

## Comparison of Four Different Ordination Methods for Patterning Water Quality of Agricultural Reservoirs

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We patterned water quality of agricultural reservoirs according to the differences of six physico-chemical environmental factors (TN, TP, DO, BOD, COD, and SS) using four different ordination methods: Principal Components Analysis (PCA), Detrended Correspondence Analysis (DCA), Nonmetric Multidimensional Scaling (NMS), and Isometric Feature Mapping (Isomap). The dataset was obtained from the water quality monitoring networks operated by the Ministry of Agriculture and Forestry and the Ministry of Environments. Chlorophyll-*a* displayed the highest correlation with COD, followed by TP, BOD, SS, and TN ( $p < 0.01$ ), while negatively correlated with altitude and bank height of the reservoirs ( $p < 0.01$ ). Although four different ordination methods similarly patterned the reservoirs according to the gradient of nutrient concentration, PCA and NMS appeared to be the most efficient methods to pattern water quality of reservoirs based on the explanation power. Considering variable scores in the ordination map, the concentration of nutrients was positively correlated with Chl-*a*, while negatively correlated with altitude and bank height. These ordination methods may help to pattern agricultural reservoirs according to their water quality characteristics.

**Key words :** agricultural reservoir, classification, ordination, multivariate analysis, water quality, reservoir management

### INTRODUCTION

Water management in agriculture has been focused mostly on the quantitative supply for irrigation without much attention to the quality of the supplied water in Korea. Recently, however, quantitative water supply as well as water quality management of agricultural reservoirs is becoming an important issue to improve quality of agricultural products as well as healthy ecosystems (Nam *et al.*, 2003; Lee *et al.*, 2007). Eutrophication has been one of the major water quality problems in lentic systems including agricultural reservoirs, as it causes turbid water with high amount of algal biomass and poor conditions

to the ecosystem (Portielje and Van der Molen, 1999). Eutrophication results in the irregularity of the nutrient cycles in aquatic ecosystem, the flourishing of microorganisms including phytoplankton, and the increase of organic matter made by the microorganisms as the high amount of nutrition is inflowed (OECD, 1982). So figuring out the relationships between related environmental variables and phytoplankton biomass variability is important to provide informative ways for determining water quality criteria and making pollution prevention plans for eutrophic reservoirs (George and Arhonditsis, 2004).

Water quality of reservoirs is influenced by various factors including physico-chemical, hydrological and geological factors. For effective

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water quality management, it is fundamental to recognize the current status of water quality, factors causing reduction of ecological function, and their mechanisms in the ecosystems. Algal growth is influenced by inflowed nutrients and nutrients released from reservoir bottoms. In addition, chemical factors have complex interactions each other in reservoirs. Therefore, different management strategies might be applied to different patterns of reservoirs.

Many studies were carried out to classify reservoirs: OECD classification (OECD, 1982), trophic state index (Carlson, 1977), and the standardization through Kratzer and Brezonik (1981) which determine categories of concerning reservoirs based on trophic state index. In Korea, Lee *et al.* (2003) classified reservoirs based on the relationship between the ratio of storage volume per water surface area (ST/WS) and Chlorophyll-*a* (Chl-*a*) concentration, and Kim and Hwang (2004) patterned reservoirs based on the relationship between Chl-*a* concentration and mean depth. However, it is not easy tasks to define reservoir patterns with single or two factors, because many different environmental factors have interactions each other. Therefore, in this study, we aimed to pattern agricultural reservoirs with four different ordination methods based on their water quality differences.

## MATERIALS AND METHODS

### 1. Ecological data

Data were obtained from the water quality monitoring networks of reservoirs operated by the Ministry of Agriculture and Forestry and the Ministry of Environment of Korea. Among the reservoirs monitored, we chose 301 agricultural reservoirs having less than 20 million m<sup>3</sup> of storage and available physical and chemical environmental factors such as total nitrogen (TN), and total phosphorous (TP), dissolved oxygen (DO), chemical oxygen demand (COD), suspended solids (SS), temperature and chlorophyll-*a* (Chl-*a*). Additionally, hydrological and geographical factors of each reservoir such as altitude, catchments, circumference, long length of reservoir, surface area, storage, bank height, and bank length were obtained from administrative records and geographical map through GIS. The variations of

**Table 1.** Variation of environmental factors in the selected reservoirs (S.D.: standard deviation).

Variables	Mean (S.D.)	Range
Altitude (m)	105.88 (98.55)	4~574
Catchment (km <sup>2</sup> )	14.14 (14.52)	0.8~93
Circumference (km)	3.98 (3.07)	0.3~19.2
Long length (km)	1.18 (0.83)	0.1~8
Surface area (km <sup>2</sup> )	0.47 (0.51)	0.1~3.3
Storage (million m <sup>3</sup> )	2.41 (2.73)	0.2~17.2
Bank height (m)	18.49 (12.35)	4~160
Bank length (m)	317.15 (322.22)	16.7~3746
TN (mg L <sup>-1</sup> )	1.54 (0.91)	0.08~6.3
TP (mg L <sup>-1</sup> )	0.07 (0.12)	0.005~1.8
DO (mg L <sup>-1</sup> )	8.2 (2.23)	3.2~17
BOD (mg L <sup>-1</sup> )	3.75 (2.63)	0.4~15.8
COD (mg L <sup>-1</sup> )	6.96 (3.69)	2.2~29.8
SS (mg L <sup>-1</sup> )	12.44 (14.64)	0.5~121.6
Temperature (°C)	16.37 (5.16)	4.2~28
Chl- <i>a</i> (mg m <sup>-3</sup> )	25.88 (44.11)	0.1~574.7

each factor were summarized in Table 1, and variations of six physical and chemical factors (TN, TP, DO, BOD, COD, and SS) used in the ordination analysis were shown in Figure 1. The selected data of the reservoirs from the monitoring networks were mostly measured in September in 2002, when data were relatively homogeneous compared with other years.

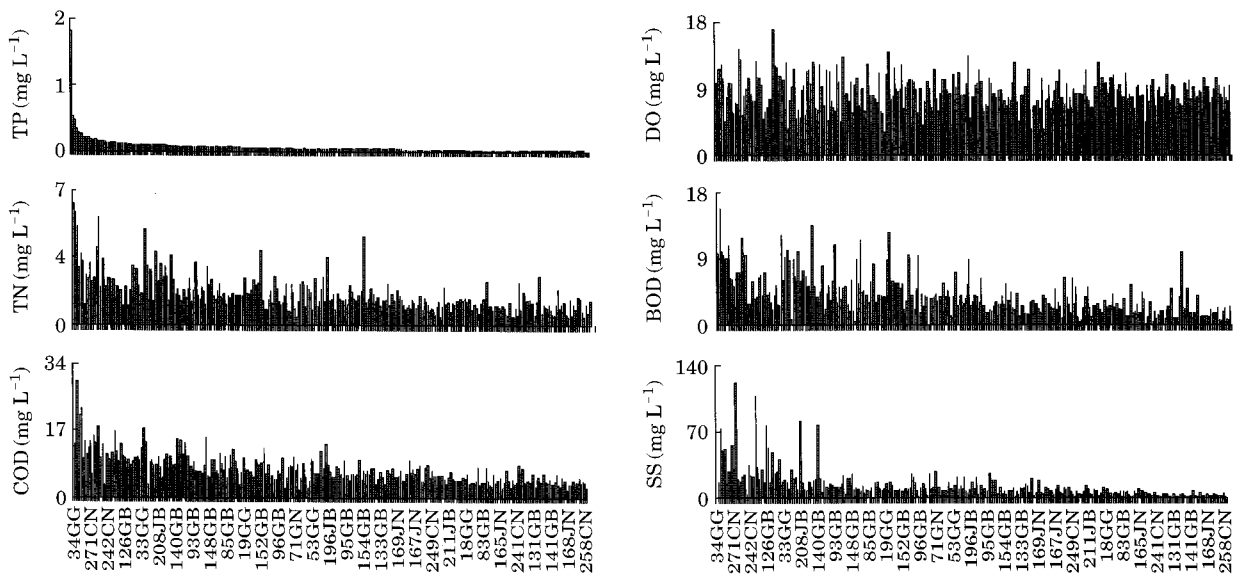
Spearman rank correlation coefficients among variables were calculated to examine the relationships between environmental variables and concentration of Chl-*a* with the statistical package, STATISTICA (StatSoft, 2004).

Carlson's trophic state index (TSI: Carlson, 1977) was calculated as equation (1) and the trophic state was evaluated based on the standardization through Kratzer and Brezonik (1981).

$$\text{TSI (Chl-}a\text{)} = 9.81 \times \ln(\text{Chl-}a\text{)} + 30.6 \quad (1)$$

### 2. Modeling procedure

To identify water quality patterns of the agricultural reservoirs based on six physical and chemical factors (TN, TP, DO, BOD, COD, and SS), we carried out four different multivariate ordination techniques: Principal Components Analysis (PCA), Detrended Correspondence Analysis (DCA), Nonmetric Multidimensional Scaling (NMS) and Isometric Feature Mapping (Isomap). PCA, DCA and NMS were conducted with the software, Pc-Ord (v.4.25) (MjM software, 1999), and Isomap was carried out with Matlab (Math-



**Fig. 1.** Differences of six physical and chemical variables of 301 reservoirs used in the ordination analyses. The numbers (1~301) in the sample names represent consecutive number and alphabets represent regions (GG: Gyeonggi; GW: Gangwon; CB: Chungbuk; CN: Chungnam; JN: Jeonnam; JB: Jeonbuk; GB: Gyeongbuk; GN: Gyeongnam).

Works, 2001). The capabilities of each ordination result were compared for patterning the water quality of the agricultural reservoirs.

Before the process of the ordinations, values of SS and TP were transformed by natural logarithm in order to reduce their variation ranges. To avoid a problem of logarithm zeros, the numeric value 1 was added to the values of each variable. Spearman rank correlation coefficients were calculated to find the relationships between the ordination axes and Chl-*a*, hydrological, and geographical factors.

### 1) Principal Components Analysis (PCA)

PCA is an indirect gradient analysis method, seeking the strongest linear correlation structure among variables (Legendre and Legendre, 1998). PCA reduces multidimensional data to lower dimensions which keep the characteristics of the raw data as much as possible. Eigen values which explain a portion of the original total variance are calculated, and then eigenvectors which contain the coefficients of the linear equation for a given axis are founded. Finally, each axis score using the eigenvector is shown in an ordination space (McCune and Grace, 2002).

### 2) Detrended Correspondence Analysis (DCA)

DCA removes arch and scaling distortions

which occur in correspondence analysis (Hill and Gauch, 1980; Legendre and Legendre, 1998). The first dimension is split into several intervals and the second axis scores are adjusted in order to make mean score within each segment zero. As individual segments of each axis are expanded or contracted, the within-sample variation of species scores is equalized (McCune and Grace, 2002).

### 3) Nonmetric Multidimensional Scaling (NMS)

NMS is a data reduction ordination method which maintains the rank ordering of the distances in a low dimensional space, expressed as a monotonic function (Shepard, 1962; Kruskal, 1964; Borg and Groenen, 1997; Cox and Cox, 2001; Mahecha *et al.*, 2007). NMS calculates the best position of the data on reduced dimensions through an iterative search that minimizes the stress of the reduced dimensions. "Stress" is a measure of departure from monotonicity in the relationship between the dissimilarity distance in the original dimensional space and distance in the reduced dimensional ordination space. The value of stress based on Kruskal's rules of thumb is between 0 and 100 (Daniel and Scott, 2007). If the value is close to 0, we can conclude NMS result is appropriate to use. In this study, we used a Monte Carlo test with 99 randomizations in order to determine whether or not the observed

**Table 2.** Spearman correlation coefficients among environmental variables in the selected reservoirs (Circum: circumference; Length: long length of reservoirs; SArea: Surface area; BHeight: bank height; BLength: bank length; Temp.: temperature; Chl- $\alpha$ : Chlorophyll- $\alpha$ ).

Variables	Altitude	Catchment	Circum	Length	SArea	Storage	BHeight	BLength	TN	TP	DO	BOD	COD	SS	Temp.	Chl- $\alpha$
Altitude	1.00	0.05	-0.32**	-0.26**	-0.48**	-0.07	0.68**	-0.38**	-0.22**	-0.44**	-0.24**	-0.45**	-0.54**	-0.31**	-0.20**	-0.56**
Catchment		1.00	0.43**	0.48**	0.50**	0.53**	0.15**	0.01	-0.01	-0.05	0.10	-0.17**	-0.25**	0.04	-0.034	-0.06
Circum			1.00	0.90**	0.8**	0.61**	-0.16**	0.22**	0.18**	0.21**	0.02	0.17**	0.21**	0.18**	0.27**	0.27**
Length				1.00	0.73**	0.59**	-0.08	0.09	0.13**	0.16**	0.02	0.11	0.14*	0.13*	0.27**	0.21**
SArea					1.00	0.67**	-0.30**	0.43**	0.18**	0.26**	0.11	0.24**	0.28**	0.20**	0.24**	0.36**
Storage						1.00	0.29**	0.22**	-0.11	-0.18**	-0.06	-0.15**	-0.11	-0.12*	0.16**	-0.05
BHeight							1.00	-0.33**	-0.37**	-0.61**	-0.19**	-0.57**	-0.59**	-0.47**	-0.199**	-0.61**
BLength								1.00	0.09	0.20**	0.07	0.21**	0.30**	0.15**	0.13*	0.24**
TN									1.00	0.62**	0.10	0.48**	0.38**	0.42**	0.11	0.48**
TP										1.00	0.01	0.59**	0.70**	0.72**	0.24**	0.64**
DO											1.00	0.12**	0.01	0.09	-0.33**	0.26**
BOD												1.00	0.60**	0.37**	0.19**	0.59**
COD													1.00	0.52**	0.31**	0.68**
SS														1.00	-0.01	0.50**
Temp.															1.00	0.20**
Chl- $\alpha$																1.00

\*p < 0.05, \*\*p < 0.01

stress value of the final solution is significantly different from the stress in randomized data.

**4) Isometric Feature Mapping (Isomap)**

Isomap (Tenenbaum *et al.*, 2000) is a new algorithm for the ordination, combining the classical techniques of PCA and NMS to a class of nonlinear manifolds (Mahecha *et al.*, 2007). The algorithm is based on a nonlinear geodesic inter-point distance matrix. The neighborhood for each point is calculated, the geodesic distance between two points is approximated by the sum of the arc lengths along the shortest path linking both points, and then classical metric MDS is applied on the approximated geodesic distance matrix. Isomap defines residual variance to characterize how well the low-dimensional Euclidean embedding captures the geodesic distances estimated from the neighborhood graph. Lower residuals indicate better-fitting solutions, with less metric distortion (Balasubramanian *et al.*, 2002).

**RESULTS**

**1. Environmental variables and trophic states**

Chl-*a* displayed the highest correlation with COD ( $r=0.68, p<0.01$ ), followed by TP, BOD, SS,

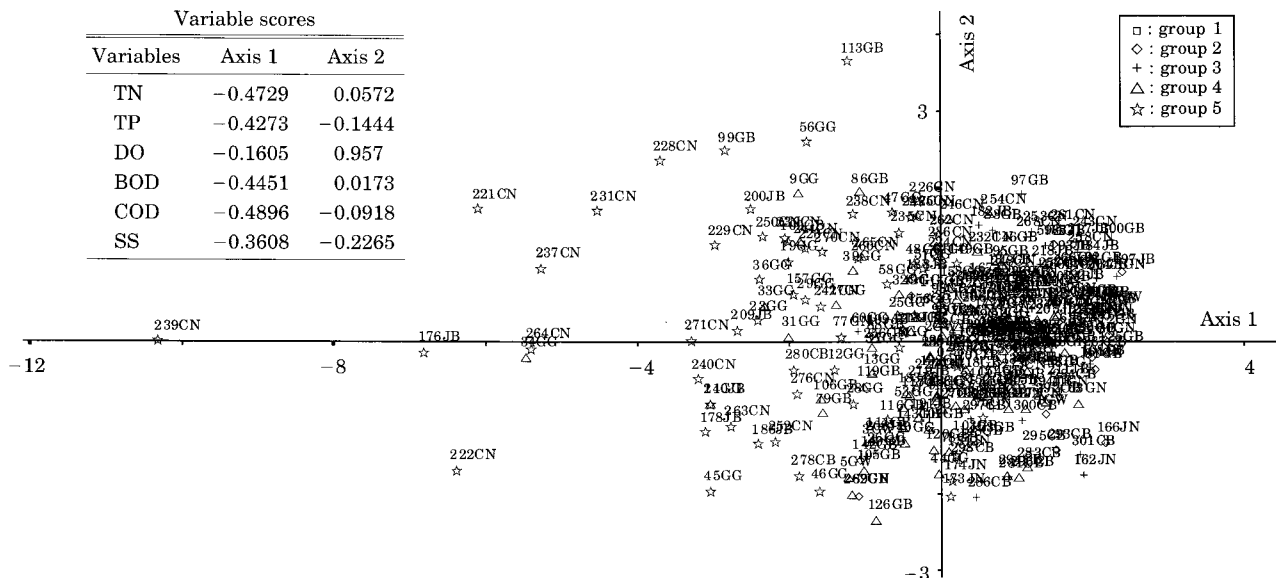
and TN ( $r=0.48, p<0.01$ ), whereas negative correlation with bank height ( $r=-0.61, p<0.01$ ) and altitude ( $r=-0.56, p<0.01$ ) (Table 2). Altitude was positively correlated with bank height ( $r=0.68, p<0.01$ ), whereas negatively correlated with physical and chemical factors COD, TP, BOD, SS, and TN ( $p<0.01$ ).

The trophic states of the reservoirs were classified into 5 groups based on Carlson's TSI (Chl-*a*) and the standardization of Kratzer and Brezonik (1981). Among 301 reservoirs, 122 (40.5%) and 71 (23.6%) of reservoirs were assigned into eutrophic and hypereutrophic states (Table 3), respectively, indicating that most Korean agricultural reservoirs are eutrophic or in the process of eutro-

**Table 3.** Classification of 301 selected reservoirs into trophic states based on the Carlson's Trophic state index (Chlorophyll-*a*) and the standardization of Kratzer and Brezonik (1981). Numbers in parentheses indicate relative abundance (%).

Groups	Trophic state index	States of nutrition	No. of reservoir (%)
1	< 20	Highly oligotrophic	2 (0.7)
2	30 ~ 40	Oligotrophic	35 (11.6)
3	45 ~ 50	Mesotrophic	71 (23.6)
4	53 ~ 60	Eutrophic	122 (40.5)
5	> 70	Hypereutrophic	71 (23.6)

Variable scores		
Variables	Axis 1	Axis 2
TN	-0.4729	0.0572
TP	-0.4273	-0.1444
DO	-0.1605	0.957
BOD	-0.4451	0.0173
COD	-0.4896	-0.0918
SS	-0.3608	-0.2265



**Fig. 2.** Principal Components Analysis (PCA) ordination of 301 reservoirs based on 6 physical and chemical variables (2.89 and 0.97 of eigen values with 48.20% and 16.16% for axes 1 and 2, respectively). The variable scores of the physical and chemical variables are listed in the figure. Reservoirs were assigned to one of five trophic states (groups 1~5) based on Carlson's trophic state index (Table 3). Sample names are explained in Fig. 1.

phication (Hwang *et al.*, 2003).

## 2. Ordination of reservoirs

Four different ordination techniques (PCA, DCA, NMS, and Isomap) were conducted to find water quality patterns concerning physical and chemical factors. Their results were compared for patterning water quality of agricultural reservoirs.

### 1) PCA

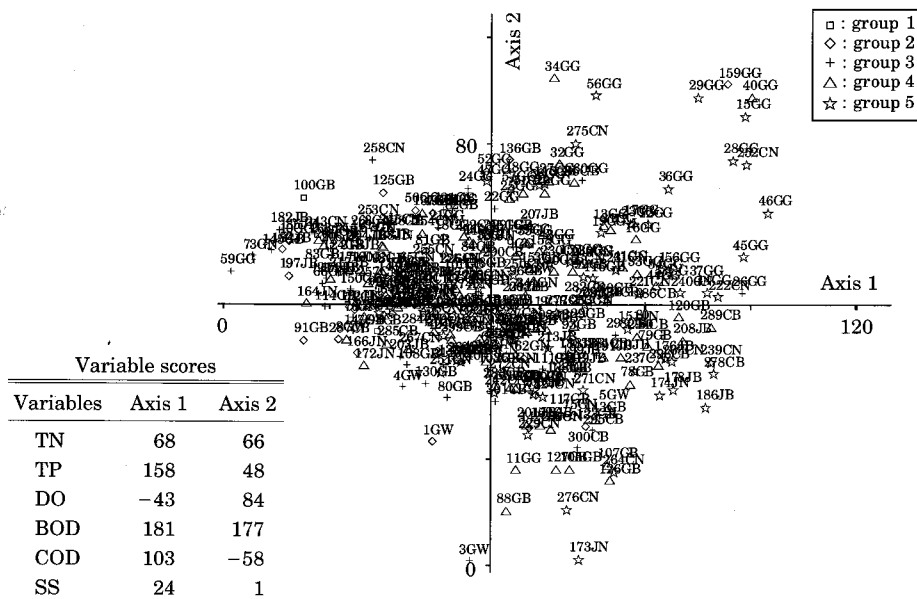
In PCA ordination, axes 1 and 2 accounted for 64.4% of the total variation in the dataset (2.89

and 0.97 of eigen values with 48.20% and 16.16% for axes 1 and 2, respectively) (Fig. 2). Overall, the reservoirs were separated according to the concentrations of nutrients in the ordination map. Concerning 5 trophic groups (Table 3) in PCA ordination, the reservoirs (i.e., 239CN, 221CN, 237CN, and 264CN) mainly from Chungnam and Gyeonggi showing eutrophic and hypereutrophic states (groups 4 and 5) were located on the left side of the ordination map, whereas oligotrophic and mesotrophic reservoirs (groups 2 and 3) were on the right area of the ordination, although the

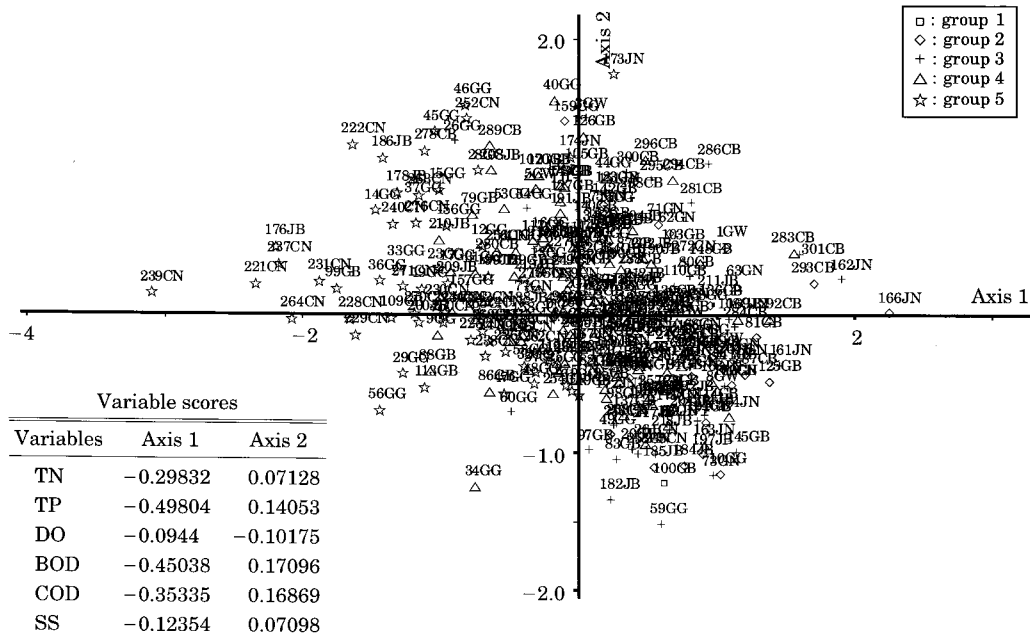
**Table 4.** Spearman correlation coefficients between the first two axes of four ordination methods and environmental factors in 301 reservoirs.

Variables	PCA		DCA		NMS		Isomap	
	Axis 1	Axis 2	Axis 1	Axis 2	Axis 1	Axis 2	Axis 1	Axis 2
Altitude	0.48**	-0.12*	-0.36**	0.14*	0.58**	-0.23**	0.58**	-0.23**
Catchment	0.10	0.11	-0.23**	0.11*	0.14*	-0.27**	0.14*	-0.27**
Circumference	-0.22**	-0.04	0.19**	-0.14*	-0.20**	0.14*	-0.20**	0.14*
Long length	-0.16**	-0.02	0.13**	-0.11	-0.15*	0.07	-0.15*	0.07
Surface area	-0.28**	-0.04	0.21**	-0.11	-0.31**	0.13*	-0.31**	0.13*
Storage	0.17**	-0.02	-0.11	-0.08	0.14*	-0.08	0.14*	-0.08
Bank height	0.62**	-0.03	-0.48**	0.09	0.65**	-0.33**	0.65**	-0.33**
Bank length	-0.23*	0.02	0.19**	-0.13*	-0.28**	0.15*	-0.28**	0.15*
Temperature	-0.20**	-0.33**	0.37**	-0.24*	-0.17**	0.33**	-0.17**	0.40**
Chl- <i>a</i>	-0.70**	0.09	0.51**	-0.13*	-0.75**	0.40**	-0.75**	0.33**

\* $p < 0.05$ , \*\* $p < 0.01$



**Fig. 3.** Detrended Correspondence Analysis (DCA) ordination of 301 reservoirs based on 6 physical and chemical variables (eigen values: axis 1=0.061, axis 2=0.029). The variable scores of the physical and chemical variables are listed in the figure. Sample names are explained in Fig. 1.



**Fig. 4.** NMS (Nonmetric Multidimensional Scaling) ordination of 301 reservoirs based on 6 physical and chemical variables (Stress value=13.4 for axes 1 and 2, Monte Carlo test;  $p < 0.01$ ). The variable scores of the physical and chemical variables are listed in the figure. Sample names are explained in Fig. 1.

samples were entangled.

Variable scores of 6 physical and chemical factors in Figure 2 indicated the magnitude of the change in the corresponding factors. The reservoirs assigned on the left side of axis 1 had the large amount of nutrients with high values of COD, TN, BOD, TP, and SS (Fig. 2). Axis 2 was highly related with DO concentration. Through Spearman rank correlation coefficients between biological, hydrological and geological factors (not used in the PCA ordination) and in the site scores of each reservoir on the axes 1 and 2, axis 1 was strongly correlated with bank height ( $r = 0.62, p < 0.01$ ) and altitude ( $r = 0.48, p < 0.01$ ) (Table 4). Meanwhile, Chl-*a* displayed negative correlation ( $r = -0.70, p < 0.01$ ) with axis 1, indicating reservoirs assigned on the left side of the ordination map (i.e. 239CN, 176JB, 34GG, and 264CN) had low altitude and bank height, and high concentrations of nutrients and Chl-*a*.

### 2) DCA

The 301 reservoirs were ordinated through the amount of nutrients in DCA ordination map with 0.061 and 0.029 of the eigen values for axes 1 and 2, respectively (Fig. 3). Overall, eutrophic and hypereutrophic (groups 4 and 5) reservoirs (i.e.,

159GG, 40GG, 29GG and 15GG) from mainly Gyeonggi (GG) were located on the right side of the ordination map, while oligotrophic (group 2) reservoirs were on the left side, although ordination of all groups tended to be entangled in the DCA map.

Considering variable scores, TN, TP, COD, BOD, and SS were positive values on the first axis, representing that reservoirs located on the right area of axis 1 had the high concentrations of nutrients. Axis 1 was negatively correlated with altitude ( $r = -0.36, p < 0.01$ ) and bank height ( $r = -0.48, p < 0.01$ ) (Table 4). Chl-*a* was positively correlated with axis 1 ( $r = 0.51, p < 0.01$ ). Therefore, the reservoirs (i.e., 40GG, 159GG, 15GG, and 29GG) on the right side of the ordination have high concentrations of nutrients and Chl-*a* at low altitude areas with low bank height of the reservoirs.

### 3) NMS

The reservoirs were ordinated based on the amount of nutrients in the NMS ordination with 13.4 of stress for axes 1 and 2 and the significant meaning of the Monte Carlo test ( $p < 0.01$ ) (Fig. 4). Overall, eutrophic and hypereutrophic reservoirs (i.e., 239CN, 221CN, 237CN, and 264CN)





inflow.

Many different methods were developed to classify trophic states of reservoirs (Carlson, 1977; OECD, 1982; Weiss, 1985; Lee *et al.*, 2003; Kim and Hwang, 2004). Mostly these methods were developed with one or two variable(s). However, the water quality assessment of reservoirs using only one or two parameter(s) may easily mislead or bias the user (Lu and Lo, 2002) because the water quality of reservoirs is influenced by a lot of environmental factors such as morphological difference based on regional climate, pollution state in catchment area, the characteristics of the region, and the scale of reservoirs, hydrological factors such as the amount of inflowed or outflowed water, and the flow of water as well as topological characteristics (EPA, 1974; Carmack *et al.*, 1979; Kim and Hwang, 2004). Lu and Lo (2002) reported a method diagnosing water quality of a reservoir with TP, Chl-*a*, and Secchi disk depth using a self-organizing maps. With this regard, we tried to pattern the water quality of the reservoirs with 6 physical and chemical environmental variables using 4 different ordination techniques. Overall, the reservoirs were scattered according to the gradients of nutrient concentrations in the ordination maps. Considering 5 groups of trophic states in the ordination maps, although hypereutrophic reservoirs were relatively clearly identified in the ordination maps, generally the reservoirs with trophic states were mixed in the ordinations (Figs. 3, 5, 6, 7). This reflected that one or two factors were not sufficient to classify water quality of the reservoirs as mentioned above. The similar results were observed in the discriminant function analysis of the trophic states of the reservoirs (Kwon *et al.*, 2008).

In addition, considering variable scores in the ordination maps, the concentrations of nutrients were positively correlated with Chl-*a*, while negatively correlated with altitude and bank height. This means that the reservoirs having a large amount of nutrients have the high concentration of Chl-*a* at low altitude and bank height of the reservoirs (i.e. 239CN, 221CN, 237CN and 231CN located in Chungnam and Gyeonggi regions).

Even though four ordination methods displayed similar ordination patterns, different methods showed different explanation power. Axes 1 and 2 of PCA explained 64.4% of the total variation. The first two axes of DCA were 0.061 and 0.029

of the eigen values, respectively. This value is too low to explain the characteristics of the raw data. In NMS, the stress of the first two axes was 13.4. Based on Kruskal's rules of thumb, the value is fair. McCune and Grace (2002) mentioned that most ecological community datasets may have solutions with stress between 10 and 20, and values in the lower half of this range are quite satisfactory, while values approaching or exceeding 20 are cause for concern. So the NMS result in this study was appropriate to be used. Significant level (*p* value) of Monte Carlo test was less than 0.01, representing that NMS result extracted stronger axes than expected by chance. Iso-map defines residual variance to evaluate the error of dimensionality reduction. The residual variance decreases to be small enough, which indicates preferable reservation of the structure of original space (Weng *et al.*, 2005). As the residual variances in the first two axes were 0.18 and 0.08, the ordination result reflected well the characteristics of raw data. In contrast to other ordination methods, the coordinates of variables such as variables scores in PCA could not be obtained. The variable scores are very efficient to evaluate their contribution in the ordination map. Therefore, this is a weakness of Isomap for the ordination of samples.

Consequently, even though similar ordination results were displayed in the results of the four different ordination methods, PCA and NMS was the most efficient to pattern reservoirs based on the explanation power. However, because different analyses have their own merits and demerits, various multivariate analyses can be used according to the objectives of the research to be solved.

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