Parameter Estimation in Continuous-Time Dynamic Models with Uncertainty

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Journal Articles

- Poyton, A.A., M.S. Varziri, K.B. McAuley, P.J. McLellan and J.O. Ramsay (2006) “Parameter estimation in continuous-time dynamic models using principal differential analysis”, *Computers & Chemical Engineering* **30**, 698-708.
- M.S. Varziri, A.A. Poyton, K.B. McAuley, P.J. McLellan and J.O. Ramsay (2008) “Selecting optimal weighting factors in iPDA for parameter estimation in continuous-time dynamic models” *Computers & Chemical Engineering* **32**, 3011-3022.
- M.S. Varziri, K.B. McAuley and P.J. McLellan (2008) “Parameter estimation in continuous-time dynamic models in the presence of unmeasured states and nonstationary disturbances” *Ind. Eng. Chem. Res.* **47**, 380-393.
- M.S. Varziri, K.B. McAuley and P.J. McLellan (2008) “Parameter and state estimation in nonlinear continuous-time dynamic models with unknown disturbance intensity” *Can. J. Chem. Eng.* **86**, 828-837.
- M.S. Varziri, K.B. McAuley and P.J. McLellan (2008) “Approximate maximum likelihood parameter estimation for nonlinear dynamic models: application to a laboratory-scale nylon reactor model” *Ind. Eng. Chem. Res.* **47**, 7274-7283.

1. Chemical engineers develop fundamental dynamic models based on knowledge of chemical and physical phenomena

2. Parameter estimation is a difficult problem
   - Two sources of uncertainty
     - Measurement noise
     - Disturbances that influence future behaviour

1. Chemical engineers develop fundamental dynamic models based on knowledge of chemical and physical phenomena

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Proposed parameter estimation techniques account for both sources of uncertainty:

- Iterative Principal Differential Analysis
- Approximate Maximum Likelihood Estimation

Why Model Chemical Reactors?

Objectives of Chemical Companies: $$$

- Produce chemicals and polymers with targeted properties
- Make different product grades efficiently in a single reactor
- Devise improved reactor operating strategies
- Bring new products to market quickly
- Develop process knowledge for trouble-shooting

Models can help companies to:

- Train operators
- Design and test automatic control schemes
- Optimize grade changeover policies
- Simulate effects of process conditions and equipment design on product properties and production rates
- Plan experiments
- Test theories about what has gone wrong
- Capture, store and distribute knowledge

Fundamental Models of Chemical Processes

Where do model equations come from?

- Material balances on chemical species, and energy balances
  - Modeler converts mythology and assumptions into mathematical expressions
  - Algebraic equations, ODEs, PDEs
- Additional equations that describe:
  - Rates of chemical reactions
  - Movement of chemical species from one phase to another

Fundamental Models of Chemical Processes

Example - Polyethylene model for INEOS (BP Chemicals)

- 22 nonlinear ODEs
- 45 parameters

– Model predicts:
  - reactant gas composition (ethylene, hexene, hydrogen)
  - polymer production rate
  - polymer properties

  using reactant feed rates and reactor temperature

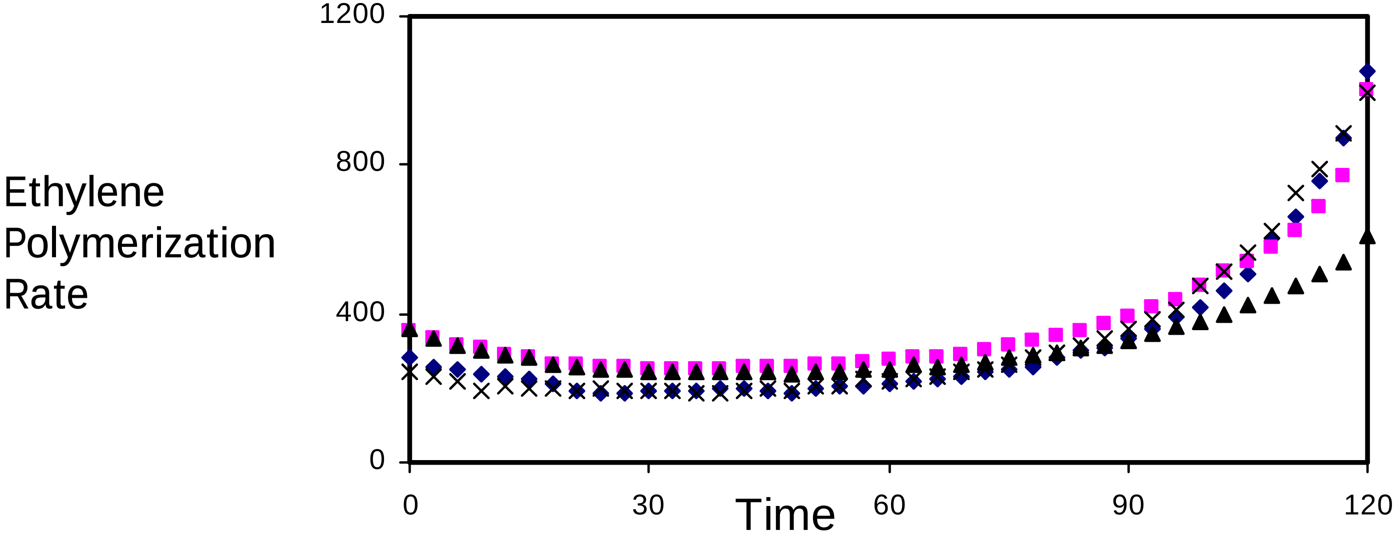
– Model for scale-up from laboratory to commercial reactors
  - Use knowledge from model to reduce the number of steps and experiments required

The Parameter Estimation Problem in Dynamic Chemical Reactor Models

- Experimental situation
  - Measurements at irregular sampling times
  - Results from replicate experiments vary due to
    - Disturbances that enter the reactor and influence future behaviour
    - Uncertainties in initial reactor conditions and input-variable trajectories

- Model equations
  - Typically 10-100 ODEs and 15-50 parameters
  - Many simplifying assumptions
  - Unknown initial values for some state variables

Four Replicates of a Dynamic Experiment



- **Any model that we fit through these data will result in correlated residuals.**
- **In dynamic systems, random errors at one time influence future responses.**
- **How should we account for this deviation from traditional least-squares assumptions during parameter estimation and model testing?**

Traditional Parameter Estimation in a Differential Equation

$$\frac{dx}{dt} = f(x, u, \theta), \quad x(0) = x_0$$

$$y_i = x_i + \varepsilon_\iota \qquad (i = 1, \ldots n) \qquad \varepsilon_\iota \sim N(0, \sigma_{\mathrm{m}}^2)$$

- Estimate the model parameters θ, given noisy observations y and known system inputs u.

$$J = \sum_{i=1}^{n} \left(y_i - \hat{x}_i(\theta) \right)^2$$

- We assume: 1) model structure is perfect
  2) u and x_0 are perfectly known
  3) measurements have random error

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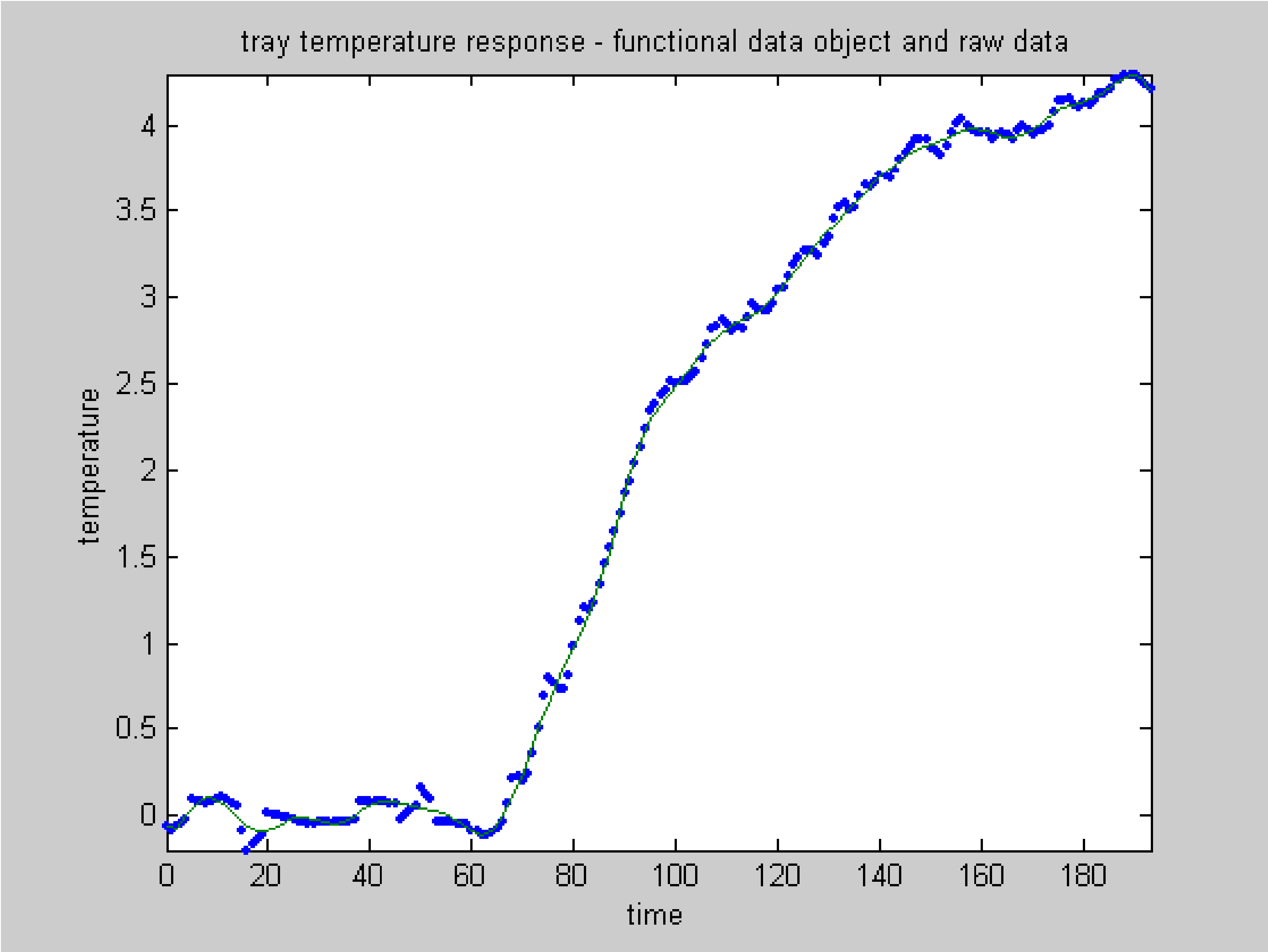
- Requires repeated numerical solution of ODE each time the optimizer guesses new parameter values
- If initial conditions are unknown, they are estimated along with the parameters

Our First Algorithm (iPDA)

- Fit an empirical curve $x_{\sim}(t)$ to the dynamic data using B-splines

$$J_1 = \sum \left(y(t_i) - x_{\sim}(t_i, \beta) \right)^2$$

Dynamic Data and B-Spline Curve



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- Determine parameter values θ to satisfy ODE as much as possible with β fixed

$$J_2 = \int_{t_0}^{t_f} \left(\frac{dx_{\sim}}{dt} - f(x_{\sim}, u, \theta) \right)^2 dt$$

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$$J_2 = \int_{t_0}^{t_f} \left(\frac{dx_{\sim}}{dt} - f(x_{\sim}, u, \theta) \right)^2 dt$$

- Adjust spline parameters β using a model-based penalty with θ fixed

$$J_3 = \sum \left(y(t_i) - x_{\sim}(t_i, \beta) \right)^2 + \lambda \int_{t_0}^{t_f} \left(\frac{dx_{\sim}}{dt} - f(x_{\sim}, u, \theta) \right)^2 dt$$

- Iterate between steps 2 and 3 until convergence

Is iPDA any good?

- No need for repeated numerical solution of ODE
  - No stability problems for bad parameter values
- No initial conditions required
- Easy to handle non-uniformly sampled data

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- No need for repeated numerical solution of ODE
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- No initial conditions required
- Easy to handle non-uniformly sampled data
- During the parameter-estimation step, minimize residuals between spline curve and fundamental model using the differentiated form of the model

$$J_2 = \int_{t_0}^{t_f} \left(\frac{dx_{\sim}}{dt} - f(x_{\sim}, u, \theta) \right)^2 dt$$

Model error

- During the spline-fitting step, minimize deviations from the data

$$J_3 = \sum \left(y(t_i) - x_{\sim}(t_i, \beta) \right)^2 + \lambda \int_{t_0}^{t_f} \left(\frac{dx_{\sim}}{dt} - f(x_{\sim}, u, \theta) \right)^2 dt$$

Measurement error

An Epiphany

- IPDA is equivalent to selecting θ and β simultaneously to minimize:

$$J = \sum \left(y(t_i) - x_{\sim}(t_i, \beta) \right)^2 + \lambda \int_{t_0}^{t_f} \left(\frac{dx_{\sim}}{dt} - f(x_{\sim}, u, \theta) \right)^2 dt$$

An Epiphany

- IPDA is equivalent to selecting θ and β simultaneously to minimize:

$$J = \sum \left(y(t_i) - \underset{\sim}{x}(t_i, \beta) \right)^2 + \lambda \int_{t_0}^{t_f} \left(\frac{d\underset{\sim}{x}}{dt} - f(\underset{\sim}{x}, u, \theta) \right)^2 dt$$

- This is the solution, but what is the underlying statistical problem?
- What is an appropriate value of λ?
- What happens in multi-response problems?
- What if some states aren't measured?
- How can we enforce known initial conditions?

AMLE, a Proposed Parameter-Estimation Technique for Stochastic DEs

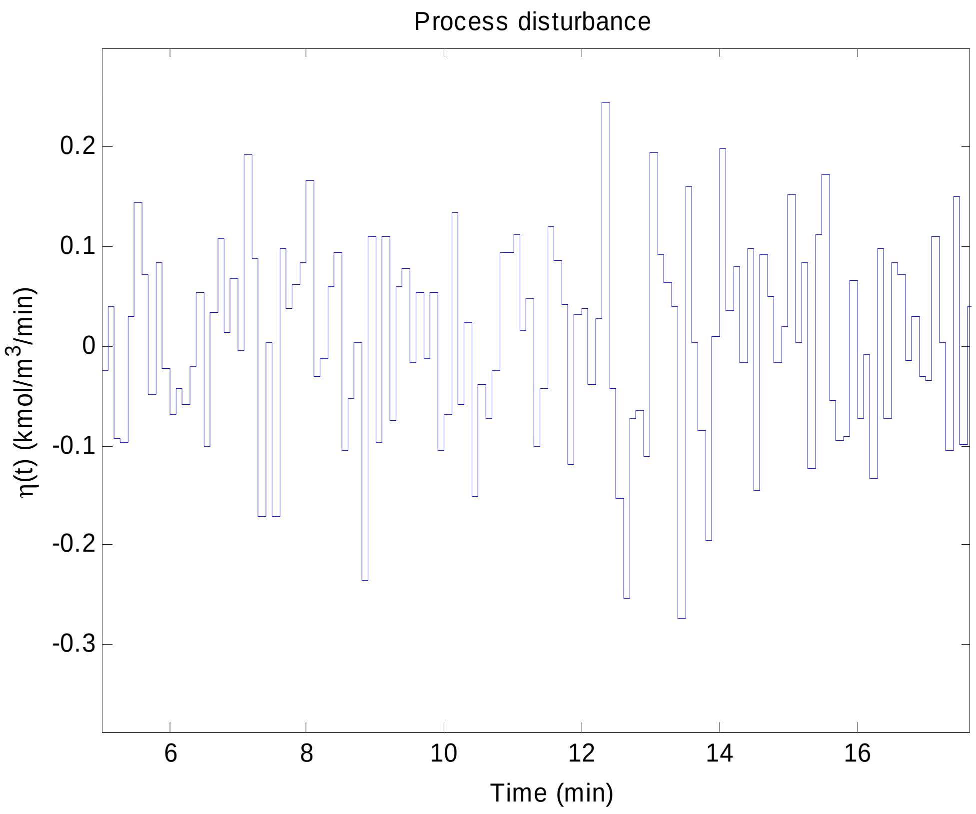
$$\frac{dx}{dt} = f(x,u,\theta) + \eta(t), \quad x(0) = x_0$$

$$y_i = x_i + \varepsilon_\iota \qquad (i = 1,\ldots n) \qquad \varepsilon_\iota \sim N(0,\sigma_{\mathrm{m}}^2)$$

$$E(\eta(t)\eta(t-\tau)) = Q\,\delta(\tau)$$

- Two noise sources
  - Measurement noise
  - Stochastic process disturbances that can account for
    - Uncertainties in u
    - Unknown or unmeasured inputs
    - Structural imperfections in model

Random Process Disturbance



AMLE, a Proposed Parameter Estimation Technique for Stochastic DEs

$$\frac{dx_{\sim}}{dt} = f(x_{\sim}, u, \theta) + \eta(t), \quad x_{\sim}(0) = x_0$$

$$y_i = x_{\sim i} + \varepsilon_\iota \qquad (i = 1, \ldots n)$$

- Our approach:
  - Assume that the solution to the differential equations can be represented using B-splines or other basis functions:

$$x(t) \cong x_{\sim}(t) = \sum_{i=1}^{b} \varphi_i(t)\beta_i$$

$\frac{dx_{\sim}(t)}{dt}$ is used to convert ODEs into algebraic equations

Approximate Maximum-Likelihood Estimation

- Assume the solution of the dynamic system can be well approximated by B-splines with unknown coefficients β
- Estimate the fundamental model parameters θ and the unknown spline coefficients β
  - Select $\hat{\theta}$ and $\hat{\beta}$ to minimize

Weighting factor

$$J = \sum_{i=1}^{n} \left(y_i - x_{i\sim} \right)^2 + \lambda \int \left(\frac{dx_{\sim}(t)}{dt} - f(x_{\sim}(t), \mathbf{u}(t), \boldsymbol{\theta}) \right)^2 dt$$

Deviations from data

Deviations from model

- Objective function arises from maximizing conditional joint density function of the states and measurements, given the parameters

What Weighting to Use?

$$J = \sum_{i=1}^{n} \left(y_i - x_{i\sim} \right)^2 + \lambda \int \left(\frac{dx_{\sim}(t)}{dt} - f(x_{\sim}(t), \mathbf{u}(t), \boldsymbol{\theta}) \right)^2 dt$$

- Heuristically
  - A large λ is appropriate when
    - Model is accurate and data are noisy
  - A small λ is appropriate when
    - Data are good and model is inaccurate

What Weighting to Use?

$$J = \sum_{i=1}^{n} \left(y_i - x_{i\sim} \right)^2 + \lambda \int \left(\frac{dx_{\sim}(t)}{dt} - f\left(x_{\sim}(t), \mathbf{u}(t), \boldsymbol{\theta}\right) \right)^2 dt$$

- Heuristically
  - A large λ is appropriate when
    - Model is accurate and data are noisy
  - A small λ is appropriate when
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$$\lambda_{opt} = \frac{\sigma_m^2}{Q}$$

Very large λ corresponds to traditional least-squares parameter estimation, which assumes a perfect model and no disturbances

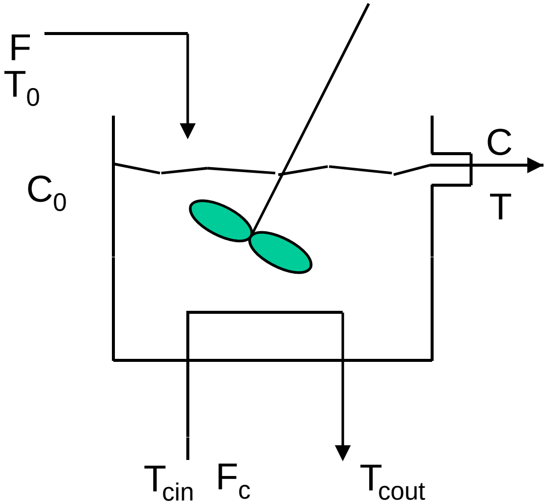
Objective Function for a Multivariate Example with Known Variances

$$J = \frac{1}{\sigma_{m1}^2}\sum_{j=1}^{n_1}\left(y_1(t_{m1j}) - x_{1\sim}(t_{m1j})\right)^2 + \frac{1}{Q_1}\int_{t=0}^{t_f}\left(\frac{dx_{1\sim}}{dt} - f_1\left(x_{1\sim}, x_{2\sim}, \mathbf{u}, \boldsymbol{\theta}\right)\right)^2 dt$$

$$+ \frac{1}{\sigma_{m2}^2}\sum_{j=1}^{n_2}\left(y_2(t_{m2j}) - x_{2\sim}(t_{m2j})\right)^2 + \frac{1}{Q_2}\int_{t=0}^{t_f}\left(\frac{dx_{2\sim}}{dt} - f_2\left(x_{1\sim}, x_{2\sim}, \mathbf{u}, \boldsymbol{\theta}\right)\right)^2 dt$$

Straightforward to write J for models with many ODEs (or DAEs) and for problems with unmeasured states

Reactor Example with Nonstationary Disturbance in Material Balance



$$\frac{dC}{dt} = f_1(C, T, \mathbf{u}, \boldsymbol{\theta}) + w + \eta_1 \qquad C(0) = 1.569 \text{ (kmol/m}^3\text{)}$$

$$\frac{dT}{dt} = f_2(C, T, \mathbf{u}, \boldsymbol{\theta}) + \eta_2 \qquad T(0) = 341.37 \text{ (K)}$$

$$\frac{dw}{dt} = \eta_3 \qquad w(0) = 0 \text{ (kmol/m}^3\text{/t)}$$

$$y_1(t_i) = C(t_i) + \varepsilon_1(t_i) \qquad (i = 1, \ldots, 64)$$

$$y_2(t_j) = T(t_j) + \varepsilon_2(t_j) \qquad (j = 1, \ldots, 213)$$

w could be a drifting flow rate or feed concentration disturbance (or a leak)

Reactor Example

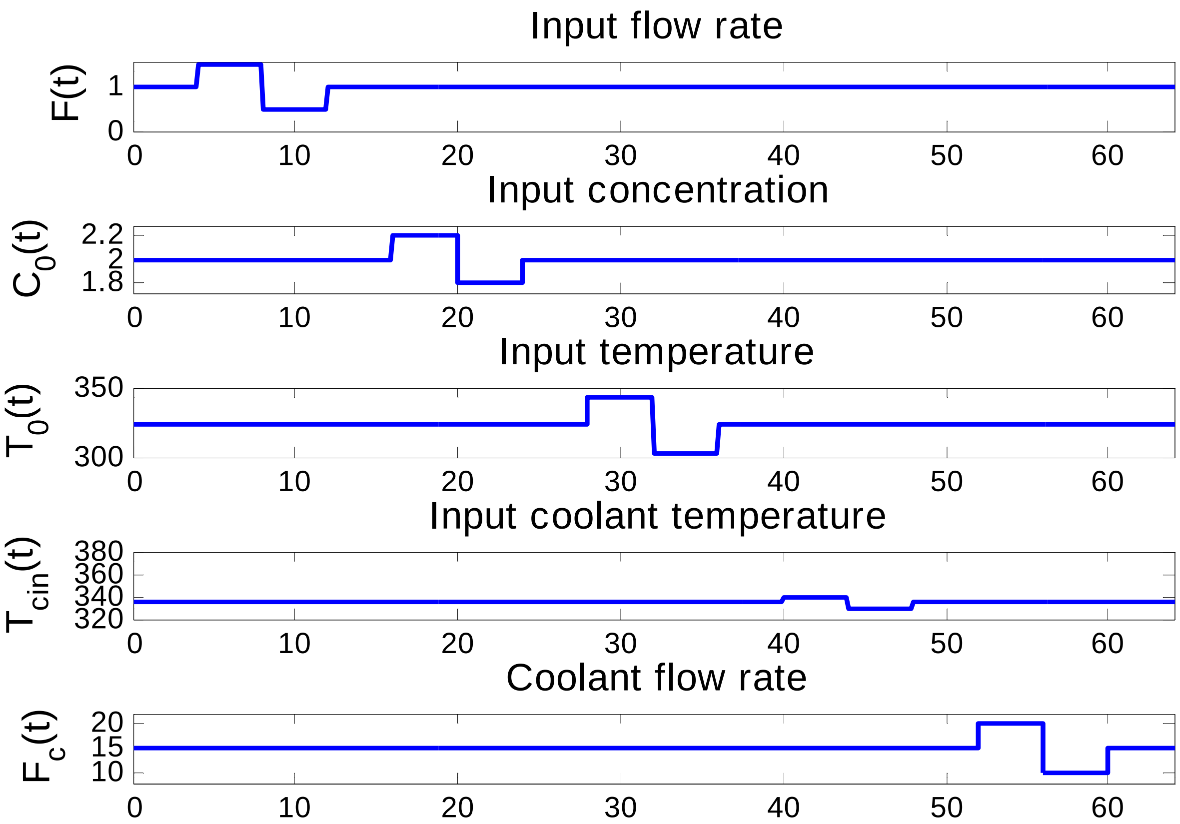
- Objective function for parameter estimation is:

$$\frac{1}{\sigma_{m1}^2}\sum_{j=1}^{64}\left(y_1(t_{m1j})-C_{\sim}(t_{m1j})\right)^2+\frac{1}{Q_{p1}}\int_{t=0}^{64}\left(\frac{dC_{\sim}}{dt}-f_1\left(T_{\sim},C_{\sim},\mathbf{u},\boldsymbol{\theta}\right)-w_{\sim}(t)\right)^2 dt$$

$$+\frac{1}{\sigma_{m2}^2}\sum_{j=1}^{213}\left(y_2(t_{m2j})-T_{\sim}(t_{m2j})\right)^2+\frac{1}{Q_{p2}}\int_{t=0}^{64}\left(\frac{dT_{\sim}}{dt}-f_2\left(T_{\sim},C_{\sim},\mathbf{u},\boldsymbol{\theta}\right)\right)^2 dt$$

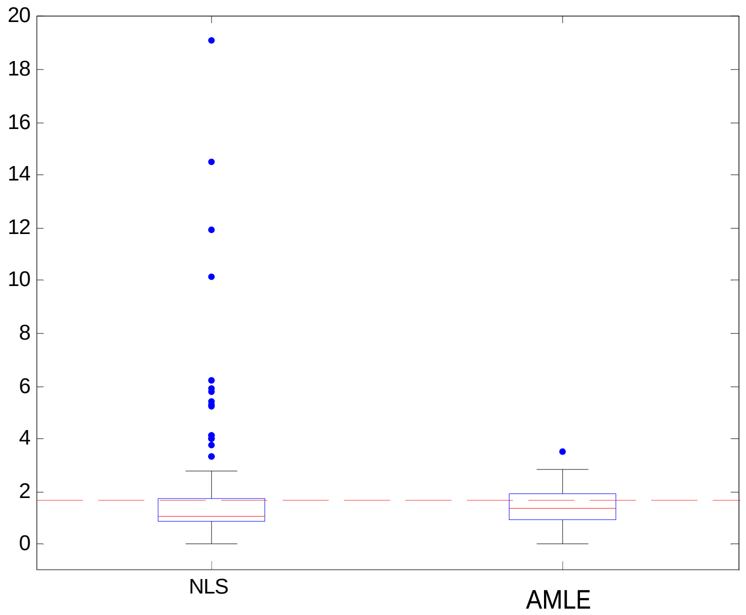
$$+\frac{1}{Q_{p3}}\int_{t=0}^{64}\left(\frac{dw_{\sim}}{dt}\right)^2 dt$$

Input Sequence u(t) for Simulated Experiments

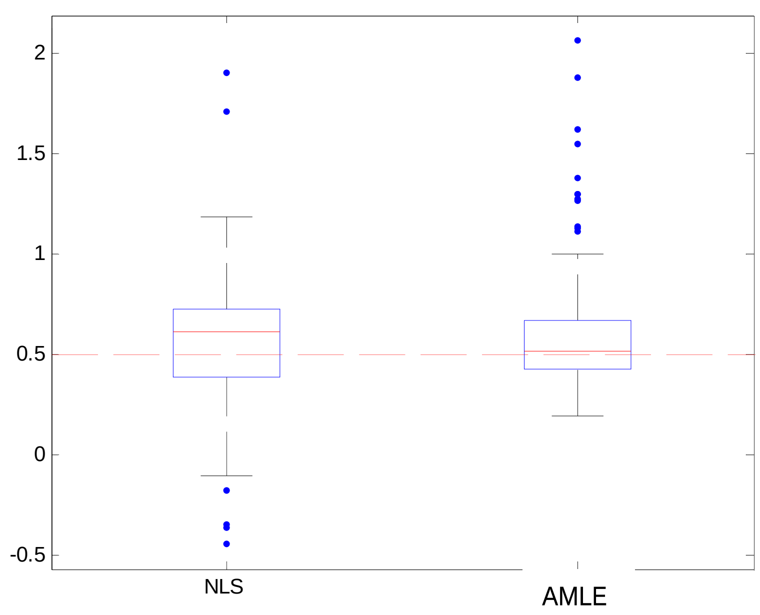


Parameter Estimation Results from Monte-Carlo Simulations of CSTR Example

- 4 parameters, a, b, E/R and k_{ref} were estimated using AMLE and traditional method nonlinear least squares (NLS)

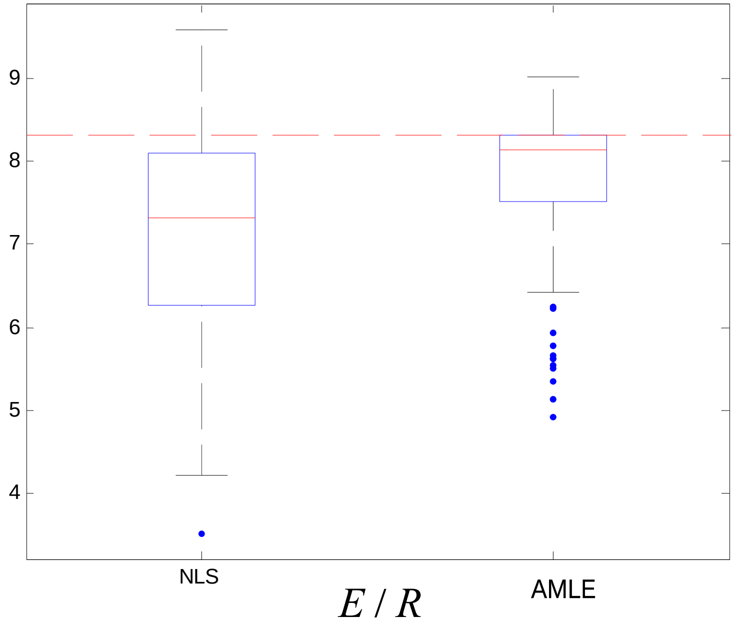


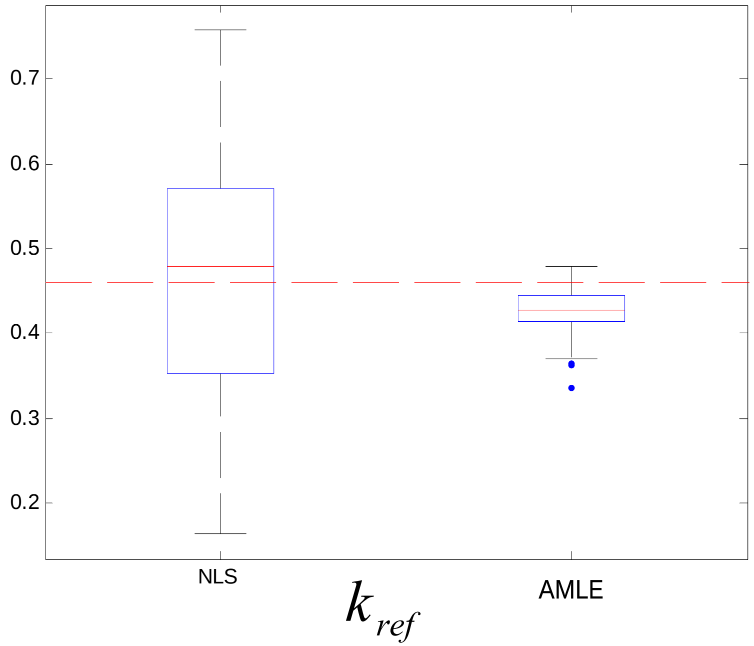
a



b

Parameter Estimation Results from Monte-Carlo Simulations of CSTR Example

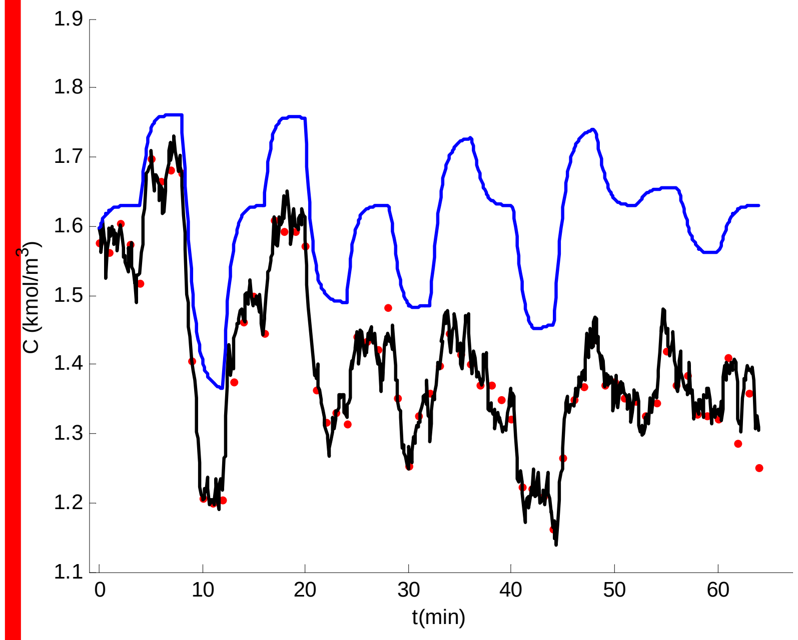




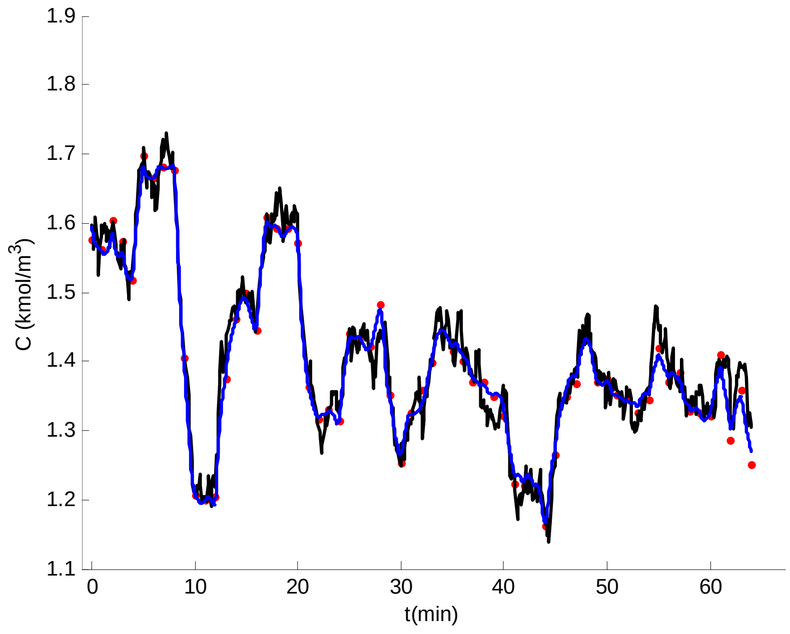
- Parameter estimates are better using AMLE
- Confidence intervals for parameter and state estimates are readily computed from inverse of FIM

State Trajectory Estimates

Concentration Trajectory



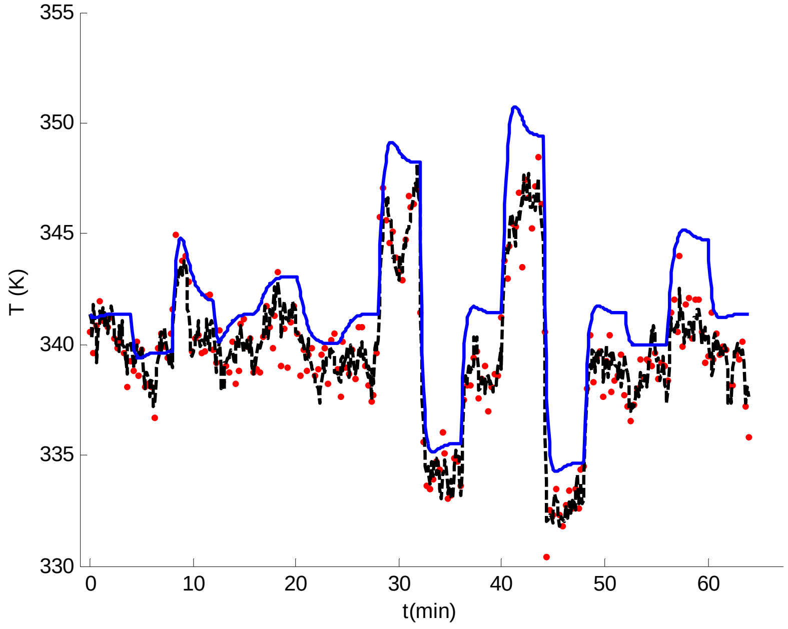
NLS



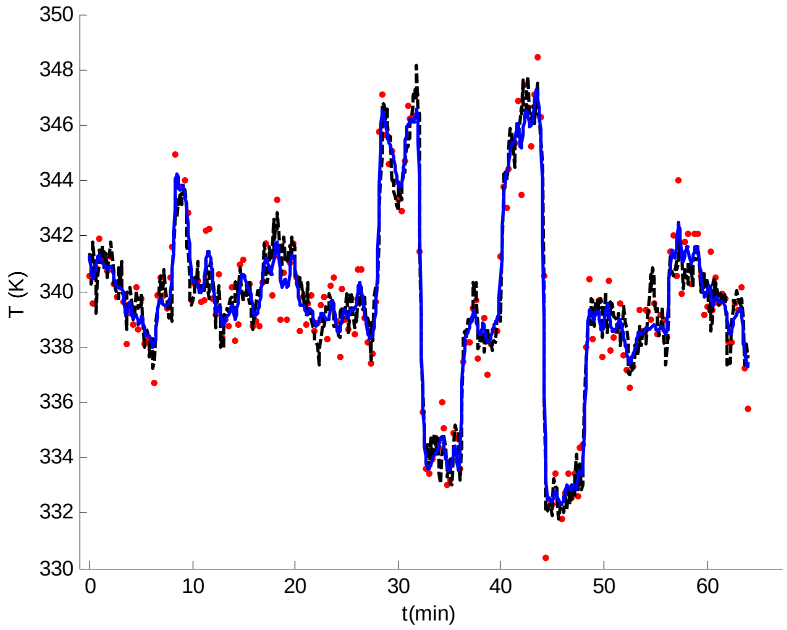
AMLE

State Estimates

- Temperature trajectory



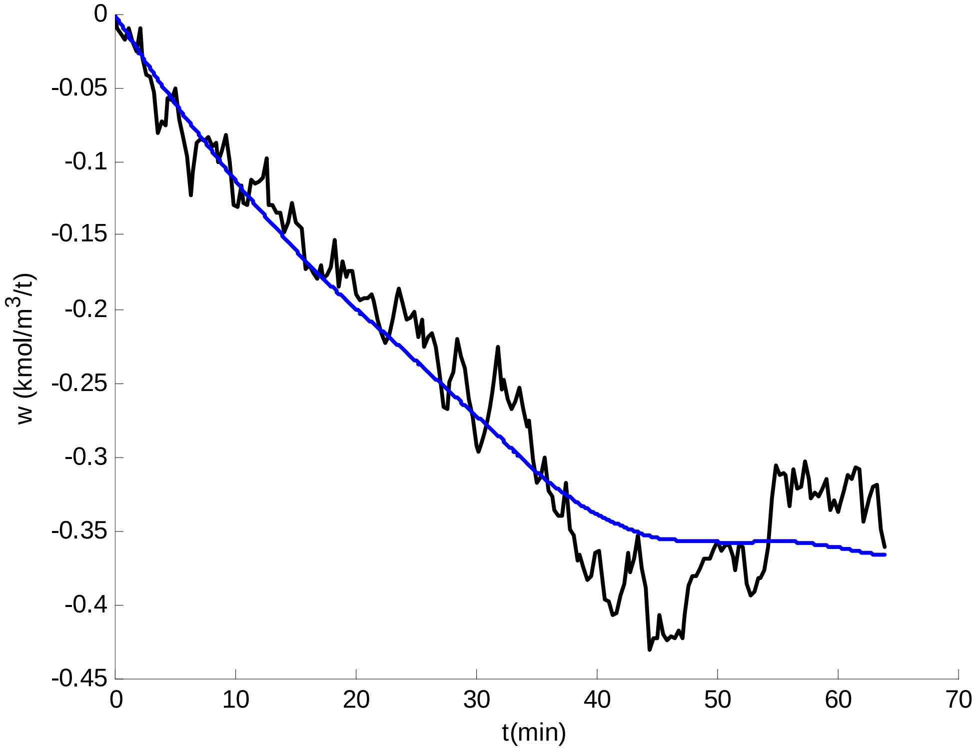
NLS



AMLE

State Estimates

- Non-stationary disturbance *w*



time

Selecting Weighting Factors in J

- Modeler can estimate σ_m^2 from repeated measurements or from information from instrument supplier

- Modeler will know that model is imperfect, and about the physical sources of disturbances, but **won't know the noise intensity Q**

- When Q is unknown, we must estimate it.
  - The correct value of Q results in spline fits that are consistent with σ_m^2
  - Iterate between parameter estimation and Q estimation until convergence

- Estimate of Q for each ODE provides information to modeler about disturbances and model mismatch

Features of iPDA and AMLE Methods

- Good for systems with
  - Unknown or uncertain initial conditions
  - Irregular sampling
  - Unmeasured states
  - Meandering (nonstationary) disturbances

- No need for repeated numerical solution of ODEs
  - Collocation methods that account for model error
  - Optimization problems readily solved in AMPL/IPOPT
  - ODEs are satisfied (or not) using soft constraints in the objective function

Testing of AMLE

- Application to a nylon polymerization reactor model with data from my lab
  - 6 unknown parameters
  - 2 measured states and 1 unmeasured state
  - unknown initial conditions
  - known measurement variances, but unknown Q values

- Seeking graduate students to estimate parameters in larger models

Acknowledgments

- Graduate Students:
  - M. S. Varziri, A. A. Poyton
- Collaborators:
  - P. J. McLellan and J. O. Ramsay
  - L.T. Biegler for advice on AMPL and IPOPT
- Funding
  - MITACS, Cybernetica, DuPont, Hatch, Matrikon, SAS, NSERC
  - BP Chemicals, MMO, Exxon, Nova Chemicals

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