Nonlinear Stochastic Modeling and State Estimation of Weakly Observable Systems: Application to Industrial Polymerization Processes

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Presentation Outline

Introduction to State Estimation

- Definition: estimate the system states (x) from measurements (y)

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- Why estimate x?
  - x is required to model the system
  - performance of an advanced feedback control system is directly affected by the quality of state estimates
  - most complex product properties are not measurable
    - ★ they must be inferred from other measurements combined with nonlinear property models
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  - most complex product properties are not measurable
    - ⋆ they must be inferred from other measurements combined with nonlinear property models
  - x is corrupted with process noise (w) and y with sensor noise (v)
- Challenge of state estimation
  - determine good estimates in the face of noisy and incomplete output measurements

Moving Horizon Estimator

- Moving Horizon Estimator (MHE)
  - optimization-based state estimator
  - robust to process disturbances and model errors
  - naturally handles nonlinear models
  - incorporates process constraints in its formulation

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  - optimization-based state estimator
  - robust to process disturbances and model errors
  - naturally handles nonlinear models
  - incorporates process constraints in its formulation
- To provide high-quality estimates, MHE requires
  - accurate dynamic model of the process
  - knowledge on noise statistics
    - ★ affecting the states and measurements
    - ★ for zero-mean Gaussian sequences, covariances specify their statistics
    - ★ Autocovariance Least-Squares (ALS) technique estimates these covariances from data

Objectives

- Apply a previously proposed design method for nonlinear state estimation [1] to build and validate state estimators for industrial polymerization processes

[1] Lima, Rawlings, and Soderstrom (2008); Lima and Rawlings (2009)

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- This design method consists of the following steps
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- This design method consists of the following steps
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  - estimator selection and implementation
- Two processes are of particular interest
  - gas-phase ethylene copolymerization process (Literature)
  - industrial gas-phase ethylene copolymerization process (ExxonMobil)

[1] Lima et al. (2008); Lima and Rawlings (2009)

Challenges of Polymerization Process Models

- Polymerization process models
  - have unobservable and weakly observable modes
  - are nonlinear and large dimensional (around 50 states and 20 measurements)
  - product properties of interest are complex nonlinear functions of states
  - stochastic disturbance structure is unknown a priori
  - may be described by differential algebraic equations

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  - product properties of interest are complex nonlinear functions of states
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  - may be described by differential algebraic equations
- In addition, industrial polymerization processes
  - have asynchronous and infrequent laboratory measurements
  - are operated over a wide range of conditions

Nonlinear Stochastic Modeling

- Modeling approach relies on the combination of
  - a nonlinear deterministic model obtained from the integration of a first principles model

$$\frac{dx}{dt} = f(x, u) \Rightarrow x_{k+1} = F(x_k, u_k)$$

  - a stochastic component estimated from process operating data
    - ★ discrete and available every $\Delta_k = t_{k+1} - t_k$
    - ★ that provides a typical sample of measurement and process disturbances affecting the system

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- Resulting nonlinear, stochastic model in discrete time (DT)

$$x_{k+1} = F(x_k, u_k) + G(x_k)w_k$$
$$y_k = h(x_k) + v_k$$

in which $w_k \sim N(0, Q)$, $v_k \sim N(0, R)$

Noise Covariance Estimation for Nonlinear Systems

Consider the Nonlinear Model

$$x_{k+1} = F(x_k, u_k) + G(x_k) w_k \qquad w_k \sim N(0, Q)$$
$$y_k = h(x_k) + v_k \qquad v_k \sim N(0, R)$$

- Noise w_k affects all the states
- Noise v_k corrupts the measurements

Idea of Autocovariances

- The state noise w_k gets propagated in time
- The measurement noise v_k appears only at the sampling times and is not propagated in time
- Taking autocovariances of data at different time lags gives covariances of w_k and v_k

Autocovariance Least-Squares (ALS) Technique

- ALS estimates covariances of system disturbances (Q, R) from data [2]

[2] Odelson, Rajamani, and Rawlings (2006); Rajamani and Rawlings (2009); Rajamani, Rawlings, and Soderstrom (2007)

[3] Rajamani et al. (2007)

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- Probabilistic approach for state estimation

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- Equivalent least-squares problem when noises are Gaussian

$$\min_{x_0, x_1 \cdots x_k} \|x_0 - \bar{x}_0\|_{P^{-1}} + \sum_{i=0}^{k-1} w_i Q^{-1} w_i^T + v_i R^{-1} v_i^T$$

s.t.: nonlinear model and constraints

- in which (Q, R) are
  - covariances of nonlinear model
  - inverse of the weights of least-squares problem

[2] Odelson et al. (2006); Rajamani and Rawlings (2009); Rajamani et al. (2007)
[3] Rajamani et al. (2007)

- For covariance estimation, a general linear time-varying process model is proposed to
  - cope with potential plant-model mismatches
  - achieve offset-free performance for outputs

[4] Francis and Wonham (1975, 1976); Pannocchia and Rawlings (2003); Rajamani, Rawlings, and Qin (2009)

Covariance Estimation: Disturbance Modeling

- For covariance estimation, a general linear time-varying process model is proposed to
  - cope with potential plant-model mismatches
  - achieve offset-free performance for outputs
- We augment the state vector with an integrated white noise component d [4]
- For a general disturbance model

$$\frac{d}{dt}\begin{bmatrix} x \\ d \end{bmatrix} = f(x, u, d)$$

- The DT version of this model is obtained by integrating $f(x, u, d)$

$$\begin{aligned} x_{k+1} &= F(x_k, u_k, d_k) + G(x_k)w_k \\ d_{k+1} &= d_k + \xi_k \\ y_k &= h(x_k, d_k) + v_k \end{aligned}$$

  and we want to estimate the covariances of w_k, ξ_k and v_k

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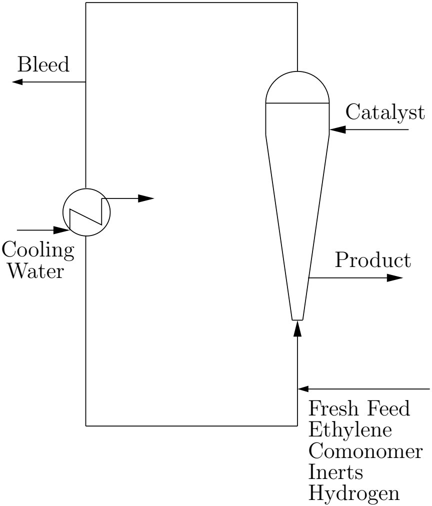
Ethylene Copolymerization Process (Literature)



Gani, Mhaskar, and Christofides (2007)

- Variables
  - 41 states
  - 17 measurements
  - 5 inputs
  - process and measurement noises
- Important variables
  - reactor temperature
  - reactor pressure
  - compositions
  - production rate
  - polymer properties
- First case study
  - noise added to temperature of recycle stream

- Simulated data are generated using published model [5]

[5] McAuley, MacGregor, and Hamielec (1990); Dadebo, Bell, McLellan, and McAuley (1997); Gani et al. (2007)

Ethylene Copolymerization Process: ALS Estimation

- Simulated data are generated using published model [5]
- Assume noise sequences $v_{\text{sim}} \sim N(0, R_{\text{sim}})$ and $w_{\text{sim}} \sim N(0, Q_{\text{sim}})$ with
  - $Q_{\text{sim}} = 2.80 \times 10^{-4}$;
  - $R_{\text{sim}} = 10^{-6} \times$ diag(5, 1, 10^4, 20, 300, 10, 200, 0.2, 0.5, 0.3, 0.04, 10^{-5}, 20, 1, 400, 300, 300)

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- Data sampling time is $\Delta_k = 60s$

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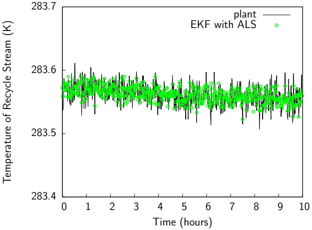
- Data sampling time is $\Delta_k = 60s$
- Applying ALS, the following covariances of w_k and v_k are estimated
  - $Q_{\text{als}} = 2.84 \times 10^{-4}$;
  - $R_{\text{als}} = 10^{-6} \times$ diag(5.03, 1, 9.7×10^3, 20.2, 308, 10.2, 198, 0.19, 0.5, 0.3, 0.04, 9.8×10^{-6}, 27.2, 0.99, 419, 289, 296)

[5] McAuley et al. (1990); Dadebo et al. (1997); Gani et al. (2007)

Ethylene Copolymerization Process (Literature): Estimator Implementation & Preliminary Conclusions

- Plot for the EKF using the ALS covariances



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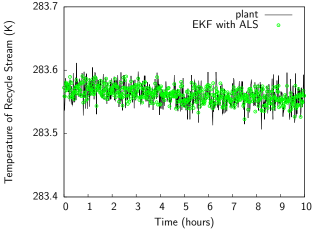

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- However, only the diagonal components of R and 1 process noise were estimated
  - due to an ill-conditioned full ALS problem

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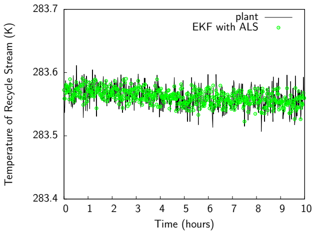

- Thus, ALS estimates the covariances accurately
- However, only the diagonal components of R and 1 process noise were estimated
  - due to an ill-conditioned full ALS problem
- Poor conditioning can be reduced or eliminated by
  - scaling of process model
  - designing a reduced-order extended Kalman filter
    - to estimate only the strongly observable system states
    - for covariance estimation

- Schmidt-Kalman filter (SKF) approach
  - originally developed for navigation systems to improve numerical stability of KF [6]
  - later used to tackle weakly observable systems [7]

[6] Schmidt (1966); Brown and Hwang (1997)
[7] Farrell and Barth (1998); Farrell (2008)

Weakly Observable Systems: Filtering Approach

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  - general idea
    - ★ remove weakly observable states in the KF gain calculation
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  - general idea
    - ★ remove weakly observable states in the KF gain calculation
    - ★ perform a well-conditioned calculation as only strongly observable modes are involved
  - resulting filter
    - ★ does not estimate the removed state variables
    - ★ still keeps track of the influences these states have on the gain applied to the other states

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Schmidt-Kalman Filter Approach

- Have system in its observability canonical form

$$\begin{bmatrix} x_o \\ \hline x_{no} \end{bmatrix}_{k+1} = \left[\begin{array}{c|c} A_o & 0 \\ \hline A_{21} & A_{no} \end{array}\right] \begin{bmatrix} x_o \\ \hline x_{no} \end{bmatrix}_k + \begin{bmatrix} G_o \\ \hline G_{no} \end{bmatrix} w_k$$

$$y_k = \begin{bmatrix} C_o & 0 \end{bmatrix} \begin{bmatrix} x_o \\ \hline x_{no} \end{bmatrix}_k + v_k$$

in which (A_o, C_o) is observable

- In this structure
  - x_o are the observable modes
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- Calculate KF gain for observable system, L_o, using A_o, C_o and G_o

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- Calculate KF gain for observable system, L_o, using A_o, C_o and G_o
- Augment L_o with zeros as $\bar{L} = \left[\begin{array}{c} L_o \\ \hline 0 \end{array}\right]$
- Physical states

$$\hat{x}_{k+1|k+1} = F(\hat{x}_{k|k}, u_k, d_k) + L[y_{k+1} - h(\hat{x}_{k+1|k}, d_{k+1})]$$

  in which $L = T\bar{L}$ and T is a similarity transformation matrix

Ethylene Copolymerization Process (Literature) Revisited: SKF Results

- Now consider the case in which 3 process noises are added to
  - hydrogen concentration
  - reactor temperature
  - cooler cooling water temperature

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  - $Q_{\mathrm{sim}} = \mathrm{diag}(5 \times 10^{-11},\ 2 \times 10^{-4},\ 0.5)$
  - $R_{\mathrm{sim}} = \mathrm{diag}(0.02, 5 \times 10^{-4}, 6 \times 10^{4}, 0.3, 80, 0.07, 40, 1.5 \times 10^{-5}, 2 \times 10^{-4}, 5 \times 10^{-5}, 1 \times 10^{-6}, 1 \times 10^{-13}, 0.2, 6 \times 10^{-4}, 100, 50, 55)$

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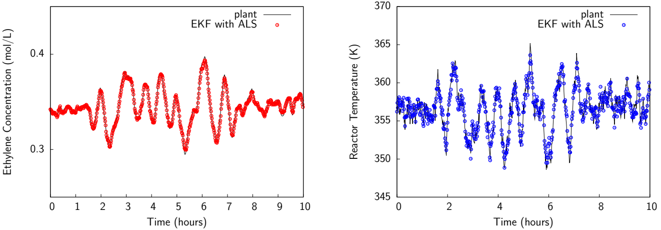
- And the ALS estimated values are
  - $Q_{\text{als}} = \text{diag}(5 \times 10^{-11},\ 1.8 \times 10^{-4},\ 0.43)$
  - $R_{\text{als}} = \text{diag}(0.03, 5.1 \times 10^{-4}, 6 \times 10^{4}, 0.3, 84, 0.07, 46, 1.9 \times 10^{-5}, 2.4 \times 10^{-4}, 5.9 \times 10^{-5}, 1 \times 10^{-6}, 1.5 \times 10^{-13}, 0.5, 6.1 \times 10^{-4}, 114, 60, 59)$

Ethylene Copolymerization Process (Literature): Estimation Results & Conclusions

- Plot for EKF with statistics determined by ALS



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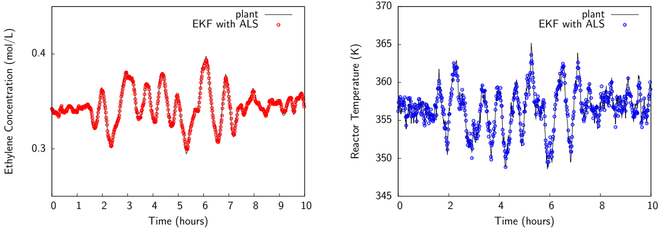

- Thus, after applying model scaling and SKF approach
  - better conditioned state and covariance estimation problems are obtained
  - ALS is now able to estimate multiple process noises
  - good results were also obtained for previous case with 1 process noise

Industrial Ethylene Copolymerization Process (ExxonMobil)

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- Project goals
  - have model predictions match process measurements
  - implement state estimators (EKF/MHE) and estimate their noise covariances

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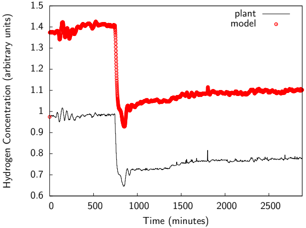
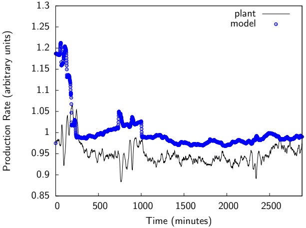
- Plots for original model predictions





Industrial Ethylene Copolymerization: Results After Disturbance Modeling

- Proposed approach to improve predictions
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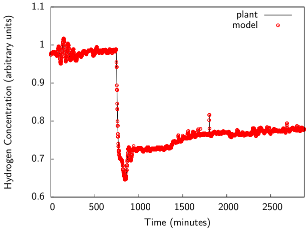

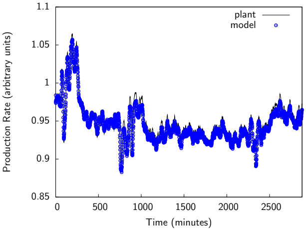

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  - NSF DDDAS grant #CNS–0540147
  - PRF grant #43321–AC9
  - TWCCC participants

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