Surrogate-assisted Global Optimization of Chemical Process Flowsheets

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Motivation

• **Design and rethink** chemical processes
  – More cost efficient
  – More CO2 efficient

• **Enhance the process design**
  – Flowsheet is designed in a process simulator
  – Most commercial process simulator act as a **black-box**, i.e. the underlying mathematical **model** is not known
Overview: Process design

- Which process is **more efficient**?
- \( \min f(x) \)
  
  \[ \text{s. t. } g_i(x) \leq 0, \quad h_j(x) = 0 \]

- \( \text{DoFs} \subset x \)

- \( x \) in-accessible if simulation fails

- MINLP Problem with in-accessible derivatives

Motivation for Flowsheet Optimization!
Case-Study: Hydroformylation of 1-dodecene in TMS

- Thermomorphic solvent system:
  - High temperature $\rightarrow$ one mixture
  - Low temperature $\rightarrow$ two liquid phases

- Flowsheet modeled in process simulator Aspen Plus
  - 10 degrees of freedom
  - 25% Non converging simulations
  - Approximately 2200 equations
  - Approx. 6 seconds per simulation
  - Purity constraint on 99% mol on product stream
Memetic Algorithm for Flowsheet Optimization

Flowsheet \rightarrow Cost function \rightarrow Evaluation \rightarrow Improvement

MA \rightarrow ES \rightarrow Meme

Process simulator: ASPEN Plus

Surrogate-assisted Optimization Techniques!
Memetic Algorithm for Flowsheet Optimization

- Train surrogate models (shallow neural networks) on the fly.
- Train first surrogate after 500 simulations
- Retrain every 200 simulations

Memetic Algorithm for Flowsheet Optimization

- Prescreen simulation candidates based on potential
- Classifier: Will the simulation converge?
- Rule on Purity: $p_e < 0.99 - p_t$

Flowsheet → Cost function → Evaluation → Surrogate Assistance

MA

ES

Meme

Process simulator: ASPEN Plus


Presentation • DoDSC Colloquium • 16th June • Lecturer: Tim Janus

Surrogate-assisted Optimization Techniques!
Memetic Algorithm for Flowsheet Optimization

- Generate candidates by optimization on surrogate models
  - Use derivative-based algorithms
  - `fmincon`

Flowsheet
- Cost function
- Evaluation

Surrogate Assistance
- Selection for reproduction
- Variation
- Recombination/mutation
- Selection for new generation

Process simulator: ASPEN Plus

- #Sim over costs
- Ten repeats
- Solid mean value
- Area is variance
- Dotted is min/max
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Problems-Challenges

- **Industrial-size case-study:**
  - 30 or more DoFs
  - Simulation times in order of minutes
  - High number of simulations due to derivative-free optimization
  - Results for an European Congress of Chemical Engineering (ECCE) contribution was based on 100,000 simulations
  - Computational time in magnitude of weeks
- **Divide and conquer**
Thank you! To get in touch scan the QR Code!