Process Identification: Some Thoughts to the Structure of the Problem

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Starting point

- Been tickled by Steinar Kolås’ promotion presentation
- Parameter identification - still a problem
- Little discussion on structure of the problem
Gas reactor – a toy example

- Fixed volume
- Gas - ideal
- No thermal effects
- Ideal valve – i.e. pulse feed – known
- Total pressure measured

\[ 2A \rightarrow B \]

Figure: Abstraction
The component mass balance:

\[ \dot{n} := s^T \tilde{n} + \hat{n} \]  \hspace{1cm} (1)

The production rate

\[ \tilde{n} := V \tilde{r} \]  \hspace{1cm} (2)

The specific production rate

\[ \tilde{r} := \frac{k}{|\nu_A|} p_A^2 \]  \hspace{1cm} (3)

The partial pressures from the equation of state, here the ideal gas law:

\[ p := n \frac{R T}{V} \]  \hspace{1cm} (4)

Finally the total pressure:

\[ p := e^T p \]  \hspace{1cm} (5)
Expand production rate

Substitution of the pressure into the specific production rate, which in turn is substituted into the production rate gives:

\[ \tilde{n} := \frac{k V}{|\nu_A|} \left( \frac{R T}{V} \right)^2 n_A^2 := a(k) n_A^2 \]  

(6)
Re-cast the model into systems notation by defining:

\[
\begin{align*}
x & := \mathbf{n} \tag{7} \\
r & := \tilde{\mathbf{n}} \tag{8} \\
u & := \hat{\mathbf{n}}_A \tag{9} \\
y & := p \tag{10} \\
f & := [1, 0]^T \tag{11} \\
\alpha & := \frac{V}{|\nu_A|} \tag{12} \\
\beta & := \frac{RT}{V} \tag{13} \\
a(k) & := k\alpha (\beta)^2 \tag{14}
\end{align*}
\]
We get the concise representation:

\[
\begin{align*}
\dot{x} & := s r + f u \\
r & := a(k) x_1^2 \\
y & := \beta (x_1 + x_2)
\end{align*}
\]
Ideal point observer/estimator

- Don’t worry about noise - worry about the structure!
- Line of development: Kalman’s observability for continuous systems
- Turns it into an algebraic problem!
Derivation

\[ y := b e^T x \] (18)
\[ \dot{y} := b e^T \dot{x} \] (19)
\[ \dot{y} := b e^T (r s + fu) \] (20)

Isolate what can be "measured":

\[ w := \dot{y} - b e^T fu := b e^T sr \] (21)
\[ \dot{w} := \ddot{y} - b e^T fu := b e^T s \ddot{r} \] (22)

Manipulate:

\[ \frac{w}{\dot{w}} := \frac{r}{\ddot{r}} \] (23)
\[ := \frac{ak x_1^2}{ak 2 x_1 \dot{x}_1} \] (24)
\[ := \frac{x_1}{\dot{x}_1} \] (25)
Get state, then reaction, then reaction const

Solve for $r$ and $x_1$:

$$r := \frac{w}{b e^T s} \quad (26)$$

$$x_1 := 2 \frac{w}{w} (s_1 r + f_1 u) \quad (27)$$

Only now nonlinearity hits: get reaction const

$$r := a(k) x_1^2 \quad (28)$$

$$a(k) := r x_1^{-2} \quad (29)$$

$$k := \frac{a(k)}{\alpha b^2} \quad (30)$$
Sequential approach

Choose conserved quantities as states
→ linear in flows and reaction
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- Acquire hydraulics, thus inflow and outflow and derivatives
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- My PhD on observing composition in batch reactors from hydraulics and temp measurements
Case: State measurable

\[
\dot{x} := F \hat{x} + S r \quad (31)
\hat{x} :: measured \quad (32)
\]
\[
r := V K g(x) \quad (33)
\]

Isolate reaction part:

\[
S r := \dot{x} - F \hat{x} \quad (34)
\]

Assume for simplicity square, invertible \( S \)

\[
r := S^{-1} (\dot{x} - F \hat{x}) \quad (35)
\]

- Regularise and use for estimation of reaction constant(s).
- If necessary differentiate
- ..etc..
Case: Observation linear in state

\[ \dot{x} := F \hat{x} + S r \]  
\[ \hat{x} :: \text{measured} \]  
\[ r := V K g(x) \]  
\[ y := C x \]

State reconstruction and estimation of reaction part is a linear problem.
Issues

- Modelling errors (dynamics) in hydraulics hurt
- Observation errors hurt
- Stochastic components can be filtered out
- Amplification of hydraulic and kinetic often very large.
Getting derivatives

- Use linear filter methods (example Schaufelberger, Maletinsky)
- Maletinsky’s - Preisig: Multi-wavelets.
- Kalman filter, extended version also does estimation job. Bad control over estimation properties as variance-covariance becomes tuning parameters
- Fixed-gain observer with jacket etc.
Given the SISO model in transfer function form

\[
\sum_{i}^{n} a_{i} D^{i} y := \sum_{i}^{n} b_{i} D^{i} u ,
\]  

(40)

elimination of the unknown initial conditions of the n integrators, except
the last one which is directly measured by the output, transforms the
model into

\[
\sum_{i}^{n} a_{i} \langle \varphi_{n,i}, y \rangle := \sum_{i}^{n} b_{i} \langle \varphi_{n,i}, u \rangle .
\]  

(41)

The functions \( \varphi_{n,0} \) are the modulating functions, B-splines of the order \( n \),
the first index, and 0-times differentiated, the second index.
Some of the important characteristics of the B-spline functions are:

- **Compact base**
  \[ \varphi_{a, \alpha}(t) = 0 \quad \text{for} \quad t \notin [0, nT]; \]

- **Derivative | Integral**
  \[ \varphi_{a, \alpha-1}(t) = \int_0^{nT} \varphi_{a, \alpha}(t) \, dt; \]

- **Stem function order n**
  \[ \varphi_{n,n}(t) = T^{-n} \sum_{i=0}^{n} (-1)^i \binom{n}{i} \delta(t - i \, T). \]
The upper triangle of functions is generated stepwise.

The first row are the Cholesky factors ± Pascal triangle entries.

Generator: consecutive convolution:
\[ \varphi_{a,a} \ast \varphi_{b,b} = \varphi_{a+b,a+b} \]

Example: convoluting \( \varphi_{1,1} \) \( n \)-times with itself \( (\varphi_{1,1})^n \) generates the first row.
Sequential approach

2 Structures

Getting derivatives: Spline-type modulating functions

Hmmm they are multi-wavelets

Back to the example

Figure: filter

Motivation

The Plant

Observer

Structure of the problem

Conclusions

\[ \tilde{x} \]

\[ \tilde{x}(1) \]

\[ \tilde{x}(2) \]

\[ \tilde{x}(3) \]
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Experiment

Experiment
Multi-Wavelet Filtered
Structure

- Structure of the observer/estimation problem is important
- Linearity of the conservation principles can be used for estimating reaction first; next regularize and then estimate parameter.
- Linearity of the state observer problem – very handy

Methods

- Linear filter methods to get derivatives
- High-gain Kalman filter – about the same
- Extended Kalman filter – do things simultaneously...may not be a good idea (modelling errors, amplification)
- Multi-wavelets – very handy as state-variable filters (also no bias problem in estimator)
- Tuning: characteristic time $\approx$ time constant to be observed
- Multi-resolution: choose parallel filters with different characteristics

Do not use methods blindly
Less sophistication in the method usually provides more insight.