



Bioprocess Data Analytics and Machine Learning July 13 – 15, 2020

Day One

| Time | Topics | Instructor(s) | Readings/ Assignments |
|---------------|---|-----------------|--------------------------------|
| 9 to 10:30 | Introduction to bioprocess data analytics: opportunities, types of data analytics problems; supervised, unsupervised, and partially supervised learning; data visualization (software tools using data from bioprocess time series, Raman spectroscopy, spectral imaging, LC-MS) | Braatz/ Anthony | Lecture notes |
| 10:30 to 11 | Coffee and networking | | |
| 11 to 12:30 | Regression: least squares, response surface methodology, ridge regression, lasso, elastic net, cross-validation, residual analysis, outlier detection, uncertainty quantification, optimal experimental design, feature engineering, nonlinearities, systematic method selection, monoclonal antibody manufacturing industrial case study | Braatz | Lecture notes |
| 12:30 to 1:30 | Lunch and networking | | |
| 1:30 to 2:30 | Tour of biopharmaceutical manufacturing labs at MIT, which includes fully automated and instrumented end-to-end continuous CHO-based monoclonal antibody production | Braatz | Lecture notes |
| 2:30 to 3:30 | Tips and traps: correlation vs. causation, inferences drawn from matching statistics, effects of feedback loops, selection among too many models, studying features for biological/ chemical/physical reasonableness, Google Flu Trends | Braatz | Lecture notes |
| 3:30 to 5 pm | Hands-on activities in visualizing and analyzing real biopharmaceutical process datasets | Anthony/ Braatz | Students use their own laptops |
| 5 to 7 | Course reception/networking | | |

Day Two

| Time | Topics | Instructor(s) | Readings/Assignments |
|---------------|---|---------------------|--------------------------------|
| 9 to 10:30 | Time series analysis: low-, high-, and band-pass filters; oscillatory data; Fourier transforms; ARMA; ARMAX; noise; AD convertors; sampling; aliasing; statistical process control (aka control charts), UV absorption for protein concentration measurement case study | Yoon/Anthony | Lecture notes |
| 10:30 to 11 | Coffee and networking | | |
| 11 to 12:30 | Latent variable methods I: PCA, multivariable statistical process control, spectral sensor calibration, PCR, PLS, spectral data artifacts, Raman spectroscopy case study | Yoon | Lecture notes |
| 12:30 to 1:30 | Lunch and networking | | |
| 1:30 to 3 | Latent variable methods II: CCA, FDA, missing data, sparse models, Raman and near-infrared case studies | Yoon | Lecture notes |
| 3 to 3:30 | Coffee and networking | | |
| 3:30 to 4:30 | Hands-on activities in visualizing and analyzing real biopharmaceutical process datasets | Yoon/Braatz/Anthony | Students use their own laptops |
| 4:30 to 5:30 | Open discussions with the instructors | Yoon/Braatz/Anthony | |
| 5:30 to 6 | Coffee and networking | | |

Day Three

| Time | Topics | Instructor(s) | Readings/Assignments |
|-------------|---|----------------|----------------------|
| 9 to 10:30 | Big data analytics: real-time video, thermal imaging, tensor data, hyperspectral imaging, LC-MS, multiway methods, multilinear subspace learning, lyophilization case studies | Anthony/Braatz | Lecture notes |
| 10:30 to 11 | Coffee and networking | | |
| 11 to 12:30 | Nonlinear analytics: support vector machines; random forests; comparisons to FDA and k-nearest neighbor classification; feature engineering revisited; kernel methods; hybrid models; autoassociative and recursive neural networks | Anthony | Lecture notes |

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|---------------------|--|--------------------|--------------------------------|
| 12:30 to 2:30 | Course lunch and networking | | |
| 2:30 to 4 pm | What can bioprocess analytics learn from other industries? | Anthony | Lecture notes |
| 4 to 4:30 | Coffee and networking | | |
| 4:30 to 5:30 | Hands-on activities in visualizing and analyzing real biopharmaceutical process datasets | Anthony/ Braatz | Students use their own laptops |
| 5:30 to 6:30 | Closing reception | Anthony/ Braatz | |