

11.8: Exercises

The file [rare_earth.csv](#) contains data for the 17 rare earth elements, which consists of the lanthanides (La → Lu) plus Sc and Y. The data is from Horovitz, O.; Sârbu, C. "Characterization and Classification of Lanthanides by Multivariate-Analysis Methods," *J. Chem. Educ.* **2005**, 82, 473-483. Each row in the file contains data for one element; the columns in the file provide values for the following 16 properties:

- mass: atomic mass (g/mol)
- density: (g/cm³)
- radius: atomic radius (pm)
- en: electronegativity (Pauling scale)
- ionenergy_1: first ionization energy (kJ/mol)
- ionenergy_2: second ionization energy (kJ/mol)
- ionenergy_3: third ionization energy (kJ/mol)
- mp: melting point (K)
- bp: boiling point (K)
- h_fusion: enthalpy of fusion (kJ/mol)
- h_atom: enthalpy of atomization (kJ/mol)
- entropy: absolute entropy (J/mol•K)
- sp_heat: specific heat (J/g•K)
- resist: electrical resistivity ($\mu\Omega$ cm)
- head_cond: heat conductivity (W cm⁻¹K⁻¹)
- gibbs: Gibbs free energy of formation (kJ/mol)

Two variables included in the original paper—the enthalpy of vaporization and the surface tension at the melting point—are omitted from this data set as they include missing values. Problems 1-3 draw upon the data in this file.

1. Perform a cluster analysis for the 17 elements in the file [rare_earth.csv](#) and comment on the results paying particular attention to the positions of Sc and Y, and the 15 lanthanides. You may wish to compare your results with those reported in the paper cited above.
2. Perform a cluster analysis for the 16 properties in the file [rare_earth.csv](#) and comment on the results. You may wish to compare your results with those reported in the paper cited above.
3. Complete a principal component analysis for the 17 elements in the file [rare_earth.csv](#). Create two-dimensional scores plots that compare PC1 to PC2, PC1 to PC3, and PC2 to PC3, and a three-dimensional scores plot for the first three principal components. Comment on your results paying particular attention to the positions of Sc and Y, and the 15 lanthanides. You may wish to compare your results to those from Exercise 11.1 and the results reported in the paper cited above. Create two-dimensional loadings plots that compare PC1 to PC2, PC1 to PC3, and PC2 to PC3, and a three-dimensional loadings plot for the first three principal components. Comment on your results. You may wish to compare your results to those from Exercise 11.2 and the results reported in the paper cited above.
4. The files [mvr_abs](#) and [mvr_conc](#) contain absorbance values for 10 samples that contain one or more the analytes Co²⁺, Cu²⁺, and Ni²⁺ at five wavelengths, and the mM concentrations of the same analytes in the 10 samples. The data are from Dado, G.; Rosenthal, J. "Simultaneous Determination of Cobalt, Copper, and Nickel by Multivariate Linear Regression," *J. Chem. Educ.* **1990**, 67, 797-800. Use the first seven samples as calibration standards and use a multivariate linear regression to determine the concentrations of the analytes in the last three samples. You may wish to compare your results with those reported in the paper cited above.

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