Invariant estimation and control of a polymerization reactor

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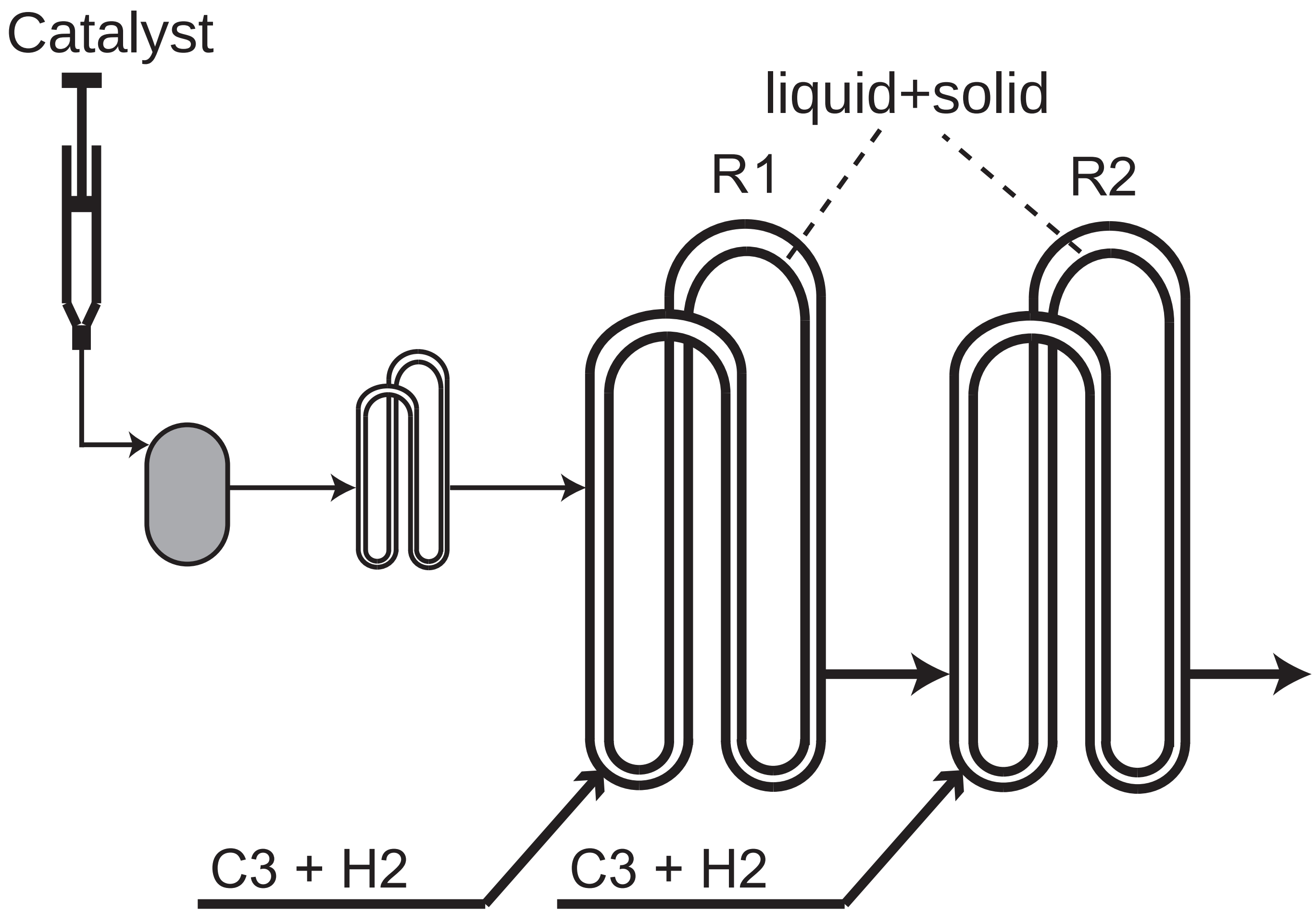
Outline :

- The poly-propylene reactor PP2 (Feluy).
- Filtering the solid fraction and choice of unit (mass-fraction or volume-fraction)...
- Invariant filtering algorithm independent of the unit: symmetries, invariant errors and observers.
- Conclusion: open issue; a geometric look on least square parameter estimation.

Loop reactors PP2 and PP3 (Feluy)

reactor loop PP2



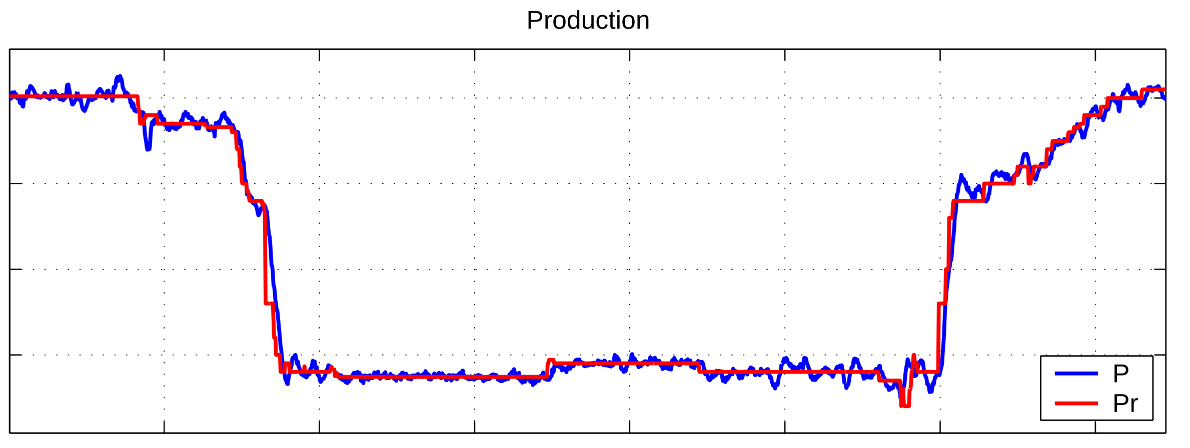
Control objectives

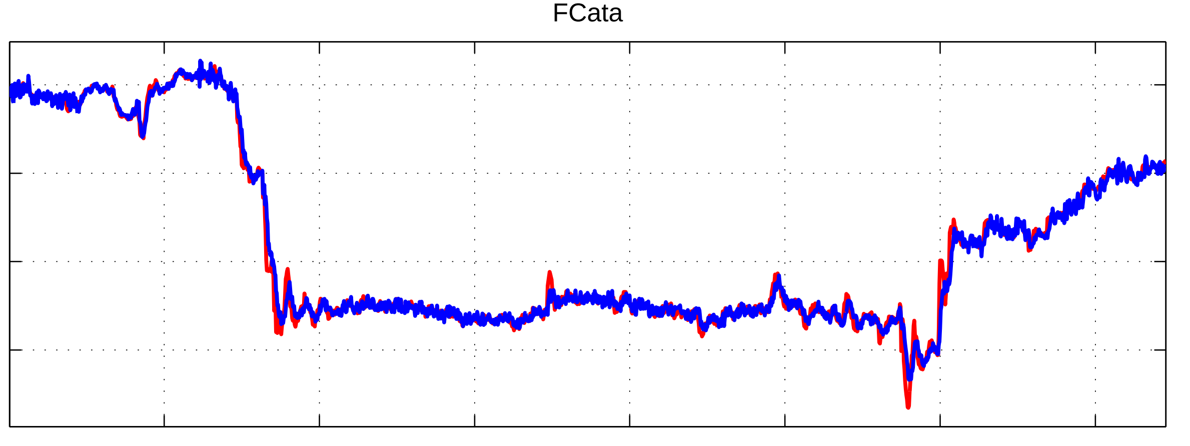
Control (manipulated) variables (input) : catalyst, C_3 input flow, H_2 input flow.

Controlled variables (output): production flow (measured via energy balance around the cooling jacket), solid fraction inside the reactor (measured with noise) , Melt-index (not measured) .

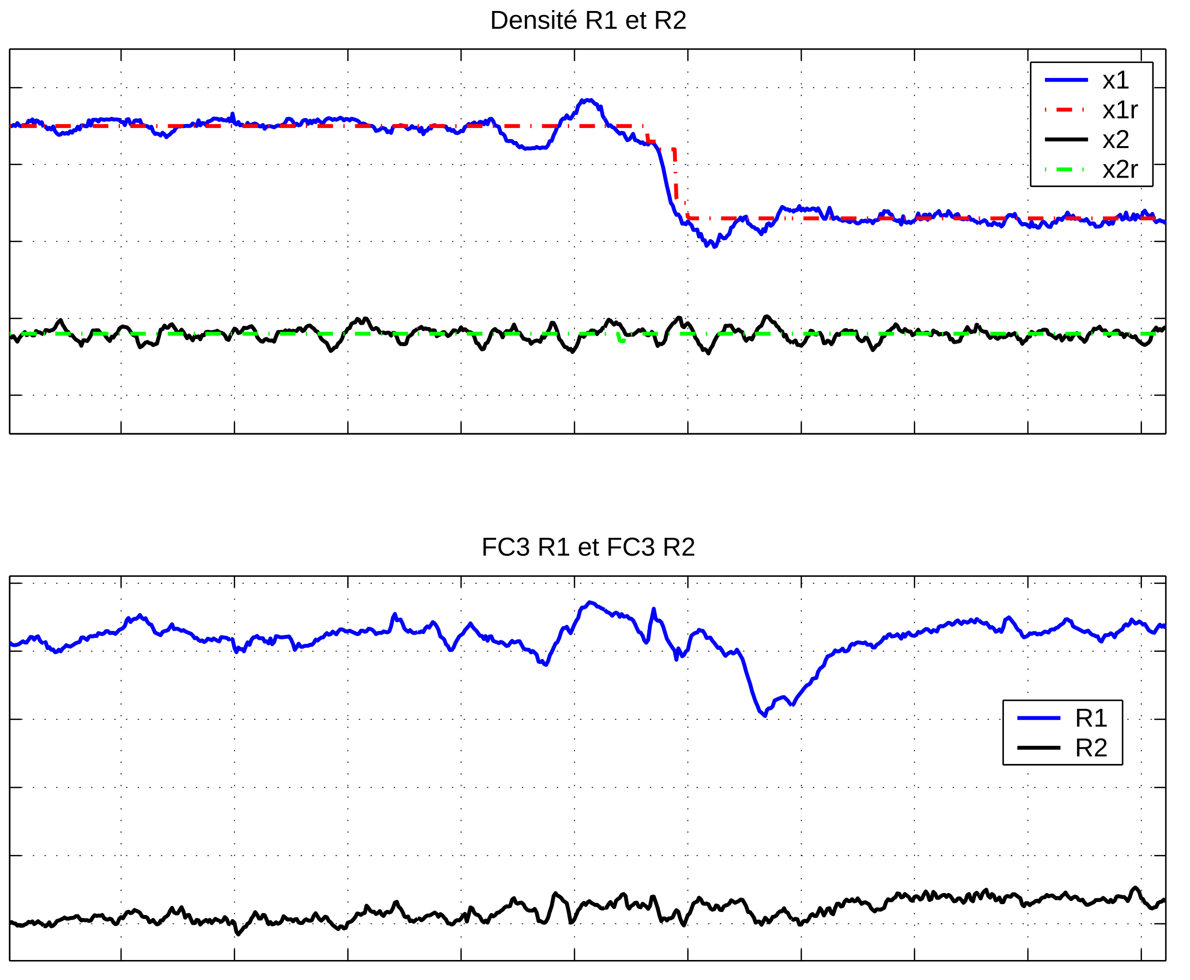
Goal: maximum production, solid fraction under a maximum hydrodynamic limit, melt-index at set-point.

Online results: production set-points tracking



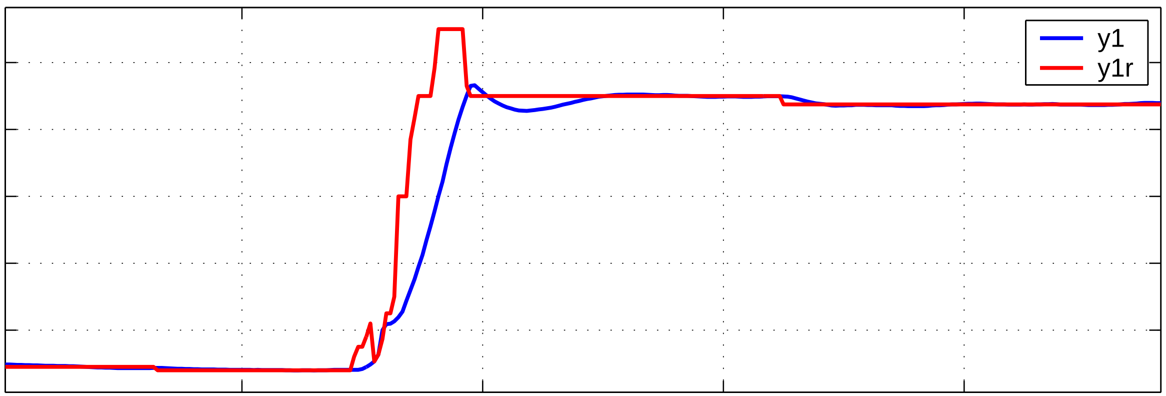


Online results: solid mass fraction set-point tracking

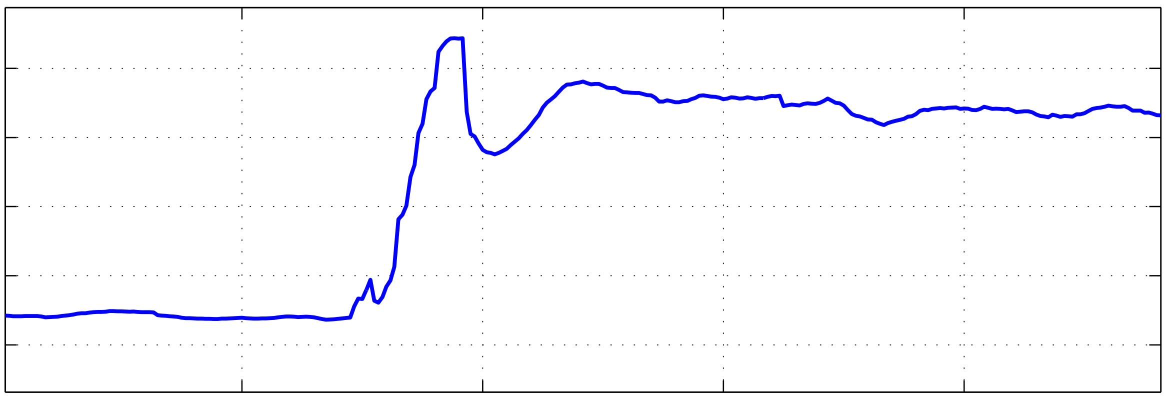


Online results: melt-index via H_2 inside the reactor

Hydrogène R1



FH2 R1



A dynamic model (DAE) of R1

Catalyst: $$\frac{d}{dt}M_{Cata} = F_{Cata} - \frac{M_{Cata}}{M_P + M_{PP}}F$$

Monomer: $$\frac{d}{dt}M_P = F_P - P - \frac{M_P}{M_P + M_{PP}}F$$

Hydrogen: $$\frac{d}{dt}M_{H_2} = F_{H_2} - \frac{M_{H_2}}{M_P + M_{PP}}F$$

Polymer: $$\frac{d}{dt}M_{PP} = P - \frac{M_{PP}}{M_P + M_{PP}}F$$

Constant volume: $$V = \frac{M_P}{\rho_P} + \frac{M_{PP}}{\rho_{PP}}$$

Catalyst activity: $$P = A\ M_{Cata}$$

solid mass-fraction: $$x = \frac{M_{PP}}{M_P + M_{PP}}$$

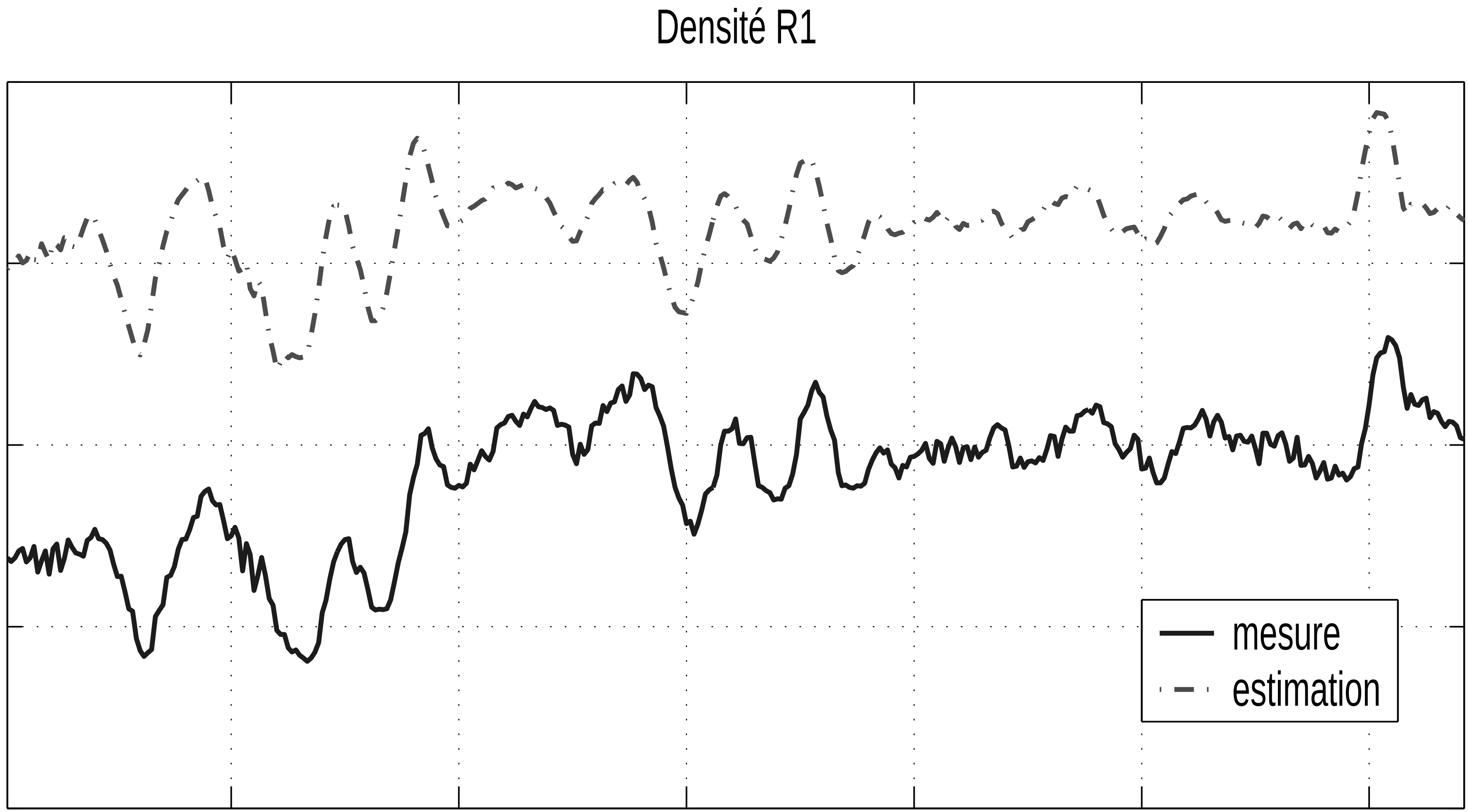
The control design for the first reactor R1

Use the triangular structure to have SISO sub-problem.

Compensate non-linearity via feedback (feedback linearization where the flat output are the controlled variables) and use PI controller on the linearized error dynamics.

Estimate unmeasured quantities (H_2 inside the reactor) and eliminate noise from the measurements (solid mass-fraction inside the reactor).

Online results: noise elimination, solid mass-fraction.



Dynamics of the solid mass-fraction x

$$\frac{d}{dt}M_P = F_P - P - \frac{M_P}{M_P + M_{PP}}F$$
$$\frac{d}{dt}M_{PP} = P - \frac{M_{PP}}{M_P + M_{PP}}F$$
$$V = \frac{M_P}{\rho_P} + \frac{M_{PP}}{\rho_{PP}}$$
$$x = \frac{M_{PP}}{M_P + M_{PP}}$$

Eliminate F (derivation of V):

$$\frac{d}{dt}x = \frac{1}{V}\left(\frac{1}{\rho_P} + x\left(\frac{1}{\rho_{PP}} - \frac{1}{\rho_P}\right)\right)(P - xF_P)$$

Noiseless estimation $\widehat{x}$ of x via an asymptotic observer

$$\frac{d}{dt}\widehat{x} = \frac{1}{V}\left(\frac{1}{\rho_P} + \widehat{x}\left(\frac{1}{\rho_{PP}} - \frac{1}{\rho_P}\right)\right)(P(t) - \widehat{x}F_P(t)) + C(x(t), \widehat{x})$$

where $x(t)$ is the noisy measure of x and $C(x, \widehat{x})$ is the correction such that $C(x, x) \equiv 0$ (no correction when the estimate $\widehat{x}$ is equal to the measure x).

Classically (extended Kalman filter) one takes $C(x, \widehat{x}) = k(x - \widehat{x})$ with a gain $k > 0$ that can vary...

Problem: such design for C depends on the unit you choose to define the solid fraction.

Dynamics of the solid volume-fraction X

$$\frac{d}{dt}V_P = F_P^{vol} - P^{vol} - \frac{\rho_P V_P}{\rho_P V_P + \rho_{PP} V_{PP}} F^{vol}$$

$$\frac{d}{dt}V_{PP} = \frac{\rho_P}{\rho_{PP}} \left(P^{vol} - \frac{\rho_{PP} V_{PP}}{\rho_P V_P + \rho_{PP} V_{PP}} F^{vol} \right)$$

$$V = V_P + V_{PP}$$

$$X = \frac{V_{PP}}{V_P + V_{PP}}$$

Eliminate F^{vol} (derivation of V):

$$\frac{d}{dt}X = \frac{1}{V} \left(\frac{1}{\rho_P} + X \left(\frac{1}{\rho_{PP}} - \frac{1}{\rho_P} \right) \right) \left(X(P^{vol} - F_P^{vol}) + (1 - X)\frac{\rho_P}{\rho_{PP}} P^{vol} \right)$$

Solid mass-fraction x or solid volume-fraction X ?

$$X = \frac{x}{x + \frac{\rho_P}{\rho_{PP}}(1-x)}, \quad x = \frac{X}{X + \frac{\rho_{PP}}{\rho_P}(1-X)}$$

and the dynamics with X reads

$$\frac{d}{dt}X = \frac{1}{V}\left(\frac{1}{\rho_P} + X\left(\frac{1}{\rho_{PP}} - \frac{1}{\rho_P}\right)\right)\left(X(P^{vol} - F_P^{vol}) + (1-X)\frac{\rho_P}{\rho_{PP}}P^{vol}\right)$$

a different expression than the dynamics with x:

$$\frac{d}{dt}x = \frac{1}{V}\left(\frac{1}{\rho_P} + x\left(\frac{1}{\rho_{PP}} - \frac{1}{\rho_P}\right)\right)(P - xF_P)$$

Problem: an extended Kalman filter with x does not correspond to an extended Kalman filter with X...

Group of transformations $\{g_\mu\}_{\mu>0}$

The map g_μ

$$[0,1] \ni x \xrightarrow{g_\mu} X = \frac{x}{x + \mu(1-x)} \in [0,1]$$

has $g_{\mu^{-1}}$ as inverse

$$[0,1] \ni X \xrightarrow{g_{\mu^{-1}}} x = \frac{X}{X + \mu^{-1}(1-X)} \in [0,1]$$

The set $\{g_\mu\}_{\mu>0}$ is a one parameter group of transformations on $[0,1]$, isomorph to multiplicative group $G = \mathbb{R}^{+*}$:

$$g_\mu \circ g_\nu = g_{\mu\nu}$$

The invariant error $E(x,\widehat{x})$

Consider the function E

$$]0,1[\times]0,1[\ni (x,\widehat{x}) \mapsto E(x,\widehat{x}) = \log\left(\frac{x(1-\widehat{x})}{\widehat{x}(1-x)}\right) \in \mathbb{R}$$

Then:

$$E(x,\widehat{x}) = E\left(\frac{x}{x+\mu(1-x)}\ ,\frac{\widehat{x}}{\widehat{x}+\mu(1-\widehat{x})}\ \right)$$

for any $\mu > 0$ and $E(x,\widehat{x}) = 0$ means that $x = \widehat{x}$.

This is no the case of $(x,\widehat{x}) \mapsto x - \widehat{x}$. Thus $E(x,\widehat{x})$ is an intrinsic way to measure the error between x and $\widehat{x}$: it is an invariant error.

The invariant observer based on the invariant error

Copy the original dynamics in x

$$\frac{d}{dt}x = \frac{1}{V}\left(\frac{1}{\rho_P} + x\left(\frac{1}{\rho_{PP}} - \frac{1}{\rho_P}\right)\right)(P - xF_P)$$

and add a correction term based on $E(x, \widehat{x})$ as follows

$$\frac{d}{dt}\widehat{x} = \frac{1}{V}\left[\frac{1}{\mu_P} + \widehat{x}\left(\frac{1}{\mu_{PP}} - \frac{1}{\mu_P}\right)\right]\left[P - \widehat{x}F_P - k\ \log\left(\frac{x(1-\widehat{x})}{(1-x)\widehat{x}}\right)\right].$$

This observer is invariant and convergent for any $k > 0$.

Dynamics invariant under a group of transformations

$$\frac{d}{dt}x = f(x), \quad y = h(x)$$

Let G be a group of transformations acting on the x-space and also on the y-space,

$$X = \varphi_g(x), \quad Y = \rho_g(y), \quad g \in G,$$

where φ_g and ρ_g are diffeomorphisms (smooth bijections).

$\frac{d}{dt}x = f(x)$ with output $y = h(x)$ is said to be G-*invariant* if for every $g \in G$ the representation of the system remains unchanged:

$$\frac{d}{dt}X = f(X), \quad Y = h(X).$$

Invariant observer

Take a G-invariant dynamics $\frac{d}{dt}x = f(x)$ with output $y = h(x)$.

The observer ($\widehat{f}(x, h(x)) \equiv f(x)$)

$$\frac{d}{dt}\widehat{x} = \widehat{f}(\widehat{x}, h(x))$$

is said G-invariant if, and only if, for all $g \in G$, for all estimated state $\widehat{x}$ and state x, we have

$$\frac{d}{dt}\widehat{X} = \widehat{f}(\widehat{X}, h(X))$$

where $\widehat{X} = \varphi_g(\widehat{x})$ and $X = \varphi_g(x)$.

Construction of invariant observer

Assume that the vector field $w(x)$ is invariant with respect to G. Take a scalar functions of the form $I(\widehat{x}, h(x))$ invariant under the action of G ($I(\widehat{x}, h(x)) = I(X, h(X))$. Then

$$\frac{d}{dt}\widehat{x} = f(\widehat{x}) + (I(\widehat{x}, y) - I(\widehat{x}, h(\widehat{x}))\ w(\widehat{x})$$

is an invariant observer. The term

$$(I(\widehat{x}, y) - I(\widehat{x}, h(\widehat{x}))\ w(\widehat{x})$$

corresponds to an invariant correction term replacing the Kalman filter correction term $k(h(x) - h(\widehat{x}))$ that does not preserve he symmetries group G.

Problem: how to compute such w and such I ?

Computation of I

Take a G-invariant dynamics $\frac{d}{dt}x = f(x)$ with output $y = h(x)$. Assume that for some x_0, the smooth map

$$G \ni g \mapsto \varphi_g(x)$$

is of rank $r = \dim G$ around $g = \mathrm{Id}$ with $r \leq n = \dim x$. Then, locally around (x_0), there exist $m = \dim y$ functionally independent invariant functions $I_i(\hat{x}, y)$, $i = 1, \dots, m$.

Proof: the Darboux-Cartan moving frame method.

The Darboux-Cartan moving frame method

The group G depends on $r \leq \dim(x) = n$ parameters $\mu = (\mu_1, ..., \mu_r)$. Its action reads

$$\mu \in \mathbb{R}^r, \quad g_\mu \in G, \quad X = \varphi_{g_\mu}(x), \quad Y = \rho_{g_\mu}(y) \quad (y = h(x)).$$

Under classical regularity conditions on the action on the x-space, one can compute a complete set of invariant errors via the following elimination algorithm.

Take any normalization $\bar{X}$. From $\bar{X} = \varphi_{g_\mu}(x)$ compute μ as function of x: $\mu = q(x)$. Then

$$I(x, \hat{x}) = \rho_{g_{q(\hat{x})}}(h(x))$$

is automatically invariant:

$$\forall \mu, \quad I(x, \hat{x}) = I(X, \hat{X})$$

.

Invariant composition error

Let

$$y = (y_1, \ldots, y_n)$$

denotes the composition of a mixture of n species. The invariant errors are given for $i \neq j$ by

$$E_{i,j}(y, \widehat{y}) = \log \left(\frac{y_i \widehat{y}_j}{\widehat{y}_i y_j} \right)$$

under the group of unit changes (same value for mass or mole fractions) (we can replace the log function by any bijection that vanishes at 1).

Conclusion

Several points remain to be fixed: computing the invariant vector field w; link between invariance and convergence (invariant does not automatically implies convergence and robustness); formalism on implicit models (DAE) where invariance is simpler.

Invariant error, normalization and parameter estimation: what is the meaning of $y_{t_k}(p) - y_{t_k}^{mesure}$ in the classical least square problem

$$\min_{\text{parameter } p} \quad \sum_{k=1}^{N} \left(y_{t_k}(p) - y_{t_k}^{mesure} \right)^2$$

where y_{t_k} corresponds to a composition at sampling time t_k.