

## 13.1: Chemometric Resources

### Books

The following small collection of books provide a broad introduction to chemometric methods of analysis. The text by Miller and Miller is a good entry-level textbook suitable for the undergraduate curriculum. The text by Massart, et. al. is a particularly comprehensive resource.

- Anderson, R. L. **Practical Statistics for Analytical Chemists**, Van Nostrand Reinhold: New York; 1987.
- Beebe, K. R.; Pell, R. J.; Seasholtz, M. B. **Chemometrics: A Practical Guide**, Wiley, 1998.
- Brereton, Richard G. **Data Driven Extraction for Science**, 2nd Edition, Wiley, 2018.
- Graham, R. C. **Data Analysis for the Chemical Sciences**, VCH Publishers: New York; 1993.
- Larose, D. T.; Larose, C. D. **Discovering Knowledge in Data: An Introduction to Data Mining**, Wiley, 2014.
- Mark, H.; Workman, J. **Statistics in Spectroscopy**, Academic Press: Boston; 1991.
- Massart, D. L.; Vandeginste, B. G. M.; Lewi, P. J.; Smeyers-Verbeke, J. **Handbook of Chemometrics and Qualimetrics: Part A and Part B**, Elsevier, 1997.
- Miller, J. N.; Miller, J. C. **Statistics and Chemometrics for Analytical Chemistry**, 7th Edition, Pearson, 2018.
- Schutt, R.; O'Neil, C. **Doing Data Science: Straight Talk From the Frontline**, O'Reilly, 2014.
- Sharaf, M. H.; Illman, D. L.; Kowalski, B. R. **Chemometrics**, Wiley-Interscience: New York; 1986.

Although not resources on chemometrics, the following books provide a broad introduction to the statistical methods that underlie chemometrics.

- Boslaugh, S. **Statistics in a Nutshell: A Desktop Quick Reference**, O'Reilly, 2013.
- Larose, D. T.; Larose, C. D. **Discovering Knowledge in Data: An Introduction to Data Mining**, Wiley, 2014.
- Schutt, R.; O'Neil, C. **Doing Data Science: Straight Talk From the Frontline**, O'Reilly, 2014.
- van Belle, G. **Statistical Rules of Thumb**, Wiley, 2008.

The following books provide more specialized coverage of topics relevant to chemometrics.

- Mason, R. L.; Gunst, R. F.; Hess, J. L. **Statistical Design and Analysis of Experiments**; Wiley: New York, 1989.
- Myers, R. H.; Montgomery, D. C. **Response Surface Methodology**, Wiley, 2002.

The following books provide guidance on the visualization of data, both in figures and in tables.

- Bertin, J. **Semiology of Graphics**, esri press, 1983.
- Few, S. **Now You See It**, Analytics Press, 2009.
- Few, S. **Show Me the Numbers**, Analytics Press, 2012.
- Few, S. **Information Dashboard Design**, Analytics Press, 2013.
- Robins, N. B. **Creating More Effective Graphs**, Charchouse, 2013.
- Tufte, E. R. **Envisioning Information**, Graphics Press, 1990.
- Tufte, E. R. **Visual Explanations** Graphics Press, 1997.
- Tufte, E. R. **The Visual Display of Quantitative Information**, Graphics Press, 2001.
- Tufte, E. R. **Beautiful Evidence**, Graphics Press, 2006.

The following textbook provides a broad introduction to analytical chemistry, including sections on chemometric topics.

- Harvey, D. T. **Analytical Chemistry 2.1** (available [here](#) and [here](#)).

### Articles

The following paper provides a general theory of types of measurements.

- Stevens, S. S. "On the Theory of Scales of Measurements," *Science*, **1946**, *103*, 677-680.

The detection of outliers, particularly when working with a small number of samples, is discussed in the following papers.

- Analytical Methods Committee "Robust Statistics—How Not To Reject Outliers Part 1. Basic Concepts," *Analyst* **1989**, *114*, 1693–1697.
- Analytical Methods Committee "Robust Statistics—How Not to Reject Outliers Part 2. Inter-laboratory Trials," *Analyst* **1989**, *114*, 1699–1702.

- Analytical Methods Committee “Rogues and Suspects: How to Tackle Outliers,” AMCTB 39, 2009.
- Analytical Methods Committee “Robust statistics: a method of coping with outliers,” AMCTB 6, 2001.
- Analytical Methods Committee “Using the Grubbs and Cochran tests to identify outliers,” *Anal. Methods*, **2015**, 7, 7948–7950.
- Efsthathiou, C. “Stochastic Calculation of Critical Q-Test Values for the Detection of Outliers in Measurements,” *J. Chem. Educ.* **1992**, 69, 773–736.
- Efsthathiou, C. “Estimation of type 1 error probability from experimental Dixon’s Q parameter on testing for outliers within small data sets,” *Talanta* **2006**, 69, 1068–1071.
- Kelly, P. C. “Outlier Detection in Collaborative Studies,” *Anal. Chem.* **1990**, 73, 58–64.
- Mitschele, J. “Small Sample Statistics,” *J. Chem. Educ.* **1991**, 68, 470–473.

The following papers provide additional information on error and uncertainty.

- Analytical Methods Committee “Optimizing your uncertainty—a case study,” AMCTB 32, 2008.
- Analytical Methods Committee “Dark Uncertainty,” AMCTB 53, 2012.
- Analytical Methods Committee “What causes most errors in chemical analysis?” AMCTB 56, 2013.
- Andraos, J. “On the Propagation of Statistical Errors for a Function of Several Variables,” *J. Chem. Educ.* **1996**, 73, 150–154.
- Donato, H.; Metz, C. “A Direct Method for the Propagation of Error Using a Personal Computer Spreadsheet Program,” *J. Chem. Educ.* **1988**, 65, 867–868.
- Gordon, R.; Pickering, M.; Bisson, D. “Uncertainty Analysis by the ‘Worst Case’ Method,” *J. Chem. Educ.* **1984**, 61, 780–781.
- Guare, C. J. “Error, Precision and Uncertainty,” *J. Chem. Educ.* **1991**, 68, 649–652.
- Guedens, W. J.; Yperman, J.; Mullens, J.; Van Poucke, L. C.; Pauwels, E. J. “Statistical Analysis of Errors: A Practical Approach for an Undergraduate Chemistry Lab Part 1. The Concept,” *J. Chem. Educ.* **1993**, 70, 776–779.
- Guedens, W. J.; Yperman, J.; Mullens, J.; Van Poucke, L. C.; Pauwels, E. J. “Statistical Analysis of Errors: A Practical Approach for an Undergraduate Chemistry Lab Part 2. Some Worked Examples,” *J. Chem. Educ.* **1993**, 70, 838–841.
- Heydorn, K. “Detecting Errors in Micro and Trace Analysis by Using Statistics,” *Anal. Chim. Acta* **1993**, 283, 494–499.
- Hund, E.; Massart, D. L.; Smeyers-Verbeke, J. “Operational definitions of uncertainty,” *Trends Anal. Chem.* **2001**, 20, 394–406.
- Kragten, J. “Calculating Standard Deviations and Confidence Intervals with a Universally Applicable Spreadsheet Technique,” *Analyst* **1994**, 119, 2161–2165.
- Taylor, B. N.; Kuyatt, C. E. “Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results,” NIST Technical Note 1297, 1994.
- Van Bramer, S. E. “A Brief Introduction to the Gaussian Distribution, Sample Statistics, and the Student’s t Statistic,” *J. Chem. Educ.* **2007**, 84, 1231.
- Yates, P. C. “A Simple Method for Illustrating Uncertainty Analysis,” *J. Chem. Educ.* **2001**, 78, 770–771.

The following articles provide thoughts on the limitations of statistical analysis based on significance testing.

- Analytical Methods Committee “Significance, importance, and power,” AMCTB 38, 2009.
- Analytical Methods Committee “An introduction to non-parametric statistics,” AMCTB 57, 2013.
- Berger, J. O.; Berry, D. A. “Statistical Analysis and the Illusion of Objectivity,” *Am. Sci.* **1988**, 76, 159–165.
- Kryzwinski, M. “Importance of being uncertain,” *Nat. Methods* **2013**, 10, 809–810.
- Kryzwinski, M. “Significance, P values, and t-tests,” *Nat. Methods* **2013**, 10, 1041–1042.
- Kryzwinski, M. “Power and sample size,” *Nat. Methods* **2013**, 10, 1139–1140.
- Leek, J. T.; Peng, R. D. “What is the question?,” *Science* **2015**, 347, 1314–1315.

The following papers provide insight into organizing data in spreadsheets and visualizing data.

- Analytical Methods Committee “Representing data distributions with kernel density estimates,” AMC Technical Brief, March 2006.
- Broman, K. W.; Woo, K. H. “Data Organization in Spreadsheets,” *The American Statistician*, **2018**, 72, 2–10.
- Frigge, M.; Hoaglin, D. C.; Iglewicz, B. “Some Implementations of the Boxplot,” *The American Statistician* **1989**, 43, 50–54.
- Midway, S. R. “Principles of Effective Data Visualizations,” *PATTER*, **2020**, 1(9).
- Schwabish, J. A. “Ten Guidelines for Better Tables,” *J. Benefit Cost Anal.* **2020**, 11, 151–178.

## Websites

- NIST Engineering Statistics HandbookST (<https://www.itl.nist.gov/div898/handbook/>)
- Rice Virtual Lab in Statistics (<https://onlinestatbook.com/rvls.html>)

- Statistics for Analytical Chemistry (<https://science.widener.edu/syb/stats/stats.html>)

---

This page titled [13.1: Chemometric Resources](#) is shared under a [CC BY-NC-SA 4.0](#) license and was authored, remixed, and/or curated by [David Harvey](#).