Tom Edgar's Contribution to Model Reduction

as an introduction to

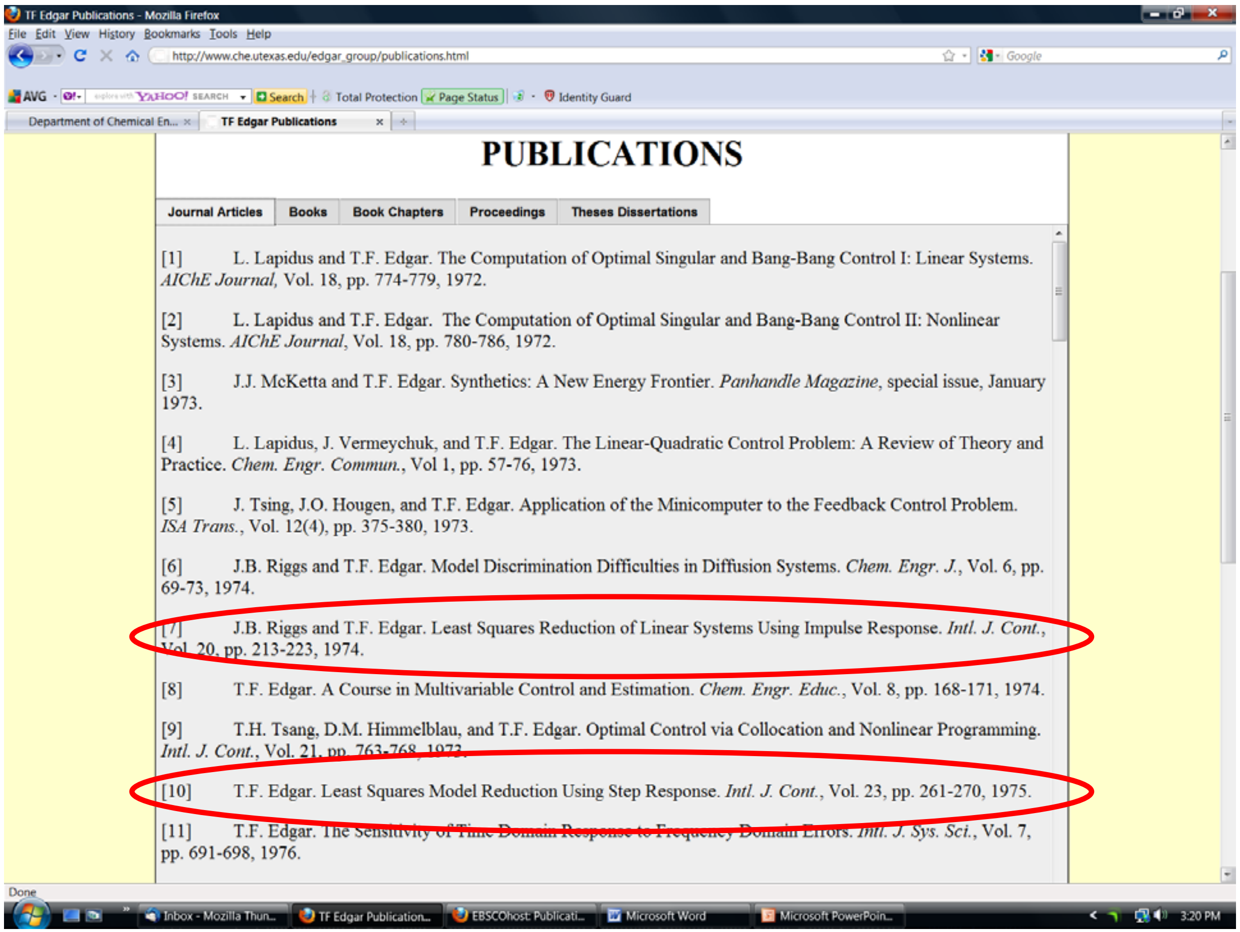
Global Sensitivity Analysis Procedure Accounting for Effect of Available Experimental Data

Yunfei Chu, Zuyi Huang, Mitchell Serpas, Juergen Hahn

Texas A& M University

Tom Edgar’s Contribution to Model Reduction

- Tom has had a long-standing interest in model reduction



PUBLICATIONS

Journal Articles | Books | Book Chapters | Proceedings | Theses Dissertations

[1] L. Lapidus and T.F. Edgar. The Computation of Optimal Singular and Bang-Bang Control I: Linear Systems. *AIChE Journal,* Vol. 18, pp. 774-779, 1972.

[2] L. Lapidus and T.F. Edgar. The Computation of Optimal Singular and Bang-Bang Control II: Nonlinear Systems. *AIChE Journal*, Vol. 18, pp. 780-786, 1972.

[3] J.J. McKetta and T.F. Edgar. Synthetics: A New Energy Frontier. *Panhandle Magazine*, special issue, January 1973.

[4] L. Lapidus, J. Vermeychuk, and T.F. Edgar. The Linear-Quadratic Control Problem: A Review of Theory and Practice. *Chem. Engr. Commun.*, Vol 1, pp. 57-76, 1973.

[5] J. Tsing, J.O. Hougen, and T.F. Edgar. Application of the Minicomputer to the Feedback Control Problem. *ISA Trans.*, Vol. 12(4), pp. 375-380, 1973.

[6] J.B. Riggs and T.F. Edgar. Model Discrimination Difficulties in Diffusion Systems. *Chem. Engr. J.*, Vol. 6, pp. 69-73, 1974.

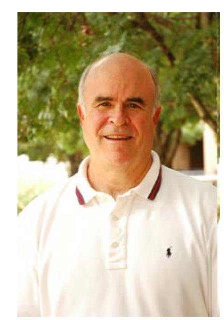
[7] J.B. Riggs and T.F. Edgar. Least Squares Reduction of Linear Systems Using Impulse Response. *Intl. J. Cont.*, Vol. 20, pp. 213-223, 1974.

[8] T.F. Edgar. A Course in Multivariable Control and Estimation. *Chem. Engr. Educ.*, Vol. 8, pp. 168-171, 1974.

[9] T.H. Tsang, D.M. Himmelblau, and T.F. Edgar. Optimal Control via Collocation and Nonlinear Programming. *Intl. J. Cont.*, Vol. 21, pp. 763-768, 1975.

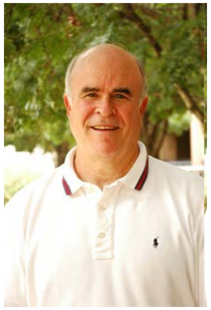
[10] T.F. Edgar. Least Squares Model Reduction Using Step Response. *Intl. J. Cont.*, Vol. 23, pp. 261-270, 1975.

[11] T.F. Edgar. The Sensitivity of Time-Domain Response to Frequency-Domain Errors. *Intl. J. Sys. Sci.*, Vol. 7, pp. 691-698, 1976.



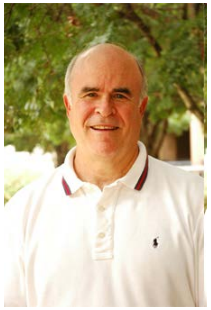
Tom Edgar's Contribution to Model Reduction

- Tom has supervised several dissertations dealing with aspects of model reduction, e.g.
  - L. S. Tung, 8/79, Analysis and Control of Large Scale Processes with Limited Measurements.
  - K. Edwards, 12/97. Kinetic Model Reduction Utilizing Optimization and Variable Selection Techniques.
  - J. Hahn, 5/02. A Balancing Approach to Analysis and Reduction of Nonlinear Systems.
  - J. Hedengren, 5/05. Real-time Estimation and Control of Large-scale Nonlinear DAE Systems.
  - S. Abrol, 8/09. Advanced Tabulation Techniques for Faster Dynamic Simulation, State Estimation and Flowsheet Optimization.



Tom Edgar's Contribution to Model Reduction

- Main motivation for model reduction was that we can build and simulate detailed models, but that they are often not suitable for real-time process control
- Fundamental models for processes involved in semiconductor manufacturing are a prime example of models that can benefit from reduction

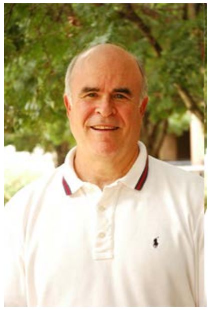


Tom Edgar's Contribution to Model Reduction

- Key to model reduction is identifying the parts of the model that contribute the most to the behavior that one is interested in

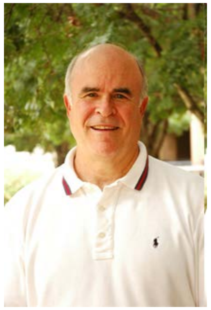
  → Sensitivity analysis

- Type of behavior is dependent upon the application



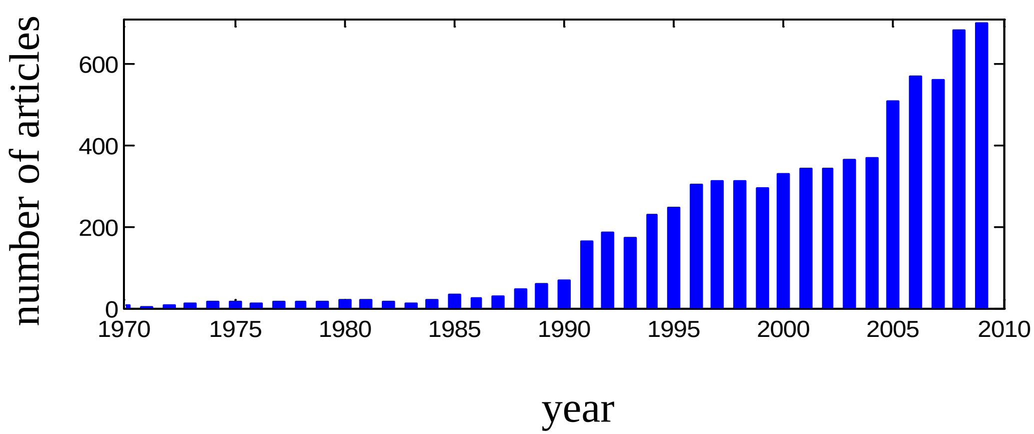
Tom Edgar's Contribution to Model Reduction

- My work under Tom's guidance ('97-'02):
  - Use balancing approach for nonlinear model reduction
  - Controllability analysis can be viewed as <u>sensitivity analysis</u> of effect that changes in inputs have on states
  - Observability analysis can be viewed as <u>sensitivity analysis</u> of effect that changes in states have on outputs
  - Balance (empirical) observability and controllability gramians to take both into account



Sensitivity Analysis

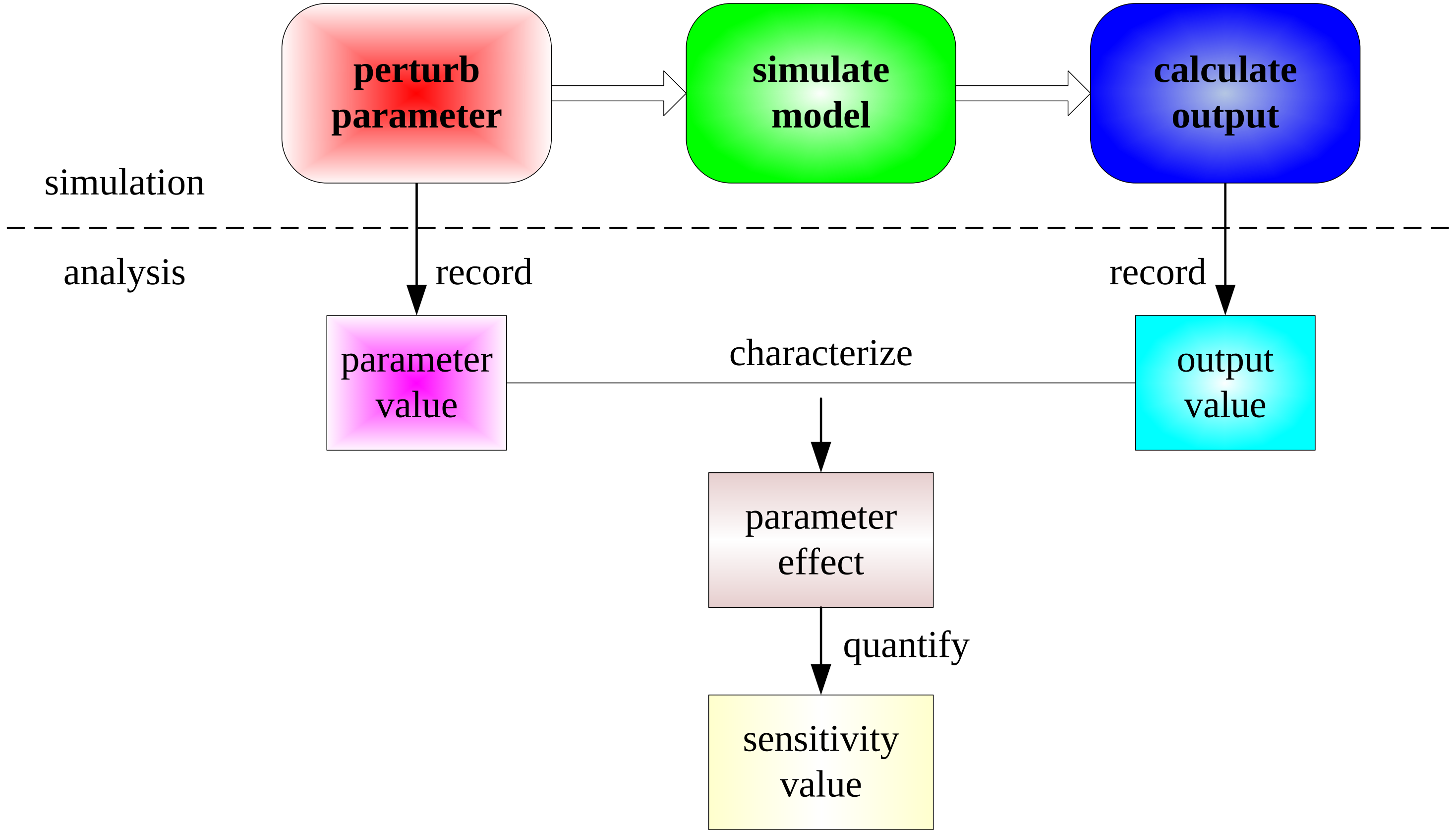
- Sensitivity analysis aims to investigate how a model component affects another component (i.e., usually output)
- Sensitivity analysis is an essential component in mathematical modeling and analysis



Data from Web of Science

Procedure of Sensitivity Analysis

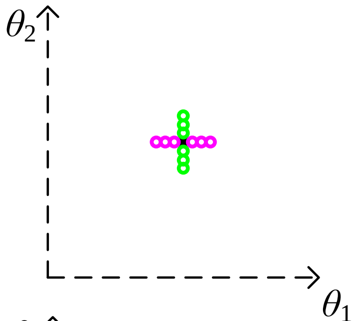
- Sensitivity analysis can be regarded as a systematic "perturbation analysis"



Ways to Perturb Parameter

- Sensitivity analysis procedures can be categorized as local sensitivity and global sensitivity analysis depending upon how parameter values are perturbed

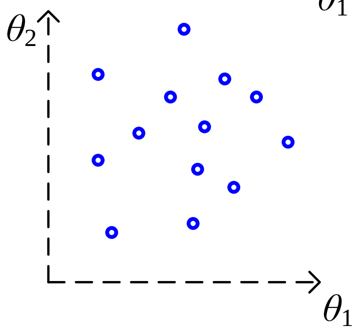
Local sensitivity analysis perturbs one parameter at a time in a small range



partial derivative:

$$s_i(t_j) = \partial y(t_j) / \partial \theta_i$$

Global sensitivity analysis perturbs multiple parameters simultaneously over a large range



conditional variance

$$s_i(t_j) = \mathrm{Var}\left[\mathrm{E}\left(y(t_j) \middle| \theta_i\right)\right]$$

It is generally acknowledged that global sensitivity is superior to local sensitivity for analyzing nonlinear models

Parameter Uncertainty

- Global sensitivity analysis varies parameter value according to information about parameter uncertainty
- Parameter uncertainty is often characterized by a probability density function
- Commonly used techniques for global sensitivity analysis use a (subjectively) assumed density function
- However, if experimental data are available it is more desirable to update parameter uncertainty from data

Challenges for Existing Global Sensitivity Analysis Techniques

- Integrating data into calculation of sensitivity value is not trivial for existing sensitivity analysis techniques
- One problem is correlation in parameter uncertainty updated from data
  - Shortcuts for uncorrelated parameters do not apply
  - Assumptions about some sensitivity measures are not met
- Another problem deals with constraints on variation of parameter value
  - Parameter values should be varied consistent with data while they are varied in a fixed specific way in many techniques

Problem Statement

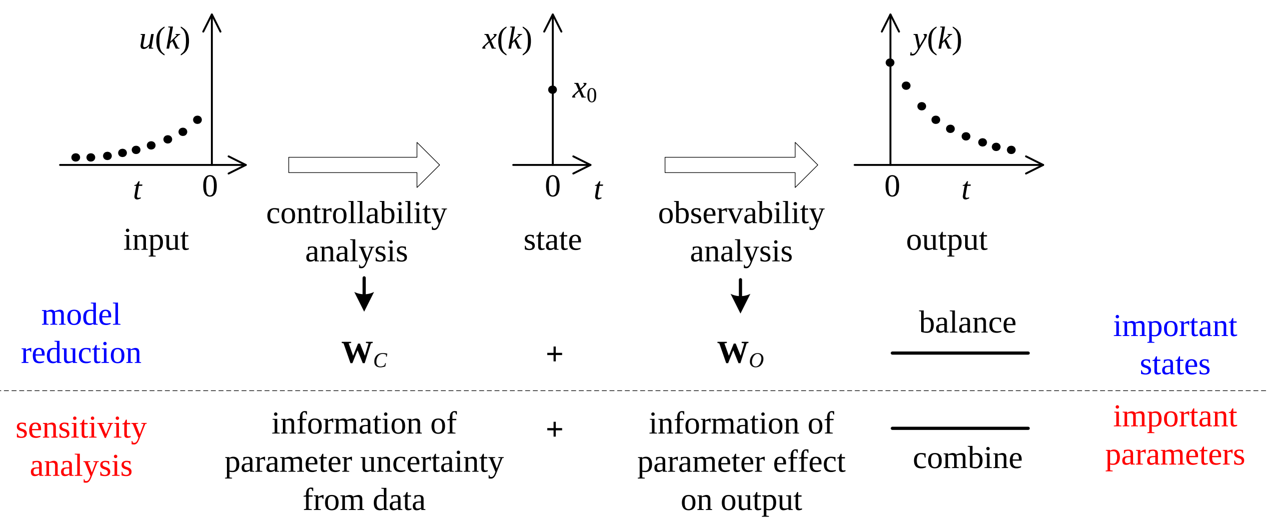
- Parameter-output relationship for sensitivity analysis is assumed to be $\mathbf{y} = \boldsymbol{\varphi}(\boldsymbol{\theta})$
- Relationship between data and parameters can be described by a regression model $\tilde{\mathbf{z}} = \mathbf{h}(\boldsymbol{\theta}) + \boldsymbol{\varepsilon}$
- Objective is to perform sensitivity analysis on output $\mathbf{y}$ with respect to parameter $\boldsymbol{\theta}$ conditioned on the data $\tilde{\mathbf{z}}$.
- Points to consider:
  - Variables of $\mathbf{y}$ are often different from those of $\tilde{\mathbf{z}}$.
  - Data are often not adequate to estimate all parameters accurately
  - Functions $\boldsymbol{\varphi}$ and $\mathbf{h}$ generally do not have an analytical solution

Presented Method

- Combination of two types of information

$$\tilde{\mathbf{z}} = \mathbf{h}(\boldsymbol{\theta}) + \boldsymbol{\varepsilon} \;\xrightarrow{\text{parameter uncertainty}}\; \boldsymbol{\theta} \;\xrightarrow{\text{parameter effect}}\; \mathbf{y} = \boldsymbol{\varphi}(\boldsymbol{\theta})$$

- Approach
  - Use a balancing approach, similar to the one used in model reduction



Formulation of Parameter Dynamic System

$$\tilde{\mathbf{z}} = \mathbf{h}(\boldsymbol{\theta}) + \boldsymbol{\varepsilon} \quad \Longrightarrow \quad \boldsymbol{\theta} \quad \Longrightarrow \quad \mathbf{y} = \boldsymbol{\varphi}(\boldsymbol{\theta})$$

characterize

$$p(\boldsymbol{\theta} | \tilde{\mathbf{z}}) = Cp(\tilde{\mathbf{z}} | \boldsymbol{\theta})\, p(\boldsymbol{\theta})$$

sample

$$\cdots \rightarrow \boldsymbol{\theta}^{k} \rightarrow \boldsymbol{\theta}^{k+1} \rightarrow \cdots \rightarrow \boldsymbol{\theta}^{m} \rightarrow \cdots$$

express

$$\boldsymbol{\theta}(k+1) = \boldsymbol{\pi}(\boldsymbol{\theta}(k), \xi(k)), \quad k < 0$$

where $\xi(k)$ is the input driving the chain

extend

$$\boldsymbol{\theta}(k+1) = \boldsymbol{\theta}(k)$$

rewrite

$$\begin{aligned} \boldsymbol{\theta}(k+1) &= \boldsymbol{\theta}(k) \\ \mathbf{y}(k) &= \boldsymbol{\varphi}(\boldsymbol{\theta}(k)) \end{aligned} \quad \text{for } k \geq 0$$

combine

$$\boldsymbol{\theta}(k+1) = \begin{cases} \boldsymbol{\pi}(\boldsymbol{\theta}(k), \xi(k)) & k < 0 \\ \boldsymbol{\theta}(k) & k \geq 0 \end{cases}$$

$$\mathbf{y}(k) = \boldsymbol{\varphi}(\boldsymbol{\theta}(k)) \qquad k \geq 0$$

Balancing Covariance Matrices

$$\boldsymbol{\theta}(k+1) = \begin{cases} \boldsymbol{\pi}(\boldsymbol{\theta}(k), \boldsymbol{\xi}(k)) & k < 0 \\ \boldsymbol{\theta}(k) & k \geq 0 \end{cases}$$

$$\mathbf{y}(k) = \boldsymbol{\varphi}(\boldsymbol{\theta}(k)) \qquad k \geq 0$$

Effect of data on parameters

$$\mathbf{W}_C = \frac{1}{n_t} \sum_{k=-n_t}^{0} \left(\boldsymbol{\theta}(k) - \boldsymbol{\mu}_\theta\right)\left(\boldsymbol{\theta}(k) - \boldsymbol{\mu}_\theta\right)^{\mathrm{T}}$$

$$\boldsymbol{\mu}_\theta = \frac{1}{n_t} \sum_{k=-n_t}^{0} \boldsymbol{\theta}(k)$$

Parameter-output effect

$$\mathbf{W}_O = \frac{1}{n_V} \sum_{i=1}^{n_V} \frac{1}{c_i^2} \mathbf{V}_i \sum_{k=0}^{n_t} \boldsymbol{\psi}_i(k) \mathbf{V}_i^{\mathrm{T}}$$

$$\boldsymbol{\psi}_i(k) = \left[\left(\mathbf{y}(k, \boldsymbol{\theta}_j^i) - \mathbf{y}(k, \bar{\boldsymbol{\theta}})\right)^{\mathrm{T}} \left(\mathbf{y}(k, \boldsymbol{\theta}_k^i) - \mathbf{y}(k, \bar{\boldsymbol{\theta}})\right)\right]_{jk}$$

Balancing

$$\mathbf{W}_C = \mathbf{L}\mathbf{L}^{\mathrm{T}}$$

$$\mathbf{L}^{\mathrm{T}} \mathbf{W}_O \mathbf{L} = \mathbf{U} \boldsymbol{\Lambda} \mathbf{U}^{\mathrm{T}}$$

$$\mathbf{T} = \mathbf{L}^{-\mathrm{T}} \mathbf{U} \boldsymbol{\Lambda}^{1/4}$$

$$\begin{bmatrix} \mathbf{t}_1 & \cdots & \mathbf{t}_n \end{bmatrix}^{\mathrm{T}}$$

combination coefficient

$$\mathrm{diag}\begin{bmatrix} \lambda_1 & \cdots & \lambda_n \end{bmatrix}^{\mathrm{T}}$$

score value

Case Study - Series Reaction

$$A \xrightarrow{\theta_1} B \xrightarrow{\theta_2} C$$

data

$$\tilde{t}_{\text{opt}} = \frac{\ln(\theta_1/\theta_2)}{\theta_1 - \theta_2} + \varepsilon$$

Effect of data on parameters

$$\mathbf{W}_C = \begin{bmatrix} 0.0477 & -0.0755 \\ -0.0755 & 0.2030 \end{bmatrix}$$

output

$$C_B(t) = \frac{\theta_1}{\theta_2 - \theta_1}\left(e^{-\theta_1 t} - e^{-\theta_2 t}\right)$$

Parameter-output effect

$$\mathbf{W}_O = \begin{bmatrix} 0.3415 & -0.0717 \\ -0.0717 & 0.2111 \end{bmatrix}$$

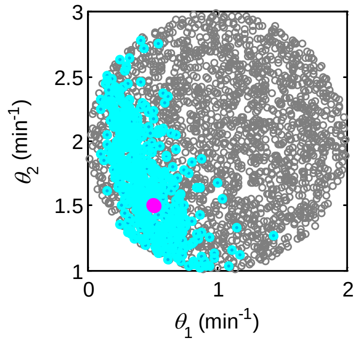
balancing

important $\bar{\mathbf{t}}_1 = [-0.6738 \quad 0.7389]^{\mathrm{T}}$ $\bar{\lambda}_1 = 0.9424$

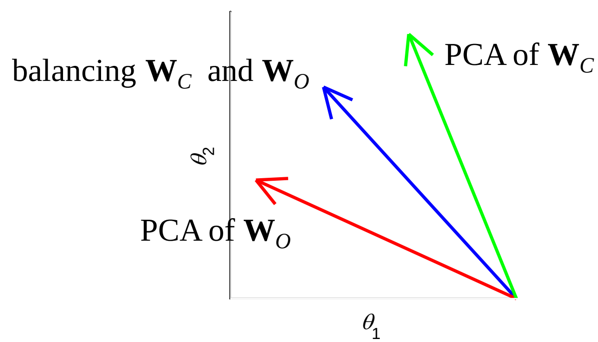
unimportant $\bar{\mathbf{t}}_2 = [0.9161 \quad 0.4010]^{\mathrm{T}}$ $\bar{\lambda}_2 = 0.0576$

combination score

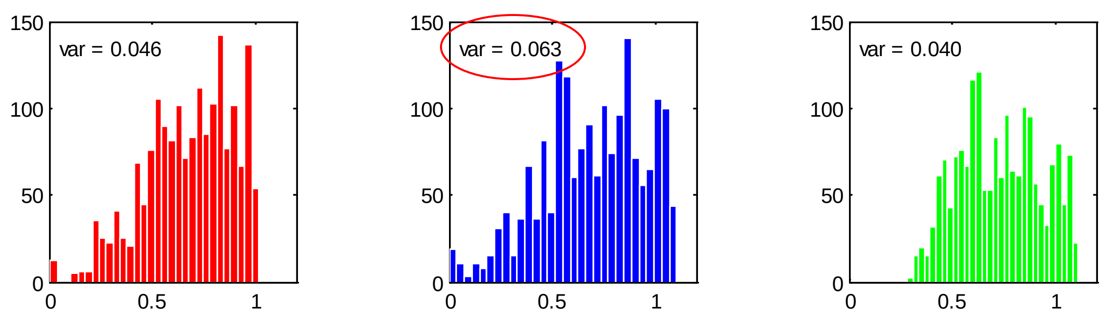
Result



sampling points from prior distribution (gray), sampling points from posterior distribution (cyan), and true parameter point (magenta)



most important directions identified from different types of information



Distribution of the norm of the output profile evaluated at each projected parameter point

Case Study - Non-isothermal CSTR

- **Model**

$$A \xrightarrow{k_1} U_1$$
$$A \xrightarrow{k_2} U_2$$
$$A \xrightarrow{k_P} P$$

- **Differential equations**

$$\frac{dC_A}{dt} = -k_1 C_A^3 - k_2 C_A^{0.5} - k_P C_A + \frac{C_{A_i} - C_A}{\tau}$$

$$\frac{dC_P}{dt} = k_P C_A - \frac{C_P}{\tau}$$

$$\frac{dT}{dt} = \frac{H_1 k_1 C_A^3 + H_2 k_2 C_A^{0.5} + H_P k_P C_A}{\rho_r c_r} + \frac{T_i - T}{\tau} + \frac{SU}{\rho_r c_r V_r}\left(T_j - T\right)$$

$$\frac{dT_j}{dt} = \frac{SU}{m_j c_j}\left(T - T_j\right)$$

$$k_1 = Z_1 \exp\left(-E_1/RT\right)$$
$$k_2 = Z_2 \exp\left(-E_2/RT\right)$$
$$k_P = Z_P \exp\left(-E_P/RT\right)$$

Problem Statement

- Parameters of interest
  - Frequency factors Z_1, Z_2, Z_3
  - Activation energies E_1, E_2, E_3
- Output for sensitivity analysis
  - Concentration of product C_P
- Data for parameter uncertainty
  - Reaction temperature T

Two Types of Information

- Parameter effect on output

$$
\mathbf{W}_O = \begin{bmatrix}
18.3 & -0.2 & -0.1 & 0.0 & 0.2 & -0.2 \\
-0.2 & 18.8 & 0.0 & 0.1 & -2.5 & 3.3 \\
-0.1 & 0.0 & 18.9 & -0.7 & 3.4 & -5.4 \\
0.0 & 0.1 & -0.7 & 20.5 & -4.9 & 12.1 \\
0.2 & -2.5 & 3.4 & -4.9 & 61.1 & -58.7 \\
-0.2 & 3.3 & -5.4 & 12.1 & -58.7 & 116.8
\end{bmatrix} \times 10^{2}
\quad
\begin{matrix} Z_1 \\ Z_2 \\ Z_P \\ E_1 \\ E_2 \\ E_P \end{matrix}
$$

$$
\begin{matrix} Z_1 & Z_2 & Z_P & E_1 & E_2 & E_P \end{matrix}
$$

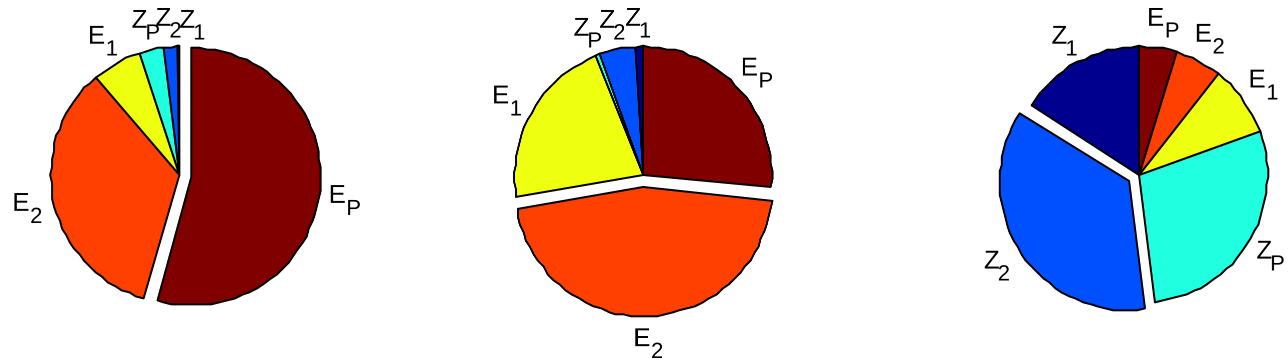
- Parameter uncertainty from data

$$
\mathbf{W}_C = \begin{bmatrix}
133.60 & -33.75 & -54.54 & 6.74 & -0.64 & -2.77 \\
-33.75 & 108.09 & -19.09 & -1.58 & 5.43 & -1.11 \\
-54.54 & -19.09 & 121.69 & -3.19 & -2.88 & 6.21 \\
6.74 & -1.58 & -3.19 & 0.37 & -0.03 & -0.16 \\
-0.64 & 5.43 & -2.88 & -0.03 & 0.40 & -0.14 \\
-2.77 & -1.11 & 6.21 & -0.16 & -0.14 & 0.32
\end{bmatrix} \times 10^{-4}
\quad
\begin{matrix} Z_1 \\ Z_2 \\ Z_P \\ E_1 \\ E_2 \\ E_P \end{matrix}
$$

$$
\begin{matrix} Z_1 & Z_2 & Z_P & E_1 & E_2 & E_P \end{matrix}
$$

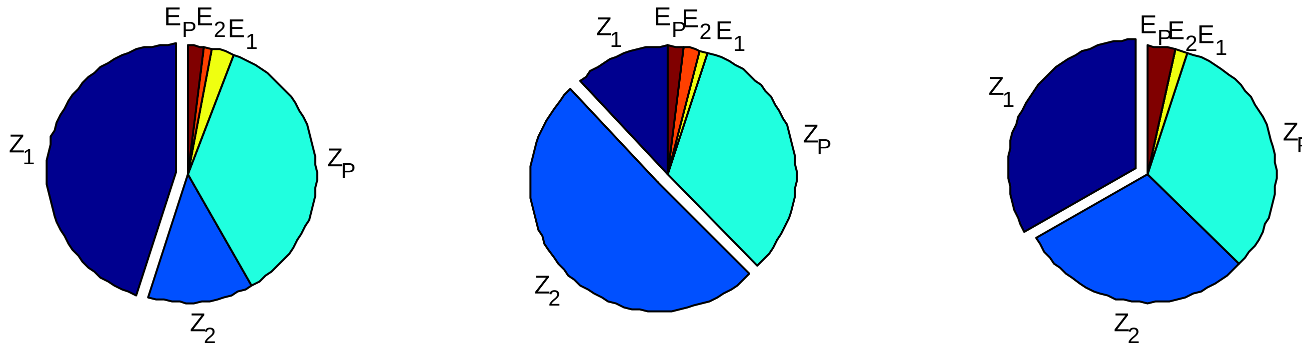
Important Parameter Combinations

- Without data



$\bar{\lambda}_1 = 0.61$ $\bar{\lambda}_2 = 0.10$ $\bar{\lambda}_3 = 0.07$

- With data



$\bar{\lambda}_1 = 0.51$ $\bar{\lambda}_2 = 0.35$ $\bar{\lambda}_3 = 0.13$

Discussion

- Important parameters without information from data
  - Activation energies E_1, E_2, E_3
- Important parameters with information from data
  - Frequency factors Z_1, Z_2, Z_3
- Uncertainty range of activation energies reduces more significantly than that of frequency factors
- Next experiment should be designed to improve the values of frequency factors

Conclusion

- Sensitivity analysis is an essential tool to identify influential parameters
- Advantage of global sensitivity over the local counterpart is that information of parameter uncertainty can be taken into account
- New global sensitivity analysis technique was introduced
- Information about parameter uncertainty from data is combined with information about parameter effect on output for calculating global sensitivity value
- Two case studies were provided to illustrate the technique

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Thank you, Tom!

DR. THOMAS F. EDGAR RESEARCH GROUP

University of Texas at Austin

Department of Chemical Engineering