



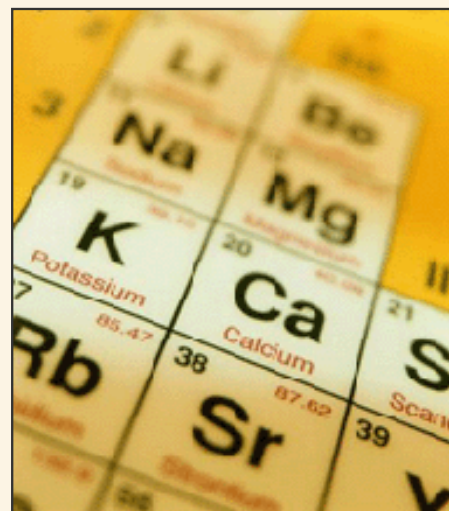
Chemometrics

Think of a chemical or biological mixture from any industry be it pharmaceutical, oil, semiconductor or clinical laboratory. To understand the composition, qualitative and quantitative analysis are essential. To know its composition (what percentages of Copper, Nickel etc are in there, identification of microorganisms in a sample etc.), we have to implore a chemist to do some chemical tests in his/her laboratory. Now imagine you are getting the required compositions while sitting in your office, where your office and Chemist's lab are like two banks of a river and is far away from acids, bases, cells or reagents. **This seemingly “out of the world” thought can be made “of the world” approach if we are aware of the word called “CHEMOMETRICS”.**

Today's automated laboratory instruments are capable of generating prodigious volumes of high-quality measurements, which in turn generates huge data volumes. Increasingly, the powerful mathematical and statistical methods of Chemometrics are being called upon to help reduce these measurements to useful information. **Broadly speaking, Chemometrics recognises the patterns for all the components from the data we have and is able to model the composition when a new sample data set is provided.**

Chemometrics is the extraction of information from multivariate chemical data using statistics and mathematics. This can be anything from calculating pH to computing a Fourier transform interpolation of a spectrum. More recently, Chemometrics refers to using linear algebra calculation methods, to make either quantitative or qualitative measurements of chemical data, primarily spectra. Like other statistical applications, Chemometrics involves extracting patterns. Patterns in the data are modeled; these models can then be routinely applied to future data in order to predict the same quality parameters. Chemometrics can be applied to a wide range of problems in chemistry, chemical engineering and related fields.

Chemometrics is not a single tool but a range of methods including – Basic Statistics, Signal Processing, Factorial Design, Calibration, Curve Fitting, Factor Analysis, Detection, Pattern Recognition and Neural Networks.



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About DecisionCraft Analytics

We provide decision-making solutions to improve operational efficiency and business responsiveness. Our consulting services employ our strengths in industry knowledge, conceptual rigor, and information technologies. Developed using concepts from decision theory; our solutions use robust optimization, simulation, and statistical engines adapted to our client's focus areas.

DecisionCraft Services

Business Diagnostics

We analyze business processes and transactional data to identify underlying patterns, unravel hidden

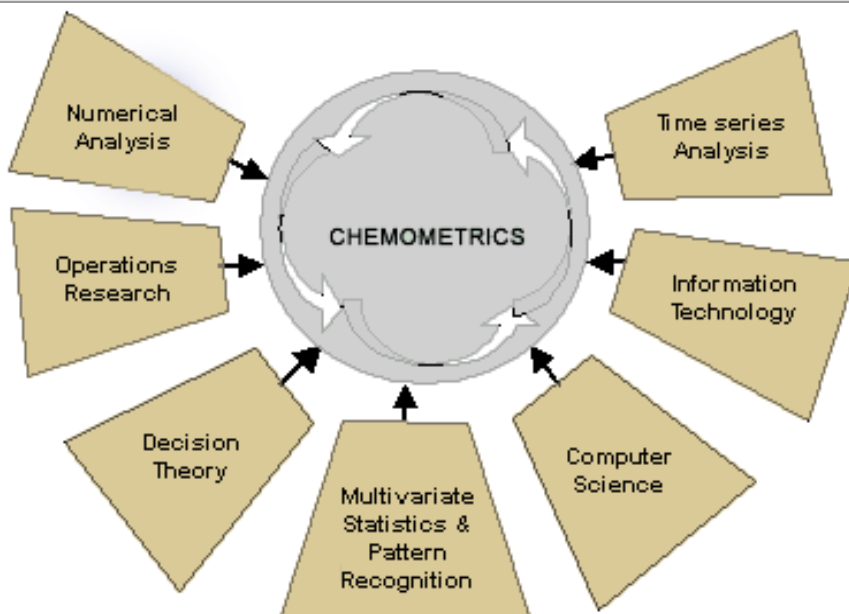


Figure 1: Methods in Chemometrics

Each of the products of the firm can be plotted on the BCG Matrix (Market Growth Rate Vs Relative Market Share) to get an idea of the cash cows and the stars in the portfolio. The products offering of the firm can be compared with that of its competitors and white spaces can be filled if that particular segment is profitable.

- Exploratory data analysis can reveal hidden patterns in complex data by reducing the information to a more comprehensible form. Such a chemometric analysis can expose possible outliers and indicate whether there are patterns or trends in the data. Exploratory algorithms such as principal component analysis (PCA) are designed to reduce large complex data sets into a series of optimized and interpretable size.
- In many applications, it is expensive, time consuming or difficult to directly measure a variable of interest. Such cases require the analyst to predict something of interest based on related properties that are easier to measure. The goal of chemometric regression analysis is to develop a model which correlates the information in the set of known measurements to the desired property. Chemometric algorithms for performing regression include partial least squares (PLS) and principal component regression (PCR). Chemometric regression is extensively used in making decisions relating to product quality in the on-line monitoring and process control industry where fast and expensive systems are needed to test.

relationships and recommend areas for improvement that can improve ROI and reduce costs.

Predictive Analytics

We use historical data intelligently to develop a view of future market trends and help our clients focus on the right audiences thereby developing their competitive edge.

Forecasting

We use advanced time-series and regression techniques for forecasting behavior of critical business variables that allows our clients to plan for their resources intelligently.

- Many applications require that samples be assigned to predefined categories. This may involve determining whether a sample is good or bad, or predicting an unknown sample as belonging to one of several distinct groups. A classification model is used to predict a sample's class by comparing the sample to a previously analyzed experience set, in which categories are already known. k-nearest neighbour (KNN) is primarily used in Chemometrics. This can be thought as separating chromatographic data set from spectroscopic data set and doing analysis. When these techniques are used to create a classification model, the answers provided are more reliable and include the ability to reveal unusual samples in the data. Therefore, Chemometrics helps in standardizing data.

Applications

Chemometric methods have been important in automating various data-intensive functions that provides support to chemical process industries, consumer product manufacturers and analytical instrument developers. **Chemometrics is widely used by semiconductor manufacturers, oil and chemical companies, pharmaceuticals and analytical instrument companies.** Although, Chemometric methods have been applied, with encouraging results, for the analysis of complex *biological data* in a number of applications including analysis of cellular images, identification of bacteria and fungi on the basis of their metabolic and chemical properties, and identification of drugs and toxic substances from their mass spectra, a lot of work remains to be done in the areas of measurement standardization, data-base collection, and user familiarity before robust statistical modeling systems are obtained for a more complete description of biological systems and their interactions. Few example applications are –

- Spectroscopic calibrations
- Process modeling for optimization
- Process models for monitoring and fault detection
- Dynamic model identification for process control
- Multivariate statistical process control
- Process analytical instrument standardization
- Analytical instrument design and development

Chemometrics is a statistical technique that can directly correlate quality parameters or physical properties to analytical instrument data collected. Chemometrics can lead to more efficient laboratory practices or automated quality control systems. The only requirements are an appropriate instrument and software to interpret the patterns in the data. Various Chemometrics softwares are now available to recognize patterns in virtually any type of multidimensional analytical data. Chemometrics is used to speed methods development and make routine the use of statistical models for data analysis.

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