



- 1 Prediction of groundwater quality index to assess suitability for drinking purpose using
- 2 averaged neural network and geospatial analysis
- 3
- 4 Seok Hyun Ahn^{1,¶}, Do Hwan Jeong^{2,¶}, MoonSu Kim², Tae Kwon Lee^{1,*}, Hyun-Koo Kim^{2,*}
- 5
- ⁶ ¹Department of Environmental Engineering, Yonsei University, Wonju 26493, South Korea
- ⁷ ²Soil and Groundwater Division, National Institute of Environmental Research, Incheon 22689,
- 8 South Korea
- 9
- 10 *Correspondence:
- 11 HK Kim, email: khk228@korea.kr,
- 12 TK Lee, email: tklee@yonsei.ac.kr
- 13 [¶]These authors contributed equally to this work.





14 Abstract

The aims of this study were to determine the groundwater quality index (GQI) using an averaged 15 neural network and evaluate its field applicability with two-dimensional (2D) spatial analysis. The 16 GQI was computed using 29 water quality parameters obtained at 3,552 portable groundwater 17 wells used as drinking water sources. The GQI was divided into the following three grades: 18 'worrisome', <0.89 (20.1% of the wells); 'good', 0.89-0.94 (62.8%); and 'very good', >0.94 19 20 (17.1%). Based on the random forest, the most important water quality parameters were general bacteria, turbidity and nitrate. The 2D spatial analysis confirmed notable differences in the GQI 21 grades among regions. The 10-year long-term groundwater quality monitoring in the 'worrisome' 22 grade showed the nitrate and chloride concentrations have continuously increased. These results 23 indicate that the coupling of the GQI with 2D spatial analysis is a promising approach that can be 24 25 applied in groundwater management and vulnerability assessment. 26

Keywords: Groundwater, Water quality index, Data-Driven modelling, 2D spatial analysis,
vulnerability assessment





29 1 Introduction

Groundwater is the preferred source of drinking water worldwide (Guppy et al., 2018). 30 Groundwater accounts for almost half of all drinking water, ~40% of irrigation water, and a third 31 32 of the water used for industrial purposes (Centre, 2018). To systematically manage groundwater and prevent contamination, the groundwater quality is monitored by using national groundwater 33 34 monitoring wells and the wells managed by the local government (Lapworth et al., 2019). Because these wells were established in consideration of the land use and hydrogeological characteristics 35 of each region and monitored for a long-time, it is easy to identify correlations between 36 groundwater pollution and environmental factors (Li et al., 2019). To analyse the groundwater 37 quality at a higher spatial resolution, the authorities classify groundwater quality categories into 38 39 microbial, chemical, acceptability, and radiological aspects and manage the groundwater quality 40 by using various parameters for each category. With the increasing accumulation of groundwater quality data reflecting the land use and hydrogeological characteristics, the number of attempts to 41 predict the water quality or derive water quality management policies has increased (Bhanja et al., 42 43 2017).

The water quality index (WQI) is an algebraic approach to evaluate the water quality by converting chemical, physical, and biological parameters with different units into a single value (Misaghi et al., 2017). Many WQIs have been established to characterise surface water such as the WQI developed by the National Science Foundation (Brown et al., 1970), the Oregon Water Quality Index (Cude, 2001), Canadian Council of Ministers of the Environment WQI (Lumb et al., 2006), and Weighted Arithmetic WQI (Brown et al., 1972). Attempts have been made to apply the WQI to other water resources, such as ground- and seawater, but in most cases, the surface water





51 indices were used (Jha et al., 2015). Because groundwater has different properties than surface water due to chemical and physical processes, including the hydrochemistry, mineralogy of 52 aquifer, and precipitation-dissolution processes, it is necessary to develop a WOI suitable for 53 54 groundwater. Although in a few groundwater quality index (GQI) studies, it has been attempted to evaluate the groundwater quality with water temperature, nitrate, pH as main parameters, it is 55 difficult to accurately determine the water quality with a limited number of parameters and data 56 (Abbasnia et al., 2019; Gao et al., 2020). Therefore, the GQI must be improved by incorporating 57 the massive amount of groundwater data, which was recently collected by the authorities. 58

Recently, many attempts have been made to predict the groundwater quality by using data-59 driven models. Data-driven models predict the output using a mathematical model of input 60 61 variables derived by the supervised learning of a given dataset. Algorithms for learning the datasets 62 include neural network, fuzzy systems, support vector machine (SVM), ensemble trees, and discriminant analysis (Wei et al., 2018). Previously, researchers predicted water quality indicators 63 such as the dissolved oxygen, turbidity, pH, and ammonia using data-driven modelling (artificial 64 neural network, ANN; random forest, RF; SVM) and yielded model prediction errors below 15% 65 66 (Antanasijević et al., 2014; Meyers et al., 2017; Najah Ahmed et al., 2019). In most previous studies using data-driven models, single water quality parameters were predicted by utilising 67 multiple water quality parameters as input variables. However, a data-driven model that can be 68 69 used to evaluate or predict the overall water quality, such as the WQI or vulnerability assessment, has not been developed. 70

The objective of this study was to test the hypothesis that data-driven models can be applied to potable groundwater in South Korea to accurately predict the groundwater vulnerability and





73 determine the groundwater quality. The prediction of the groundwater vulnerability is necessary 74 to establish policies based on prioritising regions requiring groundwater quality management. We collected water quality datasets including 47 parameters and 8,326 wells through the 'Safe 75 76 Groundwater Project in Unsupplied Areas (2017–2020)' (Fig 1). We calculated the single distance score for each well with potable groundwater by determining the difference between the water 77 78 quality parameters and water quality standards. We then created a model by using the water quality 79 datasets and distance score utilising data-driven techniques including averaged neural networks.. Regions with a high groundwater pollution vulnerability were selected by linking the binning 80 technique with two-dimensional (2D) spatial analysis, and the accuracy of the groundwater 81 pollution vulnerability was evaluated by analysing the long-term monitoring results obtained at 82 83 national groundwater monitoring wells in the selected regions. The results show that a simple WOI 84 with data-driven modelling is sufficient to select priority groundwater quality management areas. Although the focus of this study was placed on potable groundwater, our results can be used as 85 guidance for data-driven modelling efforts considering other water resources that are directly 86 related to human health (e.g., irrigation and drinking water). 87

88

89 **2 Methods**

90 2.1 Study sites

Data were acquired from 2017 to 2020 within the framework of the 'Safe Groundwater Project in Unsupplied Areas (2017–2020)' managed by the National Institute of Environmental Research, South Korea. The data included 47 drinking water quality parameters for a total of 8,326 Korean groundwater wells (2017: 2,061 wells; 2018: 2,142 wells; 2019: 2,019 wells; 2020: 2,104 wells).





95	The locations of the wells are shown in Fig. 1. All wells used in this study have been used as
96	drinking water sources by Koreans. Information about the year of the well development and land
97	use type was obtained by surveys. The groundwater quality parameters used in this study,
98	including harmful inorganics and organics, microorganisms, and substances affecting the
99	aesthetics, and standards are summarised in Table S1.

100

101 2.2 Data preprocessing

The R software (version 3.6.1) was used for data preprocessing. Because the aim of this study was to evaluate the potential use of groundwater as drinking water based on the prediction of groundwater quality, wells exceeding the groundwater quality standard were excluded from the analysis. In total, 4,774 wells had an inappropriate groundwater quality, representing 57.3% of the total groundwater (8,326 wells). Thus, 3,552 wells with potable groundwater were used for datadriven modelling.

Among the 47 water quality parameters, 18 parameters that were not detectable in the potable 108 groundwater were removed. The 18 parameters included three with the aesthetic effects (detergents, 109 110 smell, and taste), two harmful inorganic materials (cadmium and cyanide), 10 harmful organic 111 materials (phenol, diazinon, parathion, fenitrothion, carbaryl, 1,1,1-trichloroethane, 112 tetrachloroethylene, 1,2-dibromo-3-chloropropane, carbon tetrachloride, and 1.1dichloroethylene), and three microorganisms (total coliform, faecal coliform, and Escherichia coli). 113 The pH was not considered for further study because it insignificantly affects the analysis if the 114 115 drinkable level is satisfied. Therefore, the analysis and modelling were carried out with 28 parameters (general bacteria, lead, fluorine, arsenic, caesium, mercury, chromium, boron, copper, 116





- zinc, chlorine, iron, manganese, aluminium, ammonium, nitrate, sulphate, potassium
 permanganate consumption, trichloroethylene, dichloromethane, benzene, toluene, ethylbenzene,
- 119 xylene, 1,4-dioxane, total hardness, colour, and turbidity).
- 120

121 2.3 Calculation of the groundwater quality index (GQI)

To evaluate the water quality indicators used in this study in the form of a single quantitative index, the difference between each water quality indicator and the water quality criterion was calculated. First, for potable groundwater, min–max normalization (Patro and Sahu, 2015) was performed, where the water quality standard was used as max for each parameter (Fig. 2A). The following equation was used:

127
$$P_n = \frac{P_e - P_{e \min}}{P_s - P_{e \min}},$$
 (1)

where P_n denotes the normalised value, P_e represents the value of each parameter, and P_S is the groundwater quality standard for each parameter. $P_{e\ min}$ represents the minimum of P_e . Because all data used for the modelling represent potable groundwater, P_S is the maximum value.

131 Second, the deviation was calculated using the following simple equation:

132
$$P_d = 1 - P_n$$
, (2)

where P_d is the parameter's deviation value and 1 is the groundwater quality standard for each parameter. In min–max normalization, the minimum value becomes 0 and the maximum value becomes 1 because the maximum value is based on the groundwater quality.

- 136 In the third step, the distance score of the well as the single quantitative index was calculated using
- 137 the following equation:





(3)

138
$$W_d = \frac{\sum_{i=1}^{x} (P_d)^2}{x}$$
,

139 where W_d is the distance score and *x* represents the number of parameters. The calculated 140 distance score is called groundwater quality index (GQI).

Based on the GQI, the data were divided into three grades, where $W_d = 0.94$ corresponds to the

142 top 20% and $W_d = 0.89$ corresponds to the bottom 20%. A value <0.89, >0.94, and ranging

between 0.84–0.94 represents worrisome, very good, and good areas, respectively.

144

145 **2.4 Model setup**

146 Data-driven modelling was carried out using the R package 'caret' (version 6.0-86) (Kuhn, 2008). 'Caret' is an abbreviation for classification and regression training and the package contains useful 147 functions for the creation of predictive models (Fig. 2B). It focuses on simplifying training and 148 tuning processes. It also contains functions for training data preprocessing, parameter importance 149 calculation, and model visualization. It has the advantage of enabling the parallel processing of 150 151 multiple models. A total of ten classification models were chosen and used in this study. The ten 152 models were used to classify unlearned groundwater vulnerability grades by learning the previously preprocessed 28 water quality parameters. The models used include averaged neural 153 154 network, RF, SVM, ensemble trees, bagged flexible discriminant analysis, gradient boosting, penalised discriminant analysis, boosted logistic regression, ROC-based classifier, and Naïve 155 156 Bayes. The averaged neural network, an ANN model, was created by applying an averaging 157 technique to the neural network model. It is generated by modifying the functions of ordinary differential equations applied to the neural network and can be used for both regression and 158 classification analysis. Decision tree and RF are tree-based models that operate with the goal of 159





160 dividing feature space into multiple areas. The RF is a model in which the performance is improved 161 based on the use of an ensemble technique called bagging. Discriminant analysis is an analysis method that is used to identify criteria that can determine which population these samples were 162 extracted from using sample information from two populations. In this study, bagged flexible 163 discriminant analysis and penalised discriminant analysis were used. The Naïve Bayes classifier 164 is a technique prediction based on simple probabilistic and on the application of the Bayes theorem 165 (or Bayes rule) with a strong independence assumption. The SVM is one of the representative data-166 driven modelling methods, which is based on an algorithm that identifies boundaries dividing 167 groups of data by the largest margin. The ROC-based classification is a model based on ROC 168 analysis and can only be used for classification analysis. The ROC analysis is a method based on 169 170 which the below areas are compared by visualising the performance of the classifier with an ROC 171 curve. With respect to ensemble techniques, we used gradient boosting and boosted linear 172 regression models, which improve the accuracy of the model by continuously reducing the residual 173 during the learning process. The ten models described above were trained using caret's default training and all models involved 5-flod cross-validation by splitting the data into five subsets to 174 175 compare the model performance.

The classification performance of the different models was measured using common error metrics, that is, the accuracy of the confusion matrix and kappa value. Datasets with potable groundwater were divided into training sets (80%) and test sets (20%; Fig 2B). The training sets were then further divided into two parts: 80% training set and 20% validation set. The goal of these procedures was to avoid overfitting issues during the modelling process.

181





182 2.5 Feature selection

Because the groundwater quality strongly correlates with hydrogeological properties, several water quality parameter may be biased in certain areas and the water quality predictions based on the classification model may proceed with low accuracy. To better understand the effect of the water quality parameters on the data-driven model, the input feature selection was conducted by RF. The RF can be used to extract the feature importance based on how much each feature contributes to decreasing the impurity of the trees ('meandecrease gini'; MDG) (Han et al., 2016). This parameter can be used to rank the different features.

190

191 **2.6 Binning and 2D spatial analysis**

Binning is a method that is used to group a number of continuous values into a smaller number of 192 193 bins. We used binning to group multiple GQIs into one value of a grid of uniform size in the map. 194 Based on this method, a representative GQI is obtained for a region and problems caused by 195 outliers in the closed area can be alleviated. The binning was calculated and visualised using the 'stat summary 2d' function of the R package 'ggplot2' (version 3.3.3). When analysing with low 196 197 resolution using binning on national maps, the size of the bin was set to $9 \text{ km} \times 11 \text{ km}$ (longitude 198 \times latitude). When analysing with high resolution using binning for Chungcheongbuk-do, the size of the bin was set to 4.5 km \times 5.5 km (longitude \times latitude), representing one fourth of the 199 200 nationwide bin size. Each bin was coloured based on the GQI.

To compare changes in the long-term groundwater quality based on the GQI, an area with a worrisome (site A: Seangkeuk in Eumseong), good (site B: Gageum in Chungju), and very good (site C: Heoin in Boeun) GQI was selected. Water quality (nitrate and chloride concentrations)





204	datasets were collected from the national monitoring wells in the above-mentioned area. Nitrates
205	and chlorides were selected because they overlap with the water quality parameters monitored at
206	the national groundwater monitoring wells and water quality parameters used in this study.
207	
208	2.7 Statistical analysis
209	All statistical analysis were conducted using R software (version 3.6.1). To examine the
210	differences in the GQIs and water qualities of GQI grades, Kruskal-Wallis analysis was used
211	according to the normality of data. The significant differences between the GQI grades was further
212	confirmed using the 'mctp' function in the R package 'nparcomp' (version 3.0) as a nonparametric
213	post-hoc method.
214	
215	3 Results
216	3.1 Pollution characteristics of groundwater
217	Based on Korean drinking water quality standards, the water quality of 65.2% (1,344 wells) of

218 2,061 wells in 2017; 64.3% (1,377 wells) of 2,142 wells in 2018; 46.0% (928 wells) of 2,019 wells 219 in 2019; and 53.5% (1,125 wells) of 2,104 wells in 2020 was inappropriate (Fig. S1A). The major 220 sources of groundwater pollution were microorganisms (42.4%-45.9%), followed by complex pollution (24.6%-35.0%), harmful inorganics (16.1%-27.1%), substances with an aesthetic effect 221 (2.4%-6.5%), and harmful organics (one well in 2018; Fig. S1B). The complex pollution 222 containing microorganisms or nitrate accounted for 84.5% of the total proportion. Considering 223 these results, microorganisms and harmful inorganics were major groundwater pollutants in the 224 225 study area. However, it was difficult to determine specific external factors (e.g., land use and well





226 development year) causing the groundwater pollution (Fig. S2).

227

228 **3.2 Characterization of the GQI and grades**

229 The distribution of the GQI calculated in each well has been visualised in a bar graph (Fig. 3A). From the figure, a right-skewed distribution can be observed for all potable groundwater. The 230 minimum, maximum, median, and average values of the GQI were 0.7344, 0.9770, 0.9160, and 231 0.9127, respectively. These results indicate that the water quality of more than half of the wells 232 was on average within 10% of the water quality standard. Note that the GOI correlates with the 233 Weighted Arithmetic WQI, one of the well-known single indices for evaluating the surface water 234 quality (cor = -0.38, Fig. S3). The GQI was divided into three grades: 'worrisome', <0.89 (714 235 wells); 'good', 0.89–0.94 (2,229 wells); and 'very good', >0.94 (609 wells; solid line in Fig. 3A). 236 237 The GQI significantly varied depending on the grade (Kruskal test, p-value < 0.05, Fig. 3B). 238 To determine the factors that control the GOI of the wells of each grade, the water quality parameters were analysed using two approaches. First, the number of water quality parameters 239

higher than half of the water quality standards was calculated for each groundwater well (Fig. 3C). 240 241 In the 'very good' grade, one or less parameters accounted for more than 95% of the total, whereas 242 one or two parameters accounted for more than 95% of the total in the 'good' grade. In the 'worrisome' grade, more than 50% of the water quality standards of one or more parameters was 243 244 observed in all wells, and three or more water quality parameters accounted for more than 50% of the wells. As expected, when the grade changed from 'very good' to 'worrisome', many water 245 quality parameters approached the water quality standards. Second, the GQIs of the water quality 246 247 parameters contributing to the grade division were statistically compared based on the grade (Fig.





248	4). Based on the selection of the ten most important water quality parameters using the RF model,
249	the most important parameter was 'general bacteria', followed by the turbidity, nitrate, total
250	hardness, sulphate, chloride, zinc, potassium permanganate consumption, fluoride, and iron (Fig.
251	3D). The deviation value of all selected parameters significantly decreased from 'very good' to
252	'worrisome' (Kruskal test, p-value < 0.05 , Fig. 4). These results imply that various water quality
253	parameters were close to the water quality standards in the 'worrisome' grade.
254	

255 3.3 Data-driven model selection

256 The performance of ten classification models for the prediction of the GQI was compared based on the accuracy of the confusion matrix and kappa value (Fig. 5). The ANN model yielded the best 257 classification performance (96.5%–98.6%), followed by the SVM with an average classification 258 accuracy of \geq 90%. The average classification accuracy of Naïve Bayes and decision tree models 259 260 did not exceed 60%. Therefore, the ANN model with a 98.6% classification accuracy was selected 261 as the optimal classification model. We also applied the ANN model to predict the grades using individual annual datasets for additional cross-validation. The grades of all annual datasets were 262 263 predicted with an accuracy of ~99%.

264

265 3.4 Spatial analysis using GQI binning

Binning is useful for the conversion of large point-based data to a regular grid representing the
aggregation of points in the map and makes it easy to visualise the data at different map scales.
We binned the GQI and grades and plotted them on a nationwide map (each grid: 9 km × 11 km)
for South Korea (Figs S5A and S5B). Among all 1,496 grid cells, 537 (35.9% of total) grid cells





270 indicate the GQI and grades, and on average seven wells were included based on the coloured grid cells. The Chuncheongbuk-do province was selected for the visualization and analysis of the GQI 271 and grades at a higher resolution by using half of the size of the previous grid (each grid: 4.5 km 272 \times 5.5 km; Figs S5C, S5D, and 6A). Compared with other provinces, the wells are evenly spatially 273 distributed in the Chuncheongbuk-do Province. Among all 460 grid cells, 80 (17.4% of total) grid 274 275 cells indicate the GQI and grades. Among the coloured grid cells, 16 (20.0% of coloured grid), 55 (68.7%), and nine (11.3%) grid cells represent a 'worrisome', 'good', and 'very good' grade, 276 respectively. In general, the grid cells representing 'worrisome' areas are mainly distributed at the 277 edge of the province. We compared the long-term trends of the water quality of national monitoring 278 wells by selecting a representative region for each grade to confirm that our results are reliable 279 (Fig. 6A). Because the main water quality parameters used in this study and those regularly 280 monitored by the national groundwater monitoring wells are nitrate and chloride, the change of the 281 two parameters over ten years was analysed (Fig. 6B). Both the nitrate ($R^2 = 0.289$) and chlorine 282 283 $(R^2 = 0.696)$ concentrations at site A (Saengkeuk in Eumseong), which was determined to be a 'worrisome' area, have rapidly increased over the past decade. Both the nitrate ($R^2 = -0.413$) and 284 chloride ($R^2 = -0.05$) concentrations show a decreasing trend at site C; however, at site B, the 285 chloride content slightly increased ($R^2 = 0.149$), but the nitrate concentration did not change ($R^2 =$ 286 -0.02). The differences in the long-term water quality trends observed at the national groundwater 287 288 monitoring wells were confirmed based on the GQI grades.

289

290 4 Discussion

291 The 'Safe Groundwater Project in Unsupplied Areas (2017–2020)' was conducted including wells



312



292 used by citizens for which regular water quality surveys were not carried out. It is a public service 293 to provide realistic policies to citizens based on the analysis of the quality of groundwater used by citizens. In contrast to previous reports of massive water quality monitoring in South Korea, which 294 mainly included a limited number of water quality parameters monitored in national groundwater 295 monitoring wells, the data from the 'Safe Groundwater Project in Unsupplied Areas (2017–2020)' 296 297 are of great value because they include 47 water quality parameters monitored in wells that citizens 298 use as drinking water sources. More than 50% of the wells used in this study are inappropriate as 299 drinking water source (at least one water quality parameter exceeded the standard value). Considering that the ratio of wells with an inappropriate water quality was low (6.5% - 8.0%) based 300 on a previous massive survey of the groundwater quality, the number of wells with an inappropriate 301 302 water quality obtained in this study is very high (Lee and Kwon, 2016). The analysed water quality 303 parameters are significantly higher and various water quality parameters exceed the thresholds; 304 thus, the proportion of wells with an inappropriate water quality has increased. However, because 305 both studies showed that the main sources of groundwater pollution are nitrate and total coliform, it is impossible to simply explain the cause of the increase in the proportion of inappropriate wells 306 307 with the increase in the number of analysed water quality parameters (Yun et al., 2014). Because 308 the characteristics of land use or well development insignificantly affect the proportion of 309 inappropriate wells, it is necessary to analyse these data with a new approach to link them to 310 groundwater management policies. In particular, it is necessary to develop an approach by selection of areas that require groundwater management based on potable water quality data. 311 We calculated the GQI, a single index of the water quality of each groundwater well, and divided

313 it into three grades. This approach is similar to the WQI used for surface water (WHO, 2011). In





314 particular, the GQI is similar to the WQI suggested by Brown in that it is calculated as a single 315 index using the difference between the water quality standard and observed value (Seifi et al., 2020). Because the GOI calculated in this study does not include a parameter selection process nor 316 a weight determination process for the parameter, the process for calculating the GQI is very 317 simple and an index bias can be avoided. The correlation between the Weighted Arithmetic WQI 318 and GQI indicates the similarity between the two indices. However, in wells with a good water 319 quality (low WAWQI value), the GQI can be analysed with higher resolution compared with the 320 Weighted Arithmetic WOI (high variability of the GOI in the same Weighted Arithmetic WOI). 321 This indicates that the GQI is more suitable for evaluating the water quality of potable groundwater. 322 Despite the calculation for potable groundwater, the statistical differences in major water quality 323 324 parameters based on the GOI grade confirm the usefulness of the GOI. In addition, it was 325 confirmed that the difference in the number of parameters with a distance score from the standard 326 of less than 50% depends on the grade. This means that, because the GOI is calculated in 327 consideration of the effects of complex parameters rather than one parameter, it is suitable for Korea, which is facing significant groundwater pollution caused by complex pollutants. Pollution 328 329 sources change several groundwater quality parameters at the same time. Therefore, considering 330 multiple parameters at the same time is more important in tracking pollutants and characterising groundwater pollution conditions than focusing on one parameter (Menció et al., 2016). Because 331 332 the GQI has the same effect as multivariate analysis based on the simultaneous reflection of changes of multiple water quality parameters, it is of advantage in water quality surveys for both 333 complex and single pollutants (Menció et al., 2016; Wu et al., 2019). 334

335 To develop a data-driven model that can be used to predict the GQI grade, we compared the





336 predictive performance of ten classification models. The ANN performed the best, with a prediction accuracy of ~95%, followed by the SVM and bagged flexible discriminant analysis. 337 The classification performance of the ANN is high because this ensemble method uses the average 338 of the predictions from each model by fitting multiple neural network models to the same datasets 339 (Lone et al., 2021). Based on previous studies, the ANN did not have a good prediction 340 performance compared with other models (Ehteshami et al., 2016; Naghibi et al., 2018). However, 341 in most previous studies, ANNs were used for regression analysis to predict specific water quality 342 indicators rather than grades or classes, and the amount of data was considerably small for ANN 343 analysis (Ehteshami et al., 2016). In this study, a high performance was obtained because the water 344 quality parameters were divided into grades and the amount of learning data was suitable for ANN 345 applications. 346

347 Because groundwater pollution will likely quickly contaminate the groundwater in surrounding areas depending on the flow rate and hydrogeological characteristics, it is important to investigate 348 the groundwater quality of multiple wells at the regional scale to mitigate groundwater pollution 349 in a timely manner. However, because it is difficult to proceed for realistic reasons (e.g., well 350 351 selection, sampling cycle, and analysis cost), datasets are often converted into data suitable for 352 grid cell or spatial indices, and geographic areas are partitioned by using an analysis technique such as binning and displaying in maps (Shrestha et al., 2015). We recalculated the GQI by using 353 354 grid cells and binning and determined GQI grades and visualised them on a map. Although it does not completely match the existing administrative districts, the map indicates the current status of 355 the groundwater quality for Myun-sized (the second smallest administrative unit in South Korea) 356 357 grid cells (4.5 km \times 5.5 km). In the case of Chuncheonbuk-do, GQI grades were determined in





358 only 17.5% of the province because areas with an abundant water supply and unoccupied mountainous areas are not subject to water quality monitoring. These simple visualization results 359 are more intuitive and user-friendly than existing groundwater pollution vulnerability assessments 360 361 or data-driven groundwater quality models (Knoll et al., 2019; Ouedraogo et al., 2016). In addition, the data can be easily linked to groundwater management policies because water quality 362 management agencies or local governments can utilise existing groundwater quality data without 363 further monitoring processes. Because the water quality of multiple wells is converged to an 364 average value during binning, it is necessary to evaluate the reliability of the binned GOI or GOI 365 grade (Kumar and Krishna, 2018). Reliability assessment should be used to track the groundwater 366 contamination by investigating the water quality of local wells by grade in the long term. However, 367 368 it is difficult to establish a general reliability assessment because a water quality monitoring had 369 to be conducted only once in one groundwater well in this project. To indirectly evaluate the 370 reliability, we analysed the trend of the water quality changes over the past ten years based on the 371 GQI grades using the results of long-term water quality monitoring at the national groundwater monitoring wells. The water quality results significantly differ depending on the GQI grades. In 372 373 particular, in the 'worrisome' grade, the contamination of groundwater has rapidly increased over 374 the past decade, which was not observed for other grades. These results indicate that the reliability of the water quality evaluation is high, even if the GQI, which is sensitive to the changes in multiple 375 376 water quality parameters, is binned and analysed at a regional level. In addition, spatial analysis including the GQI grade can provide important information for establishing policies with respect 377 to the selection of groundwater management priority areas. 378

379





380 5 Conclusion

A method to evaluate the groundwater quality for drinking purposes based on the GQI was 381 introduced. The regional characteristics of the GQI were assessed using 2D spatial analysis. 382 Because the GQI was computed based on mass water quality data (47 water quality parameters 383 and 8,326 wells) and neural networks, the groundwater quality could be accurately determined. 384 Overall, the results show that the groundwater in a large number of wells that are currently used 385 by citizens as drinking water sources, especially in regions with low GQI (e.g., 20.1% for the 386 'worrisome' grade), is polluted. This approach can be used to predict potential groundwater 387 pollution based on the comprehensive evaluation of the groundwater quality beyond the 388 dichotomous judgement of the drinking water quality based on the water quality standard. In this 389 study, a GOI was developed based on several water quality parameters, and it only partially reflects 390 391 the water quality characteristics of the groundwater. More parameters, including hydrogeological, 392 meteorological, and land use parameters, should be added to improve the GQI and effectiveness 393 of groundwater management and risk assessment.

394





396

397 ACKNOWLEDGEMENT

- 398 We gratefully acknowledge the funding of the projects of the National Institute of Environmental
- 399 Research (NIER) in South Korea (NIER-2020-04-02-049; NIER-2021-04-02-092) by the Korean
- 400 Ministry of Environment (MOE).

401

402 AUTHOR CONTRIBUTIONS

- 403 Seok Hyun Ahn: Data curation, Data analysis, Visualization, Writing-original draft. Tae Kwon
- 404 Lee: Conceptualization, Data analysis, Writing-review & editing. Do Hwan Jeong: Validation,
- 405 Writing-review & editing, Moonsu Kim: Conceptualization, Writing-review & editing. Hyun-
- 406 Koo Kim: Conceptualization, Supervision, Writing-review & editing

407

408 COMPETING INTERESTS

- The authors declare that they have no known competing financial interests or personalrelationships that could have appeared to influence the work reported in this paper.
- 411

412 Code/Data availability

- 413 The data for this project are confidential, but may be obtained with Data Use Agreements with the
- 414 National Institute of Environmental Research (NIER) in South Korea. Researchers interested in
- 415 access to the data may contact Do Hwan Jeong at jungdh93@korea.kr.





416 **Reference**

- 417 Abbasnia, A., Yousefi, N., Mahvi, A. H., Nabizadeh, R., Radfard, M., Yousefi, M., and Alimohammadi, M.:
- Evaluation of groundwater quality using water quality index and its suitability for assessing water for
- 419 drinking and irrigation purposes: Case study of Sistan and Baluchistan province (Iran), Human and
- 420 Ecological Risk Assessment: An International Journal, 25, 988-1005, 2019.
- 421 Antanasijević, D., Pocajt, V., Perić-Grujić, A., and Ristić, M.: Modelling of dissolved oxygen in the Danube
- 422 River using artificial neural networks and Monte Carlo Simulation uncertainty analysis, Journal of
- 423 Hydrology, 519, 1895-1907, 2014.
- 424 Bhanja, S. N., Mukherjee, A., Rodell, M., Wada, Y., Chattopadhyay, S., Velicogna, I., Pangaluru, K., and
- Famiglietti, J. S.: Groundwater rejuvenation in parts of India influenced by water-policy change implementation, Scientific Reports, 7, 7453, 2017.
- 427 Brown, R., Mccleiland, N., Deiniger, R., and O'Connor, M.: Water quality index-crossing the physical 428 barrier,(Jenkis, SH, ed.) Proc, 1972, 787-797.
- Brown, R. M., McClelland, N. I., Deininger, R. A., and Tozer, R. G.: A water quality index-do we dare, Water
 and sewage works, 117, 1970.
- 431 Centre, I. G. R. A.: Groundwater Overview: Making the invisible Visible, UN WATER, 2018. 2018.
- 432 Cude, C. G.: Oregon water quality index a tool for evaluating water quality management effectiveness
- 433 1, JAWRA Journal of the American Water Resources Association, 37, 125-137, 2001.
- 434 Ehteshami, M., Farahani, N. D., and Tavassoli, S.: Simulation of nitrate contamination in groundwater 435 using artificial neural networks, Modeling Earth Systems and Environment, 2, 28, 2016.
- 436 Gao, Y., Qian, H., Ren, W., Wang, H., Liu, F., and Yang, F.: Hydrogeochemical characterization and quality
- 437 assessment of groundwater based on integrated-weight water quality index in a concentrated urban
 438 area, Journal of Cleaner Production, 260, 121006, 2020.
- Guppy, L., Uyttendaele, P., Villholth, K. G., and Smakhtin, V.: Groundwater and sustainable development
 goals: Analysis of interlinkages, 2018.
- 441 Han, H., Guo, X., and Yu, H.: Variable selection using mean decrease accuracy and mean decrease gini
- based on random forest, 2016 7th IEEE International Conference on Software Engineering and Service
 Science (ICSESS), 219-224, 2016.
- Jha, D. K., Devi, M. P., Vidyalakshmi, R., Brindha, B., Vinithkumar, N. V., and Kirubagaran, R.: Water quality
 assessment using water quality index and geographical information system methods in the coastal
 waters of Andaman Sea, India, Marine pollution bulletin, 100, 555-561, 2015.
- 447 Knoll, L., Breuer, L., and Bach, M.: Large scale prediction of groundwater nitrate concentrations from
- spatial data using machine learning, Science of The Total Environment, 668, 1317-1327, 2019.
- Kuhn, M.: Building predictive models in R using the caret package, Journal of statistical software, 28, 1-26, 2008.





- 451 Kumar, A. and Krishna, A. P.: Assessment of groundwater potential zones in coal mining impacted hard-
- 452 rock terrain of India by integrating geospatial and analytic hierarchy process (AHP) approach, Geocarto
- 453 International, 33, 105-129, 2018.
- 454 Lapworth, D. J., Lopez, B., Laabs, V., Kozel, R., Wolter, R., Ward, R., Vargas Amelin, E., Besien, T., Claessens,
- 455 J., Delloye, F., Ferretti, E., and Grath, J.: Developing a groundwater watch list for substances of emerging
- 456 concern: a European perspective, Environmental Research Letters, 14, 035004, 2019.
- Lee, J.-Y. and Kwon, K. D.: Current status of groundwater monitoring networks in Korea, Water, 8, 168, 2016.
- Li, H., Gu, J., Hanif, A., Dhanasekar, A., and Carlson, K.: Quantitative decision making for a groundwater
 monitoring and subsurface contamination early warning network, Science of The Total Environment,
 683, 498-507, 2019.
- 462 Lone, K. J., Hussain, L., Saeed, S., Aslam, A., Maqbool, A., and Butt, F. M.: Detecting basic human activities
- and postural transition using robust machine learning techniques by applying dimensionality reduction
 methods, Waves in Random and Complex Media, 2021. 1-26, 2021.
- 465 Lumb, A., Halliwell, D., and Sharma, T.: Application of CCME Water Quality Index to monitor water quality:
- 466 A case study of the Mackenzie River basin, Canada, Environmental Monitoring and assessment, 113,467 411-429, 2006.
- 468 Menció, A., Mas-Pla, J., Otero, N., Regàs, O., Boy-Roura, M., Puig, R., Bach, J., Domènech, C., Zamorano,
- M., and Brusi, D.: Nitrate pollution of groundwater; all right..., but nothing else?, Science of the total
 environment, 539, 241-251, 2016.
- 471 Meyers, G., Kapelan, Z., and Keedwell, E.: Short-term forecasting of turbidity in trunk main networks,
 472 Water Research, 124, 67-76, 2017.
- 473 Misaghi, F., Delgosha, F., Razzaghmanesh, M., and Myers, B.: Introducing a water quality index for
- 474 assessing water for irrigation purposes: A case study of the Ghezel Ozan River, Science of the Total
- 475 Environment, 589, 107-116, 2017.
- 476 Naghibi, S. A., Pourghasemi, H. R., and Abbaspour, K.: A comparison between ten advanced and soft
- 477 computing models for groundwater qanat potential assessment in Iran using R and GIS, Theoretical
- 478 and applied climatology, 131, 967-984, 2018.
- 479 Najah Ahmed, A., Binti Othman, F., Abdulmohsin Afan, H., Khaleel Ibrahim, R., Ming Fai, C., Shabbir
- 480 Hossain, M., Ehteram, M., and Elshafie, A.: Machine learning methods for better water quality prediction,
- 481 Journal of Hydrology, 578, 124084, 2019.
- 482 Ouedraogo, I., Defourny, P., and Vanclooster, M.: Mapping the groundwater vulnerability for pollution at
 483 the pan African scale, Science of The Total Environment, 544, 939-953, 2016.
- Patro, S. and Sahu, K. K.: Normalization: A preprocessing stage, arXiv preprint arXiv:1503.06462, 2015.
- 485 2015.





- 486 Seifi, A., Dehghani, M., and Singh, V. P.: Uncertainty analysis of water quality index (WQI) for groundwater
- 487 quality evaluation: Application of Monte-Carlo method for weight allocation, Ecological Indicators, 117,
- 488 106653, 2020.
- Shrestha, P., Sulis, M., Simmer, C., and Kollet, S.: Impacts of grid resolution on surface energy fluxes
 simulated with an integrated surface-groundwater flow model, Hydrol. Earth Syst. Sci., 19, 4317-4326,
- 491 2015.
- 492 Wei, Y., Zhang, X., Shi, Y., Xia, L., Pan, S., Wu, J., Han, M., and Zhao, X.: A review of data-driven approaches
- 493 for prediction and classification of building energy consumption, Renewable and Sustainable Energy
- 494 Reviews, 82, 1027-1047, 2018.
- 495 WHO, G.: Guidelines for drinking-water quality, World Health Organization, 216, 303-304, 2011.
- 496 Wu, J., Li, P., Wang, D., Ren, X., and Wei, M.: Statistical and multivariate statistical techniques to trace the
- 497 sources and affecting factors of groundwater pollution in a rapidly growing city on the Chinese Loess
- 498 Plateau, Human and Ecological Risk Assessment: An International Journal, 2019. 2019.
- 499 Yun, S. W., Choi, H.-M., and Lee, J.-Y.: Comparison of groundwater levels and groundwater qualities in
- six megacities of Korea, Journal of the Geological Society of Korea, 50, 517-528, 2014.
- 501
- 502
- 503

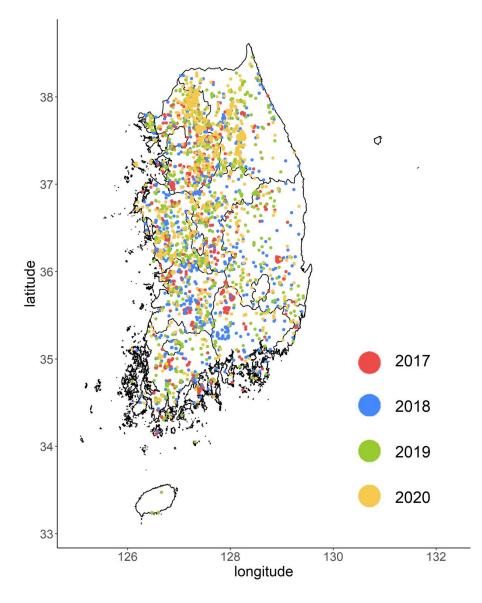




- 504 Figure list
- 505 Figure 1. Geographical information about the sampling sites in Korea.
- Figure 2. (A) Preprocessing for the calculation of the groundwater quality index including 28 water
 quality parameters and establishment of grades for data-driven modelling. (B) Workflow of the
 data-driven model.
- 509 Figure 3. (A) Visualization of the distribution based on the calculated groundwater quality index
- and grades (grey vertical line). (B) Comparison of the groundwater quality indices for the grades.
- 511 Significant differences between grades are marked by lowercase letters. (C) Proportion of each
- grade to the number of water quality parameters with a deviation value of 0.5 or less for each well.
- 513 (D) Selection of the top ten features contributing to the model performance using random forest.
- Figure 4. Boxplot of the deviation value for the top ten features contributing to the model
 performance. (A) General Bacteria, (B) Nitrate, (C) Turbidity, (D) Total hardness, (E) Chloride,
 (F) Sulphate, (G) Potassium permanganate consumption, (H) Zinc, (I) Fluorine, and (J) Iron. The
 significance of the grades was calculated with the Kruskal–Wallis test. Significant differences (P
 < 0.05) between grades are marked by lowercase letters.
- 519 Figure 5. Comparison of the data-driven model performance using the accuracy of the confusion 520 matrix and kappa value. Each classification model includes a five-fold cross validation, with ten 521 repeated values.
- 522 Figure 6. (A) The grades of the binned area for Chungcheongbuk-do are visualised in the map with
- three sites representative for the grades. Site A: Saengkeuk in Eumseong, Site B: Gageum in Chungju, Site C: Heoin in Boeun. (B) Changes in the nitrate and chloride concentrations in the last
- 524 Chungju, Site C: Heoin in Boeun. (B) Changes in the nitrate and chloride concentrations in the last 525 ten years measured at national ground monitoring wells in three representative regions.
- 526





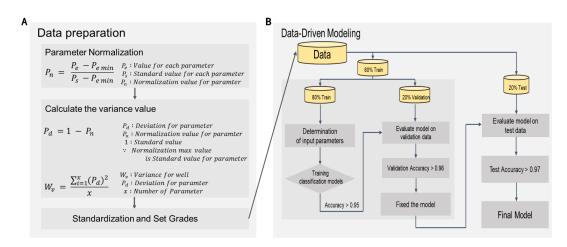


528

529 Figure 1. Geographical information about the sampling sites in Korea.







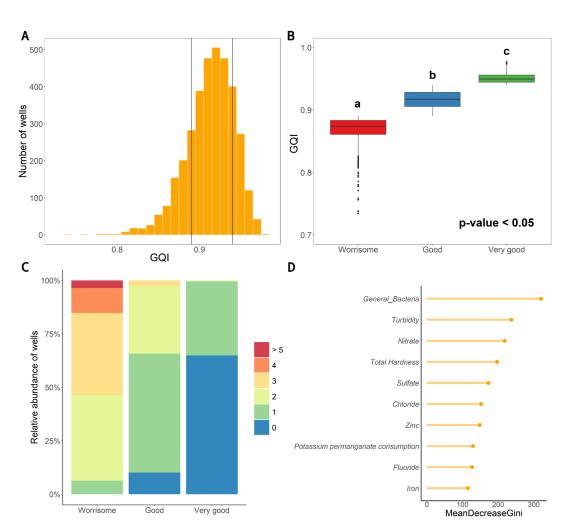
531

Figure 2. (A) Preprocessing for the calculation of the groundwater quality index including 28 water
quality parameters and establishment of grades for data-driven modelling. (B) Workflow of the

534 data-driven model.







536

Figure 3. (A) Visualization of the distribution based on the calculated groundwater quality index
and grades (grey vertical line). (B) Comparison of the groundwater quality indices for the grades.
Significant differences between grades are marked by lowercase letters. (C) Proportion of each
grade to the number of water quality parameters with a deviation value of 0.5 or less for each well.
(D) Selection of the top ten features contributing to the model performance using random forest.





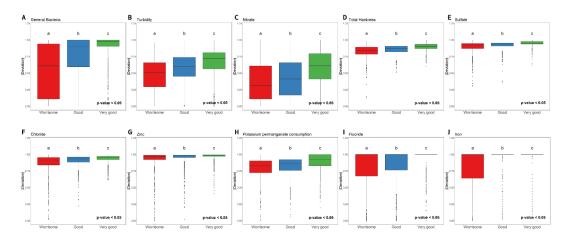
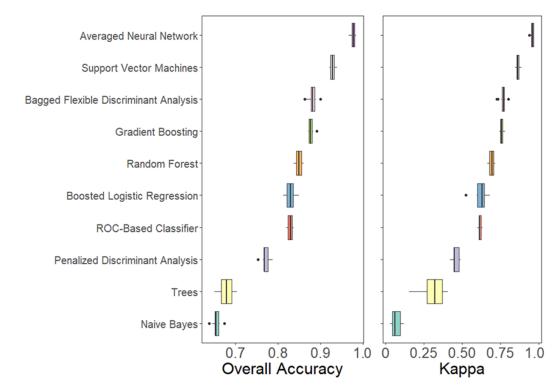




Figure 4. Boxplot of the deviation value for the top ten features contributing to the model
performance. (A) General Bacteria, (B) Nitrate, (C) Turbidity, (D) Total hardness, (E) Chloride,
(F) Sulphate, (G) Potassium permanganate consumption, (H) Zinc, (I) Fluorine, and (J) Iron. The
significance of the grades was calculated with the Kruskal–Wallis test. Significant differences (P
< 0.05) between grades are marked by lowercase letters.





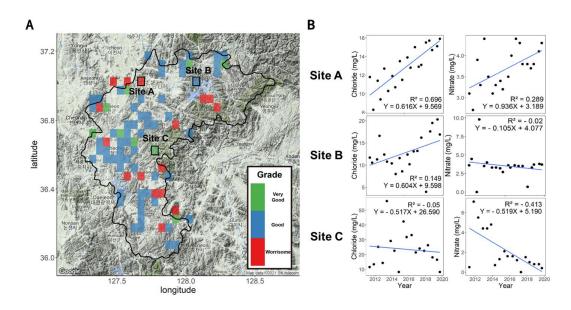


550

Figure 5. Comparison of the data-driven model performance using the accuracy of the confusion
 matrix and kappa value. Each classification model includes a five-fold cross validation, with ten
 repeated values.







555

Figure 6. (A) The grades of the binned area for Chungcheongbuk-do are visualised in the map with
three sites representative for the grades. Site A: Saengkeuk in Eumseong, Site B: Gageum in
Chungju, Site C: Heoin in Boeun. (B) Changes in the nitrate and chloride concentrations in the last

ten years measured at national ground monitoring wells in three representative regions.