화학계량학(Chemometrics)

유준 교수 (Prof. Jay Liu, jayliu@pknu.ac.kr)

2014 년 1 학기 (Spring term, 2014), 월 (Monday) 10:00 ~ 12:30, @4 공학관 210 (4-210)

강의 주제 (Topic)

Multivariate statistical methods for the analysis, monitoring and optimization of processes

강의 소개 (Course Overview)

Process and laboratory computers routinely collect massive amounts of process and quality data, yet little use is made of these data. Multivariate statistical projection methods such as Principal Components Analysis (PCA) and Projection to Latent Structures (PLS) are capable of projecting the information contained in these data down into low dimensional spaces where one can easily interpret process behaviour, establish SPC monitoring charts, and optimize process performance.

This course presents the theoretical and practical example-based background for these multivariate latent variable methods, and provides an appreciation of their potential for the analysis, monitoring and optimization of processes. Many industrial examples are analyzed and a working knowledge of the methods is provided through a series of computer assignments which utilize some of these data. These methods have a very wide range of applicability to all areas of industries and engineering where data are collected and must be interpreted.

선행과목? (Prerequisite)

공업통계 (Engineering statistics)

선형대수 (Linear algebra)

강의 목차 (Course Outline)

1. **Introduction**
   This session will present a general overview of methods and illustrate the range of problems that can be treated through applications to several industrial problems. Nature of multivariate data, concepts behind multivariate analysis, and areas of application with industrial examples will be covered.
2. Principal Component Analysis

This session will focus on methods for exploring historical process data to find and diagnose problems.

3. Partial Least Squares
   Multivariate Regression using partial least squares (PLS) and its application is addressed
4. Monitoring / SPC: Multivariate Statistical Process Control (SPC) based on PCA or PLS models will be addressed.
5. Classification Methods: A few methodologies for classification will be covered.
6. (if time permits) Product Transfer and Scale-up: Use of multivariate methods to transfer production between plants or to compare plants is the main subject. In addition, scale-up based on pilot plant & production data will be addressed.
7. (if time permits) Product Development: Use of diverse data-bases on process data and raw material data to design new products with specified properties will be addressed.

소프트웨어 (Software)

You can code your own PCA/PLS programs but use of following S/W is highly recommended.

- **ProMV (www.prosensus.ca) provides free academic version.**
- SIMCA-P (www.umetrics.com) you can use demo version for one month.
- Unscrambler (www.camo.com) you can use demo version for one month.
- PLS toolbox for MATLAB® (http://www.eigenvector.com)

This course will use ProMV in demonstration.

평가 (Evaluation)

Assignments (50%), project report (50%)

참고문헌 (References)

1. Jackson, J.E., *A user guide to principal component*, Wiley, 1991.
2. Jolliffe, I.T., *Principal component analysis*, Springer-Verlag, 1986.
3. Martens H. & Naes, T., *Multivariate calibration*, Wiley, 1991.
4. Beebe, K.R., Pell, R.J. and Seaholtz, M.B., *Chemometrics, A practical guide*, Wiley, 1998.
5. Mardia, K.V., Kent, J.T. and Bibby, J.M., *Multivariate analysis*, Academic Press, NY, 1979.
6. Martens, H. and Martens, M., *Multivariate analysis of quality, an introduction*, Wiley, NY, 2001.
7. And papers suggested during the course.

ProMV 설치 (Installation of ProMV)

1. Download ProMV 14.02 from www.promv.com and install.
2. In ProMV, go to help → about → and copy and paste your verification code (second last line).
3. Send an email to jamal.alli@prosensus.ca. Then your verification code and a license file will be sent to you. The license file will convert the 30 day trial to a one year academic license.