DATA SCIENCE FOR CHEMICAL ENGINEERING EDUCATION

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CHE 586 at USC: Process Data Analytics and Machine Learning

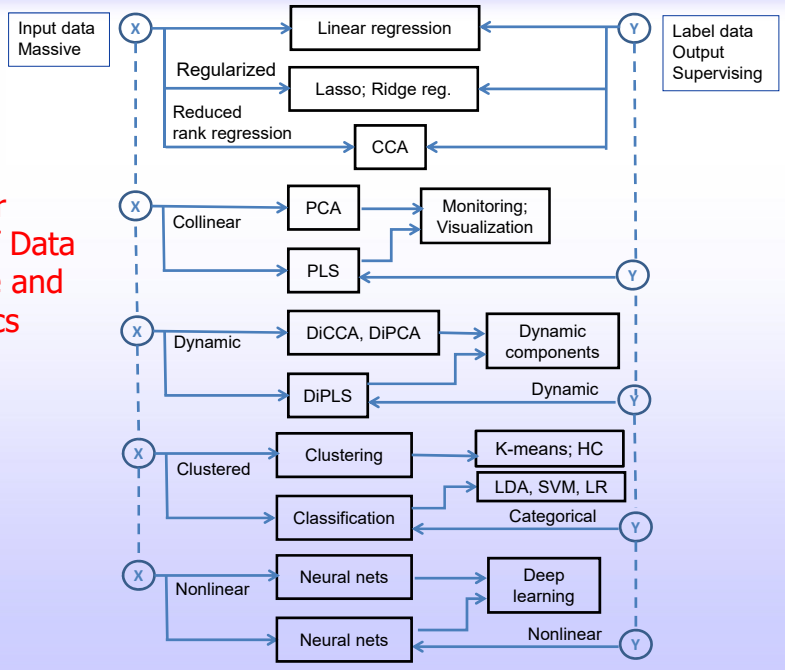
- Offered for the past three years to MS students; could be an elective for BS students
  - Topics include multi-linear regression, supervised learning, unsupervised learning, principal component analysis, partial least squares, canonical correlation analysis, clustering methods, lasso, neural networks, and deep learning.
  - Applications include analysis of chemical process data, quality data, and indirectly measured data.
  - Domain of application: industrial manufacturing data, process operation data, and data from other engineering disciplines.

Focus

- Emphasize on a *data-driven* and *linear algebraic approach* over a probabilistic approach in this course.
- Gain programming experience in R
- Textbook: An Introduction to Statistical Learning with Applications in R. Authors: James, G., Witten, D., Hastie, T., Tibshirani, R. (2013), Springer

	Topics/Daily Activities
Week 1 1/11/2019	L1. Introduction to big data, machine learning, and process data analytics
Week 2 1/18/2019	**L2. Linear regression**
Week 3 1/25/2019	L3. Principal component analysis (PCA)
Week 4 2/1/2019	**PCA**
Week 5 2/8/2019	**L4. Clustering**
Week 6 2/15/2019	**L5.** PCA for process monitoring
Week 7 2/22/2019	**L6. Fault Diagnosis**
Week 8 3/1/2019	**L6. Partial least squares**
Week 9 3/8/2019	**L7. Lasso, Ridge regression**
3/15/2019	**SPRING BREAK**
Week 10 3/22/2019	**Mid-term**
Week 11 3/29/2019	kernel methods
Week 12 4/5/2019	support vector machines
Week 13 4/12/2019	neural networks and soft sensors
Week 14 4/19/2019	deep learning
Week 15 4/26/2019	**Project report due**

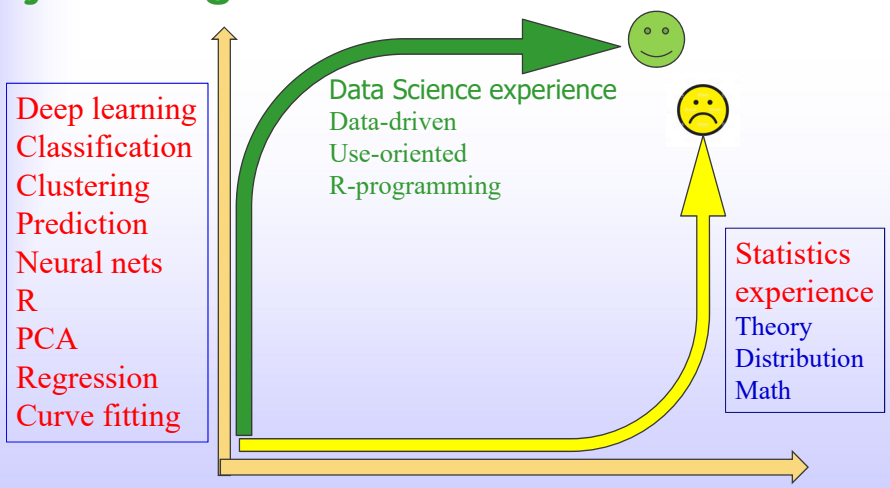
Another View of Data Science and Analytics



Statistics for Chemical Engineers Course: Sequence for Comparison

- Introduction to Probability and Statistics
- Data Collection and Analysis
- Discrete Probability Models
  - Basic probability concepts; Binomial and Poisson distributions
  - Multivariate distributions
- Continuous Probability Models
- Statistical Inference: Sampling Distribution, Confidence Intervals, p-values, and Tests of Hypotheses
- Statistical Quality Control/Statistical Process Control
- Design of Experiments with One Factor
- Design of Experiments with Two or More Factors
- Regression Analysis –
  - simple linear regression; multilinear regression

Data Science vs. Statistics experience: day and night for the student



What is Data Science Editor: Xiao-Li MENG

HDSR
HARVARD DATA SCIENCE REVIEW
A Microscopic, Telescopic, and Kaleidoscopic View of Data Science

- **Indeed, what exactly is *data science* (DS)?**
  "… the answer depends on whom you ask. Some say DS is CS (computer science). Others think DS is simply S (statistics). You may even run into someone who declares DS is just hyped-up BS (and I don't mean "Bayesian statistics")."
- **Joe Qin: Could Data Science emerge as a discipline like control theory in engineering?**
  - **What are the PID's of data science for engineers? (Qin and Chiang, 2019 overview paper)**

Essence of Data Science in ChE

- **Prediction**: Predictive Analytics
  - Predict critical but hard to measure variables from others
- **Interpretation**: Feature or knowledge discovery from data
  - Visualization
  - Diagnostics
- Decision Making

My PID for Data Science

Predict-Interpret-Decide (PID)