposed framework is that the reported variability estimations reflect methodological variability conditional on the chosen normalization scheme. In this study, normalization bounds were treated as fixed deterministic inputs and were not varied within an uncertainty propagation framework. Consequently, variability arising from expert judgment in defining normalization bounds—i.e., epistemic variability —was not explicitly parameterized or propagated in this study. As a result, the variability metrics reported (e.g., confusion index) reflect methodological uncertainty associated with weighting schemes, spatial stratification, and aggregation procedures, rather than parametric uncertainty in the normalization limits themselves. The absence of quantitative propagation of normalization-bound uncertainty is acknowledged as another limitation of the current analysis. Future work could address this by incorporating sensitivity or probabilistic

treatments of normalization parameters (e.g., Monte Carlo sampling of minimum and maximum thresholds). Overall, it is crucial that the scientific community, industry, and governmental authorities collaborate to generate detailed and high-fidelity datasets, understand the advantages and limitations of the different approaches, which can be used by policymakers to make well-informed decisions.

Additionally, PCA is designed to extract linear patterns of the associations among the criteria, neglecting the nonlinear dependencies that might be present. As a result, the resulting eigenvalues and eigenvectors might not accurately reflect the statistical correlations among the attributes, resulting in a loss of interpretability. Moreover, the outcomes of PCA are sensitive to the presence of outliers and highly skewed distributions of the input datasets, potentially leading to inaccurate conclusions with respect to variable importance. In this study, the dataset used for PCA consisted of 31,593 locations across the study area and 3–9 criteria (depending on thematic layer). Applying nonlinear PCA approaches such as kernel-PCA, to datasets of this size requires storing and manipulating very large kernel matrices, which leads to substantially higher computational costs. Standard PCA was therefore adopted as a practical and computationally feasible alternative for dimensionality reduction. In future work, kernel-PCA could be applied in this study area by reducing the dataset size through coarser spatial grids, sub-sampling locations, or focusing on key subsets of criteria, thereby making the computational requirements manageable while still capturing nonlinear patterns in the data (Jibrin et al., 2025). Nevertheless, the proposed method does not suffer from a key limitation of the AHP-PC process when handling high-dimensional datasets, which require a large number of pairwise comparisons and make it challenging to provide a fully objective and unbiased evaluation of the relative importance of each criterion.

Another limitation of the proposed method is its dependency on the number of subregions that are predicted by clustering analysis. This number varies with respect to the selected criteria and their spatio-temporal patterns, which are also subjected to sources of uncertainties. In a very recent review article, Rahbar et al. (2026) highlighted the capacity of HCA to group samples based on attribute similarity, without the necessity of predefining the number of clusters, in contrast to other clustering methods, such as K-means, K-medoids. Hence, K-means and K-medoids are expected to provide more sensitive feasibility outcomes than HCA. Nevertheless, additional work should be conducted to address this shortcoming to increase the robustness of this approach. In future work, the sensitivity of the MCDA outcomes to different choices of the optimal number of clusters could be evaluated by applying internal validation metrics (e.g., silhouette coefficient, within-cluster variance, or gap statistics) to assess how changes in cluster assignment affect the derived zone-specific PCA weights and the resulting MAR indicators. Such analyses would provide a quantitative assessment of the robustness of the weighting scheme to methodological choices and help to identify regions where indicator values are more sensitive to cluster definition.

Another option might be the development of a similar methodology that relies on the coupling of PCA with kernel smoothing methods in the decision-making process, as suggested by Ning and You, (2018), which allows the quantification of uncertainties of the data in a computationally effective manner.

5. Conclusions

The results confirm the relevance of geological and hydrogeological features in this mapping process, with higher suitability associated with areas that have aquifer characteristics favorable for MAR. Water availability is, as expected, related to the existence of potential water sources available for MAR (both natural, rivers or lakes, or non-conventional origins, such as treated wastewater), whereas WD is strongly driven by (1) the existence of relevant pressures on water resources (e.g., high water consumption such as agriculture) which may force the implementation of alternative management strategies, and (2) the evidence that the current use of those resources may not be sustainable (e.g., a noticeable trend of decreasing groundwater levels which may be related with more recurrent scarcity phenomena coupled with continuous groundwater use).

Compared with traditional MCDA methods, the current approach enables practitioners to:

- integrate multivariate statistical methods into the MCDA for the identification of feasible regions for MAR
- generate multiple realizations of the criteria weights via a semi-automatic data-driven approach that reflects the variability of site-specific characteristics
- mitigates the impact of subjectivity in stakeholders' weighting of criteria in the decision-making process
- enable the quantification of the variability associated with the criteria weights to the outcomes of the MCDA

The proposed methodology does not hinder the feedback from the stakeholders during other stages of the decision-making process (i.e., criteria selection, determination of thematic weights), which is essential to ensure that the MCDA outcomes reflect their needs. Furthermore, it does not suffer from well-known limitations of traditional MCDA methods, such as the limitation to consider no more than 9 criteria (Miller, 1956) due to the complexity of the pairwise comparison. Moreover, it enables the quantification of variability based on weights realizations that inherent spatial characteristics of the study area. In addition, it reduces the influence of potentially biased stakeholder opinions by deriving zonal-specific criterion weights directly from the data via PCA, providing a systematic and reproducible weighting scheme while preserving key spatial patterns.

The proposed approach can be applied to other hydrogeological contexts and MAR typologies, thereby supporting the design of effective large-scale water and land-use management policies. As part of future work, the inclusion of other important factors (i.e., socioeconomic, legal, institutional) that can also provide solid scientific evidence to policy-makers for the long-term positive impact of these solutions will be assessed, facilitating the further adoption of MAR on an integrated manner at river basin scale. In addition, this approach is directly applicable in other disciplines that require spatiotemporal multicriteria datasets for decision-making processes, such as flood, fire, and landslide susceptibility.

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CRediT authorship contribution statement

Constantinos F. Panagiotou: Writing – review & editing, Writing – original draft, Visualization, Software, Resources, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Tiago Martins:** Writing – review & editing, Writing – original draft, Visualization, Investigation, Data curation. **Catalin Stefan:** Writing – review & editing, Funding acquisition, Conceptualization.

Declaration of competing interest

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.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jhydrol.2026.135316.

Data availability

Data will be made available on request.

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