

(a not so) Long Problem Set 8

The file “MetalMix.RData” contains three objects: a dataframe with the name “metals” that contains absorbance values for 27 solutions at eight wavelengths, a vector with the name “score.labels” for identifying points on a scores plot, and vector with the name “rot.labels” for identifying points on a loadings plot. The 27 solutions were prepared by diluting stock solutions of 0.10 M $\text{Cu}(\text{NO}_3)_2$, 0.10 M $\text{Ni}(\text{NO}_3)_2$, and 0.10 M $\text{Co}(\text{NO}_3)_2$ to create

- three pure solutions (one each of Cu^{2+} , Ni^{2+} , and Co^{2+})
- eighteen binary mixtures (six each of Cu^{2+} and Ni^{2+} , Cu^{2+} and Co^{2+} , and Ni^{2+} and Co^{2+})
- six ternary mixtures (each containing all three metal ions)

Use this data to complete the following

- Complete a principal component analysis of the data (center the data, but do not scale the data), examine a summary of the pca model and explain why the summary is consistent with what you know about the samples.
- Examine the scores plot using the first two principal component and identify, by number, the three pure solutions, the three sets of binary mixtures, and the ternary mixtures. Be sure to explain how you arrived at your decisions.
- Examine the loadings plot using the first two principal components and identify the wavelength(s) associated with each pure solution. Using the information in the loading plot and knowing that nitrate solutions of Cu^{2+} are blue, that nitrate solutions of Ni^{2+} are green, and that nitrate solutions of Co^{2+} are pink, identify, by number, the pure solutions of $\text{Cu}(\text{NO}_3)_2$, $\text{Ni}(\text{NO}_3)_2$, and $\text{Co}(\text{NO}_3)_2$.