

Supplementary data

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SI 1 Supplementary Results

Four fitted equations for CEC_{silt} by using MLR were expressed as follows. The description of four datasets were given in Environmental variables section in the manuscript, in which the CEC_{silt} was dependent variable rather than CEC_{clay} .

$$\left\{ \begin{array}{l} \text{Dataset 1: } CEC_{silt} = 3.464 + 0.505 \times CEC_{soil} - 0.628 \times pH - 0.199 \times SOC + 0.053 \times Fe_d + 0.045 \times Sand - 0.126 \times Clay \\ \text{Dataset 2: } CEC_{silt} = 11.328 - 0.224 \times CEC_{clay} + 0.698 \times CEC_{soil} - 0.887 \times pH - 0.213 \times SOC + 0.034 \times Fe_d - 0.168 \times Clay \\ \text{Dataset 3: } CEC_{silt} = 1.258 + 0.531 \times CEC_{soil} - 0.664 \times pH - 0.228 \times SOC + 0.053 \times Fe_d + 0.037 \times Sand - 0.128 \times Clay + 0.001 \times MAT \\ \text{Dataset 4: } CEC_{silt} = 9.582 - 0.208 \times CEC_{clay} + 0.698 \times CEC_{soil} - 0.886 \times pH - 0.227 \times SOC + 0.035 \times Fe_d - 0.165 \times Clay + 0.0007 \times MAT \end{array} \right.$$

Similar with CEC_{silt} , four fitted equations for CEC_{soil} by using MLR were expressed as follows.

$$\left\{ \begin{array}{l} \text{Dataset 1: } CEC_{soil} = 6.435 + 1.342 \times pH + 1.026 \times Fe_d - 0.059 \times Sand - 0.072 \times Clay \\ \text{Dataset 2: } CEC_{soil} = -28.990 + 0.138 \times CEC_{clay} + 0.267 \times CEC_{silt} + 0.648 \times CEC_{Min} + 0.491 \times pH + 0.101 \times SOC + 0.241 \times Sand \\ \quad + 0.237 \times Silt + 0.261 \times Clay \\ \text{Dataset 3: } CEC_{soil} = 16.124 + 1.095 \times pH + 1.231 \times Fe_d - 0.048 \times Clay - 0.0002 \times MAP - 0.004 \times MAT \\ \text{Dataset 4: } CEC_{soil} = -28.990 + 0.138 \times CEC_{clay} + 0.267 \times CEC_{silt} + 0.648 \times CEC_{Min} + 0.491 \times pH + 0.101 \times SOC + 0.241 \times Sand \\ \quad + 0.237 \times Silt + 0.261 \times Clay \end{array} \right.$$

Four fitted equations for CEC_{Min} by using MLR were expressed as follows.

$$\left\{ \begin{array}{l} \text{Dataset 1: } CEC_{Min} = 40.764 + 0.974 \times CEC_{soil} - 0.403 \times Sand - 0.399 \times Silt - 0.359 \times Clay \\ \text{Dataset 2: } CEC_{Min} = 39.459 + 0.072 \times CEC_{clay} + 0.923 \times CEC_{soil} - 0.398 \times Sand - 0.404 \times Silt - 0.349 \times Clay \\ \text{Dataset 3: } CEC_{Min} = 40.764 + 0.974 \times CEC_{soil} - 0.403 \times Sand - 0.399 \times Silt - 0.359 \times Clay \\ \text{Dataset 4: } CEC_{Min} = 39.459 + 0.072 \times CEC_{clay} + 0.923 \times CEC_{soil} - 0.398 \times Sand - 0.404 \times Silt - 0.349 \times Clay \end{array} \right.$$

SI 2 Supplementary Tables

Table S1. Main soil types and diagnostic horizons with the Soil Taxonomy [3], in which the values of the CEC_{clay} (by NH_4OAc pH 7) and ECEC are required.

Diagnostic horizons	Diagnostic criteria	Soil type ^{a)}	
		Soil orders	Great groups
Kandic Horizon	Has an apparent CEC of 16 cmol(+) or less per kg clay (by 1N NH_4OAc pH 7) and an apparent ECEC of 12 cmol(+) or less per kg clay.	Alfisols	Kandiaqualfs, Palecryalfs, Ferrudalfs, Kandiudalfs, Kanhapludalfs, Kandiustalfs, Kanhaplustalfs, Rhodoxeralfs, Palexeralfs
		Oxisols	Acraquox, Acroperox, Kandiperox, Acroperox, Acrotorrox, Acrudox, Kandiudox, Acrustox, Kandiustox
		Ultisols	Albaquults, Kandiaquults, Kanhaplaquults, Kandihumults, Kanhaplohumults, Kandiudults, Kanhapludults, Kandiustults, Kanhaplustults
Oxic Horizon	Has an apparent CEC of 16 cmol(+) or less per kg clay (by 1N NH_4OAc pH 7) and an apparent ECEC of 12 cmol(+) or less per kg clay	Oxisols	Acraquox, Acroperox, Acrotorrox, Acrudox, Acrustox

^{a)} The CEC_{clay} is also used as a criterion in the Kandic and Kanhaplic subgroups of Alfisols and Ultisols, the Udoxic and Ustoxic subgroups of Quartzipsamments, and the Oxic subgroups of Inceptisols and Mollisols.

Table S2. Reference soil groups and qualifiers in the World Reference Base for Soil Resources (WRB)[4], in which the values of the CEC_{clay} (by NH_4OAc pH 7) are required.

Soil type or Qualifiers	Definitions of the criteria
<i>Reference Soil</i>	
<i>Groups</i>	
Ferralsols	Having a CEC (by 1 M NH_4OAc , pH 7) of $< 16 \text{ cmol}_\text{c} \text{ kg}^{-1}$ clay and a sum of exchangeable bases (by 1 M NH_4OAc , pH 7) plus exchangeable Al (by 1 M KCl, unbuffered) of $< 12 \text{ cmol}_\text{c} \text{ kg}^{-1}$ clay.
Acrisols	Having a CEC (by 1 M NH_4OAc , pH 7) of $< 24 \text{ cmol}_\text{c} \text{ kg}^{-1}$ clay in some part of the argic horizon.
Lixisols	Having a CEC (by 1 M NH_4OAc , pH 7) of $< 24 \text{ cmol}_\text{c} \text{ kg}^{-1}$ clay in some part of the argic horizon.
<i>Qualifiers</i>	
Acric	Having a CEC (by 1 M NH_4OAc , pH 7) of $< 24 \text{ cmol}_\text{c} \text{ kg}^{-1}$ clay
Alic	Having a CEC (by 1 M NH_4OAc , pH 7) of pH 7) of $< 24 \text{ cmol}_\text{c} \text{ kg}^{-1}$ clay
Lixic	Having a CEC (by 1 M NH_4OAc , pH 7) of $< 24 \text{ cmol}_\text{c} \text{ kg}^{-1}$ clay
Luvic	Having a CEC (by 1 M NH_4OAc , pH 7) of $\geq 24 \text{ cmol}_\text{c} \text{ kg}^{-1}$ clay
Hypersideralic	Having a CEC (by 1 M NH_4OAc , pH 7) of $< 16 \text{ cmol}_\text{c} \text{ kg}^{-1}$ clay
Sideralic	Having a CEC (by 1 M NH_4OAc , pH 7) of $< 24 \text{ cmol}_\text{c} \text{ kg}^{-1}$ clay
Ferralic	Having a CEC (by 1 M NH_4OAc , pH 7) of $< 16 \text{ cmol}_\text{c} \text{ kg}^{-1}$ clay and a sum of exchangeable bases (by 1 M NH_4OAc , pH 7) plus exchangeable Al (by 1 M KCl, unbuffered) of $< 12 \text{ cmol}_\text{c} \text{ kg}^{-1}$ clay.
Xanthic	Having a CEC (by 1 M NH_4OAc , pH 7) of $< 16 \text{ cmol}_\text{c} \text{ kg}^{-1}$ clay and a sum of exchangeable bases (by 1 M NH_4OAc , pH 7) plus exchangeable Al (by 1 M KCl, unbuffered) of $< 12 \text{ cmol}_\text{c} \text{ kg}^{-1}$ clay.

Table S3. Diagnostic subsurface horizons and diagnostic characteristics in the Chinese Soil Taxonomy (CST) [5], in which the values of the CEC_{clay} (by NH₄OAc pH 7) and ECEC are required.

Type	Soil orders	Soil groups or subgroups	Diagnostic criteria
<i>Diagnostic subsurface horizons</i>			
Ferrallic horizon	Ferralsols	Rhodi-Udic Ferralsols, Xanthi-Udic Ferralsols, Hapli-Udic Ferralsols	Having a CEC (by 1 M NH ₄ OAc, pH 7) of < 16 cmol _c kg ⁻¹ clay and an ECEC of < 12 cmol _c kg ⁻¹ clay.
LAC-ferric horizon	Ferrosols	Argi-Ustic Ferrosols, Hapli-Ustic Ferrosols, Carbonati-Perudic Ferrosols, Alliti-Perudic Ferrosols, Hapli-Perudic Ferrosols, Carbonati-Udic Ferrosols, Hi-weatheri-Udic Ferrosols, Alliti-Udic Ferrosols, Argi-Udic Ferrosols, Hapli-Udic Ferrosols	Having a CEC (by 1 M NH ₄ OAc, pH 7) of < 24 cmol _c kg ⁻¹ clay
<i>Diagnostic characteristics</i>			
Alic property		Ali-Perudic Argosols, Ali-Udic Argosols, Ali-Perudic Cambosols, Ali-Udic Cambosols, Alic Humi-Udic Andosols, Alic Hapli-Udic Andosols, Alic Acidi-Udic Argosols, Alic Bori-Perudic Cambosols, Alic Acidi-Perudic Cambosols	Having a CEC (by 1 M NH ₄ OAc, pH 7) of ≥ 24 cmol _c kg ⁻¹ clay

Table S4. Correlation coefficients between soil properties and environmental variables.

	CEC _{silt}	CEC _{soil}	CEC _{OM}	pH	SOC	Fe _d	Silt	Clay	Elevation	Slope	MRRTF	TWI	SPI	MAP	MAT
CEC _{clay}	0.272**	0.580**	0.525**	0.121	-0.067	-0.283**	0.424**	-0.263**	0.192*	0.116	-0.196*	-0.090	0.240**	-0.299**	-0.376**
CEC _{silt}	1	0.600**	0.459**	0.068	0.073	0.140	0.108	-0.337**	0.188*	0.118	-0.216*	-0.116	0.121	-0.069	-0.024
CEC _{soil}		1	0.920**	0.279**	0.048	0.258**	0.160	0.065	0.356**	0.086	-0.194*	-0.129	0.147	-0.365**	-0.310**
CEC _{OM}			1	0.238**	0.004	0.298**	0.085	0.237**	0.335**	0.046	-0.137	-0.089	0.104	-0.378**	-0.342**
pH				1	-0.001	0.048	0.225*	-0.067	0.231*	0.356**	-0.078	-0.272**	0.427**	-0.397**	-0.048
SOC					1	0.188*	0.032	-0.171	0.020	-0.018	-0.014	0.039	-0.018	0.022	0.228*
Fe _d						1	-0.130	0.541**	0.383**	-0.079	0.012	-0.025	-0.120	-0.245**	-0.077
Silt							1	-0.352**	0.120	0.145	-0.026	0.038	0.101	-0.239**	-0.213*
Clay								1	0.076	-0.225*	0.171	0.082	-0.228*	-0.163	-0.166

* Significant at the 0.05 level.

** Significant at the 0.01 level.

Table S5. Performance assessment (R^2 and RMSE) of multiple linear regression for the PTFs of CEC of silt (CEC_{silt}), CEC of the fine earth fraction (<2 mm) (CEC_{soil}) and the CEC of mineral fractions (CEC_{Min}). For each prediction case, the mean values and standard deviations of R^2 and RMSE based on 100 runs are shown.

Dataset	CEC_{silt}	CEC_{soil}	CEC_{Min}
<i>R^2</i>			
Dataset 1	0.51±0.21	0.21±0.18	0.85±0.09
Dataset 2	0.53±0.22	0.22±0.18	0.86±0.07
Dataset 3	0.54±0.23	0.21±0.21	0.85±0.08
Dataset 4	0.55±0.22	0.22±0.18	0.86±0.08
<i>RMSE</i>			
Dataset 1	2.62±0.40	4.33±0.54	1.85±0.37
Dataset 2	2.60±0.41	4.28±0.84	1.84±0.44
Dataset 3	2.58±0.41	4.27±0.99	1.83±0.44
Dataset 4	2.56±0.39	4.28±0.84	1.84±0.44

SI 3 Supplementary Figures

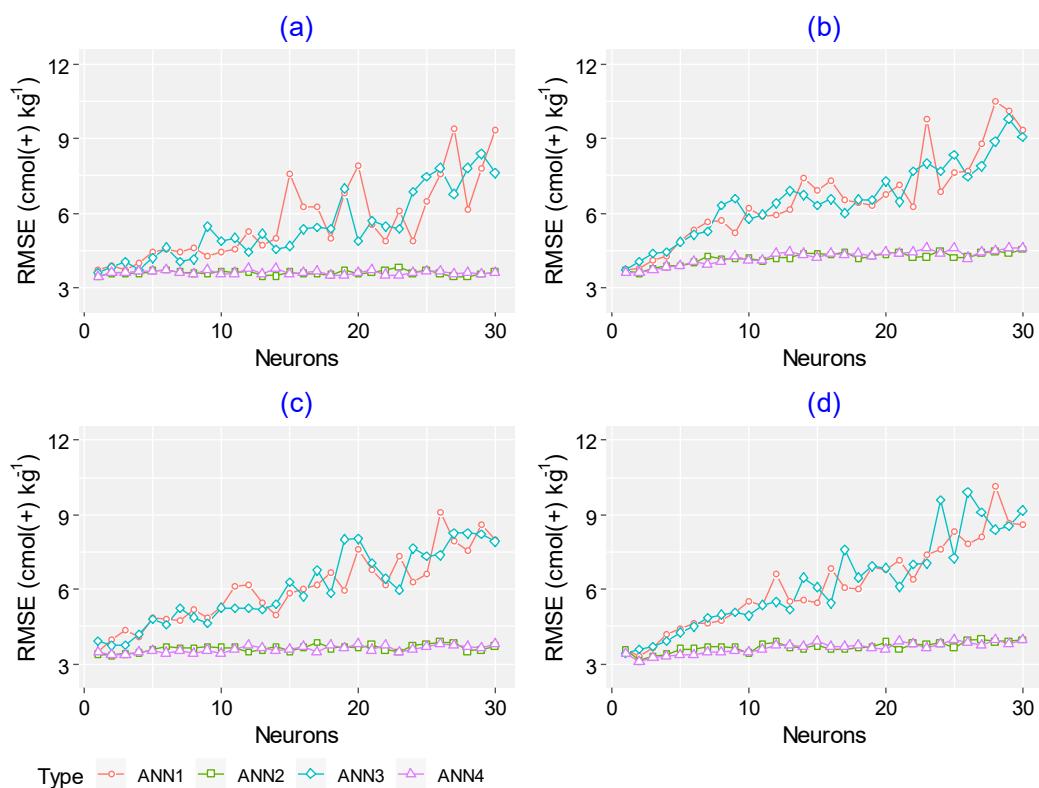


Figure S1. RMSE values of ANN models with 1 hidden layer for datasets 1 (a), 2 (a), 3 (c) and 4 (d), in which the number of neurons in the hidden layer ranged from 1 to 30. ANN1 and ANN2 refer to the resilient backpropagation algorithm with weight backtracking using hyperbolic tangent and logistic sigmoid activation functions, respectively. ANN3 and ANN4 refer to the resilient backpropagation algorithm without weight backtracking using hyperbolic tangent and logistic sigmoid activation functions, respectively.

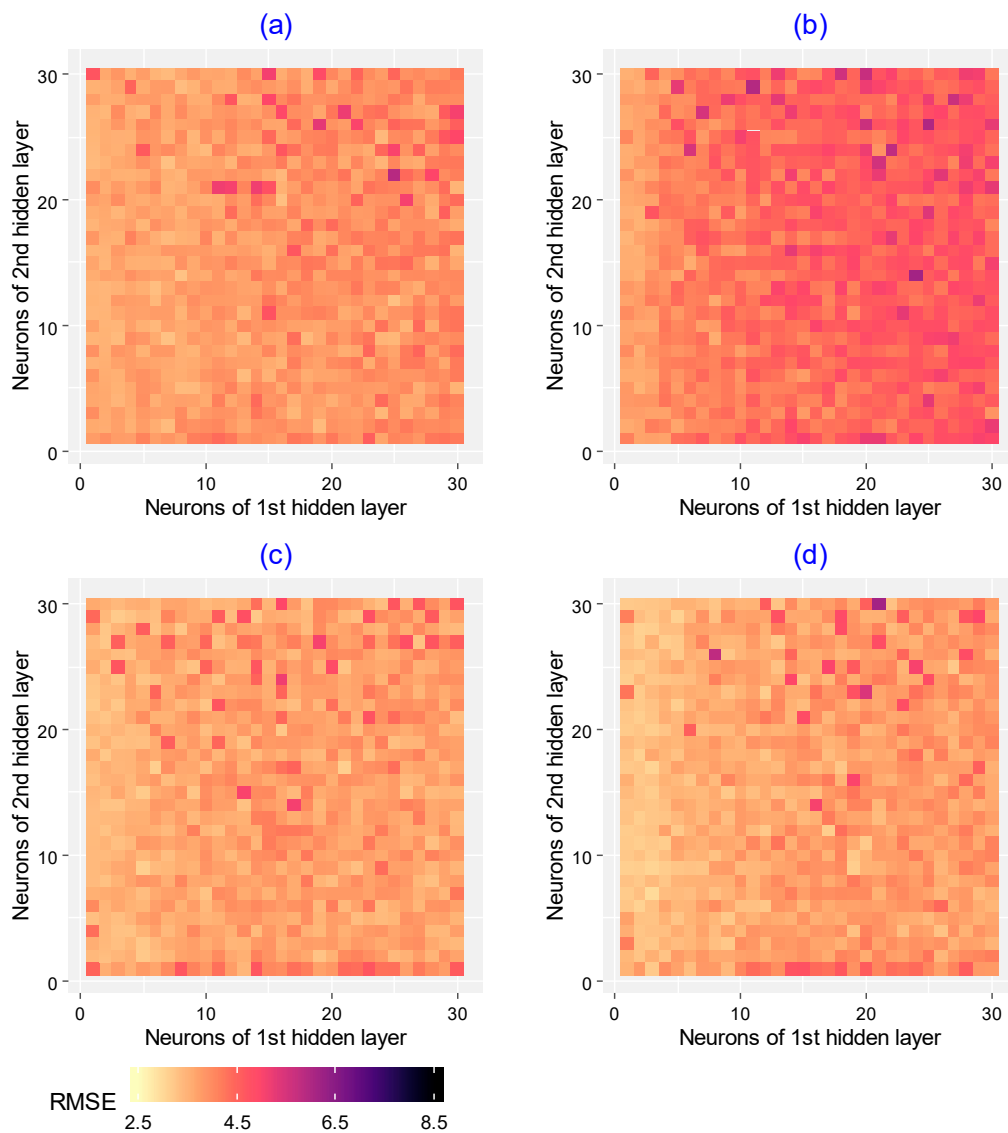


Figure S2. RMSE values of ANN models with 2 hidden layers for datasets 1 (a), 2 (a), 3 (c) and 4 (d), in which the number of neurons in the first and second hidden layer ranged from 1 to 30.

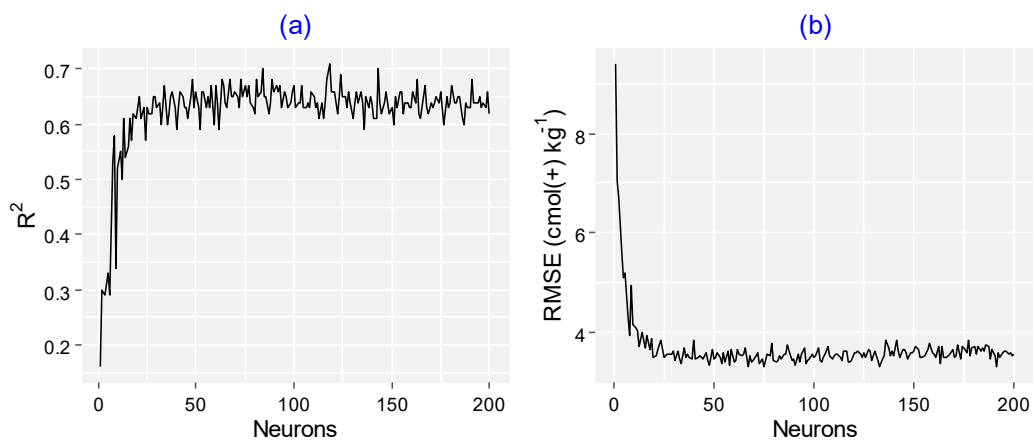


Figure S3. R^2 (a) and RMSE (b) values of DBN models with 1 hidden layer for dataset 1.

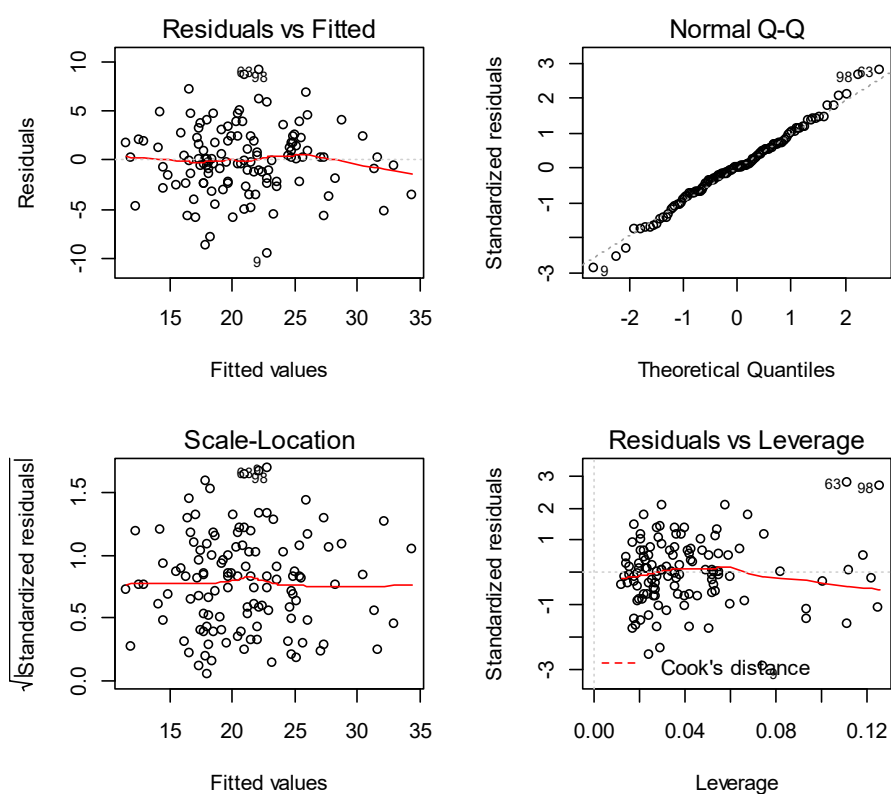


Figure S4. Residuals distribution check of dataset 1.

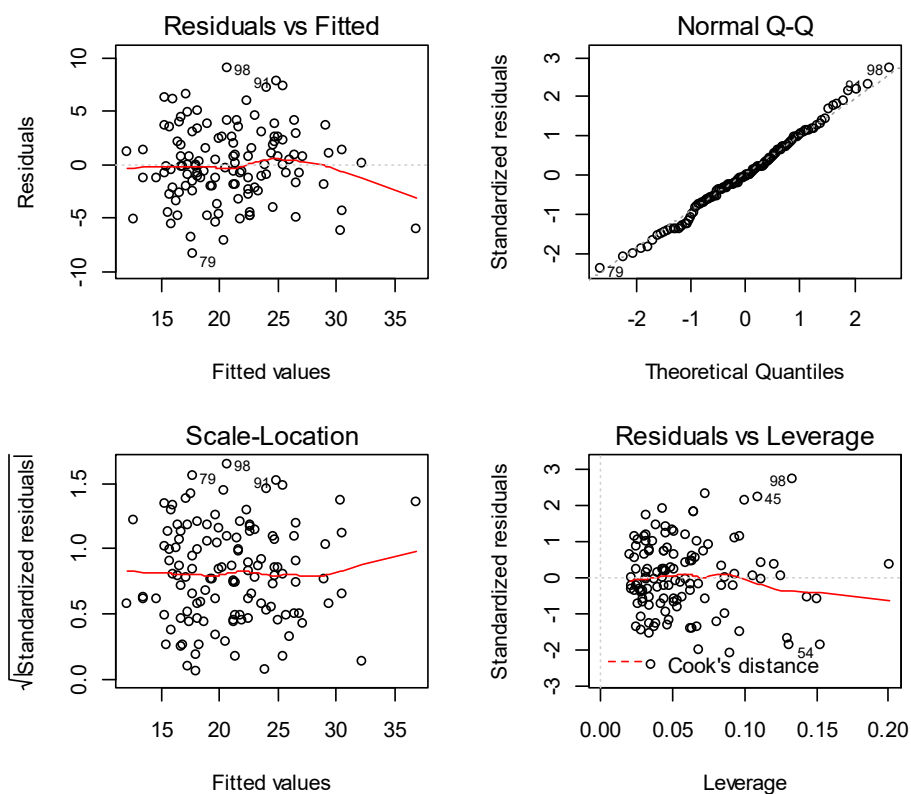


Figure S5. Residuals distribution check of dataset 2.

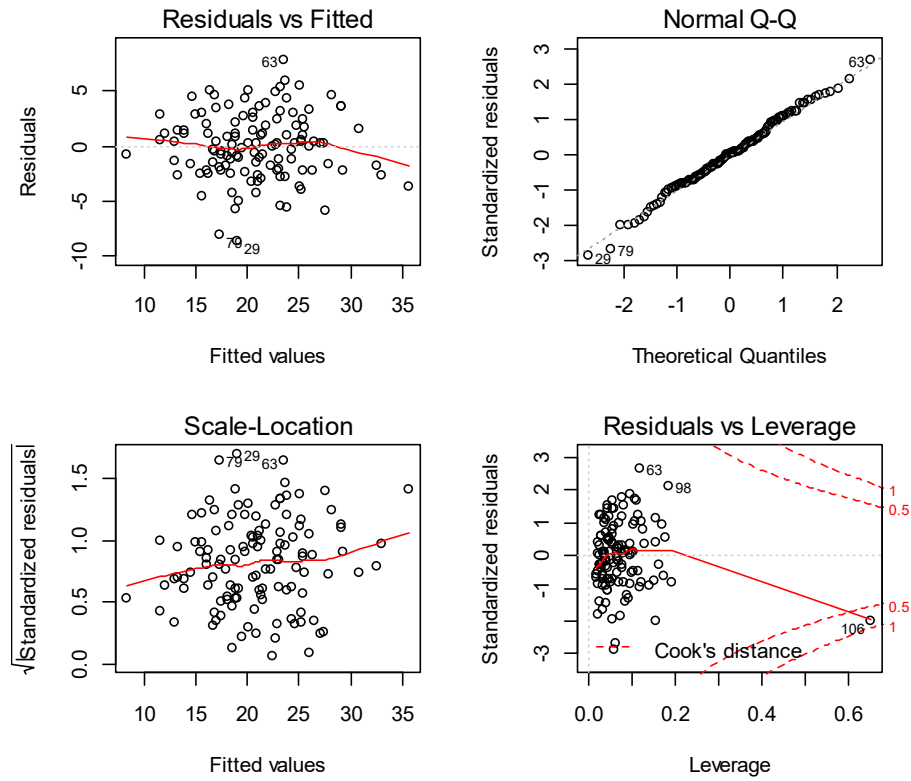


Figure S6. Residuals distribution check of dataset 3.

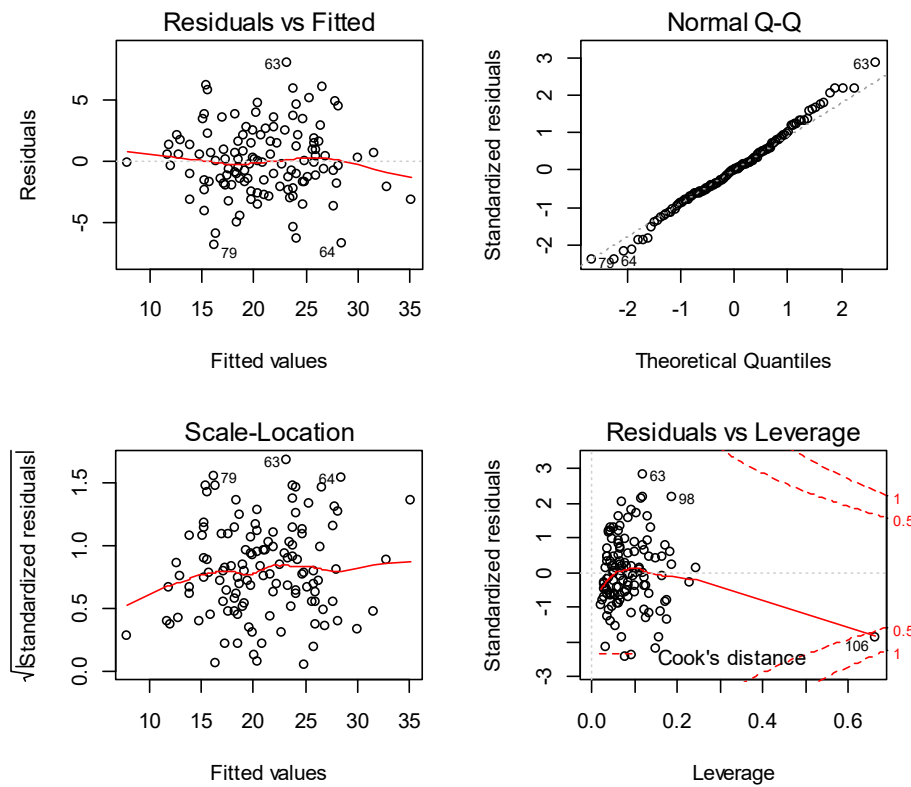


Figure S7. Residuals distribution check of dataset 4.

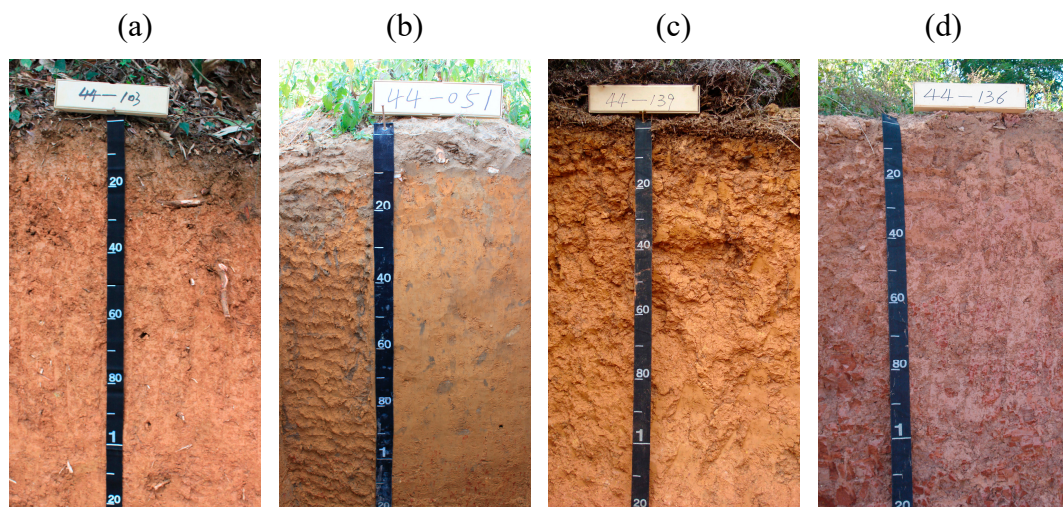


Figure S8. Representative pedons of four soil series, of which the soil type should be referenced to Ferrosols: Liangtian (a), Jinji (b), Datuo (c), and Dengta (d). The land use type of Liangtian and Datuo is forest, and that of Jinji and Dengta is upland.