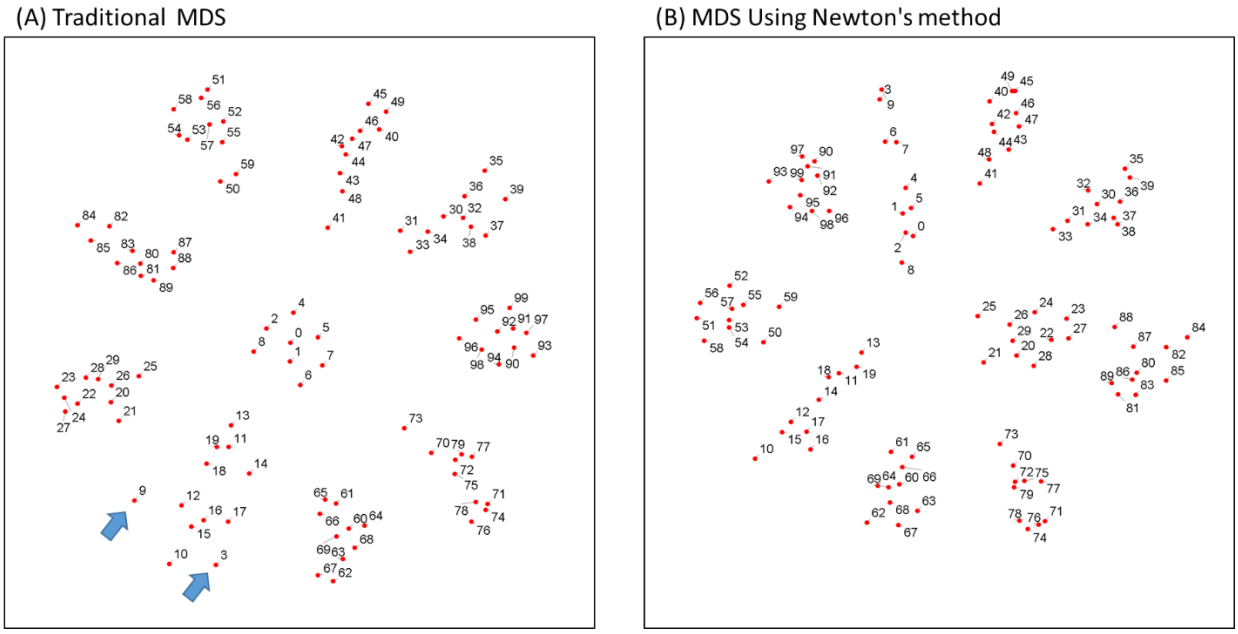


**Figure S1.** Comparison for MDS with the traditional MDS (A) and Newton's method (B). The 100 points are generated by the function genSimulationData() as shown in Supplementary Appendix B. (A) The traditional MDS is generated by Scikit-learn, which is a machine learning library for Python, as shown in Supplementary Appendix C. It can be found that the points 9 and 3 are assigned to the wrong group. (B) The MDS by using Newton's method (NMDS) can reduce the grouping errors.