Real-time Decision-making under Uncertainty in 2040

Stratos Pistikopoulos
Real-time Decision-making under Uncertainty in 2040
An Adventure in Big Data Analytics or an Opportunity for Model-based Optimization?

Stratos Pistikopoulos
Professor George Stephanopoulos

- Research inspiration & impact on my career
- Decision making under uncertainty in 2040
G. Stephanopoulos

Synthesis of process flowsheets: an adventure in heuristic design or a utopia of mathematical programming?

Research Inspiration #1

STUDIES IN PROCESS SYNTHESIS—I
BRANCH AND BOUND STRATEGY WITH LIST TECHNIQUES
FOR THE SYNTHESIS OF SEPARATION SCHEMES

ARTHUR W. WESTERBERG and GEORGE STEPHANOPoulos†
Department of Chemical Engineering, University of Florida, Gainesville, FL 32611, U.S.A.

(Received 24 June 1974; accepted 4 February 1975)

STUDIES IN PROCESS SYNTHESIS—II
EVOLUTIONARY SYNTHESIS OF OPTIMAL
PROCESS FLOWSHEETS†

GEORGE STEPHANOPoulos† and ARTHUR W. WESTERBERG
Department of Chemical Engineering, University of Florida 32611, Gainesville, FL 32067, U.S.A.

(Received 24 June 1974; accepted 23 September 1975)

A Review of Process Synthesis

NAONORI NISHIDA
Science University of Tokyo
Tokyo, Japan

GEORGE STEPHANOPoulos
University of Minnesota
Minneapolis, Minnesota 55455

and

A. W. WESTERBERG
Carnegie-Mellon University
Pittsburgh, Pennsylvania 15213

A UNIFIED APPROACH TO THE SYNTHESIS OF
CONTROL STRUCTURES FOR COMPLEX
CHEMICAL PLANTS

G. STEPHANOPoulos* and Y. ARKUN
Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455, U.S.A.

and

M. MORARI
Department of Chemical Engineering, University of Wisconsin, Madison, WI 53706, U.S.A.

(Received 1 December 1979)
Research Inspiration #2

- **March 1995 – Imperial College London**
  - External PhD examiner for my first graduating PhD student – Dr. Katerina Papalexandri
  
  "Flexibility and Controllability in the synthesis of mass/heat integrated process systems"

  - George offered encouragement/support and valuable advice
Research Inspiration #2

Encouragement to work on:

- Process Synthesis
- Process Intensification
- Interactions of design/control/operability
- Decision-making under uncertainty
Research Inspiration #2

Valuable advice (for life):

- Research question is the key
- Have an area that you publish regularly (& you become well-known)
- Have a “risky” area with long-term impact

Importance of:

From “why” to “how” to “what”:

Strategy/Philosophy is critical to research innovation

(First - get the Big Picture right!)
Professor George Stephanopoulos

- Research inspiration & impact on my career
- Decision making under uncertainty in 2040
Decision-making under uncertainty in 2040

How far have we advanced between 1980-2017?
Decision-making under uncertainty in 2040

How far have we advanced between 1980-2017?

Advances in:

- Computing power
  - ×10E08 faster!
Decision-making under uncertainty in 2040

How far have we advanced between 1980-2017?

Advances in:

- Computing power
  - ×10E08 faster!
- Simulation
  - ×10E04 bigger problems!

Simulation of flows in industrial compressors*

Decision-making under uncertainty in 2040

How far have we advanced between 1980-2017?

Advances in:

- Computing power
  - \( \times 10^{10} \) faster!
- Simulation
  - \( \times 10^{10} \) bigger problems!

Similar trends in:

- Optimization
- Data Analytics
Decision-making under uncertainty in 2040

How far have we advanced between 1980-2017?

A word-usage relative frequency plot in Google Books

*Data is adopted from Google Ngrams*
Decision-making under uncertainty in 2040

How far have we advanced between 1980-2017?

A word-usage relative frequency plot in Google Books

- Uncertainty quantification
- Decision making under uncertainty
- Robust Optimization
- Stochastic Programming
- Big Data
- Data driven
- Model free
- Derivative free
- Data analytics

*Data is adopted from Google Ngrams*
Decision-making under uncertainty in 2040

Adventure in Big Data Analytics or Opportunity for Model-based Optimization?

- Model-free
- Equation-free
- Variable-free
- Derivative-free

Myths & misconceptions?
Perception or Reality?
Decision-making under uncertainty in 2040

Adventure in Big Data Analytics or Opportunity for Model-based Optimization?

1. Can we innovate / propose new designs with data only?
   - Role of discrete 0-1 choices?

2. Can Causality be fully expressed through data only?
   - For example, biomedical applications

3. Can we tackle decision making under uncertainty with data only?
   - Two-stage stochastic/robust optimization
Motivating “thought” experiment
Two-stage decision-making under uncertainty

“here-and-now” decisions: Must be taken prior the realization of the uncertainty
“wait-and-see” decisions: Can be taken after the realization of the uncertainty

Application Areas:

1. Design and Scheduling:
   • Design decisions: “here-and-now”
   • Scheduling decisions: “wait-and-see”
   • Demand: uncertainty

2. Scheduling and Control:
   • Scheduling decisions: “here-and-now”
   • Control decisions: “wait-and-see”
   • Process disturbances: uncertainty

3. Design and Control
4. Facility location and transportation
5. Dynamic pricing and revenue management
6. Energy generation and distribution
7. Project management
Motivating “thought” experiment
Adjustable Robust Optimization

\[
\min_{x} c^T x + \max_{u \in U} \min_{y \in \Omega(x,u)} b^T y
\]

s.t. \(Ax \geq d, \ x \in S_x\)

\[
\Omega(x,u) = \{y \in S_y : Wy \geq h - Tx - Mu\}
\]

x: “here-and-now” decisions
y: “wait-and-see” decisions
u: uncertainty
Motivating “thought” experiment
Adjustable Robust Optimization

Model-Based Approaches:

1. One key approach – Assume linear decision rules:
   \[ y = q + Qu \]
   - Set \( y \) as an affine function of the uncertainty – simplifies the problem.
   - Can be solved as Static Robust Optimization

2. Generalized decision rules through multi-parametric programming:
   \[
   y = \begin{cases} 
   Q_1 u + P_1 x + q_1 & \text{if} & G_1 u + H_1 x \leq h_1 \\
   Q_2 u + P_2 x + q_2 & \text{if} & G_2 u + H_2 x \leq h_2 \\
   \vdots \\
   Q_n u + P_n x + q_n & \text{if} & G_n u + H_n x \leq h_n 
   \end{cases}
   \]
   - Solve the lower level problem multi-parametrically considering \( u \) and \( x \) as parameters
   - Arrive to a set of (exact) affine decision rules valid for the whole feasible space of \( u \) and “here-and-now” decisions \( x \).
   - Use M-POP to get the exact global solution
Motivating “thought” experiment
Adjustable Robust Optimization

Data-Driven Approaches:

3. Surrogate Modeling and Optimization within ARGONAUT
   • Development of surrogate approximations that correlate input data to the problem objective.
   • Use of derivative-based global optimization techniques to solve the optimization problem.

   • Used to express $y$ as an explicit function of $x$ and $u$.
   • $\epsilon$-SVR: Supervised learning algorithm.
   • Kernel functions transform nonlinear data to a higher dimensional space where there is a linear explanation of the input data.
   • Kernel function used:
     \[ e^{-\gamma |x-x_i|^2} \]
     Parameters: $\gamma$ ($\& C, \epsilon$)
Motivating “thought” experiment
Adjustable Robust Optimization
Sampling and Output Handling – Method 3

“Unsupervised”
- Solution via GAMS

\[
\begin{align*}
\min_{y \in \Omega(x,u)} & \quad b'y \\
\text{s.t.} & \quad Ax \geq d, \quad x \in S_x \\
\Omega(x,u) & = \{y \in S_y : Wy \geq h - Tx - Mu\}
\end{align*}
\]

“Supervised”
- Solution via B-POP

\[
\begin{align*}
\max_{x \in U} & \quad \min_{y \in \Omega(x,u)} b'y \\
\text{s.t.} & \quad Ax \geq d, \quad x \in S_x \\
\Omega(x,u) & = \{y \in S_y : Wy \geq h - Tx - Mu\}
\end{align*}
\]

**x**: “here-and-now” decisions  
**y**: “wait-and-see” decisions  
**u**: uncertainty
Motivating “thought” experiment

Adjustable Robust Optimization

Sampling and Output Handling – Method 4

---

**“Unsupervised”**
- Solution via GAMS
  \[
  \min_{y \in \Omega(x,u)} b'y
  \]
  \[
  \text{s.t. } Ax \geq d, \ x \in S_x
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**“Supervised”**
- Solution via B-POP
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  \max_{u \in U} \min_{y \in \Omega(x,u)} b'y
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  \Omega(x,u) = \{ y \in S_y : Wy \geq h - Tx - Mu \}
  \]

---

x: “here-and-now” decisions
y: “wait-and-see” decisions
u: uncertainty

Machine Learning via Support Vector Machines

y as a function of x and u
Motivating “thought” experiment

Instances:

<table>
<thead>
<tr>
<th>Linear/Non-Linear</th>
<th>Instance 1</th>
<th>Instance 2</th>
<th>Instance 3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Linear</td>
<td>Linear</td>
<td>Non-linear</td>
</tr>
<tr>
<td># of “here-and-now” variables</td>
<td>2 - continuous</td>
<td>3 - continuous 3 - binary</td>
<td>1 - continuous 2 - binary</td>
</tr>
<tr>
<td># of “wait-and-see” variables</td>
<td>2 - continuous</td>
<td>9 - continuous</td>
<td>3 - continuous</td>
</tr>
<tr>
<td># of sampling points used by the data-driven techniques</td>
<td>41 – Unsupervised 21 - Supervised</td>
<td>728 – Unsupervised 488 - Supervised</td>
<td>244 – Unsupervised 124 - Supervised</td>
</tr>
</tbody>
</table>
Motivating “thought” experiment

Results:
Value of the objective function:

<table>
<thead>
<tr>
<th></th>
<th>Instance 1</th>
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</thead>
<tbody>
<tr>
<td>Exact</td>
<td>451</td>
<td>30.536</td>
<td>7,320</td>
</tr>
<tr>
<td>Affine rules</td>
<td>451</td>
<td>33,680</td>
<td>----</td>
</tr>
</tbody>
</table>

Affine rules:

\[ y = q + Qu \]

Exact – Multi-parametric approach:

\[
y = \begin{cases} 
  Q_1 u + P_1 x + q_1 & \text{if } G_1 u + H_1 x \leq h_1 \\
  Q_2 u + P_2 x + q_2 & \text{if } G_2 u + H_2 x \leq h_2 \\
  \vdots \\
  Q_n u + P_n x + q_n & \text{if } G_n u + H_n x \leq h_n 
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Motivating “thought” experiment

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</tr>
<tr>
<td>“Unsupervised” (ARGONAUT)</td>
<td>860</td>
<td>Infeasible</td>
<td>Infeasible</td>
</tr>
<tr>
<td>“Supervised” (ARGONAUT)</td>
<td>452.8</td>
<td>Infeasible</td>
<td>8,150</td>
</tr>
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Surrogate Modeling and Optimization (ARGONAUT):
Motivating “thought” experiment

Results:
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</tr>
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- Approximations (such as Affine rules) may be sub-optimal
- Affine rules cannot be derived for non-linear problems – Instance 3
- Data-driven techniques (could) arrive to near optimal solutions only for continuous problems with “Supervised” data
- “Unsupervised” data resulted in infeasible solutions for mixed-integer problems
Motivating “thought” experiment
Results of the Machine Learning method:

<table>
<thead>
<tr>
<th>Instance 1</th>
<th>“Unsupervised”</th>
<th>“Supervised”</th>
</tr>
</thead>
<tbody>
<tr>
<td>y1</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>y2</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>y11</td>
<td>0.0313</td>
<td>1024</td>
</tr>
<tr>
<td>y12</td>
<td>0.0313</td>
<td>1024</td>
</tr>
<tr>
<td>y13</td>
<td>0.0313</td>
<td>512</td>
</tr>
<tr>
<td>y21</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>y22</td>
<td>0.0313</td>
<td>512</td>
</tr>
<tr>
<td>y23</td>
<td>0.0625</td>
<td>512</td>
</tr>
<tr>
<td>y31</td>
<td>0.0313</td>
<td>512</td>
</tr>
<tr>
<td>y32</td>
<td>0.0313</td>
<td>1024</td>
</tr>
<tr>
<td>y33</td>
<td>0.0313</td>
<td>1024</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Instance 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>y1</td>
</tr>
<tr>
<td>y2</td>
</tr>
<tr>
<td>y3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Instance 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>y1</td>
</tr>
<tr>
<td>y2</td>
</tr>
<tr>
<td>y3</td>
</tr>
</tbody>
</table>

Parameters of the function of $y$ in terms of $x$ and $u$

Root-Mean-Square Error

Machine Learning via Support Vector Machines

$y$ as a function of $x$ and $u$
Motivating “thought” experiment

Results of the Machine Learning method:

<table>
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<tbody>
<tr>
<td></td>
<td>$\gamma$</td>
<td>C</td>
<td>$\epsilon$</td>
<td>RMSE</td>
</tr>
<tr>
<td>Instance 1</td>
<td>$y_1$</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$y_2$</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$y_{11}$</td>
<td>0.0313</td>
<td>1024</td>
<td>0.1</td>
</tr>
<tr>
<td></td>
<td>$y_{12}$</td>
<td>0.0313</td>
<td>1024</td>
<td>0.1</td>
</tr>
<tr>
<td></td>
<td>$y_{13}$</td>
<td>0.0313</td>
<td>512</td>
<td>0.1</td>
</tr>
<tr>
<td></td>
<td>$y_{21}$</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Instance 2</td>
<td>$y_{22}$</td>
<td>0.0313</td>
<td>512</td>
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<td></td>
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<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$y_2$</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$y_3$</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

- Using “Unsupervised” data - we cannot form expression for $y$
- Using “Supervised” data - expressions for $y$ can be obtained for all cases (and are accurate)
Decision-making under uncertainty in 2040 – some remarks

- Data are important and useful provided that . .
  - The right type of data . .
  - The right amount of data . .
  - The right timing of data . .

- “Model-free”, “Variable-free”, “Equation-free” or “derivative-free” - a “myth”
  - A ‘model’ is always generated (with ‘variables’, ‘equations’ and use of ‘derivatives’!! – *within an algorithm*)

- Innovation/Design/Novel type of decisions *cannot* be obtained only by data!
  - Knowledge is essential

“Intelligent” data is the key
Decision-making under uncertainty in 2040 – some remarks

- Importance of
  - Algorithms
  - Hypothesis testing

- Big-Data Analytics
  - “virtual reality” modeling
  - “training” the algorithm (to create ‘intelligence’)

- Model-based Optimization
  - “reality” modelling
  - “training” the model (to create ‘intelligence’)

- Optimization is central in both!
  (Parameter estimation)

- Hybrid approach (?)

\[\text{Data} + \text{Models} + \text{Algorithms} \rightarrow \text{Solution}\]
Professor George Stephanopoulos

Happy 70th Birthday!
&
Happy Retirement!

Thank you for being such an Inspirational Intellectual Leader to all of us!!