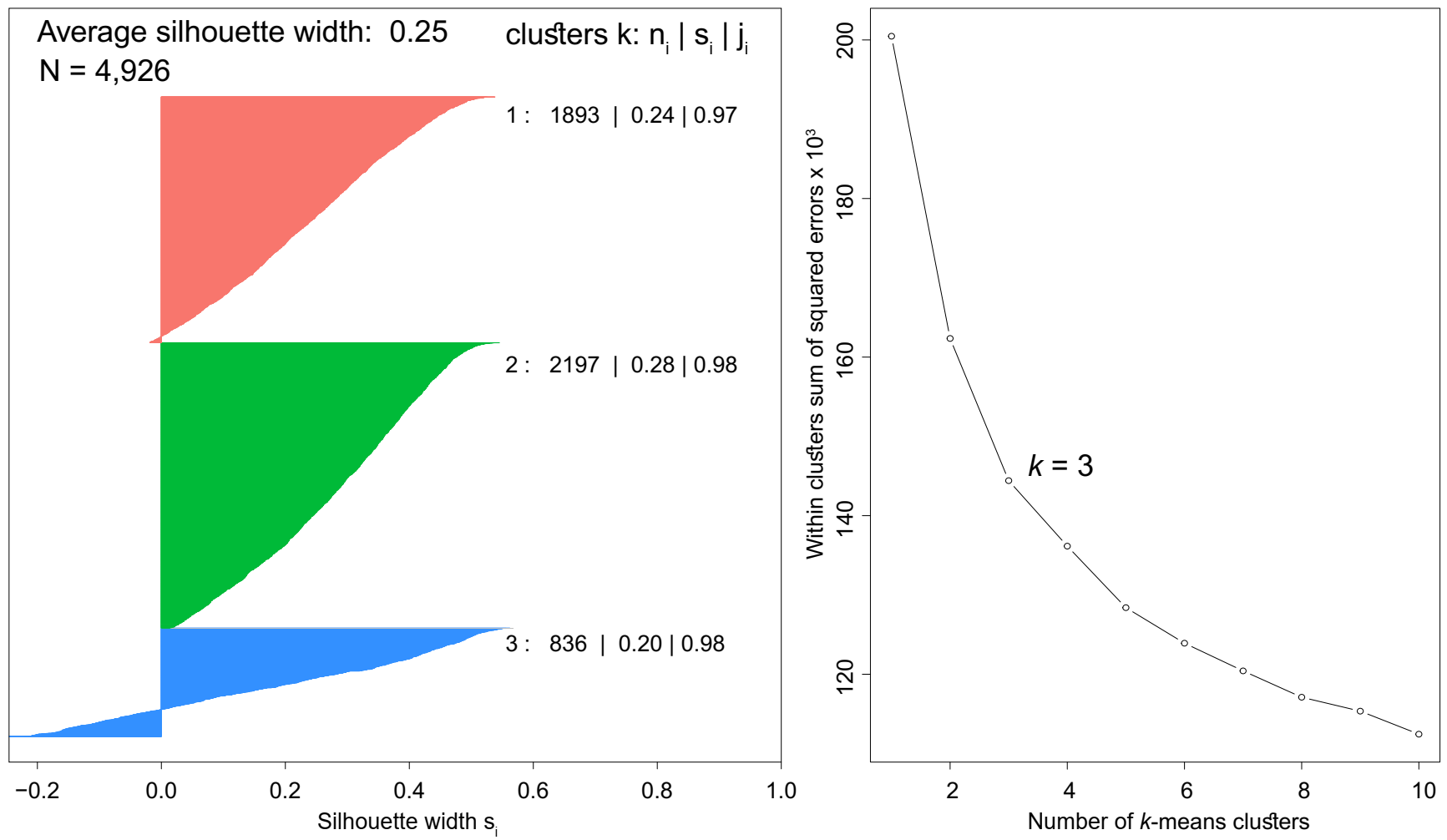
**Table S1.** Sequential binary partitioning used to obtain 17 ilr-coordinates of 18 geochemical variables of N = 4926 dataset. The procedure of partitioning is based on the hierarchical dendrogram (Figure 3d). Composite variables within a balance are the geometric mean of all components.

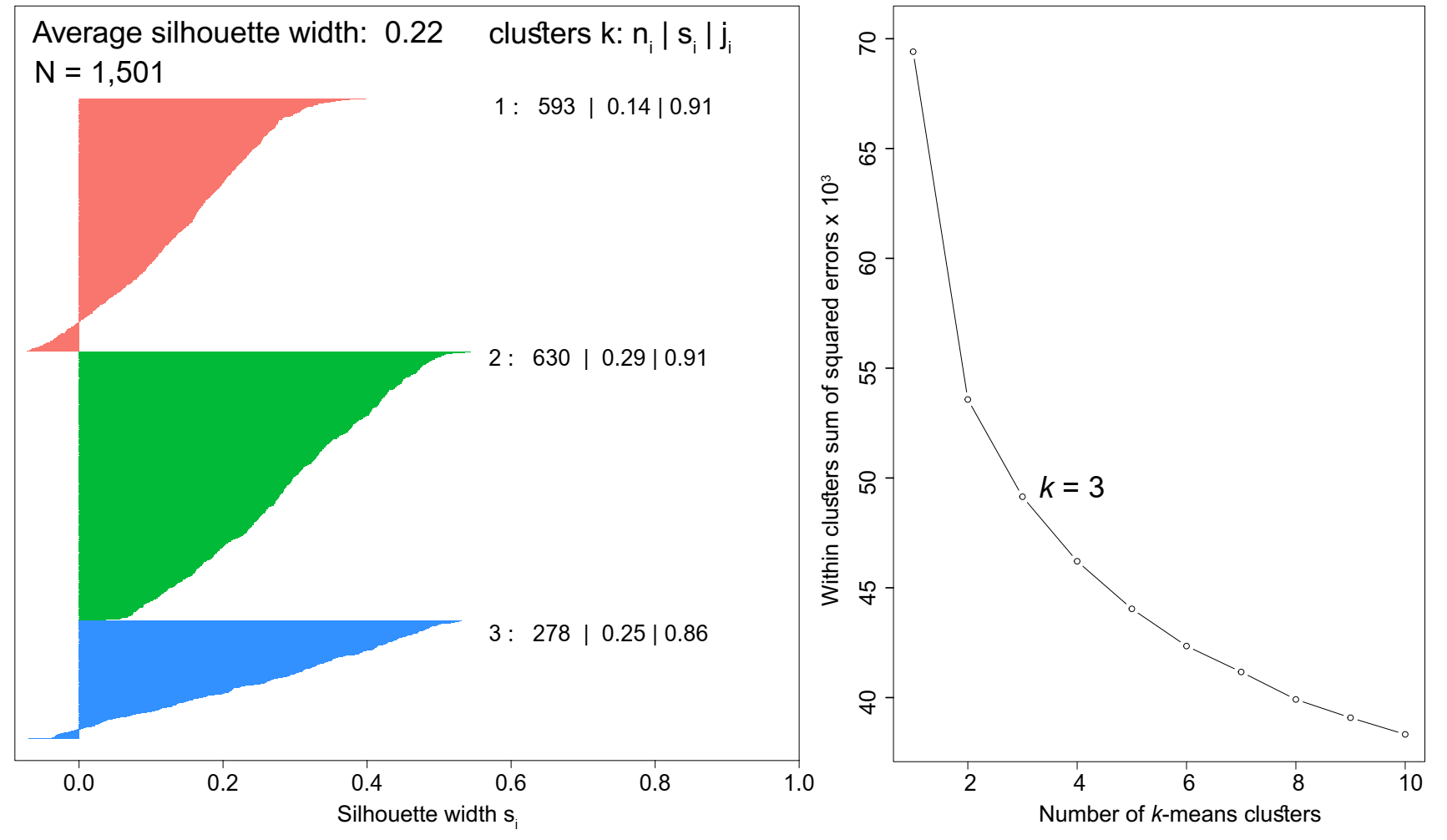
|  |  |
| --- | --- |
| **Balance** | **Binary partition** |
| b1 | [Bi, 206Pb, 207Pb, 208Pb | Ni, Te, Co, Re, Au, Cu, Ag, As, 204Pb, Mn, Sn, Zn, Se, Ti] |
| b2 | [Bi | 206Pb, 207Pb, 208Pb] |
| b3 | [206Pb | 207Pb, 208Pb] |
| b4 | [207Pb | 208Pb] |
| b5 | [Ni | Te, Co, Re, Au, Cu, Ag, As, 204Pb, Mn, Sn, Zn, Se, Ti] |
| b6 | [Te | Co, Re, Au, Cu, Ag, As, 204Pb, Mn, Sn, Zn, Se, Ti] |
| b7 | [Co | Re, Au, Cu, Ag, As, 204Pb, Mn, Sn, Zn, Se, Ti] |
| b8 | [Re | Au, Cu, Ag, As, 204Pb, Mn, Sn, Zn, Se, Ti] |
| b9  b10  b11 | [Au, Cu, Ag | As, 204Pb, Mn, Sn, Zn, Se, Ti]  [Au | Cu, Ag]  [Cu | Ag] |
| b12 | [As | 204Pb, Mn, Sn, Zn, Se, Ti] |
| b13 | [204Pb | Mn, Sn, Zn, Se, Ti] |
| b14 | [Mn, Sn, Zn | Se, Ti] |
| b15  b16 | [Mn | Sn, Zn]  [Sn | Zn] |
| b17 | [Se |Ti] |



**Figure S1.** Silhouette widths values (s) within a cluster . Cluster number i, a number of analyses (ni), average si and Jaccard similarity value ji per cluster are given. Sum of squared errors versus and the number of clusters k = 1, …, 10 showing that 3 clusters are sufficient for k-means clustering.

**Table S2.** Sequential binary partitioning used to obtain 17 ilr-coordinates of 18 geochemical variables of N = 1501 dataset. The procedure of partitioning is based on the hierarchical dendrogram (Figure 4d). Composite variables within a balance are the geometric mean of all components.

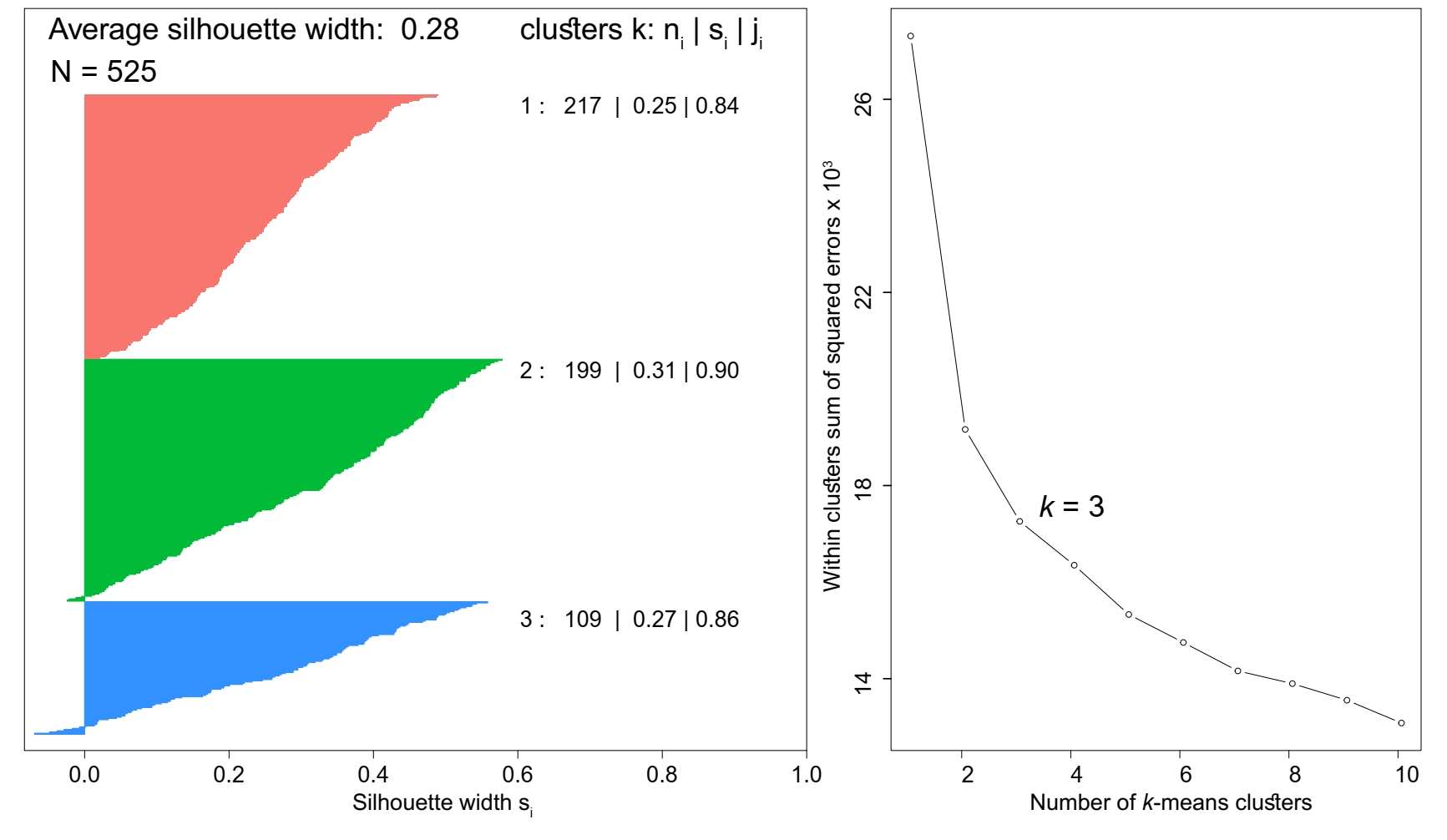
|  |  |
| --- | --- |
| **Balance** | **Binary partition** |
| b1 | [Au, 206Pb, 207Pb, 208Pb, 204Pb, Ag, Bi, Cu | Ni, Co, Re, Te, As, Mn, Se, Ti, Sn, Zn] |
| b2 | [Au | 206Pb, 207Pb, 208Pb, 204Pb, Ag, Bi, Cu] |
| b3 | [206Pb, 207Pb, 208Pb, 204Pb, Ag | Bi, Cu] |
| b4 | [Bi | Cu] |
| b5 | [206Pb, 207Pb, 208Pb | 204Pb, Ag] |
| b6 | [206Pb | 207Pb, 208Pb] |
| b7 | [207Pb | 208Pb] |
| b8 | [204Pb | Ag] |
| b9  b10  b11 | [Ni | Co, Re, Te, As, Mn, Se, Ti, Sn, Zn]  [Co | Re, Te, As, Mn, Se, Ti, Sn, Zn]  [Re | Te, As, Mn, Se, Ti, Sn, Zn] |
| b12 | [Te | As, Mn, Se, Ti, Sn, Zn] |
| b13 | [As | Mn, Se, Ti, Sn, Zn] |
| b14 | [Mn | Se, Ti, Sn, Zn] |
| b15  b16 | [Se, Ti | Sn, Zn]  [Se | Ti] |
| b17 | [Sn | Zn] |
|  |  |



**Figure S2.** Silhouette widths values (s) within a cluster . Cluster number i, a number of analyses (ni), average si and Jaccard similarity value ji per cluster are given. Sum of squared errors versus and the number of clusters k = 1, …, 10 showing that 3 clusters are sufficient for k-means clustering.

**Table 3.** Sequential binary partitioning used to obtain 17 ilr-coordinates of 18 geochemical variables of N = 525 dataset. The procedure of partitioning is based on the hierarchical dendrogram (Figure 5d). Composite variables within a balance are the geometric mean of all components.

|  |  |
| --- | --- |
| **Balance** | **Binary partition** |
| b1 | [204Pb, 206Pb, 207Pb, 208Pb, Bi, Ag, Au, Cu | Ni, Re, Co, Mn, Se, Ti, Sn, Zn, As, Te] |
| b2 | [204Pb, 206Pb, 207Pb, 208Pb, Bi, Ag | Au, Cu] |
| b3 | [Au | Cu] |
| b4 | [204Pb, 206Pb, 207Pb, 208Pb | Bi, Ag] |
| b5 | [Bi |Ag] |
| b6 | [204Pb | 206Pb, 207Pb, 208Pb] |
| b7 | [206Pb | 207Pb, 208Pb] |
| b8 | [207Pb | 208Pb] |
| b9  b10  b11  b12 | [Ni, Re | Co, Mn, Se, Ti, Sn, Zn, As, Te]  [Ni | Re]  [Co | Mn, Se, Ti, Sn, Zn, As, Te]  [Mn, Se, Ti, Sn, Zn | As, Te] |
| b13 | [As | Te] |
| b14 | [Mn | Se, Ti, Sn, Zn] |
| b15 | [Se, Ti | Sn, Zn] |
| b16  b17 | [Se | Ti]  [Sn | Zn] |



**Figure S3.** Silhouette widths values (s) within a cluster . Cluster number i, a number of analyses (ni), average si and Jaccard similarity value ji per cluster are given. Sum of squared errors versus and the number of clusters k = 1, …, 10 showing that 3 clusters are sufficient for k-means clustering.