CL205: Artificial Intelligence and Data Science in Chemical Engineering

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AI in Chemical Engineering

- Has a long history
- $\sim$40 years old atleast !!
- Even older if you consider various correlations used in heat transfer, fluid flow, mass transfer, thermo, etc. (early 1900s onwards) !

Problems in Chemical Engineering

- Material Design
  - Design of product: Rubber with desired properties
  - Design of catalyst: To improve certain routes of production
- Process Synthesis and Design: How to assemble a flowsheet and design equipment and operating conditions
- Process Operation
  - Process control: Process operates as desired
  - Monitoring and fault diagnosis: Identify problems as and when they occur
  - Prognosis (predictive monitoring), condition based monitoring: Identify problems about to occur
  - Process systems engineering

Most material in remaining slides from:

Venkat Venkatasubramanian, The promise of artificial intelligence in chemical engineering: Is it here, finally?, AIChE Journal, Volume 65, Issue 2, p. 466-478, year 2019.

Chemical Engineering

- Is undergoing major changes
- Significant opportunities and challenges
  - Modeling
  - Sensing and Automated decision making
- Changes driven by confluence of
  - Cheap, widely accessible, powerful computing, measurements and low cost communications: IIOT
  - Significant progress in molecular engineering: products, catalysts
  - Increasing automation of globally integrated operations
  - Tightening of environmental constraints
  - Demand for speedy, cost efficient, customized products/services
- Led to generation, use, and management of massive amounts of diverse data, and other sources of information
- In short Industry 4.0

AI in Chemical Engineering (AICE): History

Phase 0: Early Attempts

- Attempts started as early as in late 1960s.
- Adaptive Initial Design Synthesizer System:
  - Developed in 1971 for process synthesis: Finding the best flowsheet (different units and connections between them) to produce a desired product
  - Used symbolic manipulation, linked data structures, etc.
- Those days computers were not in vogue and computing was hard

AICE: Phase I- (1)

- Phase I: Expert Systems Era, 1983 to 1995
- Expert Systems
  - Knowledge based or rule based systems
  - Mimic problem-solving of humans by incorporating domain knowledge
  - Separated knowledge base and execution strategy
  - Different from conventional programming
  - Not data heavy at all

AICE: Phase I- (2)

- Expert system examples
  - CONPHYDE 1983, CMU: Predicting thermophysical properties of complex fluid mixtures
  - DECADE 1985, CMU: Catalyst design
  - PROSPECTOR for mineral prospecting
  - MYCIN for diagnosing infectious diseases
  - R1 for configuring Vax computers
  - ⋮

AICE: Phase I- (3)

- Other contributions as well
- Stephanopoulos and coworkers (MIT):
  - MODELL.LA: Language for developing process models
- Venkatasubramanian and coworkers (Columbia, Purdue):
  - Causal model based diagnostic expert systems
  - Idea of automated learning of expert systems
- Abnormal Situation Management (ASM) consortium:
  - Industry and academia joint program
- Courses on AI in Process System Engineering included in Che curriculum
  - Stephanopoulos G., Artificial intelligence in process engineering: a research program. Chem Eng Educ. 1986, 182-185.
  - Venkatasubramanian V. Artificial intelligence in process engineering: experiences from a graduate course. Chem Eng Educ. 1986, 188-192.

AICE: Phase I Pitfalls

- Despite promise, Expert Systems based approach did not take-off as anticipated.
- Too costly (time, manpower, money) to develop, and
- Even harder to maintain
- Approach did not scale to larger (practical) problems

AICE: Phase II

- The Neural Networks Era (1990 to 2008)
- Modeling (nonlinear function approximation) from data
- Feedforward neural networks
- Single layer
- Some success in modeling, fault diagnosis, control, and product design
  - Examples: Venkatasubramanian and coworkers (Purdue): gasoline additives, rubber design, etc.
- But not great impact once again

AICE: Phase II Pitfalls

- Neural networks were not deep
  - Not possible to train deep networks: Computational issues
- Challenging problems in vision, natural language processing (NLP), and speech understanding were unsolved
- Organizational and people acceptance not high: Do we really need it?
- Maturing of mathematical programming based approaches: optimization based planning/scheduling, system identification, control, estimation.
  - Relatively easier to apply and led to significant gains.

AICE: Phase III

- Deep Learning and the Data Science Era (2005 onwards)
- Key ideas
  - Better NN architectures: Convolution neural networks, recurrent neural networks, deep networks
  - Reinforcement learning: Reward based learning
  - Machine Learning: Incorporation of mathematical methods from probability and statistics with typical AI techniques, such as: Support Vector Machines, Random Forests, Bayesian Belief Networks,...
- Coupled with advances in hardware: Computing, storage, and communication
- Good success in material science community: Use of simulation data, catalytic reaction data

AICE: So have the stars finally aligned?

- *Has the moment where AI can affect chemical engineering in a game-changing way finally arrived?*
- A guarded Yes!
- Why yes:
  - Issues related to hardware sorted out
  - Issues related to demand and acceptability in market (and industry) sorted out
  - Interest in AI, acceptability, and training amongst academic researchers and students at all time high
  - Plenty of funding available to pursue tough problems

Then Why the Hesitancy- 1

- Important challenges remain
- Hybrid modeling challenges
  - Be able to use multiple mathematical modeling and knowledge representation approaches: graphs, ODEs, rule based representations, data driven models, etc.
  - Essentially develop AI based models in Chemical Engineering: ChatGPT or Watson for Chemical Engineering
- Issues related to lack of data in some domains: Need public datasets akin to those available in image processing and natural language processing

Then why the Hesitancy- 2

- Who will do this?
- Not realistic to expect computer scientists to do this
  - Just like it is not realistic to expect mathematicians who understand ODEs to solve process control problems
- Need manpower educated in fundamentals of both
  - Chemical Engineering, and
  - AI
  - Going beyond the ability to merely use existing tools

The Opportunities

- Deeper, research challenges related to hybrid modeling
- Relatively low hanging fruits
  - Use of image processing and natural language processing in chemical process industry
  - Increasingly being used
  - Poised for exponential take-off
- Fantastic career opportunities

AI@ Chemical Engg IIT Bombay

- A rich history
- CL688 (AI in Process Engineering) (or its equivalent) started in late 1990s
- Several faculty working in different areas
  - Process systems engineering: control, estimation, design, soft-sensing, condition based monitoring
  - Bioinformatics
  - Molecular simulations
- Courses/expertise in estimation, statistics, and optimization

References

- Venkat Venkatasubramanian, The promise of artificial intelligence in chemical engineering: Is it here, finally?, AIChE Journal, Volume 65, Issue 2, p. 466-478, year 2019.

Thank You