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A review of macroinvertebrate- and fish-based stream health modelling techniques

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Abstract

During the last three decades, explaining cause–effect relationships between natural and anthropogenic disturbances with measures of stream health have motivated the growing application of statistical, machine learning, and soft computing methods. The aim of this review is to provide insight into the most widely used methods for predicting biological variables based on macroinvertebrate and fish species in riverine ecosystems. Therefore, we describe several methods including multiple linear regression, generalized linear models, generalized additive models, boosted regression trees, random forests, artificial neural networks, fuzzy logic-based, and Bayesian belief networks along with recent applications of these. Moreover, issues regarding variable selection, model interpretability, ensemble modelling, and model evaluation and overfitting are discussed. Recent advances have suggested the need for integrated modelling systems to enhance the predictive ability and improve interpretability. However, trade-offs between model complexity and accuracy demand research efforts in uncertainty quantification/propagation in model ensembles. Additionally, models should be perceived as complementary tools that require further validation with field measurements. Therefore, a consensus regarding monitoring and modelling practices for stream health applications is recommended.

KEYWORDS

habitat suitability, machine learning, soft computing, species distribution models, statistical methods, stream health

1 | INTRODUCTION

Current and future threats to freshwater ecosystems due to changes in environmental conditions and impacts of anthropogenic activities require urgent and well-informed actions (Strayer & Dudgeon, 2010; Vörösmarty et al., 2010; Waldron et al., 2017). Therefore, health assessments of these ecosystems are critical to promoting their protection and restoration (Beechie et al., 2010). During the last few decades, many environmental legislations have been increasingly supportive of the introduction of biological assessments in local, regional, and national monitoring programs (Hering et al., 2010; Hill et al., 2017). Typically, different metrics and indices are derived from biological assessments to represent the stream health condition. The stream health concept comprises the physical, chemical, and biological capacity to maintain

the structure and functioning of freshwater ecosystems, required for supporting living systems (Karr, 1999; Maddock, 1999). The stream health indices are generally classified into biotic indices, multimetric indices, and multivariate methods (Herman & Nejadhashemi, 2015). Biotic indices use only one metric to describe stream health, whereas more than one metric are used for multimetric indices (Herman & Nejadhashemi, 2015). Biotic metrics are individual characteristics describing species abundance, biomass and condition, species richness and composition, or trophic composition. Multivariate methods use a reference condition to predict ratios of taxa observed versus expected (O/E). By implementing statistical and modelling, the multivariate methods relate environmental features with observed organisms.

Biological measurements in aquatic ecosystems can be obtained from several biological assemblages, and their selection is usually

subjected to the type of study being performed. Benthic macroinvertebrates are preferred when studying localized effects of habitat and water quality alterations, due to their limited movement within a water body (Kerans & Karr, 1994). Meanwhile, fish communities are preferred when evaluating changes in flow regime and spatial connectivity (Karr, 1981). Benefits of stream health evaluation include the possibility to explore the environmental mechanisms driving ecosystem alterations (Herman & Nejadhashemi, 2015). Likewise, indicators of stream health can help with the identification of degraded areas and the provision of necessary inputs to design protection and restoration projects (Walters, Roy, & Leigh, 2009).

In this study, the stream health modelling approaches were defined in the concept of predicting stream health indices in freshwater systems. Stream health models are developed for establishing reference conditions (Feio & Poquet, 2011; Hawkins, Norris, Hogue, & Feminella, 2000), predicting biological variables and indicators in unsampled locations (Merriam, Petty, Strager, Maxwell, & Ziemkiewicz, 2015; Waite et al., 2010), classifying streams by impairment condition (Brown et al., 2012; Maloney, Weller, Russell, & Hothorn, 2009), and predicting biological variables and indicators given the implementation of conservation practices (Hall et al., 2017; Herman et al., 2015; Sowa et al., 2016) and changes in environmental and landscape stressors (Einheuser et al., 2012; Einheuser, Nejadhashemi, Wang, Sowa, & Woznicki, 2013; Einheuser, Nejadhashemi, & Woznicki, 2013). These models have been enhanced by the advances in landscape methods for studying freshwater ecosystems (Johnson & Host, 2010; E. A. Steel et al., 2010), species distribution models (SDMs; Elith & Graham, 2009; Li & Wang, 2013; Van Echelpoel et al., 2015), and habitat suitability models (Ahmadi-Nedushan et al., 2006; Yi et al., 2017). Still, due to the complexity and nature of the problem, stream health models are mainly empirical-based rather than mechanistic or process-based. However, hierarchical approaches incorporating climate, hydrologic, hydraulic, water quality, and/or physical habitat models have been suggested to improve the current models' predictability, interpretability, and accuracy (Daneshvar, Nejadhashemi, Herman, & Abouali, 2017; Einheuser et al., 2012; Einheuser, Nejadhashemi, Wang, et al., 2013; Einheuser, Nejadhashemi, & Woznicki, 2013; Guse et al., 2015; Herman et al., 2015; Holguin-Gonzalez et al., 2013; Holguin-Gonzalez et al., 2014; Holguin-Gonzalez, Everaert, Boets, Galvis, & Goethals, 2013; Jähnig et al., 2012; Kail et al., 2015; Kennen, Kauffman, Ayers, Wolock, & Colarullo, 2008; Woznicki et al., 2016; Woznicki, Nejadhashemi, Tang, & Wang, 2016; Yi et al., 2017).

Modelling approaches include traditional regression models (e.g., multiple linear regression [MLR] and generalized linear models [GLM]), multivariate statistics methods (e.g., discriminant analysis, principal component analysis [PCA], and redundancy analysis [RDA]), clustering methods (e.g., self-organizing maps and *k*-nearest neighbours), structural equation modelling, machine learning, and soft computing techniques (e.g., fuzzy logic, neural networks, and evolutionary computation). In this paper, we review the most widely used modelling approaches for predicting unimetric and multimetric stream health indices related to macroinvertebrates and fish assemblages in freshwater ecosystems. The methods discussed herein are able to model both continuous and categorical data and comprise traditional

statistical approaches, machine learning, and soft computing methods. The goal of this paper is to identify advantages and drawbacks of these methods in predicting stream health indices in the context of variable selection, model interpretability, and model evaluation and overfitting. The specific objectives of this study are to (a) summarize the main characteristics of the selected modelling methods and their applications and (b) identify features requiring further research for improving stream health modelling practices.

2 | MODELLING METHODS

In this section, we describe the most widely used methods for stream health modelling. In general, the approaches presented herein are data-driven because we are dealing with natural systems; however, soft computing methods are more suitable for incorporating expert elicitation. In addition, both soft computing and machine learning methods are more flexible regarding statistical assumptions than traditional statistical modelling approaches.

2.1 | Statistical methods

A statistical model is a specification of probability distributions reproducing observed data, establishing mathematical relationships between explanatory and response variables (Nelder & Baker, 2006). Multivariate statistics methods can be used for either ordination or classification purposes. Ordination is the arrangement of biological data samples along one or more gradients (Austin, 1976), whereas classification is the assignment of biological data samples into groups based on a measure of similarity (or dissimilarity; Mitteroecker & Bookstein, 2011).

2.1.1 | Linear statistical methods

Linear statistical methods have been applied mainly to elucidate relationships between landscape, habitat, and water quality factors and biological variables. In this category, there are methods with different complexity levels such as MLR, GLMs, and generalized additive models (GAMs), which have been widely implemented in ecological applications (Leathwick, Elith, & Hastie, 2006). MLR fits a linear equation using the observed data to model the relationship between a set of explanatory variables and a response variable, assuming independent and identically normal distributed errors. Meanwhile, GLMs introduce some flexibility allowing different error distributions, selected from the exponential family of sampling models (e.g., normal, binomial, Poisson, and gamma), and relate the response variable *Y* with the explanatory variables *X* using a prespecified link function *g* (McCullagh & Nelder, 1989). The link function provides the relationship between the linear predictor η and the expected value (i.e., mean) of the response variable *Y* given the set of explanatory variables *X*:

$$g[E(Y|X)] = \eta = \alpha + X\beta, \quad (1)$$

where *E* is the expectation operator and α and β are the intercept and the vector of linear weights, respectively. When selecting different link functions, GLMs comprise linear, logistic, and Poisson regressions, among others. For instance, logistic regression is preferred when

modelling species presence/absence, whereas Poisson regression is more suitable when modelling the count data (Li & Wang, 2013). In order to further account for nonlinearities, GAMs extend GLMs, expressing η as the sum of unspecified nonparametric linear or nonlinear smoothing functions f_j , applied over the set of p explanatory variables X_i (Hastie, Tibshirani, & Friedman, 2009):

$$g[E(Y|X)] = \alpha + f_1(X_1) + \dots + f_p(X_p). \quad (2)$$

To ensure that the smoothing functions are identifiable, they are restricted to have zero mean (Maloney, Schmid, & Weller, 2012). These functions are commonly estimated using a scatter plot smoother (e.g., cubic spline) as the basic building block (Hastie et al., 2009; Zuur, Ieno, Walker, Saveliev, & Smith, 2009).

Linear statistical models were initially introduced to build empirical associations between landscape and stream health attributes. Early efforts were mostly concerned in identifying the main stressors and landscape components (i.e., riparian buffer and watershed) affecting water quality, physical habitat, and/or freshwater biological communities (Van Sickle et al., 2004). Many of these works are reviewed by Ahmadi-Nedushan et al. (2006), Johnson and Host (2010), and E. A. Steel et al. (2010). Linear statistical models have also been continuously applied as benchmarks for comparison with other statistical methods and machine learning approaches. For macroinvertebrate communities, traditional regression models are still used to relate abiotic stressors with species occurrence in order to explore habitat and water quality preferences, especially in headwaters (Pond, Krock, Cruz, & Ettema, 2017) and tropical regions (Damanik-Ambarita et al., 2016; Everaert et al., 2014; Jerves-Cobo et al., 2017). However, prediction of the biological condition under different spatial and temporal domains and scales have been also addressed in some studies for both macroinvertebrate and fish assemblages (Frimpong, Sutton, Engel, & Simon, 2005; Johnson & Host, 2010; Van Sickle & Burch Johnson, 2008).

Representative studies employing MLR for stream health prediction include models developed by Waite et al. (2010) to predict several macroinvertebrate metrics using watershed- and riparian-scale variables. Results showed that the best models explained 41–74% of the variation requiring only two or three explanatory variables after stepwise selection using the Akaike information criterion (AIC) estimator. Likewise, Merriam, Petty, Strager, Maxwell, and Ziemkiewicz (2013, 2015) employed linear regression and deletion tests to predict two indices based on benthic macroinvertebrate abundance as a function of surface mining, underground mine permit density, residential development, and location attributes. The results suggested that the interactions between different land uses are more important than a single land use effect.

On the other hand, GLMs have been very popular for predicting species occurrence and distribution in freshwater ecosystems (Ahmadi-Nedushan et al., 2006). Van Sickle et al. (2004) implemented a linear regression and a negative binomial GLM for projecting fish and macroinvertebrate biological indices as a function of landscape and streamflow variables under different timeline scenarios, including reference conditions. Donohue, McGarrigle, and Mills (2006) employed a stepwise binary logistic regression and logarithmic and quadratic

regressions to obtain national-wide relationships between catchment and water quality attributes and stream ecological status based on an index representing the structure of benthic macroinvertebrate communities. Other studies have implemented GLMs in an integrated ecological modelling framework involving hydrodynamic, water quality and stream habitat suitability models to predict macroinvertebrate-based stream health at a reach scale (Holguin-Gonzalez, Boets, et al., 2013; Holguin-Gonzalez, Everaert, et al., 2013; Kuemmerlen et al., 2014). Sui, Iwasaki, Saavedra Valeriano, and Yoshimura (2014) developed a predictive model employing a geomorphology-based hydrological model to determine ten flow indices. Then a GLM was implemented in order to relate those indices to the occurrence probabilities of 50 fish species at a watershed scale. In a recent study, Gieswein, Hering, and Feld (2017) used GLM to quantify the pairwise stressor interactions (strength and significance). This was performed following implementation of a decision tree-based model for identifying stressor hierarchy. A boosted regression trees (BRT) model was used when analysing the relationships between several factors (i.e., riparian land use, physical habitat quality, nutrients, and natural variables) and fish, macroinvertebrates, and macrophytes assemblages.

With respect to GAMs, Maloney et al. (2012) compared the standard and boosted versions of this method for macroinvertebrate and fish metrics prediction, using watershed, stream, and site attributes as explanatory variables. Results indicated that gradient boosting applied to GAMs avoids overfitting and provides interpretable relationships, which is an advantage in comparison with traditional machine learning techniques. Additionally, regular GAM has been also compared with a GAM based on PCA for fish richness and diversity prediction (Zhao et al., 2014). Results showed different selected explanatory variables for each approach, generating different outcomes for the response variables. However, PCA-based GAM performed better during cross-validation tests and was found to be more suitable when predictors are highly correlated (Zhao et al., 2014). More recently, Almeida, Alcaraz-Hernández, Merciai, Benejam, and García-Berthou (2017) evaluated the effect of sampling effort in terms of transect length on fish metrics. This was performed for a large Mediterranean watershed using a GAM with sampling area as a predictor. Results indicated that fish indices that are obtained using predictive models are more sensitive to sampling strategies than simpler biotic metrics that are model-independent, showing a decrease in their values with increasing sampling area, despite observed higher richness.

Regarding spatial-scale effects, Johnson and Host (2010) listed representative studies from 2000 to 2008 involving invertebrates and fish assemblages. For each study, the authors reported the scales (e.g., habitat, reach, local, ecosystem, watershed, regional, and ecoregion) at which explanatory variables explained the instream biological response. Johnson and Host (2010) showed meaningful differences in the scale's importance among the reviewed studies, due to the different region sizes and disturbance levels for each case. A study by Frimpong et al. (2005) used linear and piecewise regression to compare the performance of stream habitat indices obtained at the watershed scale and observations at the reach scale for fish metrics prediction. Results indicated that watershed-scale variables provided better predictions for stream health than reach-scale variables.

Additionally, predictive ability decreased with the spatial extent, which might be attributed to the increase of the attributes' heterogeneity. In another study, Van Sickle and Johnson (2008) developed a distance weighting model based on linear regression for estimating specific land use areas within watersheds that best explain fish index of biotic integrity (IBI). With this approach, it is possible to compare different scales of landscape influence on stream health. Furthermore, linear models have been also used for multimetric indices formulation. Pont, Hughes, Whittier, and Schmutz (2009) implemented a procedure involving stepwise, multilinear, logistic, and Poisson regressions to build a predictive IBI for aquatic vertebrates (fish and aquatic amphibians). Particularly, this procedure was developed to discriminate natural and anthropogenic effects over the biotic metrics computation. Implementing the same approach, Moya et al. (2011) developed a multimetric index for macroinvertebrate assemblages. This index based on predictive models successfully discriminated between the reference and disturbed sites.

2.1.2 | Shrinkage methods

In general, the interpretability of models decreases when the number of predictors (and regression coefficients) is large. This condition may result in multicollinearity/redundancy, low bias, and large variance, which reduce the model accuracy (Hastie et al., 2009). In general, variable selection methods are based on discrete processes that retain a subset of predictors while discarding the rest. However, the reduced number of regression coefficients may result in high variances that significantly increase prediction errors. Variable selection based on shrinkage methods attempts to reduce the number of regression coefficients while reducing variance and increasing model bias (Dormann et al., 2013; Hastie et al., 2009; Hastie, Tibshirani, & Wainwright, 2015; Reineking & Schröder, 2006). Furthermore, shrinkage methods are based on continuous processes attempting to solve the following problem:

$$\min_{\alpha, \beta} \left[\sum_{i=1}^N \left(y_i - \alpha - \sum_{j=1}^p x_{ij} \beta_j \right)^2 + k \|\beta_j\|_q \right], \quad (3)$$

where $k \geq 0$ is the parameter controlling the amount of shrinkage (a larger number corresponds to a greater amount of shrinkage), N is the number of observations of a response variable (y_i) and p corresponding predictor variables, $x_i = (x_{i1}, \dots, x_{ip})^T$, and $\|\beta_j\|_q$ is the ℓ_q norm of β . In the ridge regression method (Hoerl & Kennard, 1970), $q = 2$, and therefore, $\ell_2 = \sum_{j=1}^p \beta_j^2$. For this condition, it is possible to derive a closed-form expression to obtain the linear intercept (α) and linear model weights (β), while minimizing the residual sum of squares (RSS):

$$\text{RSS}(k) = (Y - X_N \beta)^T (Y - X_N \beta) + k \beta^T \beta, \quad (4)$$

where X_N is the set of explanatory variables, which have been standardized by subtracting the sample average.

By minimizing Equation (4), the regression coefficients β are shrunk toward zero (Hastie et al., 2009). Meanwhile, in the least absolute shrinkage and selection operator (LASSO; Tibshirani, 1996), $q = 1$, with $\ell_1 = \sum_{j=1}^p |\beta_j|$, resulting in a quadratic programming problem. For this case, solving Equation (3) provides a reduced number of nonzero

parameters. For $q < 1$, the problem also results in some nonzero parameters, but it is not a convex problem and thus much more computationally demanding (Hastie et al., 2015). Optimal values for k are generally obtained by minimizing cross-validation prediction errors. Shrinkage methods are generally suitable when the number of observations is not large compared with the number of explanatory variables (Ahmadi-Nedushan et al., 2006).

LASSO has shown more reliability than stepwise methods for variable selection in ecology applications (Elith & Graham, 2009). Recent applications of the LASSO method include modelling stream health using indices based on macroinvertebrate assemblages (Berger et al., 2017; Kaelin & Altermatt, 2016) and distributions of freshwater fish species (Huang & Frimpong, 2015; Huang, Frimpong, & Orth, 2016). For instance, Berger et al. (2017) used PCA and LASSO to describe the relationship between six macroinvertebrate indices and environmental variables including water quality (micropollutants, toxic units, physiochemistry, nutrients, and major ions), land use, and wastewater exposure. Results regarding variable importance using LASSO were very similar when using weight of evidence (i.e., large statistically significant regression coefficients) and hierarchical partitioning (Berger et al., 2017). In addition, results showed that the instream water quality measurements are better predictors than surrogates such as distance to Wastewater Treatment Plant (WWTPs) and land uses. Meanwhile, Kaelin and Altermatt (2016) developed a nationwide landscape-scale model for Switzerland using Ephemeroptera, Plecoptera, and Trichoptera (EPT) species richness and family richness in response to environmental variables such as land use and topology. They found that EPT and family richness responded oppositely. Regarding fish-based modelling applications, Huang and Frimpong (2015) compared a LASSO-regularized logistic regression model with BRT and maximum-entropy (MaxEnt) models. Results indicated that the presence-absence LASSO model outperformed the MaxEnt presence-only model while being very similar to BRT during validation. Moreover, LASSO outperformed the BRT model for small sample sizes because BRT was prone to overfitting. In addition, Huang et al. (2016) showed that the LASSO model for fish species prediction (presence-absence) outperformed among the three methods in 13 out of 16 cases. They also recommended that the underfitting in LASSO models can be prevented by loosening the penalization (i.e., decreasing k magnitude for increasing model complexity) when simulating species distribution over time.

2.1.3 | Multivariate methods

Ordination refers to multivariate statistical methods commonly classified into indirect (unconstrained ordination) and direct gradient analysis (constrained ordination, also known as canonical ordination; De'ath, 1999; Guo, Park, Liu, & Lek, 2015). Ordination methods are generally preferred when analysing multiple species at multiple sites (Ahmadi-Nedushan et al., 2006). The main objective of ordination is to reduce dimensionality to identify patterns in the data while describing relationships with explanatory variables (e.g., environmental gradients). As a result, data samples are ordered in such a way that similar points are placed together (Ahmadi-Nedushan et al., 2006).

Indirect gradient analysis only uses samples collected in one data matrix, extracting dominant or orthogonal axes of variation. Any

additional information regarding explanatory variables is used afterwards to enhance results' interpretation. These methods can be classified into distance-based techniques (e.g., polar ordination, principal coordinate analysis, and nonmetric multidimensional scaling [NMDS]) and eigen analysis-based techniques, which can be derived from linear models (e.g., PCA) or from unimodal (nonlinear) models (e.g., correspondence analysis [CA] and detrended CA). Contrariwise, in direct gradient analysis, variables of interest are directly related to explanatory variables. Therefore, these techniques are preferred for habitat modelling (Ahmadi-Nedushan et al., 2006). Direct gradient methods can also be based on linear models (e.g., RDA) or unimodal models (e.g., canonical CA [CCA] and detrended CCA). It is worth noting that linear models are preferred for short gradients, whereas unimodal models are, in general, more suitable for aquatic habitat modelling (Ahmadi-Nedushan et al., 2006).

Multivariate methods for biological assessments, such as the River Invertebrate Prediction and Classification System (RIVPACS) and its variants (Abbasi & Abbasi, 2012; Feio & Poquet, 2011), are mainly based on ordination methods. These multivariate methods attempt to predict ratios of taxa observed versus expected (O/E), carefully choosing reference sites while using categorical (e.g., presence/absence) rather than continuous biological data. Some recent applications of ordination methods within stream health modelling were reported by Gazendam, Gharabaghi, Ackerman, and Whiteley (2016), indicating that the integration with other techniques is needed for identifying relationships between environmental variables and stream health using PCA or CCA. For instance, D'Ambrosio, Williams, Williams, Witter, and Ward (2014) used CCA and variance partitioning to evaluate the relationships between instream habitat, spatial location, and geomorphic characteristics on fish- and macroinvertebrate-based stream health indices. This study was conducted considering highly modified drainage channels as a consequence of agricultural activities. Results provided key ecological drivers for each biological community, under different stream geomorphic condition and location. Additionally, it is worth noting that ordination methods have been mainly implemented to assess the influence of explanatory variables on response variables before implementing more complex approaches for predicting stream health indicators (Lin, Chen, Chen, & Yang, 2016). In other cases, ordination has been used for model interpretation. For instance, Leigh, Stewart-Koster, Sheldon, and Burford (2012) used NMDS after implementing Bayesian belief networks (BBNs) to compare the attributes of macroinvertebrates assemblages for different scenarios of streamflow regulation. Variables modelled in this study included functional groups abundances, richness and evenness, species diversity, site variability, and beta-diversity.

Additional applications of multivariate statistics methods include the spatial analysis of ecological data. For example, spatial analysis can be used to model the structure of stream health data by discriminating different sources of variation such as gradients, scale effects, and random noise (Borcard, Gillet, & Legendre, 2011). Multivariate methods for modelling species patterns and distributions include trend-surface analysis with CCA (Bertolo & Magnan, 2006; Mykrä, Heino, & Muotka, 2007), principal coordinates of neighbour matrices and Moran's eigenvector maps (Dray, Legendre, & Peres-Neto,

2006), partial analysis (Aguiar, Ferreira, & Pinto, 2002; Beasley & Kneale, 2003; Magalhaes, Batalha, & Collares-Pereira, 2002), variation partitioning (Peres-Neto, Legendre, Dray, & Borcard, 2006), and multiscale ordination (Wagner, 2004). Further details regarding ordination techniques and spatial analysis of ecological data can be found in Borcard et al. (2011), Kent (2006), Legendre and Legendre (2012), and Zuur, Ieno, and Smith (2007).

2.2 | Machine learning

Machine learning is a form of artificial intelligence employing statistical, probabilistic, and optimization algorithms to identify relationships and patterns from datasets. The resulting outcomes can be used for data analysis, visualization, and prediction (Mitchell, 1999).

2.2.1 | Decision tree-based methods

The decision tree family of models are hierarchical structures also known as classification and regression trees (CART; Breiman, Friedman, Stone, & Olshen, 1984). These models divide the predictor space into regions with a homogenous response and then fitting a constant to each region. A decision tree grows using binary splits, resulting in a dendrogram with varying numbers of branches (De'ath, 2007). Each split is defined by threshold values accompanying the explanatory variables. Regression trees fit the mean response to observations, whereas classification trees, which are used for categorical data, fit the most frequent class as the constant. Usually, CART are grown to a maximum and then pruned using cross-validation approaches to prevent overfitting (Hastie et al., 2009). CART have been applied in several stream health applications and nowadays are commonly used as a benchmark approach for comparison with other methods (Ambelu, Lock, & Goethals, 2010; He, Wang, Lek-Ang, & Lek, 2010; Holguin-Gonzalez et al., 2014; Holguin-Gonzalez, Boets, et al., 2013; Maloney et al., 2009; Ocampo-Duque, Schuhmacher, & Domingo, 2007; Waite et al., 2012; Wang, Robertson, & Garrison, 2007). Known drawbacks of CART are the difficulty in modelling smooth functions and producing very different results when making small changes to the training data (Elith, Leathwick, & Hastie, 2008). However, ensemble methods based on computational intensive procedures such as boosting and bootstrap aggregation (aka bagging) have shown better and promissory results in ecological applications (De'ath, 2007). Thus, two ensemble methods, BRT and random forests (RFs), are further described in the next sections.

Boosted regression trees

The BRT method is an advanced form of regression that combines a large number of regression trees using the boosting technique to increase predictive performance (De'ath, 2007; Friedman, 2001; Hastie et al., 2009). Boosting is a forward sequential procedure that aims to find and merge results from multiple models (e.g., decision trees), emphasizing on observations poorly represented by an existing combination of models (Brown et al., 2012). For BRT, boosting works as an optimization technique, minimizing the difference between predicted and observed values, adding at each step a new tree that best reduces this difference (Elith et al., 2008). The technique updates the residuals in each iteration, preserving the existing trees while

extending the overall model. Hence, the final BRT model is a linear combination of several decision trees. Like other regression methods, it is possible to define the error distribution in BRT models in order to consider different response types (e.g., Gaussian, Poisson, and binomial).

BRT models are controlled by two important parameters: the learning rate (lr), which determines the contribution of each tree, and the tree complexity (tc), which controls the number of terminal nodes and interactions. Both lr and tc define the required number of trees (nt) for an optimal prediction (Elith et al., 2008). In addition, the stochasticity of BRT models is controlled by the "bag fraction," which refers to the observations that are randomly drawn to train each new tree, with optimal values between 0.5 and 0.75 (Elith et al., 2008). In ecological applications, small values for lr (<0.001), and therefore high nt ($>1,000$), are preferred in order to avoid overfitting, reduce the contribution of each tree, and increase predictive reliability (Elith et al., 2008). Values for tc are defined depending on the data availability and are restricted to the desired computing time. High values for tc imply a slower lr to keep a similar optimal nt (Elith et al., 2008).

Works conducted by Moisen et al. (2006), Elith et al. (2006), and Leathwick, Elith, Francis, Hastie, and Taylor (2006) are among the first studies employing BRT models for ecological applications. Particularly, they showed that BRT models are more flexible and outperform regression models such as GLM or GAM in variable selection, higher variance explanation, and lower prediction error. Moreover, BRT models are suitable for handling nonlinear relationships and can model smooth functions and interactions (Elith et al., 2008). Applications in stream health modelling include the determination of quantitative relationships between landscape variables and instream biological response (Chee & Elith, 2012; Gieswein et al., 2017; Golden, Lane, Prues, & D'Amico, 2016; Pilière et al., 2014; A. E. Steel, Peek, Lusardi, & Yarnell, 2017; Tonkin, Stoll, Sundermann, & Haase, 2014; Waite & Van Metre, 2017), prediction (Brown et al., 2012; Clapcott et al., 2017; Elias et al., 2016; Leclerc, Oberdorff, Belliard, & Leprieur, 2011; J. T. May et al., 2015; Waite et al., 2012, 2014), multimetric indices formulation (Clapcott, Goodwin, Young, & Kelly, 2014; Esselman et al., 2013), and setting of instream water quality/ecological objectives and disturbance thresholds (Clapcott et al., 2012; Clapcott, Young, Goodwin, & Leathwick, 2010; Wagenhoff et al., 2016). Moreover, the most of recent studies involving BRTs implementation have dealt with regional and national scales (Clapcott et al., 2017; Waite & Van Metre, 2017).

Nonlinear relationships using BRTs have been explored using different explanatory and response variables and distinct objectives. For instance, Chee and Elith (2012) analysed the patterns of occurrence for 17 native and alien riverine fish species. In that study, the explanatory variables comprised 20 environmental predictors including physiographic, bioclimatic, edaphic, and land cover attributes. The survey method was also considered as a categorical explanatory variable. Results showed that several, but not all, of the developed models are transferable to adjacent regions. Meanwhile, Tonkin et al. (2014) explored the effects of distance and barriers on the occurrence of macroinvertebrate assemblages. Hence, four different BRT models (i.e., considering different factors driving invertebrate colonization) were evaluated. In another study, Golden et al. (2016) addressed the

relationship between landscape variables at the watershed and riparian buffer scales with instream nutrient concentration and fish IBI under low flow conditions. Landscape variables included temporal and geographic position attributes and indicators of run-off and point and nonpoint nutrient sources. Similarly, Pilière et al. (2014) explored the relationships between environmental stressors and freshwater invertebrates represented by the Invertebrate Community Index. Predictors included geography, water quality, physical-habitat quality, and toxic pressure variables. The results suggested that it is necessary to fit explanatory variables interactions to increase predictive ability and model interpretability. In a recent study, Waite and Van Metre (2017) used BRTs to identify the most important stressors explaining the macroinvertebrate condition in streams. The final model was determined sequentially eliminating variables according to cross-validation performance. Three macroinvertebrate metrics and a multimetric index were used as response variables. Results indicated that watershed-scale stressors acted as surrogate variables for instream stressors. However, given the performance metrics for model validation, the authors did not recommend using the fitted BRT models for prediction in unsampled sites. On the other hand, there are several studies that implemented BRTs for understanding instream processes that affect species distribution. For instance, a study by A. E. Steel et al. (2017) explored the relationship between streamflow regime and water temperature metrics with the Shannon-Wiener diversity index, total richness, and total density per square metre of benthic macroinvertebrate assemblages. Results indicated that macroinvertebrate diversity and total richness showed the best predictive performances, with metrics related to spring snowmelt recession and variability in summer water temperature having the greatest relative influence. Meanwhile, the total density per square metre of benthic macroinvertebrates showed the poorest fitness, limiting the interpretability of the modelling results (A. E. Steel et al., 2017).

In general, studies using BRTs concerned with predicting the stream health condition using fish and macroinvertebrate communities are recent. Leclerc et al. (2011) attempted to select an appropriate statistical method for predicting nine fish species occurrence in large river systems at a reach scale. Compared methods were CART, GLM, and BRT, where the latter showed the best performance because BRT is especially suitable for fitting nonlinear relationships and continuous data. Specified predictors comprised qualitative (occurrence of shallow waters and shelters), semiquantitative (range of coverage/magnitude of bottom substrate, current velocity, shade, macrophytes, and complexity structures), and quantitative (value for depth, stream width, substrate diversity, and cover of bed sediment) variables. The results showed that the BRT method selected a greater number of variables, giving more importance to continuous variables. Furthermore, this method provided a better ecological interpretability and consistency in the obtained response curves. Other studies have used BRT models to predict benthic macroinvertebrate metrics at a regional scale. For instance, Waite et al. (2012) used land use and land cover explanatory variables to obtain richness and O/E ratios. In addition, the study compared MLR, CART, RF, and BRT predictive performances. Results indicated that BRT outperformed the other methods and provided additional information regarding potential interaction among explanatory variables. Meanwhile, Brown et al. (2012) used benthic

macroinvertebrate IBI (I-IBI) as the response variable. Landscape variables at the watershed and riparian-buffer scales were selected as explanatory variables. In the study, population density and agricultural and urban land use were the predictors with the highest influence on the response. However, the final BRT model was not able to capture the minimum and maximum values of the observed data. Therefore, the results suggested that the outcomes from BRT models should not be used to predict index values at specific sites. Instead, the model is recommended to be used to predict impairment condition due to watershed disturbance (Brown et al., 2012).

In a more recent study, Elias et al. (2016) implemented a two-level nested model to predict macroinvertebrate occurrence. The first level attempted to predict four water quality variables (dissolved oxygen, phosphates, ammonium, and nitrates) with a BRT model. Then these variables were used to predict reference conditions of stream health employing a different modelling approach. However, results showed that the BRT model was only successful in predicting nitrates. Other studies have addressed related fields to stream health modelling such as surface water and groundwater interactions and water quality modelling (Poor & Ullman, 2010; Smucker, Becker, Detenbeck, & Morrison, 2013). For instance, Johnson, Snyder, and Hitt (2017) successfully estimated the effects of groundwater seepage on stream temperature in unsampled sites at headwaters. Hence, landform and precipitation covariates, representing spatial and temporal variables, respectively, were selected as explanatory variables. During the modelling process, these variables were sequentially eliminated using ranking, clustering, and model simplification approaches.

The impacts of the scale of study on model predictability have been also addressed with BRT models, in which depending on the size and location of study, the importance of natural gradients and anthropogenic stressors is different (J. T. May et al., 2015; Waite et al., 2014). However, it was suggested that using BRT models for small spatial scales provide more accurate predictions compared with large-scale studies (Waite et al., 2014). A study by Clapcott et al. (2017) attempted to estimate site-specific contemporary and reference values for a macroinvertebrate index, evaluating spatial-scale effects on the predictions. Models at national and regional scales were tested for comparison. In general, the proportion of native vegetation in upstream catchments was the primary predictor, whereas the remaining relevant predictors varied regionally. The main environmental predictor at large scales also included flow variability, habitat category, substrate composition, summer temperature, and average upstream slope. Regional models showed that low flow remaining downstream after daily water allocation and calcium concentration of rocks in the catchments were relevant. Other methods (i.e., analysis of covariance and RF) were also evaluated. Results indicated that models at different scales were equally informative. However, the authors recommended using finer-scale predictors to improve the model accuracy. These variables include substrate size, nutrient concentrations, streamflow, and temperature. Additionally, it was shown that regression tree-based methods did not overestimate biological condition scores because the methods do not extrapolate beyond the range of observations. Meanwhile, these methods are able to predict stream classes that are unrepresented in the available observations (Clapcott et al., 2017).

BRT model interpretability has been found to be suitable for defining disturbance thresholds and setting instream objectives. Particularly, functional indicators for ecosystem processes are often used as response variables for the task mentioned above (Clapcott et al., 2012, 2010; Wagenhoff et al., 2016). Functional indicators include variables related to primary production, ecosystem respiration, organic matter breakdown, and cellulose decomposition potential, among others (Clapcott et al., 2010). Furthermore, it has been suggested that statistical analysis based on single-stressor models has the tendency to provide spurious thresholds for management purposes (Wagenhoff et al., 2016). Meanwhile, the use of sediment-specific macroinvertebrate metrics has been encouraged for improving prediction and threshold definition (Wagenhoff et al., 2016). Other findings include the importance of spatial variation of the predictors for increasing predictive power (Clapcott et al., 2012). Finally, additional applications of BRT models at national and continental scales comprise the definition of multimetric indices. Examples include the formulation of fish community indicators in large regions (Esselman et al., 2013) and multimetric indices development based on water quality-based predictive modelling, measurements of macroinvertebrate and fish assemblages, and indicators for ecosystem processes (Clapcott et al., 2014).

Random forests

Similar to BRT, RFs are collections of individual CART (Breiman, 2001). This method fits several trees using bootstrap samples of the training data while employing a small number of randomly selected predictors from the explanatory variables (Snelder, Booker, & D., 2013). The bootstrapping process attempts to reduce the variance of estimated outputs (Hastie et al., 2009), which is typically high for single large regression trees. For each bootstrapped sample, the largest tree is grown but not pruned, and aggregation is made by averaging or majority voting the trees (Carlisle, Falcone, Wolock, Meador, & Norris, 2009; Cutler et al., 2007). The size of randomly selected predictors is usually $\sqrt{p}$ or $\log(p)$, being p the number of explanatory variables (De'ath, 2007). This method requires a large number of trees to ensure convergence (Booker, Snelder, Greenwood, & Crow, 2015). Additionally, because of the bootstrap sampling, RF excludes over 37% of observed data for growing the regression or classification trees. This nondrawn portion is called out-of-bag samples (Prasad, Iverson, & Liaw, 2006), and error estimates are computed using these samples. Then these error estimates are used for regression trees aggregation (Carlisle, Falcone, Wolock, et al., 2009). When used for classification, RF determines the most frequent class across all trees for each observation within the out-of-bag portion. Estimating the error using the out-of-bag samples is almost equivalent to perform k -fold cross-validation, in which once the error stabilizes, the training is terminated (Hastie et al., 2009). Therefore, because a large number of trees provides limited generalization errors, RF method prevents overfitting (Prasad et al., 2006).

RF applications include predicting the instream biological condition and simulating ecologically relevant hydrologic indices in undisturbed sites and ungauged locations. Most of the studies have been developed at regional and national scales. Some RF models have attempted to evaluate the effects of human activities and relevant environmental factors on natural aquatic ecosystems (He et al.,

2010), whereas others have addressed the prediction of instream biological condition in ungauged locations (Carlisle, Falcone, & Meador, 2009; Hill et al., 2017). Many of these studies have been focused on predicting macroinvertebrate taxa richness and composition (Álvarez-Cabria, González-Ferreras, Peñas, & Barquín, 2017; Booker et al., 2015; Carlisle, Falcone, & Meador, 2009; Chinnayakanahalli, Hawkins, Tarboton, & Hill, 2011; Patrick & Yuan, 2017; Vander Laan, Hawkins, Olson, & Hill, 2013; Waite et al., 2014). Other studies have addressed the RIVPACS-type approach for determining biological condition (Carlisle, Falcone, & Meador, 2009; Chinnayakanahalli et al., 2011). Moreover, fish assemblages composition and richness (He et al., 2010; Patrick & Yuan, 2017) and fish biomass (Álvarez-Cabria et al., 2017) have also been modelled. Other applications include determining reference conditions (Clapcott et al., 2017). For biological condition prediction, common explanatory variables comprise geospatial datasets including land cover, land use, topography, climate, soils, societal infrastructure, and hydrologic modification. Some of these studies have addressed natural flow regime and water quality and temperature roles on biological condition predictability (Booker et al., 2015; Chinnayakanahalli et al., 2011; Patrick & Yuan, 2017; Vander Laan et al., 2013). For instance, Patrick and Yuan (2017) used the 171 Hydrologic Index Tool indices as predictors, which were obtained with statistical modelling. Other studies have identified variables describing natural and human activities as important predictors (Carlisle, Falcone, & Meador, 2009; He et al., 2010), especially land use changes and flow modification. Regarding ecologically relevant hydrologic indices, common explanatory variables are related to geospatial data describing natural watershed characteristics. However, RF models usually include a reduced number of indices (between one and 36), and prediction errors range from 15% to 40% (Carlisle, Falcone, Wolock, et al., 2009). Other applications include river classification (Dhungel, Tarboton, Jin, & Hawkins, 2016; Snelder et al., 2013), where classification success has ranged from 34% to 75%. Additionally, there are studies that have analysed potential effects of climate change (Dhungel et al., 2016), environmental flow, and flow–ecology relationships, for environmental impact assessment (Buchanan et al., 2017).

2.2.2 | Artificial neural networks

Artificial neural networks (ANNs) are nonlinear models with many parameters flexible enough to approximate any smooth function. ANN is a learning method based on the idea of building linear combinations of the specified explanatory variables and then modelling the response variables as nonlinear functions of these linear combinations (Hastie et al., 2009). ANNs are labelled as “black box” models and are known for being useful for prediction but not very useful for producing understandable models (i.e., provide limited insight into the relative influence of explanatory variables). However, multiple methods for understanding ANN results are available, including sensitivity analysis and randomization tests (Gevrey, Dimopoulos, & Lek, 2003; Olden & Jackson, 2002).

A typical two-stage regression or classification network model is known as a feed-forward neural network. Under this approach, linear combinations of explanatory variables X are transformed into Z elements called “hidden units” using a nonlinear function σ , known as

the “activation function.” Usually, σ is the sigmoid function, which is a smooth version of the step function. However, Gaussian radial basis functions are also commonly used (Hastie et al., 2009; Mathon et al., 2013). For ANN setting, more than one layer of hidden units can be used (Lek & Guégan, 1999). Afterwards, these Z elements are linearly combined. Then the linear combinations are transformed using an output function to provide the response variables. The constants involved in the linear combinations are known as “weights.” The aforementioned ANNs are called multilayer perceptrons (MLPs) and are very popular among ecological applications. In order to fit ANNs with observed data, a two-pass procedure known as back-propagation, which is a gradient descent algorithm, is typically employed in order to determine the weights (Hastie et al., 2009). Hence, key MLP parameters include the number of times that the training data is used to update the weights of the hidden units (i.e., epochs) and the number of hidden layers and units. Alternatives to MLP, such as the generalized regression neural network, have been recently applied for stream health modelling (Mathon et al., 2013; Sutela, Vehanen, & Jounela, 2010).

ANNs were first introduced in ecological applications during the 1990s (Lek et al., 1996; Lek & Guégan, 1999); however, since then, the method has been widely used. Goethals, Dedeker, Gabriels, Lek, and De Pauw (2007) presented a review of 26 representative studies addressing macroinvertebrate prediction, covering a period from 1998 to 2006. In those studies, the response variables were usually presence/absence, abundance and derived indicators (e.g., richness, average score per taxon, exergy), using landscape, instream, and water quality attributes as explanatory variables (i.e., inputs). Studies using fish biological data have been also implemented for evaluating restoration projects and understanding the effects of changes in physical habitat and water quality variables (Olaya-Marín, Martínez-Capel, Soares Costa, & Alcaraz-Hernández, 2012; Olaya-Marín, Martínez-Capel, & Vezza, 2013; Olden, Lawler, & Poff, 2008).

Other studies have reported an increased use of self-organizing maps (SOMs) for predicting macroinvertebrate and fish distributions and exploring relationships with landscape and environmental variables (Chon, 2011; Tsai, Chang, & Herricks, 2016). SOMs, also known as the Kohonen networks, are unsupervised ANNs that are implemented for pattern classification, clustering, and ordering purposes (Kalteh, Hjorth, & Berndtsson, 2008) and are also known for approximating probability density functions of the input data (Chon, 2011). Recent works have addressed variable selection and uncertainty analysis to gain insight into the results interpretability, which is one of the main ANN's drawbacks. For instance, Mouton, Dedeker, Lek, and Goethals (2010) compared six different methods reviewed by Gevrey et al. (2003) for evaluating explanatory variables' individual contribution in predicting macroinvertebrates abundance. The results indicated that some techniques are more sensitive and less stable than others. However, it was shown that the different methods were able to provide consistent results regarding the order of importance for the explanatory variables. Likewise, Grenouillet, Buisson, Casajus, and Lek (2011) and Guo et al. (2015) evaluated the variability and uncertainty of an ensemble of several models including GLM, GAM, CART, RF, and ANNs, among others, in the prediction of fish distributions in streams and lakes at a national level. This evaluation included the

comparison between the individual predictions provided by every single model and an average of ensemble models. Results indicated that ensemble modelling results improve accuracy when modelling different species and revealed uncertainty dependence upon geographical extent. In addition, Gazendam et al. (2016) developed an ANN model to predict two macroinvertebrate indices (Hilsenhoff's Biotic Index and richness) while testing combinations of physically based input variables (geomorphic, riparian, hydrology, and watershed level). Results showed that considering both watershed and reach scales (geomorphic and riparian), inputs can improve model performance and are consistent with findings using ordination techniques (D'Ambrosio et al., 2014; D'Ambrosio, Williams, Witter, & Ward, 2009).

2.2.3 | Other methods

Additional statistical and machine learning methods that have been implemented for SDM and habitat suitability include multivariate adaptive regression splines (MARSs), support vector machines (SVMs), and partial least squares regression (PLSR). Other methods such as MaxEnt (Phillips, Aneja, Kang, & Arya, 2006) and genetic algorithm for rule set production (Stockwell & Peters, 1999) are not further described herein because they are intended for using presence-only data. It is worth noting that these two methods are especially suitable when working with small sample sizes and incomplete datasets (Xinhai Li & Wang, 2013; Yi et al., 2017).

MARSs (Friedman, 1991) are multidimensional extensions of GAMs that build up from basis functions fitting separate splines for different intervals (with extremes known as *knots*) of the predictor variables. MARS algorithm finds the location and number knots using an exhaustive search procedure in a forward/backward stepwise fashion (Prasad et al., 2006). MARS models are better suited than CART for continuous variables, can handle large numbers of explanatory variables with low-order interactions, and automatically quantify interaction effects (Xinhai Li & Wang, 2013; Prasad et al., 2006). However its interpretability is limited when analysing species–environmental relationships, its parameter identification is not straightforward, and it is highly sensitive to extrapolation (Prasad et al., 2006). MARS method is mainly implemented for multispecies modelling (Guo, Lek, et al., 2015) and is considered as an alternative to other regression methods such as GLM and GAM (Barry & Elith, 2006; Xinhai Li & Wang, 2013; Yi et al., 2017).

On the other hand, SVM (Vapnik, 2000) is a machine learning algorithm that also uses basis functions known as *kernels* to map data into a new nonlinear feature hyperspace attempting to simplify data patterns. Then the data are classified, whereas the margins between hyperplanes that are used to define classes are maximized. These hyperplanes are determined by a set of support vectors using quadratic programming. An advantage of SVMs is the reduced number of tuning parameters. Also, SVM models are not prone to overfitting. However, because this method does not provide a simple representation or a pictorial graph, the interpretation of modelling results is difficult (Cutler et al., 2007), the algorithm is computationally demanding, and the tuning parameters are poorly identifiable when data are not linearly separable (Guo, Park, et al., 2015). SVMs have been applied mainly for modelling species–habitat relationships for fish

communities (Fukuda & De Baets, 2016; Fukuda, De Baets, Waegeman, Verwaeren, & Mouton, 2013; Muñoz-Mas, Fukuda, Pórtolles, & Martínez-Capel, 2018; Muñoz-Mas, Vezza, Alcaraz-Hernández, & Martínez-Capel, 2016) and for predicting the occurrence and macroinvertebrate-based stream health indices using landscape and water quality attributes (Ambelu et al., 2010; Fan et al., 2017; Hoang, Lock, Mouton, & Goethals, 2010; Lin et al., 2016; Sor, Park, Boets, Goethals, & Lek, 2017). In general, the studies have indicated similar performances between ANN and SVM when predicting continuous variables, although SVM usually performs slightly better than ANN. Meanwhile, methods such as RF have shown better results than SVM for classification purposes.

PLSR (Wold, Sjöström, & Eriksson, 2001) is a method that projects explanatory and response variables into a new space where MLR is performed. PLSR is known for handling multicollinearity and strong correlation of predictors while allowing a high interpretability of the resulting regression coefficients (Villeneuve, Souchon, Usseglio-Polatera, Ferréol, & Valette, 2015). Moreover, this method is suitable when the number of explanatory variables is greater than the number of observations (Abouali, Nejadhashemi, Daneshvar, & Woznicki, 2016). PLSR method has been used as an explicative method for quantifying relationships between several stressors and stream health indicators. This method is especially suitable for identifying the most relevant input variables before any predictive model training (Abouali et al., 2016; Einheuser, Nejadhashemi, Wang, et al., 2013; Villeneuve et al., 2015).

In an attempt to facilitate the integration with expert elicitation regarding causal relationships, different approaches are being integrated within the SEM framework for stream health modelling (Riseng, Wiley, Black, & Munn, 2011; Surridge, Bizzi, & Castelletti, 2014). For instance, a recent study by Villeneuve, Piffady, Valette, Souchon, and Usseglio-Polatera (2018) shows an application of the aforementioned framework using PLS for evaluating the direct and indirect effects of multiple stressors on macroinvertebrate indices in nested spatial scales (watershed, reach, and site). Results showed that the direct effects of instream water quality conditions decrease when indirect effects from land use and hydromorphological alterations are considered for macroinvertebrate assemblages.

2.3 | Soft computing methods

Soft computing is a collection of paradigms that attempt to represent complex systems in an environment of imprecision, uncertainty, and partial truth, resembling human mind and biological systems' learning. Soft computing approaches include fuzzy logic, neurocomputing, evolutionary computation, and probabilistic reasoning (Zadeh, 1994, 1998).

2.3.1 | Fuzzy logic-based methods

Fuzzy logic-based methods are used to model nonlinear relationships employing linguistic terms instead of numeric values. These methods incorporate membership functions, fuzzy set operations, and *if-then* rules for mapping from a given input to an output. This process is also called "fuzzy inference" (Ocampo-Duque, Ferré-Huguet, Domingo, & Schuhmacher, 2006). The membership functions are curves with values

between 0 and 1 that represent the degree of membership of an input variable's value (element) to a certain fuzzy set, where 0 and 1 represent nonmembership and full membership, respectively (Adriaenssens, Goethals, & De Pauw, 2006). Given that the same element may belong to several sets at the same time, expert knowledge is necessary to define the overlap between different membership functions for the same variable. Then the obtained membership values are combined for different variables using fuzzy *if-then* rules incorporating fuzzy set operations. Outcomes from different fuzzy rules are then aggregated into a final fuzzy score. Fuzzy set operations include union, intersection, and additive complement. Following Adriaenssens, De Baets, Goethals, and De Pauw (2004), fuzzy *if-then* rules consist of antecedent and consequent parts, which mainly rely on expert knowledge. The antecedent part states conditions for the explanatory variables (i.e., input), whereas the consequent describes the corresponding values of the response variables (i.e., output). When both parts are concerned with statements that define the value of the variables without considering any explicit function relating the explanatory and response variables, the model belongs to the Mamdani-Assilian type. On the other hand, when the consequent part establishes a linear or nonlinear relationship between the explanatory and response variables, the model belongs to the Takagi-Sugeno type. It would be necessary to implement a weighting operation using a specified decision-making method (e.g., analytic hierarchy process) to define the influence of each input variable in the final fuzzy score (Ocampo-Duque et al., 2006). Once the fuzzy rules are implemented, the defuzzification operation is performed, if necessary, in order to obtain a numerical output under no-fuzzy contexts (Ocampo-Duque et al., 2006). Fuzzy logic models are generally trained employing optimization routines based on the Shannon-Waver entropy (tuning the fuzzy set parameters looking for entropies values greater than 0.85) or genetic algorithms to generate uniformly distributed fuzzy sets (Yi et al., 2017). Then the nearest ascent hill-climbing algorithm can be used for optimizing the consequent part of each fuzzy rule (Yi et al., 2017).

Compared with ANNs, fuzzy logic-based methods provide a more transparent insight into the influence and interactions of input variables. Moreover, the analysis of the model is more intuitive and can be performed in a semiquantitative manner, whereas uncertainty quantification can be easily integrated. However, setting the membership functions and fuzzy rules, which are jointly referred as the knowledge database, is not an easy task (Adriaenssens, De Baets, et al., 2004). In order to address this issue, several techniques such as adaptive neuro-fuzzy inference systems (ANFIS; Jang, 1993) were introduced. ANFIS is a hybrid method that combines ANNs and fuzzy logic. An adaptive network is a multilayer feed-forward neural network where the hidden units may or may not have parameters. These parameters are determined during the training process using observed data by minimizing the predictive error. Therefore, the membership functions are introduced in the first hidden layer of parameterized units. Successive layers, which contain nonparameterized units, represent the *if-then* fuzzy rules while incorporating the fuzzy set operations. Each successive layer attempts to represent the different specified fuzzy rules. The last layer before computing the overall fuzzy score comprises parameterized units. In this layer, the linear and nonlinear relationships for Takagi-Sugeno type models are introduced. These relationships

are referred as "output membership functions" (Jang, 1993). The number of parameters in the ANFIS model depends on the number of explanatory variables, the number of membership functions per variable, the membership functions shape, and the output membership function type. Thus, the number of parameters should not be greater than the number of available observations for model training in order to avoid overfitting (Woznicki, Nejadhashemi, Tang, & Wang, 2016).

Early fuzzy logic applications for predictive modelling and ecosystem management were reviewed by Adriaenssens, Goethals, Charles, and De Pauw (2004). The integration of expert knowledge, the use of qualitative data, and the capacity to incorporate uncertainty assessments have motivated the growing use of fuzzy logic-based methods in ecological applications (Adriaenssens, De Baets, et al., 2004; Ocampo-Duque et al., 2006). Recent studies include the prediction of macroinvertebrate abundance (Adriaenssens et al., 2006; A. M. Mouton, De Baets, & Goethals, 2009; Van Broekhoven, Adriaenssens, De Baets, & Verdonchot, 2006), ecological status classification (Ocampo-Duque et al., 2007), the development of multimetric stream health indices (Marchini, Facchinetti, & Mistri, 2009), and the prediction of fish species occurrence, distribution, or derived indices (Boavida, Dias, Ferreira, & Santos, 2014; Muñoz-Mas, Martínez-Capel, Schneider, & Mouton, 2012). When applied for prediction, fuzzy logic-based models typically use water quality and hydrologic and hydromorphological attributes and knowledge based on species preferences and tolerances. In an attempt to implement fuzzy logic in a more data-driven fashion, ANFIS has been recently implemented using process-based models to evaluate the impacts of conservation practices and environmental changes on stream health indices at a watershed scale (Einheuser et al., 2012; Einheuser, Nejadhashemi, Wang, et al., 2013; Einheuser, Nejadhashemi, & Woznicki, 2013). For instance, the Soil and Water Assessment Tool (SWAT) has been employed to simulate streamflow series in order to obtain ecologically relevant hydrologic indices. Those hydrologic indices are later used to predict stream health indices using ANFIS (Herman et al., 2015; Herman et al., 2016). Other studies have also incorporated water quality simulations (sediment and nutrients) for predicting stream health indicators (Woznicki, Nejadhashemi, Abouali, et al., 2016; Woznicki, Nejadhashemi, Tang, & Wang, 2016). Moreover, Abouali et al. (2016) employed the same integrated framework to develop a two-phase approach coupling PLSR and ANFIS for predicting macroinvertebrate and fish-based indices. Results showed a significant improvement in the prediction power while omitting the need for variable selection. It is worth noting that ensemble modelling frameworks integrating process-based models are especially suitable for evaluating climate change effects on biological assemblages (Daneshvar, Nejadhashemi, Herman, & Abouali, 2017). Recently, Yi et al. (2017) presented a detailed revision of fuzzy logic integration with process-based models intended for habitat modelling. Remarkable applications include micro-habitat selection/evaluation for fish and macroinvertebrate assemblages and dam operation/removal assessments (e.g., CASiMiR model).

2.3.2 | Bayesian belief networks

BBN is directed acyclic graphs having nodes linked by probabilities (Pearl, 1986). Each node represents constants, discrete or continuous

variables, or continuous functions in the model, whereas the arrowed links indicate direct correlation or causal relationships between nodes (McCann, Marcot, & Ellis, 2006). There are two types of nodes: parent or independent nodes (nodes that do not have arrows incoming or outgoing) and child nodes (with one or both incoming and outgoing arrows). Each node has an associated probability distribution, which is unconditional for parent nodes and conditional for child nodes. The outcomes of each node are known as *states* (McDonald, Ryder, & Tighe, 2015). Probability distributions are usually defined for each node in terms of the *states* (i.e., conditional probability tables [CPTs]; McCann et al., 2006). Consequently, a BBN is composed of a qualitative component referring to the network structure and a quantitative component given by the CPTs within each node (Phan, Smart, Capon, Hadwen, & Sahin, 2016).

The structure of the network is iteratively determined using expert knowledge and/or prior data, where metrics such as correlation coefficients are often used to define causal links. It is important to note that causal links should be carefully defined in order to prevent high levels of uncertainty in the model's outputs (McDonald et al., 2015). Conditional independence tests are often used for learning the BBN structure. However, when multiple BBNs are tested, model selection using the Bayesian information criterion (BIC) or optimization routines is also employed (Aguilera, Fernández, Fernández, Rumí, & Salmerón, 2011). Determining relevant variables is usually addressed by knowing that the nodes within a network can be unconditionally separated, or conditionally separated/connected if prior knowledge is given in other nodes (Aguilera et al., 2011). On the other hand, determining the probability values populating CPTs is usually done using prior data and the Bayes' theorem for probabilities propagation from parent nodes. Training algorithms have been developed in accordance with the BBN description of the joint probability distribution of the nodes within the network (Pérez-Miñana, 2016). CPTs, which are marginal probability distributions, are often parameterized and calculated using approaches based on Monte Carlo simulation (Phan et al., 2016), Gibbs sampling or dynamic discretization (Nojavan, Qian, & Stow, 2017; Pérez-Miñana, 2016), maximum likelihood or the Laplace correction (Aguilera et al., 2011), or the expectation maximization algorithm for small and incomplete datasets and the gradient learning algorithm for large incomplete datasets and continuous data (McDonald et al., 2015). In general, populating CPTs requires expert knowledge, the use of several data-based methods, or both (Phan et al., 2016).

There are recent reviews covering BBN applications in areas such as environmental modelling (Aguilera et al., 2011), ecosystem services modelling (Landuyt et al., 2013; Pérez-Miñana, 2016), ecological risk assessment (McDonald et al., 2015), and water resources management (Phan et al., 2016), which also include some early studies related to stream health modelling (Adriaenssens, Goethals, et al., 2004; Marcot, Holthausen, Raphael, Rowland, & Wisdom, 2001). The aforementioned reviews addressed different aspects of BBN model development/application such as data preprocessing, complexity, training, optimization, validation methods, variations and extensions (e.g., dynamic Bayesian networks for time series modelling and hidden Markov models for higher order relationships; Tucker & Duplisea, 2012), integration with other modelling techniques, and software comparison. Moreover, given the extensive application of BBN in ecology

and environmental science, there are guidelines addressing good modelling practices (Chen & Pollino, 2012; Marcot, Steventon, Sutherland, & McCann, 2006), overfitting, uncertainty quantification, and salient issues (Marcot, 2012, 2017).

Representative BBN applications in stream health modelling include the evaluation of cumulative environmental impacts of multiple stressors on ecosystem health using traditional and scientific knowledge (Mantyka-Pringle et al., 2017). The study incorporated biotic factors describing wildlife health, food webs, wildlife populations, fish health, and macroinvertebrate metrics (density, richness, and diversity), among others. Other recent studies have also addressed the estimation of the interactive effect of land use and climate change (considering its influence on water quality, physical factors, and habitat characteristics) on fish population success (Turschwell et al., 2017), EPT macroinvertebrates indices integrating SEM (Xue Li, Zhang, Guo, Gao, & Wang, 2018), and both fish and macroinvertebrate richness (Mantyka-Pringle, Martin, Moffatt, Linke, & Rhodes, 2014). Likewise, BBN models have been developed for predicting macroinvertebrate indices using land use, physicochemical, and hydromorphological factors (Allan et al., 2012; Forio et al., 2015; McLaughlin & Reckhow, 2017). However, McLaughlin and Reckhow (2017) could not find strong causal relationships or a high predictive power when relating water quality parameters (e.g., nutrients, chlorophyll, and dissolved oxygen) and habitat attributes to benthic macroinvertebrates in streams. The results may indicate that the BBN model is reflecting associations rather than strict causal relationships between variables. In addition, low predictive power might be a consequence of not considering all relevant factors affecting the response variable. However, other studies have been able to identify relevant stressors. For instance, Forio et al. (2015) indicated that flow velocity is a major variable determining stream health, which is highly sensitive to natural streamflow alterations by dams and water abstractions. In addition, Dyer et al. (2014) ended up with a similar conclusion when analysing the effects of climate change and stream regulation on ecologically relevant hydrologic indices and water quality attributes using BBN. Moreover, there are studies implementing BBN for environmental flows decision-making processes using macroinvertebrate assemblages (Leigh et al., 2012; Shenton, Hart, & Chan, 2014) and water management for fish species conservation (Peterson, Wenger, Rieman, & Isaak, 2013; Vilizzi et al., 2013). On the other hand, Death, Death, Stubbington, Joy, and van den Belt (2015) compared BBN with logistic regression, ANN, classification trees, and RF while predicting a macroinvertebrate-based stream health index at a national scale. Results indicated that BBN moderately outperformed the other methods; however, the model preparation is more time-consuming. BBN has been also implemented for evaluating the habitat suitability of invasive macroinvertebrate species using purely data-driven and expert knowledge-based approaches (Boets, Landuyt, Everaert, Broekx, & Goethals, 2015).

3 | KNOWLEDGE GAP ANALYSIS

Explaining cause-effect relationships between environmental and anthropogenic factors with measures of ecological integrity or health

in freshwater ecosystems is not a straightforward task because of the complex, nonlinear, and uncertain nature of these systems (Niemi & McDonald, 2004). However, growing applications of statistical and soft computing methods have been employed to address the aforementioned challenges. When selecting a modelling approach, aspects regarding variable selection, interpretability of modelling results, modelling ensembles for increasing predictive ability, and model evaluation and overfitting should be considered. Particularly, we have identified the need for developing guidelines regarding three main aspects of stream health modelling practice: variable selection, model evaluation, and data acquisition and uncertainty analysis for modelling ensembles. In this section, we briefly describe the aspects mentioned above and indicate the corresponding research priorities.

Strategies for variable selection include trial and error, expert knowledge, statistical analysis, heuristics, or combinations of these methods (Falcone, Carlisle, & Weber, 2010; R. J. May, Maier, Dandy, & Fernando, 2008). However, there is not an agreement on how to proceed with variable selection when developing stream health models (Woznicki et al., 2015). Variable selection is a critical step in any empirical modelling exercise, compromising performance, efficiency, and interpretability (Xuyuan Li, Maier, & Zecchin, 2015). Moreover, the number of selected input variables defines the number of model parameters to be calibrated, the computational effort, and is critical for overfitting prevention (Galelli et al., 2014). The process of preventing excessive model complexity while maintaining predictive performance is known as regularization (Reineking & Schröder, 2006). According to the studies reviewed in this paper, ordination and classification methods, nonparametric rank correlations, and Bayesian methods (e.g., O'Hara & Sillanpää, 2009) are usually implemented. For instance, Woznicki et al. (2015) compared PCA, Spearman's rank correlation, and Bayesian variable selection when modelling macroinvertebrates- and fish-based indices with ANFIS. Results showed that Bayesian variable selection provided the best final models (Woznicki et al., 2015). Other variable selection approaches are based on stepwise procedures using relative quality (e.g., using AIC; Clapcott et al., 2017), backward elimination (Fox et al., 2017), clustering employing SOMs (Bowden, Dandy, & Maier, 2005), partial mutual information (Fernando, Maier, & Dandy, 2009), penalized estimation (e.g., LASSO and ridge regression; Section 2.1.2) and using interpretability tools based on sensitivity and perturbation analysis and the relative importance of the predictors (Elith et al., 2008; Gevrey et al., 2003). Nevertheless, there is a lack of studies comparing different variable selection methods with different stream health modelling approaches. Thus, further research in this area is encouraged to gain insight into the influence of different ensembles of variable selection approaches and modelling methods over predictive ability and model parsimony.

Traditional statistical methods based on linear regression (e.g. MLR, GLM) are generally transparent, and their coefficients can be well interpreted (Xinhai Li & Wang, 2013). However, those methods usually show the lowest predictive power. For more complex models, there have been initiatives introducing expert elicitation into the model formulation and training. In those cases, fuzzy logic and BBN approaches have played an important role (Mantyka-Pringle et al., 2017; A. M. Mouton et al., 2009). On the other hand, when working

with data-driven approaches, some alternatives have been formulated depending on the implemented modelling method. For instance, in decision tree-based methods (e.g., CART, BRT, and RF), results are interpreted estimating the relative influence of predictor variables and are visualized and examined using partial dependence plots (Hastie et al., 2009). Relative influence in single trees can be measured based on the number of times a variable is selected for splitting. The number of times is weighted by a squared sum measure of model improvement as a result of adding each split to the individual tree. The final relative influence is obtained by averaging the corresponding results for the individual trees and then standardizing the final values (Elith et al., 2008). A similar option for obtaining relative influence measures can be applied using the out-of-bag samples, assuming that relative decrease in prediction accuracy is related to the variable influence (Carlisle, Falcone, & Meador, 2009). The out-of-bag samples observations are used to obtain a decrease in prediction accuracy when the explanatory variables are randomly permuted in each tree. Then the decrease is averaged and standardized across all trees (Carlisle, Falcone, & Meador, 2009). Partial dependence plots attempt to represent the effect of a variable when assigning average values for all other variables in the model. The plots can reveal strong interactions when using multiple variables and are especially suitable for detecting disturbance thresholds or ranges. However, these plots are limited to low-dimensional views (Hastie et al., 2009). Other methods for analysing the contribution of input variables are based on partial derivatives, perturbation of the input variables, and successive variation in a certain input variable, whereas the remaining are kept constant, among others, that are specifically designed for ANNs (e.g., neural interpretation diagram, Garson's algorithm, randomization test, and stepwise methods; Gevrey et al., 2003; Olden & Jackson, 2002). However, to significantly improve the interpretability of modelling results, it is necessary to advance towards frameworks that incorporate process-based models to describe disturbance factors (Araújo & New, 2007).

Ensemble modelling frameworks have been introduced to improve predictive ability while understanding cause-effect and multiscale dynamics driving instream changes due to alterations in landscape and environmental factors. The inclusion of process-based modelling approaches into integrated stream health modelling frameworks has been developed for different scales (i.e., macro-, meso-, and micro-scales). For instance, at a macro-scale (e.g., watershed and ecoregion), main advancements are related to the representation of bioclimatic and hydrologic factors using climatic, hydrologic, hydraulic, and water quality models. At meso- (e.g., river segments and hydromorphologic units: pool, riffle, run, ...) and micro-scales (e.g., point locations and substrate), computational fluid dynamics, hydraulic, water quality, and physical habitat models predicting local velocities, depths, and physic-chemical constituents are often implemented (Daneshvar, Nejadhashemi, Woznicki, & Herman, 2017; Yi et al., 2017). For instance, Jähnig et al. (2012) proposed a framework following the driver-pressure-state-impact concept. Drivers include main watershed and instream stressors (e.g., climate, land use, and river alteration). Pressures on freshwater ecosystems comprise hydrologic and hydraulic stress, sediment intake, and substrate stability, among others, which can be represented by process-based models developed in

TABLE 1 Summary of advantages, disadvantages, and applications for the methods described in this study

Method	Advantages	Disadvantages	Prediction power	Difficulty of variable selection	Applications
Multiple linear regression	• Straightforward implementation and interpretation • Computational effort is low	• Low predictive power • Method assumptions (i.e., normality and homoscedasticity) are usually violated • Parameter estimation is unstable under multicollinearity and strong correlated variables	Low	Low	Merriam et al., 2013, 2015; Pond et al., 2017; Waite et al., 2010, 2012 Frimpong et al., 2005; Van Sickle & Burch Johnson, 2008
Generalized linear models	• Straightforward implementation and interpretation • Flexible with the selection of error distributions • Computational effort is low	• Low predictive power • Model structure (distributions selection) must be defined a priori	Low	Low	Damanik-Ambarita et al., 2016; Death et al., 2015; Donohue et al., 2006; Everaert et al., 2014; Gieswein et al., 2017; Holguin-Gonzalez, Boets, et al., 2013; Holguin-Gonzalez, Everaert, et al., 2013; Jerves-Cobo et al., 2017; Kuemmerlen et al., 2014; Moya et al., 2011; Pont et al., 2009; Sauer, Domisch, Nowak, & Haase, 2011; Van Sickle et al., 2004 Fukuda et al., 2013; Gieswein et al., 2017; Grenouillet et al., 2011; Guo, Lek, et al., 2015; Hermoso, Linke, Prenda, & Possingham, 2011; Kwon, Bae, Hwang, Kim, & Park, 2015; Ledere et al., 2011; Patrick & Yuan, 2017; Sui et al., 2014
Generalized additive models	• Suitable for modelling nonlinear relationships • Uses nonparametric basis functions	• Prone to overfitting • Reduced interpretability of modelling results	Medium	Medium	Almeida et al., 2017; Fukuda et al., 2013; Grenouillet et al., 2011; Guo, Lek, et al., 2015; Maloney et al., 2012; Zhao et al., 2014
Shrinkage methods	• Straightforward implementation and interpretation • Suitable for cases when the number of observations is not large compared with the number of explanatory variables	• Prone to underfitting • Limited predictive power	Medium	Low	Berger et al., 2017; Kaelin & Altermatt, 2016 Huang & Frimpong, 2015; Huang et al., 2016
Ordination methods	• Suitable when analysing multiple species in multiple sites • Straightforward interpretation • Computational effort is low • Suitable for variable selection and exploratory analysis	• Methods' assumptions (e.g., linearity and unimodality) are likely to be violated • Interpretability is compromised when high correlations are present without clear causal relationships • Some methods are sensitive to the relative scaling and noise of the explanatory variables	Medium	Low	Aguiar et al., 2002; Beasley & Kneale, 2003; D'Ambrosio et al., 2014; Lin et al., 2016; Leigh et al., 2012; Mykrä et al., 2007; Pond et al., 2017 Bertolo & Magnan, 2006; D'Ambrosio et al., 2014, 2009; Kwon et al., 2015; Magalhaes et al., 2002; Patrick & Yuan, 2017
Classification and regression trees	• Do not require assumptions about data distribution	• Smooth functions are poorly modelled	Low	Medium	Ambelu et al., 2010; Death et al., 2015; Holguin-Gonzalez et al., 2014; Holguin-Gonzalez, Boets, et al., 2013; Maloney et al., 2011; Guo, Lek, et al., 2015; He et al., 2010; Kwon et al., 2015;

(Continues)

TABLE 1 (Continued)

Method	Advantages	Disadvantages	Prediction power	Difficulty of variable selection	Applications
	Interactions between predictors are modelled and can be easily visualized	- Provide very different results when making small changes to the training data - Large trees are poorly interpretable - Not suitable for modelling continuous datasets (e.g., temporal dynamics) - They are often not transferable to another location or time domain			Macroinvertebrates al., 2009; Ocampo-Duque et al., 2007; Sauer et al., 2011; Waite et al., 2012; Wang et al., 2007
Boosted regression trees	- Suitable for modelling smooth functions and interactions between predictors - Insensitive to outliers - Exclude irrelevant predictor variables - Do not extrapolate beyond the range of observations	- Time consuming for large number of trees or low learning rates - Prone to overfitting - Maximum and minimum values for response variables are poorly reproduced - Interactions between multiple (more than three) explanatory variables are difficult to visualize and interpret - Model interpretability is limited - They are often not transferable to another location or time domain	High	Medium	Brown et al., 2012; Clapcott et al., 2012, 2017, 2014; J. T. May et al., 2015; Pilière et al., 2014; A. E. Steel et al., 2017; Tonkin et al., 2014; Wagenhoff et al., 2016; Waite et al., 2012, 2014; Waite & Van Metre, 2017
					Chee & Elith, 2012; Clapcott et al., 2014; Esselman et al., 2013; Golden et al., 2016; Leclere et al., 2011; Huang & Frimpong, 2015; Huang et al., 2016.
Random forests	- Resistant to overfitting - Cross-validation is not necessary because a similar approach is automatically performed during model training - Good for classification purposes	- Time consuming for large number of trees - Less accurate than BRT - Interactions between multiple (more than three) explanatory variables are difficult to visualize and interpret - Model interpretability is limited - Cannot be extrapolated beyond the range of observations - They are often not transferable to another location or time domain	High	Medium	Álvarez-Cabria et al., 2017; Booker et al., 2015; Carlisle, Falcone, & Meador, 2009; Chinnayakanahalli et al., 2011; Clapcott et al., 2017; Death et al., 2015; Fox et al., 2017; Hill et al., 2017; Patrick & Yuan, 2017; Vander Laan et al., 2013; Waite et al., 2012
					Álvarez-Cabria et al., 2017; Fukuda & De Baets, 2016; Fukuda et al., 2013; Grenouillet et al., 2011; Guo, Lek, et al., 2015; He et al., 2010; Kwon et al., 2015; Olaya-Marin et al., 2013; Patrick & Yuan, 2017; Tuulaikhuu, Guasch, & García-Berthou, 2017; Vezza, Muñoz-Mas, Martínez-Capel, & Mouton, 2015
Artificial neural networks	- Suitable for modelling nonlinear relationships - Vast literature addressing aspects such as variable selection, sensitivity analysis, model ensembles, and optimal design - Good performance when modelling continuous data	- Model interpretability is limited - Relative importance of predictor variables is more difficult to determine than other approaches - They are often not transferable to another location or time domain	High	High	Chon, 2011; Gazendam et al., 2016; Goethals et al., 2007; Mathon et al., 2013; Ans M. Mouton et al., 2010; Sauer et al., 2011
					Chon, 2011; Fukuda et al., 2013; Grenouillet et al., 2011; Guo, Lek, et al., 2015; Mathon et al., 2013; Olaya-Marin et al., 2012, 2013; Olden et al., 2008; Sutela et al., 2010; Tsai et al., 2016

(Continues)

TABLE 1 (Continued)

Method	Advantages	Disadvantages	Prediction power	Difficulty of variable selection	Applications	Fish
Multivariate adaptive regression splines	• Suitable for modelling smooth functions • Can handle a large number of explanatory variables with low-order interactions • Automatically quantify interaction effects	• Model interpretability is limited • Highly sensitive to extrapolation (prone to under and overestimation) • Model parameters are difficult to identify	Medium	Medium	Sauer et al., 2011	Hermoso et al., 2011; Kwon et al., 2015; Leathwick, Elith, & Hastie, 2006
Support vector machines	• Suitable for modelling nonlinear relationships • Reduced number of algorithm parameters. • Overfitting is unlikely • Good performance when modelling continuous data	• Model interpretability is limited • Algorithm is computationally expensive • Model parameters are difficult to identify when data are not linearly separable • They are often not transferable to another location or time domain	High	High	Ambelu et al., 2010; Fan et al., 2017; Hoang et al., 2010; Lin et al., 2016; Sor et al., 2017	Fukuda & De Baets, 2016; Fukuda et al., 2013; Kwon et al., 2015; Muñoz-Mas et al., 2018
Partial least squares regression	• Handles multicollinearity and strong correlation of predictors • Straightforward interpretation • Suitable when the number of explanatory variables is greater than the number of observations	• Interpretability is compromised when high correlations are present without clear causal relationships • Sensitive to the relative scaling and noise of the predictor variables	Medium	Medium	Abouali et al., 2016; Riseng et al., 2011; Surridge et al., 2014; Villeneuve et al., 2018, 2015	Abouali et al., 2016; Einheuser, Nejadhashemi, Wang, et al., 2013; Villeneuve et al., 2015
Fuzzy logic-based	• Provides insight into the influence and interactions of explanatory variables. • Uncertainty quantification is easily integrated into the models • Suitable for including expert elicitation and partial information along data	• Computational effort rapidly increases with the number of predictors • Introduction of expert elicitation into models can be time consuming • They are often not transferable to another location or time domain	High	High	Adriaenssens et al., 2006; Herman et al., 2016; Herman & Nejadhashemi, 2015; Marchini et al., 2009; A. M. Mouton et al., 2009; Ocampo-Duque et al., 2007; Van Broekhoven et al., 2006; Woznicki, Nejadhashemi, Abouali, et al., 2016; Woznicki, Nejadhashemi, Tang, & Wang, 2016	Abouali et al., 2016; Boavida et al., 2014; Einheuser et al., 2012; Einheuser, Nejadhashemi, Wang, et al., 2013; Einheuser, Nejadhashemi, & Woznicki, 2013; Fukuda & De Baets, 2016; Fukuda et al., 2013; Herman et al., 2015, Herman et al., 2016; Muñoz-Mas et al., 2012; Woznicki, Nejadhashemi, Abouali, et al., 2016; Woznicki, Nejadhashemi, Tang, & Wang, 2016; Yi et al., 2017
Bayesian belief networks	• Uncertainty quantification is easily integrated into the models • Suitable for including expert elicitation and partial information with data • Able to handle missing values in input dataset	• Computational effort and data demand rapidly increases with the number of variables • Loss of accuracy and information because of variable discretization • Model performance greatly depends on the qualitative network definition (i.e.,	High	High	Allan et al., 2012; Boets et al., 2015; Death et al., 2015; Forio et al., 2015; Xue Li et al., 2018; Mantyka-Pringle et al., 2014; McLaughlin & Reckhow, 2017	Mantyka-Pringle et al., 2017, 2014; Peterson et al., 2013; Turschwell et al., 2017; Vilizzi et al., 2013

(Continues)

TABLE 1 (Continued)

Method	Advantages	Disadvantages	Prediction power	Difficulty of variable selection	Applications	
					Macroinvertebrates	Fish
	• Can be extended to account for feedback loops and time series modelling	• network formulation itself is an important source of error • Time series modelling is computationally demanding				

several areas such as ecohydrology and ecohydraulics. State refers to the outputs driven by the aforementioned pressures (e.g., extreme events, sediment, velocity, depth, substrate, and nutrients). Finally, to evaluate the impact of the different state variables, species distribution, aquatic biodiversity, and stream health measures can be obtained (Jähnig et al., 2012). A similar comprehensive framework was recently proposed by Kail et al. (2015), introducing a module for simulating stream channel geomorphological evolution. Other authors have put more attention on states describing the flow regime, using ecologically relevant hydrologic indices (Woznicki, Nejadhashemi, Abouali, et al., 2016) and linkages with climate change scenarios (Daneshvar, Nejadhashemi, Herman, & Abouali, 2017; Guse et al., 2015). It is also worth noting that there is a trade-off between model complexity and uncertainty. In ensemble stream health modelling, gaining model predictive power and interpretability implies multiple information sources, an elevated number of model parameters, and the persistence of epistemic errors in model formulation. Hence, higher outcome uncertainties might be expected. Therefore, increased efforts studying uncertainty propagation and shrinking in ensemble modelling must be addressed to promote more transparent decision-making processes. On the other hand, with the advent of big data sources and applications, including image processing and long-term monitoring data (Kuemmerlen, Stoll, Sundermann, & Haase, 2016), recent advances in deep learning are encouraged to be implemented and integrated within existing modelling frameworks (Babbar-Sebens, Mukhopadhyay, Singh, & Piemonti, 2015; Lecun, Bengio, & Hinton, 2015). Furthermore, it is necessary to evaluate how the current strategies for biological data acquisition are compatible with data derived from remote sensing products and traditional environmental information systems and networks and how these strategies can help us to better understand the health of a stream. In summary, stream health modelling should be seen as complementary tools that require continuous validation with field measurements (Kuehne, Olden, Strecker, Lawler, & Theobald, 2017). Therefore, clear guidelines regarding monitoring stream health for modelling purposes should be considered in future studies.

With respect to *model evaluation and overfitting*, the commonly used performance measures depend on the type of response variable. When categorical variables are predicted (e.g., presence/absence and impairment condition), the percentage of correctly classified observations, true statistical skills, sensitivity, specificity, Cohen's kappa, and the area under receiver operating characteristic curve are commonly calculated (Manel, Williams, & Ormerod, 2001; Sor et al., 2017). Meanwhile, using several performance measures when conducting modelling exercises is recommended (Maloney et al., 2009). When predicting continuous response variables (e.g., a stream health index and biomass), commonly used performance measures are the correlation coefficient (r), the coefficient of determination (R^2), the Nash-Sutcliffe efficiency, the root mean squared error (RMSE), and the deviance between observed and predicted values (Goethals et al., 2007). On the other hand, the application of the algorithm's formulation and the k -fold cross-validation techniques can be used to minimize model's overfitting as they were widely used in studies reviewed here. Likewise, other approaches for preventing overfitting include variable selection, regularization, pruning of decision trees, and early stopping

of boosting algorithms (optimizing the number of trees, learning rate, and tree complexity). However, to the best of our knowledge, there are no standard guidelines for evaluating the stream health model performance, even though, for other aspects of environmental modelling, several guidelines have been developed including Bennett et al. (2013), Moriasi et al. (2007), and Moriasi, Gitau, Pai, and Daggupati (2015). Therefore, for stream health modelling, a combination of the aforementioned criteria or new criteria should be further evaluated with respect to their applicability/usefulness.

4 | SUMMARY AND CONCLUSION

In this study, we provided an overview of different statistical, machine learning, and soft computing methods widely used in ecological applications and stream health modelling based on data describing macroinvertebrates and fish assemblages. The main advantages and disadvantages for the reviewed methods are summarized in Table 1. It is worth noting that statistical methods are simpler and more interpretable than other methods, whereas their prediction power is sometimes low. However, if the major process components are incorporated and a correct model structure is chosen, statistical models can represent the principles of an environmental/ecological system (e.g., ubiquitous power laws in nature). On the other hand, models based on machine learning techniques sometimes provide a better accuracy in reproducing observed stream health indices and are in general more suitable for representing nonlinear systems. Nevertheless, models developed with these methods generally have poor or no transferability beyond the place and/or time domain of data that were used. Furthermore, it can be difficult to interpret and hardly provide insight into model parameters' meaning and relative importance. Thus, soft computing methods, which can be integrated with machine learning techniques, are favourable because they allow the insertion of expert elicitation and partial information, enhancing interpretability of ecological models. However, model formulation is usually time consuming, especially for very complex models. Meanwhile, soft computing models that are structured based on expert knowledge are susceptible to misrepresenting causal relationships and consequently are likely to provide higher structural uncertainties. This can be due to the fact that models developed using soft computing techniques are subject to significant judgements of modellers. In addition, they are often not transferable to another location or time domain.

Therefore, frameworks supporting the integration of process-based models for driving multiscale stressors and employing ensembles of different empirical modelling techniques are being recommended. Meanwhile, these types of modelling techniques are vulnerable to uncertainty propagation resulted from the modelling process and components and data sources, which can affect the consistency and reliability of the modelling results. Meanwhile, there is a growing amount of literature providing better practices for data preparation, optimal model design, model interpretation, performance evaluation, and variables relative importance, among others, for specific methods such as decision trees, ANN, fuzzy logic, and BBN. Therefore, it is crucial to develop guidelines addressing the aforementioned aspects for stream health modelling practice.

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