Model-based Fault Diagnosis

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Overview

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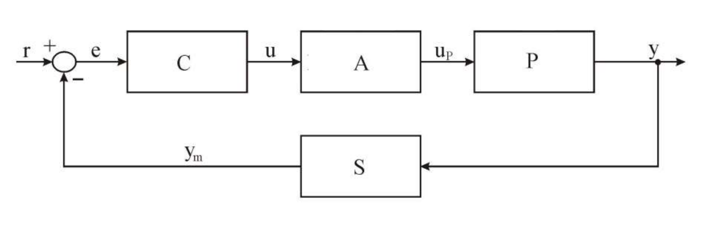
2. Residual Generators
3. Observer-based Fault Diagnosis
4. Case Study - Fault Diagnosis in Chemical Reaction Networks

Introduction to Fault Diagnosis

The control loop



- P - Controlled Plant
- A - Actuator
- S - Sensor
- C - Controller

The fault

- A *fault* is a phenomena that changes the behavior of the technological process system such that it no longer satisfies its original purpose.
- *Fault vs. disturbances*: The disturbances also change the the system's behavior, like the faults. The distinction can be made from the control point of view. The disturbances can be handled by the original control strategy applied to the nominal system. The faults are more severe changes, the control strategy has to be changed to deal with it.
- *Fault vs. failure*: The fault causes an undesired change in the system behavior such that the system performance changes in an undesired way. However, by control engineering methods the system is remediable such that it still remains functional. Failure is the inability of the system to accomplish its function. The system has to be shut down, the failure is an irrecoverable event.

Types of faults

- *Process Faults*: Such faults that change the dynamical behavior of the controlled system.
- *Sensor Faults*: The sensor measurements suffer substantial errors.
- *Actuator faults*: The influence of the controller on the plant is modified or interrupted.

Types of faults

Faults can be also differentiated on the basis of their behaviour over time.

- *Intermittent faults*: have short duration malfunctions, which can still induce long-lasting effects.
- *Persistent faults*: have a long-range time evolution

- *Incipient faults*: slowly evolving faults effects.
- *Abrupt faults*: abrupt change with permanent character

Fault Diagnosis

- *Fault Diagnosis* a subfield of control engineering which deals with monitoring of a process system to identify whether the fault has occurred, and to determine the location and type of fault.
- *Why it is necessary?* Monitoring highly automated technological processes (lights out manufacturing)
- *Why it is necessary?* Based on the obtained fault information, adapt the control strategy to the faulty situation.

Fault Diagnosis

The essential tasks of the fault diagnosis:

- *Fault detection*: Detection of the presence of faults in the process system
- *Fault isolation*: Localization of different faults
- *Fault identification*: Fully characterize the type, size and nature of the faults

Instead of identification we often do *fault estimation*: approximate reconstruction of fault signals from the available measurements.

Model of the fault-free system

- Let a Linear Time-Invariant (LTI) process described by the input-output model:

$$y(s) = G_u(s)u(s),\ \ y \in \mathbb{R}^p,\ \ u \in \mathbb{R}^m.$$

  $G_u(s)$ is the *rational transfer function matrix (transfer matrix)* of the process model.

- Let a minimal state-space realization of the process system model:

$$\begin{aligned} \dot{x} &= Ax + Bu,\ \ x(0) = x_0 \\ y &= Cx + Du \end{aligned}$$

  $x \in \mathbb{R}^n$, $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{p\times n}$, $D \in \mathbb{R}^{p\times m}$.

- The relation between a state-space and the input-output model ($x_0 = 0$) by applying the inverse Laplace transform:

$$y(s) = (C(sI - A)^{-1}B + D)u(s)$$

Equations of transfer matrices

- The columns $G_i(s)$ of a transfer matrix $G(s) = [G_1(s) \ \ldots \ G_n(s)]$, $i = 1 \ldots n$ are *linearly dependent* if there exists n transfer functions $h_i(s) \neq 0$ such that $\sum_{i=1}^{n} h_i(s) G_i(s) = 0$. If this equation is true only for $h_i(s) = 0, \ i = 1 \ldots n$ then the column of $G(s)$ are *linearly independent*.
- Normal rank (*rank*) of a transfer matrix: the maximal number of independent columns of $G(s)$. It can be shown that the rank is the largest possible rank of the complex matrix $G(\lambda)$ for all values of $\lambda \in \mathbb{C}$ if $G(s)$ has finite norm.
- Equation with transfer matrices with $G_x(s)$ unknown, $G_A(s)$, $G_B(s)$ known.

$$G_A(s) G_X(s) = G_B(s) \quad (1)$$

$$G_X(s) G_A(s) = G_B(s) \quad (2)$$

- *Lemma 1*: Equation (1) is solvable if $rank[G_A] = rank\,[G_A \ G_B]$
- *Lemma 2*: Equation (2) is solvable if $rank[G_A] = rank \begin{bmatrix} G_A \\ G_B \end{bmatrix}$

- The fault in a dynamical system is modeled as an input signal ($f \in \mathbb{R}^{m_f}$) which deviates the transient and steady state behavior of the system states or outputs from the nominal situation. f is a deterministic time function. In the fault-free case $f = \underline{0}$.
- The model of the LTI system with *additive* fault

$$y(s) = G_u(s)u(s) + G_f(s)f(s).$$

- In the state-space representation:

$$\dot{x} = Ax + Bu + E_f f, \; x(0) = x_0$$
$$y = Cx + Du + F_f f$$

- Then it yields:

$$G_f(s) = C(sI - A)^{-1}E_f + F_f$$

Model of the faulty system

- Actuator faults (f_A):

$$\dot{x} = Ax + B(u + f_A)$$
$$y = Cx + D(u + f_A)$$

- Process faults (f_P):

$$\dot{x} = Ax + Bu + E_P f_P$$
$$y = Cx + Du + F_P f_P$$

- Sensor faults (f_S):

$$\dot{x} = Ax + Bu$$
$$y = Cx + Du + f_S$$

Model of the faulty system

- System model with sensor-, actuator- and process faults:

$$\dot{x} = Ax + Bu + E_f f$$
$$y = Cx + Du + F_f f$$

- The fault vector:

$$f = \begin{pmatrix} f_A \\ f_P \\ f_S \end{pmatrix}$$

- $E_f = [B\ E_P\ 0]$ and $E_f = [D\ F_P\ I\ ]$

Model with fault and disturbance

- The disturbance (d) is also modeled as a deterministic, unknown input signal. The model of the LTI system with additive fault and disturbance:

$$\Sigma \ : \ y(s) = G_u(s)u(s) + G_f(s)f(s) + G_d(s)d(s).$$

- The state space representation

$$\begin{aligned} \dot{x} &= Ax + Bu + E_f f + E_d d \\ y &= Cx + Du + F_f f + F_d d \end{aligned}$$

Residual Generators

Residual generator for fault diagnosis

- The *residual signal* (r) provides information about the presence or location and properties of the fault.
- The *residual generator* is a procedure which computes the residual signal based on the available information about the process (model, measurements).
- Recall the faulty system model:

$$y(s) = G_u(s)u(s) + G_f(s)f(s) + G_d(s)d(s).$$

- The general form of a *linear residual generator (RG)*:

$$RG \ : \ r(s) = Q(s) \begin{bmatrix} y(s) \\ u(s) \end{bmatrix} = Q_y(s)y(s) + Q_u(s)u(s)$$

  where $Q(s)$ is a proper and stable transfer matrix.
- The *internal form* of the residual generator

$$r(s) = R_u(s)u(s) + R_f(s)f(s) + R_d(s)d(s).$$

  where

$$[R_u(s) \ R_f(s) \ R_d(s)] = Q(s) \begin{bmatrix} G_u(s) & G_f(s) & G_d(s) \\ I & 0 & 0 \end{bmatrix}.$$

- The jth component of f is detectable, if the occurrence (deviation from zero) of a fault entry f_j produces an interpretable change in r regardless to u and d.
- The desired residual:

$$r(s) = 0u(s) + R_{fj}(s)f_j(s) + 0d(s), \text{ where } R_{fj} \neq 0$$

- *Definition (Fault Detectability)*: The j component of f in Σ is detectable with RG if $\exists\ Q(s)$ such that $R_{fj} \neq 0,\ R_u = 0,\ R_d = 0$.
- *Theorem*: f_j in Σ is detectable iff $rank[G_d\ G_{fj}] > rank[G_d]$.
- *Proof* (sufficiency):
  The general transfer matrix equation:

$$Q(s)\begin{bmatrix} G_u(s) & G_{fj}(s) & G_d(s) \\ I & 0 & 0 \end{bmatrix} = [0\ R_{fj}(s)\ 0].$$

- *Proof (ctd.)*:
  The rank condition:

$$rank \begin{bmatrix} G_u(s) & G_{fj}(s) & G_d(s) \\ I & 0 & 0 \end{bmatrix} = rank \begin{bmatrix} G_u(s) & G_{fj}(s) & G_d(s) \\ I & 0 & 0 \\ 0 & R_{fj}(s) & 0 \end{bmatrix}.$$

  Since $rank\,[R_{fj}] = 1$

$$rank\,[G_u] + rank\,[G_{fj}\ G_d] = rank\,[G_u] + 1 + rank\,[G_d]$$

- *Corollary*: If $d = 0$, the fault f_j is detectable whether $rank\,[G_{fi}(s)] > 0$, i.e. $G_{fi}(s) \neq 0$
- *Definition*: The system Σ is *completely fault detectable* with *RG* if all the components of *f* are detectable.

Fault Isolability

- To isolate the fault, we need to deal with the interactions among the entries of f.
- Let a *bank of residual generators*

$$r^{(j)}(s) = Q^{(j)}(s)\begin{bmatrix} y(s) \\ u(s) \end{bmatrix}, \; i = 1 \dots m_f$$

$$r^{(j)}(s) = R_u(s)u(s) + R_{fj}^{(j)}(s)f_j(s) + \sum_{k \neq j} R_{fk}^{(j)}(s)f_k(s) + R_d d(s)$$

- *Definition (Strong Fault Isolability)*: The jth component of f in Σ is strong isolable with RG if $\exists$ $Q^{(j)}(s)$ such that $R_{fj}^{(j)} \neq 0$, $R_u = 0$, $R_d = 0$, $R_{fk}^{(j)} = 0$, $\forall k \neq j$.

Fault Isolability - Structure Matrix

- Consider all the fault gain terms in the bank of residual generators. Let

$$R_f = \begin{bmatrix} R_{f1}^{(1)} & \dots & R_{fm}^{(1)} \\ \dots & \dots & \dots \\ R_{f1}^{(m)} & \dots & R_{fm}^{(m)} \end{bmatrix}$$

- Define the *structure matrix*

$$S_f(i,j) = 1 \text{ if } R_{fj}^{(i)} \neq 0$$
$$S_f(i,j) = 0 \text{ if } R_{fj}^{(i)} = 0$$

Fault Isolability - Structure Matrix

Prescribed structure matrices:

- Strong isolability

$$S_P = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

- Strong block isolability

$$S_P = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- Weak isolability (cannot isolate simultaneous faults)

$$S_P = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$$

- Complete fault detection

$$S_P = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}$$

- Let

$$Q = \begin{bmatrix} Q^{(1)} \\ \dots \\ Q^{(m)} \end{bmatrix}$$

- *Definition*: For a prescribed structure matrix the system Σ is S-fault isolable if $\exists Q$ such that $S = S_P$, where S is the structure matrix of R_f, $R_u = 0$, $R_d = 0$.
- *Theorem*: The system Σ is S-fault isolable for S_P with RG iff $\forall i, j$ $rank[G_d \ \widehat{G}_f^{(i)} \ G_{fj}] > rank[G_d \ \widehat{G}_f^{(i)}] \ \forall \ S_P(i,j) = 1$. Here $\widehat{G}_f^{(i)}$ is formed from those the columns of G_f for which $S_P(i,j) = 0$.

- *Definition (Complete strong fault identifiability)*: The system Σ is called strongly fault identifiable with RG if $\exists Q$ such that $r = f$.
- The equation to be solved:

$$Q(s)\left[\begin{array}{ccc} G_u(s) & G_f(s) & G_d(s) \\ I & 0 & 0 \end{array}\right] = [0 \ I \ 0].$$

- By detailing the equation (recall that $Q(s) = [Q_y(s) \ Q_u(s)]$)

$$\begin{aligned} Q_y(s)G_u(s) &= -Q_u(s) \\ Q_y(s)G_f(s) &= I \\ Q_y(s)G_d(s) &= 0 \end{aligned}$$

- In order to solve the problem, $G_f(s)$ has to be invertible. The problem is NOT solvable for $d \neq 0$ (except if the process model satisfies $G_f(s)^{-1}G_d(s) = 0$).

- *Definition (Complete weak fault identifiability)*: The system Σ is called weekly identifiable with RG if $\exists Q$ such that $r(s) = R_{fP}(s)f(s)$, where $R_{fP}(s)$ is proper, stable and $R_{fP}(0)$ is invertible.
- If the system Σ weakly identifiable,
  then $f = R_{fP}(0)^{-1} lim_{t \to \infty} r$ if f constant.
- The system of equation to be solved

$$Q_y(s) G_u(s) = -Q_u(s)$$
$$Q_y(s) G_f(s) = R_{fP}(s)$$
$$Q_y(s) G_d(s) = 0$$

Solving the Fault Diagnosis problem

- The equation to be solved in a general case:

$$[Q_y(s)\ Q_u(s)]\begin{bmatrix} G_u(s) & G_f(s) & G_d(s) \\ I & 0 & 0 \end{bmatrix} = [0\ R_f(s)\ 0].$$

- Check the rank condition of the targeted fault diagnosis problem.
- Depending on the problem to be solved, $R_f(s)$ can be prescribed, partially prescribed or it can also be designed. In all cases it is desirable to be proper and stable.
- If the problem is solvable, compute $Q_y(s)$ based on the equation

$$Q_y(s)\begin{bmatrix} G_f(s) & G_d(s) \\ 0 & 0 \end{bmatrix} = [R_f(s)\ 0].$$

- Choose

$$Q_u(s) = -Q_y(s)G_u(s)$$

Analytical Redundancy

- Reconstruction of the nominal system output based on the system model and the known input.
- The fault induces a deviation form the nominal input, which can be determined based on the difference between the measured output and reconstructed nominal output.
- The solution of the fault diagnosis problem implicitly applies the *analytical redundancy*:

$$r(s) = Q_y(s)\,(y(s) - G_u(s)u(s))$$

- $Q_y(s)$ is the *postfilter*. It ensures the compensation of the disturbances, the proper and prescribed response of the residual generator.

- Let a faulty SISO system without disturbances given by:

$$y(s) = \frac{K_u}{T_u s + 1} u(s) + \frac{K_f}{T_f s + 1} f(s).$$

- Design: $[Q_y(s)\ Q_u(s)] \begin{bmatrix} \frac{K_u}{T_u s+1} & \frac{K_f}{T_f s+1} \\ I & 0 \end{bmatrix} = [0\ R_f(s)].$
- Let $Q_y(s) = R_f(s) \frac{T_f s+1}{K_f}$
- $R_f(s)$ has to have a relative degree at least 1. Let $R_f(s) = \frac{1}{T_r s+1}$ (fault estimation).
- The obtained residual generator: $r(s) = \frac{1}{T_r s+1} \frac{T_f s+1}{K_f} \left(y(s) - \frac{K_u}{T_u s+1} u(s) \right)$
- Remark: The fault estimation problem in the SISO case cannot be solved in the presence of disturbances (i.e. $G_d \neq 0$), since $rank[G_f\ G_d] = rank G_d = 1$.

Another Example

- Let a faulty, two output system with disturbance:

$$y_1(s) = \frac{K_{u1}}{T_{u1}s+1}u(s) + \frac{K_f}{T_f s+1}f(s) + \frac{K_{d1}}{T_{d1}s+1}d(s).$$
$$y_2(s) = \frac{K_{u2}}{T_{u2}s+1}u(s) + \frac{K_{d2}}{T_{d2}s+1}d(s).$$

- Design:

$$[Q_{y1}(s)\ Q_{y2}(s)\ Q_u(s)] \begin{bmatrix} \frac{K_{u1}}{T_{u1}s+1} & \frac{K_f}{T_f s+1} & \frac{K_{d1}}{T_{d1}s+1} \\ \frac{K_{u2}}{T_{u2}s+1} & 0 & \frac{K_{d2}}{T_{d2}s+1} \\ I & 0 & 0 \end{bmatrix} = [0\ R_f(s)\ 0].$$

- The fault diagnosis problem is solvable as $rank[G_f\ G_d] = 2,\ rank G_d = 1$.
- The system of equations

$$Q_{y1}(s)\frac{K_{u1}}{T_{u1}s+1} + Q_{y2}(s)\frac{K_{u2}}{T_{u2}s+1} = -Q_u(s)$$
$$Q_{y1}(s)\frac{K_f}{T_f s+1} = R_f(s)$$
$$Q_{y1}(s)\frac{K_{d1}}{T_{d1}s+1} + Q_{y2}(s)\frac{K_{d2}}{T_{d2}s+1} = 0$$

- The solution of the fault estimation problem:

$$
\begin{aligned}
R_f(s) &= \frac{1}{T_r s + 1} \\
Q_{y1}(s) &= \frac{1}{T_r s + 1} \frac{T_f s + 1}{K_f} \\
Q_{y2}(s) &= -\frac{1}{T_r s + 1} \frac{T_f s + 1}{K_f} \frac{K_{d1}}{T_{d1} s + 1} \frac{T_{d2} s + 1}{K_{d2}} \\
Q_u(s) &= \frac{1}{T_r s + 1} \frac{T_f s + 1}{K_f} \left(\frac{K_{d1}}{T_{d1} s + 1} \frac{T_{d2} s + 1}{K_{d2}} \frac{K_{u2}}{T_{u2} s + 1} - \frac{K_{u1}}{T_{u1} s + 1} \right)
\end{aligned}
$$

Another Example

The engineer's solution:

- Recall the system model

$$y_1(s) = \frac{K_{u1}}{T_{u1}s+1}u(s) + \frac{K_f}{T_f s+1}f(s) + \frac{K_{d1}}{T_{d1}s+1}d(s).$$
$$y_2(s) = \frac{K_{u2}}{T_{u2}s+1}u(s) + \frac{K_{d2}}{T_{d2}s+1}d(s).$$

- Step 1: Estimate the disturbance based on the second output

$$\widehat{d}(s) = \frac{1}{T_{r2}s+1}\frac{T_{d2}s+1}{K_{d2}}\left(y_2(s) - \frac{K_{u2}}{T_{u2}s+1}u(s)\right)$$

- Step 2: Estimate the fault based on the first output and estimated disturbance

$$r(s) = \widehat{f}(s) = \frac{1}{T_r s+1}\frac{T_f s+1}{K_f}\left(y_1(s) - \frac{K_{u1}}{T_{u1}s+1}u(s) - \frac{K_{d1}}{T_{d1}s+1}\widehat{d}(s)\right)$$

Residual generation in the presence of noise

- Assume the faulty system model in the form

$$y(s) = G_u(s)u(s) + G_f(s)f(s) + G_d(s)d(s) + G_w(s)w(s).$$

- The noise signal w is considered unmeasurable. However, we could have information about some (frequency domain) properties of the noise signal.
- In the residual generator replace $y(s)$ with $y(s) - G_w(s)w(s)$ to obtain the noise-affected residual signal

$$r_w(s) = Q_y(s)(y(s) - G_u(s)u(s) - G_w(s)w(s)).$$

- If we have information about the frequency domain behavior of the noise signal, we could apply extend $Q_y(s)$ with a properly design filter $Q_w(s)$ attenuate the effect of noise in the frequency domain affected by noise.

$$r(s) = Q_w(s)Q_y(s)(y(s) - G_u(s)u(s)).$$

- Warning: The influence of the fault signal in the corresponding frequency domain on the residual signal will also be attenuated!

Threshold computation

- The influence of the noise on residual signal:

$$r_w(s) = r(s) - Q_y(s)G_w(s)w(s).$$

- Let $w_\infty = \|w(t)\|_\infty$
- Compute $Q_\infty^{(w)} = \|Q_y(s)G_w(s)\|_\infty$
- It yields the *threshold* of the residual generation: $th = Q_\infty^{(w)} w_\infty$.
  It satisfies: $\|r_w(t) - r(t)\|_\infty \leq th$.
- The *decision signal*:

$$\delta = \begin{cases} 1, & \textit{if } |r_w(t)| > th \\ 0, & \textit{otherwise.} \end{cases}$$

- Warning: Fault signals with smaller magnitude than the threshold cannot be detected!

Observer-based Fault Diagnosis

- Let a minimal state-space realization of an LTI process system:

$$\dot{x} = Ax + Bu, \;\; x(t_0) = x_0$$
$$y = Cx + Du$$

$x \in \mathbb{R}^n$, $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{p\times n}$, $D \in \mathbb{R}^{p\times m}$.

- *Definition (Observability)*: The ability to determine the initial state (x_0) of the system based on the observation of the output in a finite time domain $(t_0, \;\; t_f)$.
- *Definition (Observability Matrix)*:

$$M_O = \begin{bmatrix} C \\ CA \\ \dots \\ CA^{n-1} \end{bmatrix}$$

- *Theorem (Observability)*: The LTI process system is observable if $rank(M_O) = dim(x)$.
- *Note*: Because the effect of the known input may be subtracted out during the observation process, it is sufficient to consider the homogeneous response to determine observability.

Observability

- The response of the system from initial condition x_0 is:

$$y(t) = Ce^{At}x_0 = [\xi_1(t) \dots \xi_n(t)] \begin{bmatrix} x_{01} \\ \dots \\ x_{0n} \end{bmatrix}$$

- In the complex domain:

$$y(s) = C(sI - A)^{-1}x(s) = [\zeta_1(s) \dots \zeta_n(s)] \begin{bmatrix} x_1(s) \\ \dots \\ x_n(s) \end{bmatrix}$$

- The system is *unobservable* if any column of $[C(sI - A)^{-1}]$ is 0.
- The system is *unobservable* if there exists a linear dependence between the columns of $[C(sI - A)^{-1}]$ (e.g. $\zeta_1 = \alpha\zeta_2$).

Observability - Example

- Let an mechanical system described by the equation $m\ddot{p} = u$, where p is the position, m - mass parameter, u - control input. The velocity of the system is $v = \dot{p}$.
- The state space model $x = (p\ v)^T$:

$$\begin{pmatrix} \dot{p} \\ \dot{v} \end{pmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{pmatrix} p \\ v \end{pmatrix} + \begin{bmatrix} 0 \\ 1/m \end{bmatrix} u$$

- Case 1: Let the measured output $y = p$, i.e. $C = (1\ 0)$.
  The observability matrix:

$$M_O = \begin{bmatrix} C \\ CA \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},\ rank(M_O) = 2$$

  The system is observable.
- Case 2: Let the measured output $y = \dot{p} = v$, i.e. $C = (0\ 1)$.
  The observability matrix:

$$M_O = \begin{bmatrix} C \\ CA \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix},\ rank(M_O) = 1.$$

  The system is NOT observable.

Observer design

- *Definition*: A *state observer* is a system that provides an estimate of the internal state of a given real system, from measurements of the system input and output.
- The common form of a state observer for an LTI system:

$$\dot{\widehat{x}} = A\widehat{x} + Bu + K(y - C\,\widehat{x} - Du),\ \widehat{x}(t_0) = \widehat{x}_0$$

  where $K \in \mathbb{R}^{n\times p}$ is the observer gain matrix.
- Observation error: $e = x - \widehat{x}$. It is desirable that $lim_{t\to\infty} e(t) = 0$.
- Observation error dynamics:

$$\dot{e} = (A - KC)e,\ e(t_0) = x_0 - \widehat{x}_0$$

- *Theorem*: If the LTI system is observable, then $\exists\ K$ such that $A - KC$ is Hurwitz.

State observers in the presence of faults

- Let an observable LTI system with faults and without disturbances

$$\begin{aligned} \dot{x} &= Ax + Bu + E_f f \\ y &= Cx + Du + F_f f \end{aligned}$$

- Let the same state observer:

$$\dot{\hat{x}} = A\hat{x} + Bu + K(y - C\,\hat{x} - Du)$$

  such that $A - KC$ Hurwitz.

- The observer error dynamics:

$$\dot{e} = (A - KC)e + E_f f - KF_f f$$

State observers for residual generation

- Define the residual signal

$$r = y - C\,\widehat{x}$$

- The residual generator:

$$\begin{aligned}\dot{e} &= (A - KC)e + (E_f - KF_f)f \\ r &= Ce + F_f f\end{aligned}$$

- In the complex domain:

$$r(s) = R_f(s)f(s) = (\underbrace{C}_{C_R}(sI - (\underbrace{A - KC}_{A_R}))^{-1}(\underbrace{E_f - KF_f}_{B_R}) + \underbrace{F_f}_{D_R})f(s)$$

State observers for residual generation

- The residual generator:

$$r(s) = R_f(s) f(s) = (C_R(sI - A_R)^{-1} B_R + D_R) f(s)$$

- The jth component of the fault is detectable if the jth column of $R_f \neq 0$.
- To improve the performance of the residual generator, it can be extended with a postfilter, i.e. $r(s) = Q_f(s) R_f(s) f(s)$.

- Let an LTI System with disturbances

$$\dot{x} = Ax + Bu + E_d d$$
$$y_d = C_d x + Du + F_d d$$

- E_d has full column rank. Otherwise, rewrite $E_d d = EE^{(2)}d$, where E has full column rank and $E^{(2)}d$ is the new disturbance input.
- Output transformation: Let the new output $y = T_d(y_d - Du)$, where $T_d F_d = 0$. It yields that

$$y = Cx$$

where $C = T_d C_d$.

Unknown Input Observers

- *Definition*: An observer is defined as an *unknown input observer* for the system

$$\dot{x} = Ax + Bu + Ed$$
$$y = Cx,$$

if its output ($\widehat{x}$) approaches asymptotically to the system's state regardless of the presence of the unknown input (disturbance) in the system.

- The structure of the full order unknown input observer

$$\dot{z} = A_O z + TBu + Ky$$
$$\widehat{x} = z + Hy,$$

- The matrices $A_O, \ T, \ K, \ H$ has to be chosen such that $lim_{t\to\infty}(x - \widehat{x}) = 0$.

- The estimation error ($e = x - \widehat{x}$) is governed by the following dynamics

$$\begin{aligned}\dot{e} &= (A - HCA - K_1 C)e + [K_2 - (A - HCA - K_1 C)H]y \\ &+ [A_O - (A - HCA - K_1 C)]z + [T - (I - HC)]Bu + (HC - I)Ed\end{aligned}$$

where $K = K_1 + K_2$.

- If one can make the following relations hold true

$$\begin{aligned}&(HC - I)E = 0 \\ &T = I - HC \\ &A_O = A - HCA - K_1 C \\ &K_2 = A_O H\end{aligned}$$

the state estimation error will then be

$$\dot{e} = A_O e$$

Unknown Input Observers

- *Lemma*: The matrix equation $XA = B$ has a solution if $rank[A] = rank\begin{bmatrix} A \\ B \end{bmatrix}$. A solution is $X = BA^{+}$ where A^{+} is the pseudo-inverse (generalized inverse) of A.
- If A has full column rank then $X = B(A^T A)^{-1} A^T$.
- *Theorem*: The system

$$\dot{z} = A_O z + TBu + Ky$$
$$\widehat{x} = z + Hy,$$

is an unknown input observer for

$$\dot{x} = Ax + Bu + Ed$$
$$y = Cx,$$

if $(A - HCA, C)$ observable and $rank[CE] = rank\begin{bmatrix} CE \\ E \end{bmatrix}$ where $H = E(CE)^{+}$ and K_1 is chosen such that $A - HCA - K_1 C$ is Hurwitz.

Unknown Input Observers for Fault Diagnosis

- Let an LTI system with sensor- and actuator faults and disturbances:

$$\dot{x} = Ax + B(u + f_A) + Ed$$
$$y = Cx + f_S,$$

- Define the residual signal

$$r = y - C\,\widehat{x} = (I - CH)y - Cz$$

- The residual generator:

$$\dot{e} = A_O e + TBf_A + K_1 f_S - H\,\dot{f}_S$$
$$r = Ce + f_S \qquad (3)$$

Unknown Input Observers for Sensor Fault Isolation

- Let a system with sensor faults and disturbances:

$$\begin{aligned} \dot{x} &= Ax + Bu + Ed \\ y^{(j)} &= \widehat{C}^{(j)} x + f_S^{(j)}, \\ y_j &= C_j x + f_{Sj},\ j = 1 \dots m \end{aligned} \tag{4}$$

  where f_{Sj} is the jth fault, $\widehat{C}^{(j)}$ contains the columns of C except C_j
- The residual generator

$$\begin{aligned} \dot{z}^{(j)} &= A_O^{(j)} z^{(j)} + T^{(j)} Bu + K^{(j)} y^{(j)} \\ r^{(j)} &= (I - H^{(j)} \widehat{C}^{(j)}) y^{(j)} - \widehat{C}^{(j)} z^{(j)},\ j = 1 \dots m \end{aligned}$$

Unknown Input Observers for Sensor Fault Isolation

- The residual signal

$$\begin{aligned} \dot{z}^{(j)} &= A_O^{(j)} z^{(j)} + T^{(j)} Bu + K^{(j)} y^{(j)} \\ r^{(j)} &= (I - \widehat{C}^{(j)} H^{(j)}) y^{(j)} - \widehat{C}^{(j)} z^{(j)}, \; j = 1 \dots m \end{aligned}$$

- If one can make the following relations hold true

$$\begin{aligned} (H^{(j)} \widehat{C}^{(j)} - I) E &= 0 \\ T^{(j)} &= I - H^{(j)} \widehat{C}^{(j)} \\ A_O^{(j)} &= A - H^{(j)} \widehat{C}^{(j)} A - K_1^{(j)} \widehat{C}^{(j)} \\ K_2^{(j)} &= A_O^{(j)} H^{(j)} \end{aligned}$$

then weak fault isolability can be achieved with the following decision logic:
if $\|r^{(j)}\| < th^{(j)}$ and $\|r^{(k)}\| > th^{(k)}$ $\forall k \neq j$, then there is a fault in the jth sensor.

Unknown Input Observers for Actuator Fault Isolation

- Let an LTI system with actuator faults and disturbances:

$$\begin{aligned}\dot{x} &= Ax + \widehat{B}^{(j)}(u^{(j)} + f_A^{(j)}) + B_j(u_j + f_{Aj}) + Ed \\ &= Ax + \widehat{B}^{(j)}u^{(j)} + \widehat{B}^{(j)}f_A^{(j)} + E^{(j)}d^{(j)} \\ y_j &= Cx,\ j = 1 \dots m\end{aligned}$$

  where f_{Aj} is the jth actuator fault, $\widehat{B}^{(j)}$ contains the columns of B except the jth column B_j.
- The newly defined disturbance terms

$$\begin{aligned}E^{(j)} &= [E\ B_j] \\ d^{(j)} &= [d^T\ u_j + f_{Aj}]^T\end{aligned}$$

Unknown Input Observers for Actuator Fault Isolation

- The residual signal

$$\dot{z}^{(j)} = A_O^{(j)} z^{(j)} + T^{(j)} \widehat{B}^{(j)} u^{(j)} + K^{(j)} y$$
$$r^{(j)} = (I - CH^{(j)}) y^{(j)} - Cz^{(j)}, \; j = 1 \ldots m$$

- If one can make the following relations hold true

$$(H^{(j)} C - I) E^{(j)} = 0$$
$$T^{(j)} = I - H^{(j)} C$$
$$A_O^{(j)} = A - H^{(j)} CA - K_1^{(j)} C$$
$$K_2^{(j)} = A_O^{(j)} H^{(j)}$$

then weak fault isolability can be achieved with the following decision logic:
if $\|r^{(j)}\| < th^{(j)}$ and $\|r^{(k)}\| > th^{(k)}, \; \forall k \neq j$, then there is a fault in the jth actuator.

Case Study - Fault Diagnosis in Chemical Reaction Networks

Chemical Reaction Networks (CRNs)

The dynamic model of a CRN is built upon the following elements:

- Species: $\mathcal{S} := \{S_1 \dots S_n\}$ are constituent molecules undergoing (a series of) chemical reactions.
- Complexes: $\mathcal{C} := \{\mathcal{C}_1 \dots \mathcal{C}_m\}$ are formally linear combinations of the species with integer coefficients, i.e. $\mathcal{C}_k := \sum_{i=1}^{n} \alpha_{k,i} S_i$, where $\alpha_{k,i}$ are the stoichiometric coefficients. If S_i is not present in $\mathcal{C}_k$, then $\alpha_{k,i} = 0$.
- Reactions: $\mathcal{R} := \{\mathcal{R}_1 \dots \mathcal{R}_r\}$ where $\mathcal{R}_k : \; \mathcal{C}_i \to \mathcal{C}_j$. Here $\mathcal{C}_i$ is the reactant (or source) complex, and $\mathcal{C}_j$ is the product complex for $k = 1, \dots, r$.
- Reaction rate coefficients: $\kappa_k > 0$ that is associated to $\mathcal{R}_k$ for $k = 1, \dots, r$.

Example of chemical reaction

$$A + B \underset{\kappa_2}{\overset{\kappa_1}{\rightleftharpoons}} C$$
$$C \xrightarrow{\kappa_3} D$$
$$3B \xrightarrow{\kappa_4} E$$

- Species: A, B, C, D, E
- Reactant complexes: A+B, C, 3B
- Product complexes: C, D, E

The Stoichiometric Matrix

- We associate vectors $\mathbf{y}_k \in \mathbb{R}^n$ to the complexes $\mathcal{C}_k$ composed of their stoichiometric coefficients α_{ki} such that $\mathbf{y}_{k,i} = \alpha_{ki}$ for $k = 1, \ldots m$.
- Let us denote by $\mathbf{y}_{kR} \in \mathbb{R}^n$ the so-called complex vector associated to a reactant complex, and by $\mathbf{y}_{kP} \in \mathbb{R}^n$ the vector associated to the product complex of the kth reaction, i.e. $\mathcal{R}_k : \mathcal{C}_{kR} \to \mathcal{C}_{kP}$.
- The stoichiometric matrix $N \in \mathbb{R}^{n \times r}$ contains all the vectors $\mathbf{y}_{kP} - \mathbf{y}_{kR}$ of a CRN in its columns.

Example of chemical reaction

$$A + B \underset{\kappa_2}{\overset{\kappa_1}{\rightleftharpoons}} C$$

$$C \xrightarrow{\kappa_3} D$$

$$3B \xrightarrow{\kappa_4} E$$

$$\underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 3 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}_{N_R} \quad \underbrace{\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}}_{N_R} \quad \underbrace{\begin{pmatrix} -1 & 1 & 0 & 0 \\ -1 & 1 & 0 & -3 \\ 1 & -1 & -1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}}_{N = N_P - N_R}$$

Dynamic model of the CRN

- The CRN model describes the dynamics of the species' concentrations $\mathbf{c} = \begin{pmatrix} c_1 & c_2 & \dots & c_n \end{pmatrix}^T \in \mathbb{R}_+^n$.
- The reaction rate of the kth reaction $\mathcal{R}_k: \ \sum_{i=1}^{nS} \alpha_{kR,i} S_{ki} \to \sum_{i=1}^{nP} \alpha_{kP,i} P_{ki}$

$$r_k(\mathbf{c}, \mathbf{k}) = \kappa_k \prod_{i=1}^{n} c_i^{\alpha_{kR,i}}$$

- Vector of reaction rate coefficients $\mathbf{k} = \begin{pmatrix} \kappa_1 & \kappa_2 & \dots & \kappa_r \end{pmatrix}^T \in \mathbb{R}_+^r$.
- Monomial vector $p_k(\mathbf{c}) = \prod_{i=1}^{n} c_i^{\alpha_{kR,i}}$
- Now we can form the reaction rate vector $\mathbf{r}(\mathbf{c}, \mathbf{k}) = \begin{pmatrix} r_1 \dots r_r \end{pmatrix}^T$ in the form

$$\mathbf{r}(\mathbf{c}, \mathbf{k}) = \mathrm{diag}(\mathbf{k})\mathbf{p}(\mathbf{c}) = \mathrm{diag}(\mathbf{p}(\mathbf{c}))\mathbf{k}$$

- With these notations the model of a CRN reads as:

$$\dot{\mathbf{c}} = N\,\mathbf{r}(\mathbf{c}, \mathbf{k}), \quad \mathbf{c}(0) = \mathbf{c}_\circ.$$

Example of chemical reaction

$$A + B \underset{\kappa_2}{\overset{\kappa_1}{\rightleftharpoons}} C$$

$$C \xrightarrow{\kappa_3} D$$

$$3B \xrightarrow{\kappa_4} E$$

- The CRN model describes the dynamics of the species' concentrations $\mathbf{c} = (c_A \ c_B \ c_C \ c_D \ c_E)^T$
- The reaction rate coefficients: $\mathbf{k} = (\kappa_1 \ \kappa_2 \ \kappa_4 \ \kappa_4)^T$
- Monomial vector: $\mathbf{p} = \left(c_A c_B \ c_C \ c_C \ c_B^3\right)^T$
- The dynamic model:

$$\begin{pmatrix} \dot{c}_A \\ \dot{c}_B \\ \dot{c}_C \\ \dot{c}_D \\ \dot{c}_E \end{pmatrix} = \begin{pmatrix} -1 & 1 & 0 & 0 \\ -1 & 1 & 0 & -3 \\ 1 & -1 & -1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} k_1 c_A c_B \\ k_2 c_C \\ k_3 c_C \\ k_4 c_B^3 \end{pmatrix}$$

Rate change estimation as a fault diagnosis problem

- Faults are assumed to act through the change of reaction rate coefficients. For chemical systems, this can be the result of e.g. unexpected change of temperature or chemical composition of a catalyst. In the case of mass convection networks which are formally kinetic, change in the 'rate coefficients' can be caused by altered flow conditions.
- The effect of the fault on the reaction rate: Consider that in the case of a fault event a number of $q \leq r$ elements of the reaction rate coefficient vector $\mathbf{k}$ suffer changes.

$$\mathbf{k}_f = \mathbf{k} + \boldsymbol{f}$$

- If the kth rate is not affected by the disturbance, $f_k = 0$.
- If $f_k > 0$, the reaction rate increases.
- If $f_k = -\kappa_k$, the reaction vanishes.

Rate change estimation as a fault diagnosis problem

- Consider the truncated fault vector $\mathbf{f} = (f_1 \dots f_q)^T \in \mathbb{R}^q$ containing only the elements that could take piecewise constant non-zero values in the case of a fault event. The corresponding truncated monomial vector is denoted as $\mathbf{p}_t(\mathbf{c}_t) \in \mathbb{R}^q$. Here $\mathbf{c}_t$ represents the concentration vector of such species that take part in fault-influenced reactions.
- The truncated stoichiometric matrix ($N_t \in R^{n \times q}$) contains those columns of N that describe such reactions that could be influenced by the faults. With the appropriately ordered N_t, $\mathbf{p}_t$, $\mathbf{f}$, the CRN model with faults can be written as:

$$\dot{\mathbf{c}} = N\mathbf{r}(\mathbf{c}) + N_t P_t(\mathbf{c}_t)\mathbf{f}$$

where $P_t(\mathbf{c}_t) = \mathrm{diag}(\mathbf{p}_t(\mathbf{c}_t))$.

Rate change estimation as a fault diagnosis problem

- Consider the fault-affected CRN model given by the equation $\dot{\mathbf{c}} = N\mathbf{r}(\mathbf{c}) + N_t P_t(\mathbf{c}_t)\mathbf{f}$. The aim of the observer design is to compute an estimate of $\mathbf{f}$ based on which the changes in the dynamics of the CRN can be anticipated.
- Let Σ_Δ be a dynamic system which has the estimated fault vector $(\widehat{\mathbf{f}} \in \mathbb{R}^q)$ as output, and its input is $\mathbf{c}_m \in \mathbb{R}^m$, a vector which contains the measurable entries of the state vector $\mathbf{c}$.
- Σ_Δ is a fault estimator for $\dot{\mathbf{c}} = N\mathbf{r}(\mathbf{c}) + N_t P_t(\mathbf{c}_t)\mathbf{f}$ if its internal state vector is bounded and its output satisfies $\widehat{\mathbf{f}} \to \mathbf{f}$ as $t \to \infty$ for bounded inputs and finite initial conditions.
- If no fault is present in the system $(\mathbf{f} = \mathbf{0})$, then $\widehat{\mathbf{f}} \to \mathbf{0}$.

Rate change estimation
Example: Edelstein Network

$$S_1 \underset{\kappa_2}{\overset{\kappa_1}{\rightleftharpoons}} 2S_1$$

$$S_1 + S_2 \underset{\kappa_4}{\overset{\kappa_3}{\rightleftharpoons}} S_3 \underset{\kappa_6}{\overset{\kappa_5}{\rightleftharpoons}} S_2$$

- Stoichiometric matrix of the Edelstein network:

$$N = \begin{pmatrix} 1 & -1 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 1 & -1 \\ 0 & 0 & 1 & -1 & -1 & 1 \end{pmatrix}$$

- Reaction rate vector of the Edelstein network:

$$\mathbf{r}(\mathbf{c}) = \begin{pmatrix} \kappa_1 c_1 & \kappa_2 c_1^2 & \kappa_3 c_1 c_2 & \kappa_4 c_3 & \kappa_5 c_3 & \kappa_6 c_2 \end{pmatrix}^T$$

Example - Rate change estimation in Edelstein Network

$$S_1 \underset{\kappa_2}{\overset{\kappa_1}{\rightleftharpoons}} 2S_1$$

$$S_1 + S_2 \underset{\kappa_4}{\overset{\kappa_3}{\rightleftharpoons}} S_3 \underset{\kappa_6}{\overset{\kappa_5}{\rightleftharpoons}} S_2$$

Consider that the reactions 1, 3 are affected by disturbances.
In this case:

$$\mathbf{c}_t = (c_1 \;\; c_2)^T,$$

$$P_t(\mathbf{c}_t) = \operatorname{diag}(c_1 \;\; c_1 c_2),$$

$$N_t = \begin{pmatrix} 1 & -1 \\ 0 & -1 \\ 0 & 1 \end{pmatrix}.$$

- LaSalle's invariance principle is a criterion for the asymptotic stability of an autonomous (possibly nonlinear) dynamical system.
- Consider an autonomous nonlinear dynamical system $\dot{x} = f(x(t))\ x(0) = x_0$. Suppose f has an equilibrium at x_e so that $f(x_e) = 0$. The equilibrium of the above system is said to be *asymptotically stable* if there exists $\delta > 0$ such that if $\|x(0) - x_e\| < \delta$, then $x(t)$ is bounded and $\lim_{t\to\infty} \|x(t) - x_e\| = 0$.
- If a function $L(\mathbf{x}) \geq 0$ can be found such that $\dot{L}(\mathbf{x}) \leq 0$ for all $\mathbf{x}$ (negative semidefinite), then all the trajectories of the system converge into the set $\{\mathbf{x} : \dot{L}(\mathbf{x}) = 0\}$.

- *Theorem:* If the matrix $N_t P_t(\mathbf{c}_t)$ has full column rank $\forall \mathbf{c}_t$, then

$$\begin{cases} \dot{\widehat{\mathbf{c}}} = N\mathbf{r}(\mathbf{c}) + N_t P_t(\mathbf{c}_t)\widehat{\mathbf{f}} + \Gamma_c(\mathbf{c} - \widehat{\mathbf{c}}) \\ \dot{\widehat{\mathbf{f}}} = P_t(\mathbf{c}_t) N_t^T \Gamma_f(\mathbf{c} - \widehat{\mathbf{c}}) \end{cases}$$

  is a residual generator for the system $\dot{\mathbf{c}} = N\mathbf{r}(\mathbf{c}) + N_t P_t(\mathbf{c}_t)\mathbf{f}$.

- *Sketch of the Proof:* Define the Lyapunov function candidate

$$L(t) = \frac{1}{2}\widetilde{\mathbf{c}}^T\Gamma_f\widetilde{\mathbf{c}} + \frac{1}{2}\widetilde{\mathbf{f}}^T\widetilde{\mathbf{f}}.$$

  where $\widetilde{\mathbf{c}} = \mathbf{c} - \widehat{\mathbf{c}}$, $\widetilde{\mathbf{f}} = \mathbf{f} - \widehat{\mathbf{f}}$.
- The dynamics of the observation errors ($\widetilde{\mathbf{c}} = \mathbf{c} - \widehat{\mathbf{c}}$, $\widetilde{\mathbf{f}} = \mathbf{f} - \widehat{\mathbf{f}}$) yields as

$$\begin{pmatrix} \dot{\widetilde{\mathbf{c}}} \\ \dot{\widetilde{\mathbf{f}}} \end{pmatrix} = \begin{pmatrix} -\Gamma_c & N_t P_t(\mathbf{c}_t) \\ -P_t(\mathbf{c}_t) N_t^T \Gamma_f & 0 \end{pmatrix} \begin{pmatrix} \widetilde{\mathbf{c}} \\ \widetilde{\mathbf{f}} \end{pmatrix}.$$

- The time-derivative of it reads as $\dot{L}(t) = -\widetilde{\mathbf{c}}^T\Gamma_f\Gamma_c\widetilde{\mathbf{c}} \leq 0$.
- By LaSalle invariance principle, the estimation error trajectories converge to the invariant set $\widetilde{\mathbf{c}} = \mathbf{0}$. Accordingly, $\widetilde{\mathbf{c}}, \dot{\widetilde{\mathbf{c}}} \to \mathbf{0}$ as $t \to \infty$. We obtain that $N_t P_t(\mathbf{c}_t)\widetilde{\mathbf{f}} \to \mathbf{0}$ as $t \to \infty$. The matrix $N_t P_t(\mathbf{c}_t)$ admits left inverse. Then we conclude that $\widehat{\mathbf{f}} \to \mathbf{f}$ as $t \to \infty$.

Extended observer for input disturbance compensation

- Consider the model of an open chemical reaction, with input and output flows

$$\dot{\mathbf{c}} = N\mathbf{r}(\mathbf{c}) + \mathbf{i} - V_o\mathbf{c}.$$

  The vector of the rate of supply is $\mathbf{i}$, $V_o\mathbf{c}$ is the rate of removal. $V_o = \mathrm{diag}(v\ v\ \dots\ v)$
- The rate of supply can be modelled as

$$\mathbf{i} = \left(v_{I1}c_{I1}\ \ v_{I2}c_{I2}\ \ \dots\ \ v_{In}c_{In}\right)^T$$

  where c_{Ii} is the ith inlet concentration and $v_{Ii} \geq 0$ is the ith input flow rate.

Extended observer for input disturbance compensation

- The input disturbance is considered as a change in the inlet concentration and it is modeled as an additive term in the open CRN model in the form $E\mathbf{d}$, where $\mathbf{d} \in \mathbb{R}^p$ is the input disturbance vector and $E \in \mathbb{R}^{n \times p}$ is the input disturbance matrix, containing p standard basis vectors with dimension n, indicating that which species' concentrations are influenced by the disturbance.
- The open CRN model with rate- and input disturbance has the form:

$$\dot{\mathbf{c}} = N\mathbf{r}(\mathbf{c}) + N_t P_t(\mathbf{c}_t)\mathbf{f} + \mathbf{i} + E\mathbf{d} - V_o\mathbf{c}.$$

Extended observer for input disturbance compensation

- *Theorem:* If $N_E(\mathbf{c}_t) = [N_t P_t(\mathbf{c}_t)\ E]$ has full column rank $\forall \mathbf{c}_t$, then

$$\begin{cases} \dot{\widehat{\mathbf{c}}} = N\mathbf{r}(\mathbf{c}) + N_t P_t(\mathbf{c}_t)\widehat{\mathbf{f}} + \mathbf{i} - V_o\mathbf{c} + E\widehat{\mathbf{d}} + \Gamma_c(\mathbf{c} - \widehat{\mathbf{c}}) \\ \dot{\widehat{\mathbf{f}}} = P_t(\mathbf{c}_t)N_t^T\Gamma_f(\mathbf{c} - \widehat{\mathbf{c}}) \\ \dot{\widehat{\mathbf{d}}} = E^T\Gamma_f(\mathbf{c} - \widehat{\mathbf{c}}). \end{cases}$$

  is a disturbance observer of the open CRN. Moreover, $\lim_{t\to\infty}\widehat{\mathbf{d}} = \mathbf{d}$.
- The Lyapunov function candidate for the convergence analysis is chosen as

$$L(t) = \frac{1}{2}\widetilde{\mathbf{c}}^T\Gamma_f\widetilde{\mathbf{c}} + \frac{1}{2}\widetilde{\mathbf{f}}_t^T\widetilde{\mathbf{f}}_t + \frac{1}{2}\widetilde{\mathbf{d}}^T\widetilde{\mathbf{d}}.$$

- The estimation error dynamics has the form:

$$\begin{pmatrix} \dot{\widetilde{\mathbf{c}}} \\ \dot{\widetilde{\mathbf{f}}}_t \\ \dot{\widetilde{\mathbf{d}}} \end{pmatrix} = \begin{pmatrix} -\Gamma_c & N_t P_t(\mathbf{c}_t) & E \\ -P_t(\mathbf{c}_t)N_t^T\Gamma_f & 0 & 0 \\ -E^T\Gamma_f & 0 & 0 \end{pmatrix} \begin{pmatrix} \widetilde{\mathbf{c}} \\ \widetilde{\mathbf{f}}_t \\ \widetilde{\mathbf{d}} \end{pmatrix}.$$

Fault Estimation

- Consider the Edelstein network:

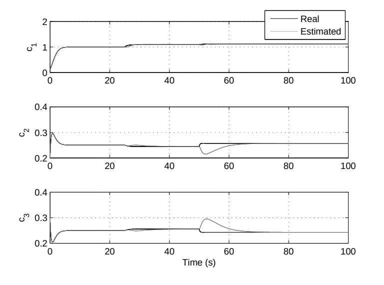
$$S_1 \underset{\kappa_2}{\overset{\kappa_1}{\rightleftharpoons}} 2S_1$$

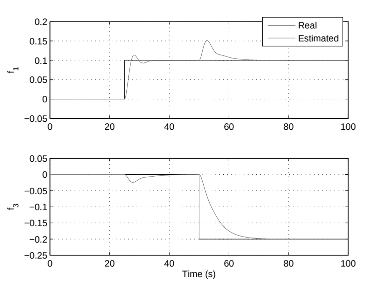
$$S_1 + S_2 \underset{\kappa_4}{\overset{\kappa_3}{\rightleftharpoons}} S_3 \underset{\kappa_6}{\overset{\kappa_5}{\rightleftharpoons}} S_2$$

  The reaction rate coefficients were chosen $\kappa_k = 1,\ k = 1 \ldots 6$.

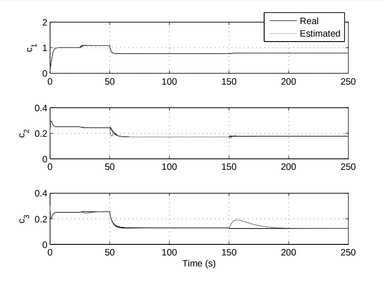
- For the first experiment in the Edelstein network the following reaction rate changes were assumed:
  $\kappa_{f1} = \kappa_1 + f_1,\ f_1 = 0.1 \cdot \mathbf{1}(t - 25)$,
  $\kappa_{f3} = \kappa_3 + f_3,\ f_3 = -0.2 \cdot \mathbf{1}(t - 50)$.

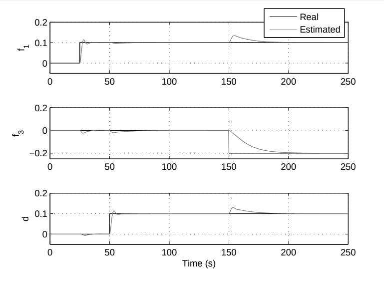
Fault Estimation





Fault and Disturbance Estimation





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