

Supplementary materials:

Akaike Information Criterion

To select the optimal model, the Akaike Information Criterion (AIC) is applied. AIC is defined as follows:

$$AIC = 2K - 2 \log(L(\hat{\theta}|D))$$

where K is the number of parameters in the model and $\log(L(\hat{\theta}|D))$ is the maximized log-likelihood of the model $\hat{\theta}$ given the data D . The lower the AIC, the better the model.

Deviance explained (DE)

The deviance D_v of a proposed model is the difference of the log-likelihoods between the proposed model and the perfect model, which is defined as:

$$D_v = 2 \log(L(\hat{\theta}_s|D)) - 2 \log(L(\hat{\theta}|D))$$

where $\log(L(\hat{\theta}_s|D))$ and $\log(L(\hat{\theta}|D))$ are the maximized log-likelihoods of the perfect model $\hat{\theta}_s$ and the proposed model $\hat{\theta}$, respectively, given the data D . Here $\hat{\theta}_s$ is the saturated model with one parameter for each data point.

Deviance explained (DE) refers to the proportion of the total deviance explained by $\hat{\theta}$.

Detecting the influential data

We applied to Cook's distance D_i to validate the influential observations. Cook's distance D_i of observation i is defined as follows:

$$D_i = \frac{\sum_{j=1}^n (\bar{y}_j - \bar{y}_{j(i)})^2}{K \frac{1}{n} \sum_{j=1}^n (y_j - \bar{y})^2}$$

where \bar{y}_j is the j th fitted value, $\bar{y}_{j(i)}$ is the j th fitted value excluding observation i , and K is the number of parameters in the regression model. Those Cook's distances of arsenic in groundwater in Chiayi city were well above three times mean Cook's distance, suggesting arsenic in groundwater in Chiayi city are influential observations.

Table S1. Descriptive statistics for groundwater in Taiwan

Item	n	Mean±STD	Min	Q1	Median	Q3	Max
Metal and Inorganics							
As (mg/L)	9,048	$6.72 \times 10^{-3} \pm 2.34 \times 10^{-2}$	0.0003	0.0004	0.0006	0.0035	0.612
Ca (mg/L)	6,148	87.7 ± 72.7	0.5	39.1	74.9	113.0	630.0
Cd (mg/L)	9,048	$1.05 \times 10^{-3} \pm 4.18 \times 10^{-4}$	0.001	0.001	0.001	0.001	0.014
Cl (mg/L)	7,323	$6.63 \times 10^2 \pm 3.12 \times 10^3$	1.5	12.7	24.3	54.6	40,600
Cr (mg/L)	9,045	$2.08 \times 10^{-3} \pm 2.30 \times 10^{-3}$	0.001	0.001	0.001	0.003	0.161
Cu (mg/L)	9,048	$2.27 \times 10^{-3} \pm 3.45 \times 10^{-3}$	0.001	0.001	0.002	0.003	0.211
Fe (mg/L)	9,048	1.35 ± 4.82	0.005	0.016	0.059	0.662	140
K (mg/L)	6,148	17.3 ± 66.8	0.10	1.80	3.33	7.84	1,160
Mg (mg/L)	6,148	$56.4 \pm 2.05 \times 10^2$	0.48	12.3	17.6	30.2	3,880
Mn (mg/L)	9,048	$5.13 \times 10^{-1} \pm 8.76 \times 10^{-1}$	0.005	0.014	0.196	0.675	13.9
Na (mg/L)	6,148	$3.41 \times 10^2 \pm 1.51 \times 10^3$	0.8	16.4	28.8	62.7	17,600
NH ₃ -N (mg/L)	9,048	1.05 ± 3.44	0.01	0.02	0.07	0.63	123
NO ₃ -N (mg/L)	9,048	2.25 ± 3.81	0.01	0.03	0.43	3.17	65.4
Pb (mg/L)	9,045	$4.20 \times 10^{-3} \pm 2.48 \times 10^{-3}$	0.003	0.003	0.003	0.005	0.097
SO ₄ (mg/L)	9,048	$1.62 \times 10^2 \pm 4.35 \times 10^2$	1.0	41.3	69.1	115	6,510
Zn (mg/L)	9,048	$1.77 \times 10^{-2} \pm 4.99 \times 10^{-2}$	0.002	0.002	0.007	0.016	1.410
Physicochemical and biological properties							
Alk (mg/L)	6,148	$2.36 \times 10^2 \pm 1.42 \times 10^2$	0	132	218	321	1120
EC (µmho/cm @25°C)	9,048	$2.36 \times 10^3 \pm 8.08 \times 10^3$	58	459	664	1,020	97,300
pH (-)	9,046	6.73 ± 0.58	3.6	6.4	6.8	7.1	10.8
TDS (mg/L)	9,048	$1.64 \times 10^3 \pm 6.01 \times 10^3$	40.5	294	432	668	80,400
TH (mg/L)	9,048	$4.70 \times 10^2 \pm 1.08 \times 10^3$	5.5	159	269	393	17,600
TOC (mg/L)	9,048	1.88 ± 1.89	0.10	0.84	1.43	2.30	71.30
WT (°C)	9,046	26.5 ± 1.7	18.6	25.4	26.6	27.7	34.7

Abbreviations: Alk: Alkalinity; EC: Electrical conductivity; Q1: Lower Quartile; Q3: Upper Quartile; STD: Standard deviation; TDS: Total Dissolved Solids; TH: Total Hardness; TOC: Total Organic Carbon; WT: Water Temperature

Table S2. Descriptive statistics for reservoirs in Taiwan

Item	n	Mean±STD	Min	Q1	Median	Q3	Max
Inorganics							
NH ₃ -N (mg/L)	4,492	1.08x10 ⁻¹ ± 4.84x10 ⁻¹	0.01	0.01	0.02	0.05	7.35
NO ₂ -N (mg/L)	2,986	2.05x10 ⁻² ± 7.80x10 ⁻²	0.001	0.002	0.004	0.008	0.722
NO ₃ -N (mg/L)	4,448	4.54x10 ⁻¹ ± 5.77x10 ⁻¹	0.01	0.14	0.34	0.55	8.09
Physicochemical and biological properties							
Alk (mg/L)	4,492	94.1 ± 44.2	0.2	70.1	93.7	119	345
Chl_A (µg/L)	4,492	10.3 ± 25.4	0.0	1.2	3.0	8.0	685
COD (mg/L)	4,480	10.5 ± 13.8	4.0	4.0	5.3	10.1	287
DO (ml/min · m ²)	3,776	7.75 ± 2.45	0.0	7.0	8.0	9.0	23.7
EC (µmho/cm@25°C)	4,492	3.67x10 ² ± 2.66x10 ²	52	228	301	426	4,650
pH (-)	4,492	8.13 ± 0.56	5.2	7.8	8.2	8.4	10.2
SD (m)	2,176	1.62 ± 1.12	0.1	0.8	1.3	2.2	8.2
SS (mg/L)	4,491	8.96 ± 20.5	1.0	2.4	4.3	9.1	702
TB (NTU)	4,492	9.69 ± 25.2	0.3	2.2	4.1	8.9	750
TH (mg/L)	4,492	1.24x10 ² ± 60.2	13.9	92.9	122	156	783
TOC (mg/L)	4,492	2.68 ± 3.56	0.14	1.09	1.55	2.50	84.7
WT (°C)	4,492	23.5 ± 5.1	6.9	19.7	23.6	27.4	35.4

Abbreviations: Alk: Alkalinity; Chl-A: Chlorophyll-A; COD: Chemical Oxygen Demand; DO: Dissolved Oxygen; EC: Electrical conductivity; Q1: Lower Quartile; Q3: Upper Quartile; SD: Secchi Depth (Transparency); STD: Standard deviation; SS: Suspended Solids; TB: Turbidity; TH: Total Hardness; TOC: Total Organic Carbon; WT: Water Temperature

Table S3. Descriptive statistics for rivers in Taiwan

Item	n	Mean±STD	Min	Q1	Median	Q3	Max
Metal and Inorganics							
Ag (mg/L)	7,632	1.83x10 ⁻³ ± 1.13x10 ⁻³	0.001	0.001	0.001	0.003	0.015
As (mg/L)	7,622	3.57x10 ⁻³ ± 4.80x10 ⁻³	0.0003	0.0009	0.0020	0.0043	0.1020
Cd (mg/L)	7,738	1.03x10 ⁻³ ± 9.68x10 ⁻⁴	0.001	0.001	0.001	0.001	0.067
Cr (mg/L)	7,738	2.85x10 ⁻³ ± 1.34x10 ⁻²	0.002	0.002	0.002	0.003	1.05
Cu (mg/L)	7,632	2.62x10 ⁻² ± 2.21x10 ⁻¹	0.001	0.002	0.003	0.009	13.7
Hg (mg/L)	6,141	3.22x10 ⁻⁴ ± 1.15x10 ⁻⁴	0.0003	0.0003	0.0003	0.0003	0.0041
Mn (mg/L)	7,632	1.76x10 ⁻¹ ± 4.18x10 ⁻¹	0.005	0.030	0.084	0.181	12.2
NH ₃ -N (mg/L)	22,652	3.54 ± 9.46	0.01	0.05	0.32	2.82	193
NO ₂ -N (mg/L)	7,738	1.41x10 ⁻¹ ± 2.58x10 ⁻¹	0.001	0.008	0.044	0.175	8.01
NO ₃ -N (mg/L)	7,738	1.3 ± 2.15	0.01	0.36	0.74	1.40	56.0
Pb (mg/L)	7,738	6.70x10 ⁻³ ± 1.99x10 ⁻²	0.003	0.003	0.005	0.005	1.28
Se (mg/L)	4,807	1.02x10 ⁻³ ± 1.96x10 ⁻⁴	0.001	0.001	0.001	0.001	0.006
Zn (mg/L)	7,632	1.41x10 ⁻¹ ± 1.95	0.002	0.010	0.019	0.037	95.7
Physicochemical and biological properties							
BOD (mg/L)	22,652	4.86 ± 9.39	1.0	1.0	1.8	5.0	341
COD (mg/L)	22,649	20.7 ± 40.3	4.0	4.5	10.1	24.0	3,180
Coliform (CFU/100mL)	22,652	4.45x10 ⁵ ± 4.99x10 ⁷	10	1,100	11,000	75,000	6.20x10 ⁸
DO (ml/min · m ²)	19,074	6.96 ± 2.76	0.0	5.5	7.7	8.8	23.0
EC (µmho/cm@25°C)	22,652	2.29x10 ³ ± 6.89x10 ³	31	305	465	751	52,800
pH (-)	22,652	7.83 ± 0.59	2.4	7.5	7.9	8.2	11
SS (mg/L)	22,652	1.76x10 ² ± 2.05x10 ³	1.0	8.6	21.1	54.25	241,000
TKN (mg N/L)	1,758	4.71 ± 12.9	0.05	0.32	0.89	3.86	256
TOC (mg/L)	10,556	4.51 ± 7.37	0.10	1.19	2.38	5.15	292
WT (°C)	22,652	24.4 ± 4.8	4.6	20.9	24.6	28.1	37.3

Abbreviations: Biochemical Oxygen Demand; COD: Chemical Oxygen Demand; DO: Dissolved Oxygen; EC: Electrical conductivity; Q1: Lower Quartile; Q3: Upper Quartile; SS: Suspended Solids; STD: Standard deviation; TKN: Total Kjeldahl nitrogen; TOC: Total Organic Carbon; WT: Water Temperature;

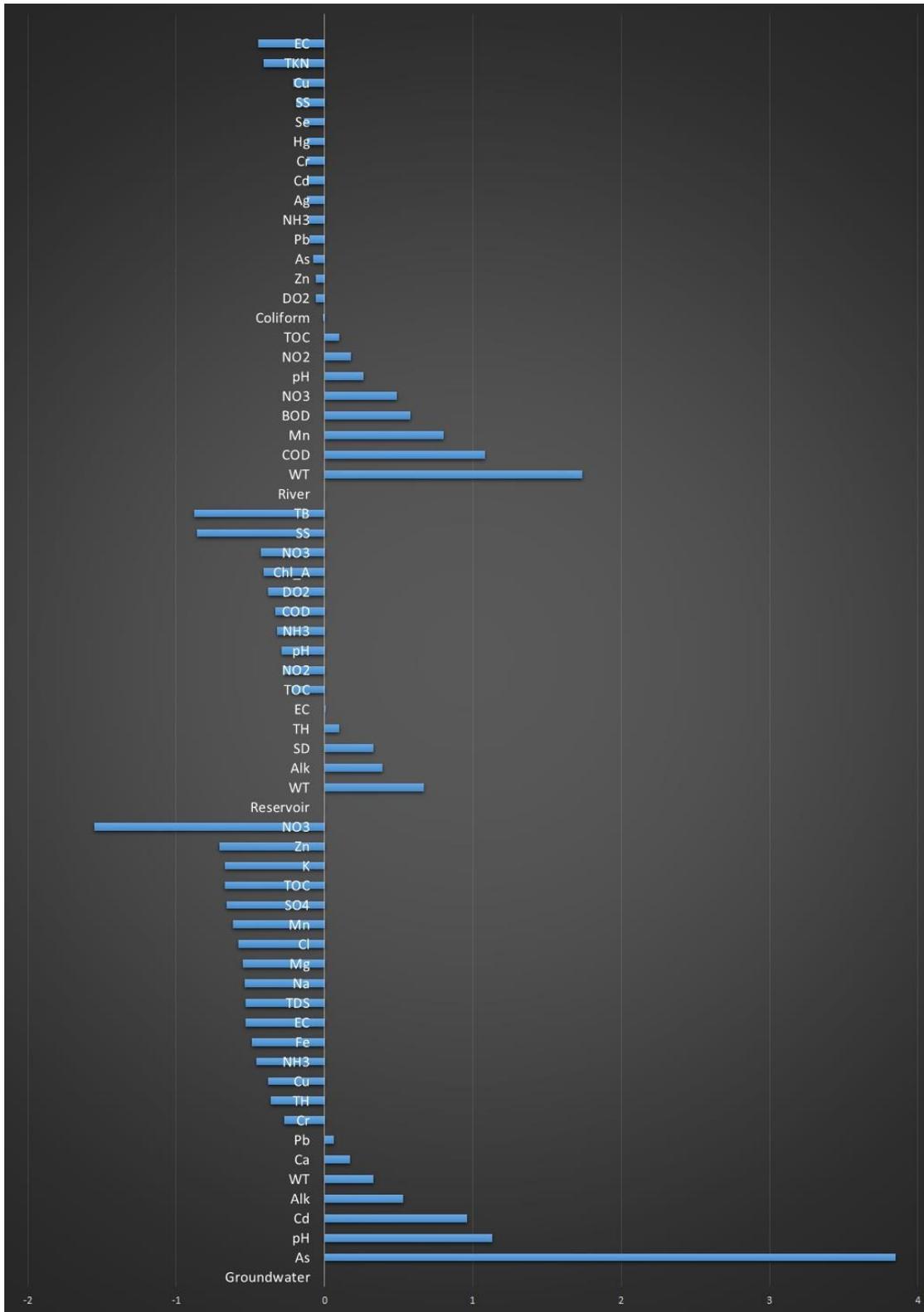


Figure S1. The Z-score bar chart of monitoring water attributes of Chiayi city, Taiwan.