**Motivation**

- Identification of Active Metabolic Pathways
  - Angles Between Subspaces
  - Correlation Distances between treatments

**Data-Driven Stoichiometric and Kinetic Modeling of Complex Reaction Systems**

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- Advisor: Prof. Christos Georgakis

**Modeling Approach**

- Assumptions
  - 1st Step: Stoichiometric Identification
  - 2nd Step: Kinetic Model Construction

- Stoichiometric Modeling
  - Reaction Mechanism Unknown
  - Based on Concentration over Time Data
  - Approximation of Stoichiometric Models

- Kinetic Modeling
  - Start Point: Library of Kinetic Models
  - Parameter Estimation
  - Structural Iteration on the Model

**Stoichiometric Identification Algorithm**

- Data Matrix
- Determination of Independent Reaction Number: r
- Tests on Targets
- Accuracy Calculation (average RMSE)
- Models Selection

**Assumptions**

- Angles between the Target Stoichiometries and the OSS
- Angles between the Target Stoichiometries
- Positive Reaction Extents, through Rotation of the Matrices

**Library of Kinetic Models**

- Power Law Model
  - Several Chemical Systems
- Inhibition Terms
  - Michaelis Menten
  - Biological Systems
  - Langmuir-Hinshelwood
  - Heterogeneous Catalytic Reactions

**Parameter Estimation**

- Estimation of Reaction Orders and Kinetic Rate Constants

**Software Tools:**

- Matlab (Mathworks Inc.)
- JACOBIAN (Numerica Technology Inc.)
- CVODES (MIT PSE lab)

**Conclusions**

- Industrial Impact:
  - Significant Reduction of the Time to the Market for New Pharmaceuticals
  - Tighter Control of the Production Process
  - Implementation of PAT - FDA demands

- Biological Systems:
  - Generate Specific Cellular Responses
  - Reverse Engineer Protein-to-Protein Reaction Networks

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**Figures**

- **Fig 1. Angles**
  - $\theta = \arccos \frac{t_1}{t_2}$
  - $\varphi = \arccos \frac{t_3}{t_4}$

- **Fig 2. Reaction Extents & Rotations**
  - Chart showing correlation distances between the subspaces.

- **Fig 3. Correlation Distances**
  - Chart illustrating the correlation distances between the subspaces for different treatments.

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