Part 2

QR for nonlinear black-box SI

A qualitative-fuzzy framework

Outline

- The method:

  qualitative behaviors $\rightarrow$ fuzzy rules

- An application to medical domain

  Kinetics of Thiamine (vitamin B_1)

  in the cells of the intestine tissue

- Results

- Open problems

Motivations

Goal: to exploit QR techniques to improve the performances of black-box approaches to SI of nonlinear systems

- Statistical approaches: nonlinear regression
  - paucity of directly applicable results
- Neural networks
  - may be extremely inefficient
  - the result does not capture any structural knowledge

QR for exploiting all available *prior* knowledge to provide for:

- a proper identifier
- a proper initialization of the parameter estimation procedure

Why Fuzzy Systems ?

- capability to deal with linguistic description (IF-THEN rules) of the system dynamics
- universal approximator
- better performance over the neural networks when prior knowledge is available
- understandable results in terms of the fuzzy rule base

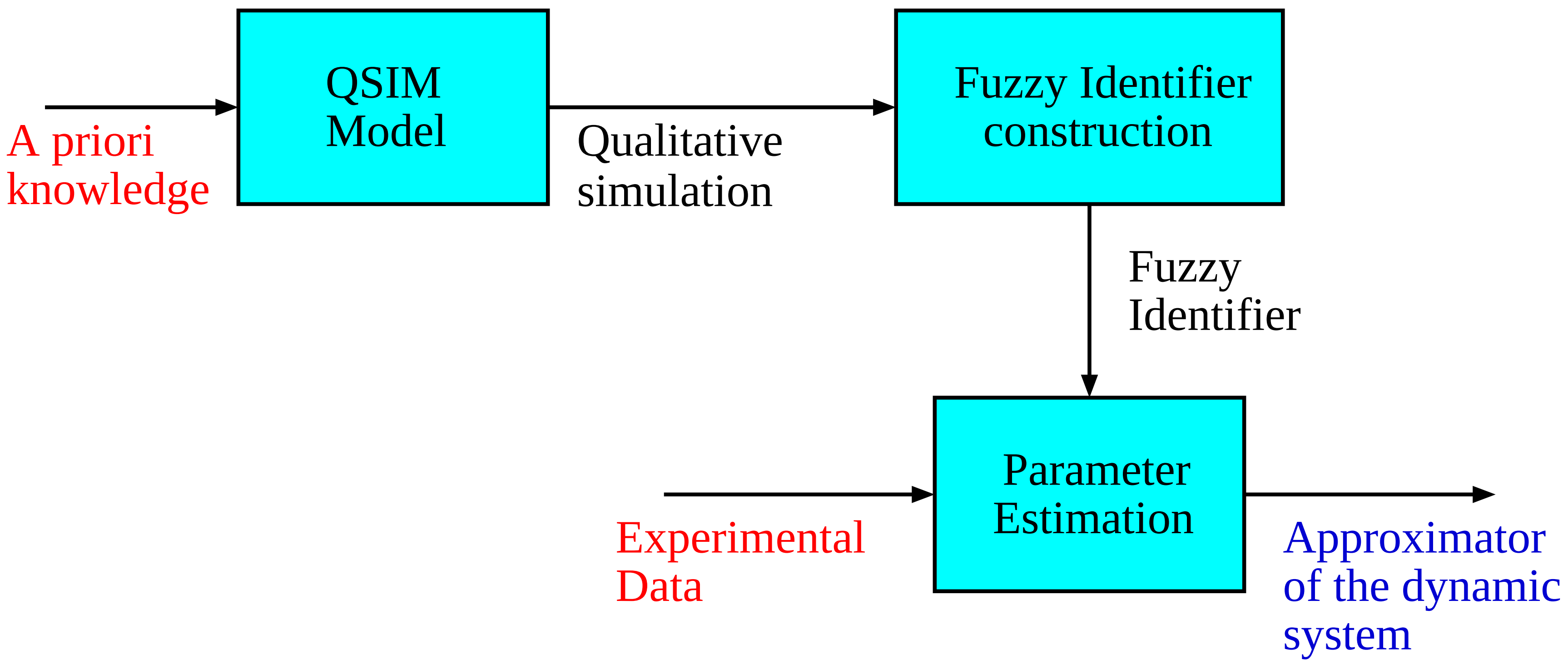
BUT

To define a *meaningful* rule base on complex dynamic systems is *quite difficult*

$\Downarrow$

IDEA: automatically build a meaningful rule base from QSIM models

Main steps

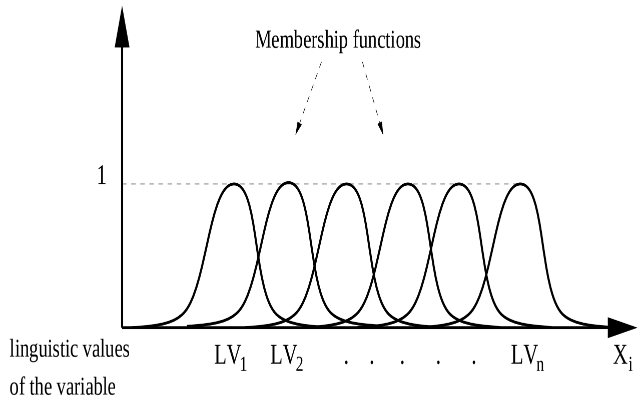


A priori knowledge
QSIM Model
Qualitative simulation
Fuzzy Identifier construction
Fuzzy Identifier
Experimental Data
Parameter Estimation
Approximator of the dynamic system

Fuzzy Systems

- A fuzzy set F in U, the universe of discourse, is defined by a membership function μ_F

$$\mu_F : \quad U \rightarrow [0, 1]$$



- Fuzzy rules: IF x_i is μ_i AND $\ldots$ x_j is μ_j THEN y is μ_k

  For function approximation $y = f(\underline{x})$: the value $y \in V \subset R$ is inferred by rules with n input variables $x_i \in U_i \subset R$

- Inference engine
  - singleton fuzzifier
  - product-inference rule
  - centered average defuzzifier

Fuzzy Identifier

$$y(\underline{x}, \underline{\theta}) = \frac{\sum_{j=1}^{M} \overline{y}^j (\prod_{i=1}^{n} \mu_i^j(x_i))}{\sum_{j=1}^{M} (\prod_{i=1}^{n} \mu_i^j(x_i))}$$

$\underline{\theta}$ vector of parameters, M number of rules

- Gaussian μ_i: $y(\underline{x}, \underline{\theta}) = \frac{\sum_{j=1}^{M} \overline{y}^j (\prod_{i=1}^{n} exp(-(\frac{x_i - \overline{x}_i^j}{\sigma_i^j})^2))}{\sum_{j=1}^{M} (\prod_{i=1}^{n} exp(-(\frac{x_i - \overline{x}_i^j}{\sigma_i^j})^2))}$

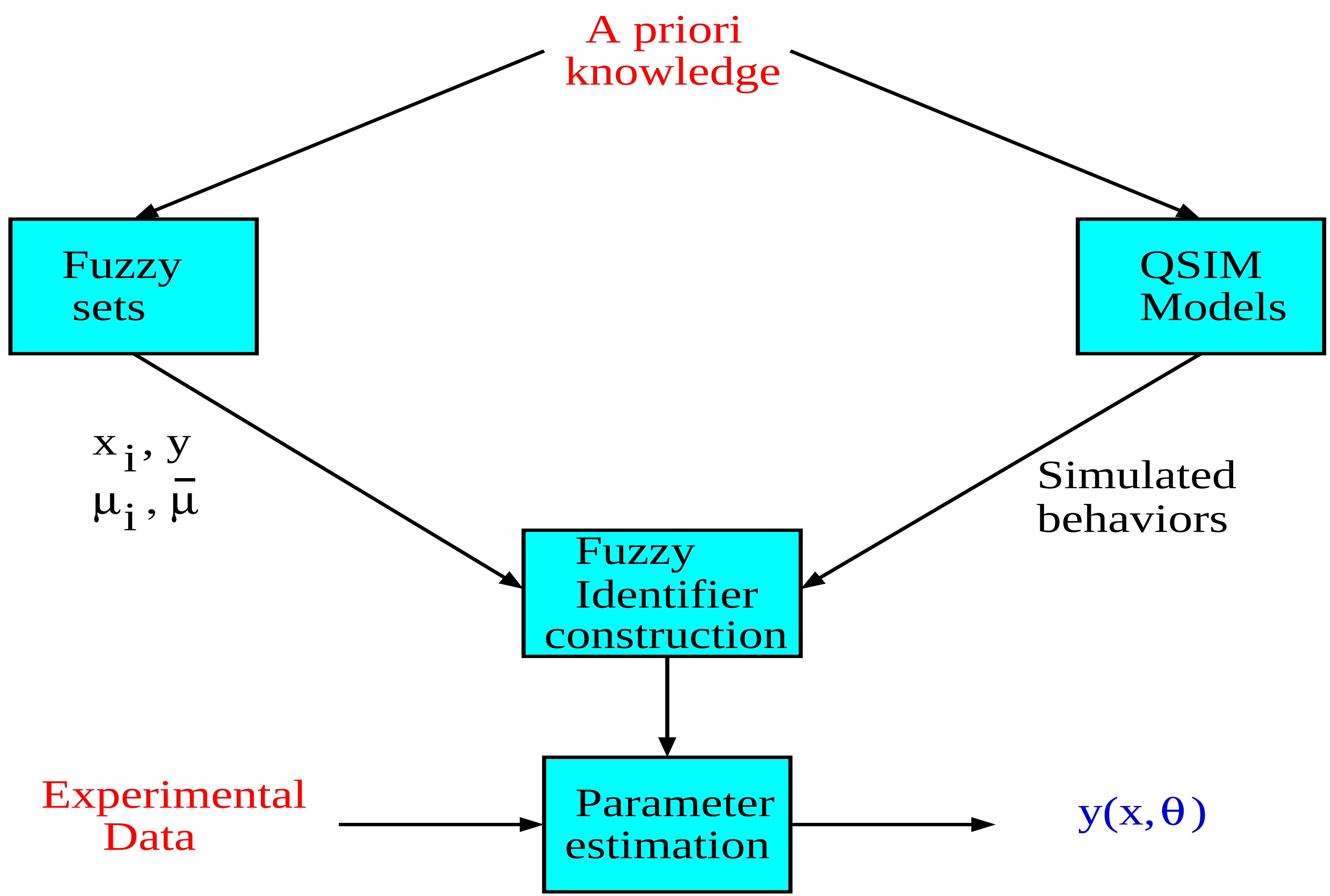
$$\underline{\theta} = (\overline{y}^j,\ \overline{x}_i^j, \sigma_i^j,),\ \ i = 1, .., n,\ j = 1, .., M$$

- We are interested in an approximator of the kind:

$$\boxed{y_{k+1} = y(\underline{x}_k, \underline{\theta})}$$

  – k is a discrete time index
  – $\underline{x}_k = \{\underline{u}_k, y_k\}$, $\underline{u}_k$, y_k current inputs and output

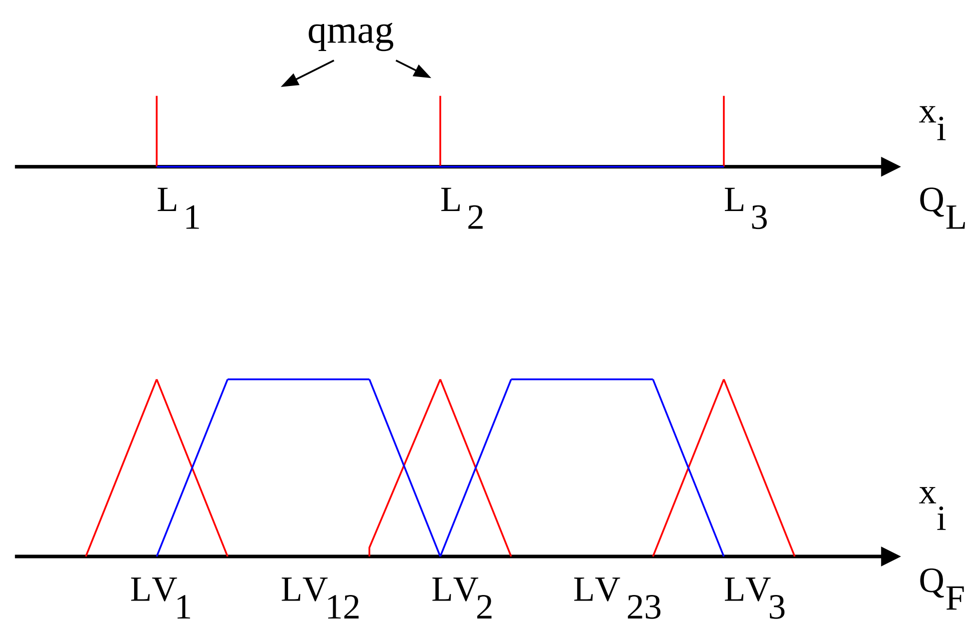
The method: basic steps



Analogies between QSIM and FS (1)

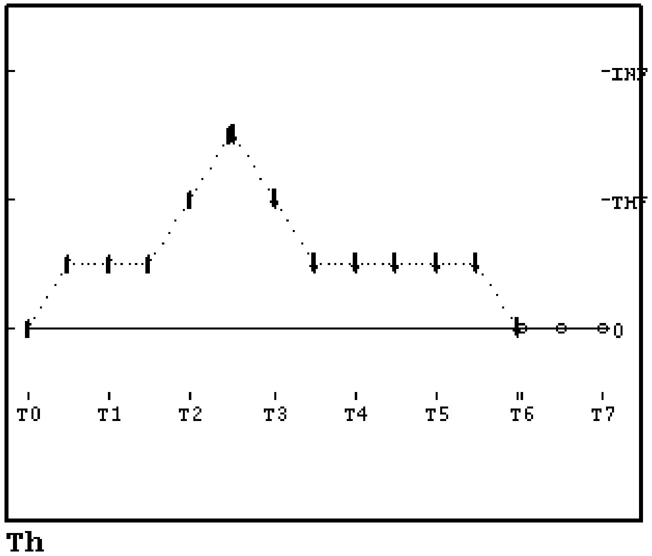
- system model level

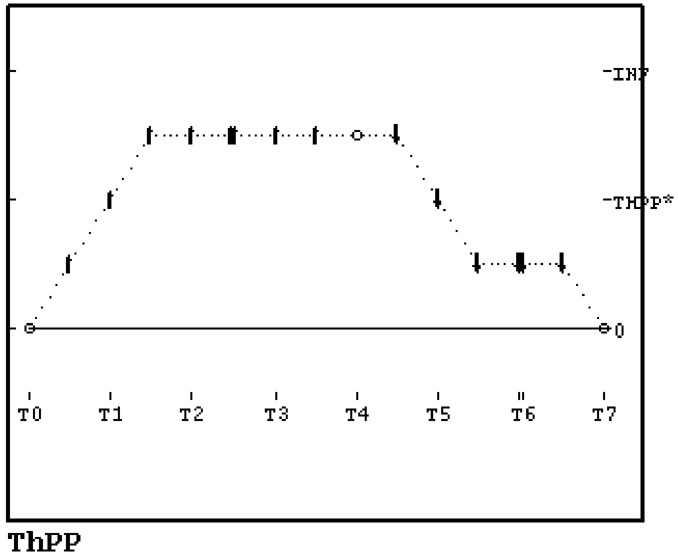
$$
\begin{tikzcd}
 & & \boldsymbol{R} \arrow[dl] \arrow[dr] & & \\
qmag & Q_L \arrow[l] \arrow[rr, leftrightarrow] & & Q_F \arrow[r] & \mu
\end{tikzcd}
$$



Analogies between QSIM and FS (2)

System behavior level



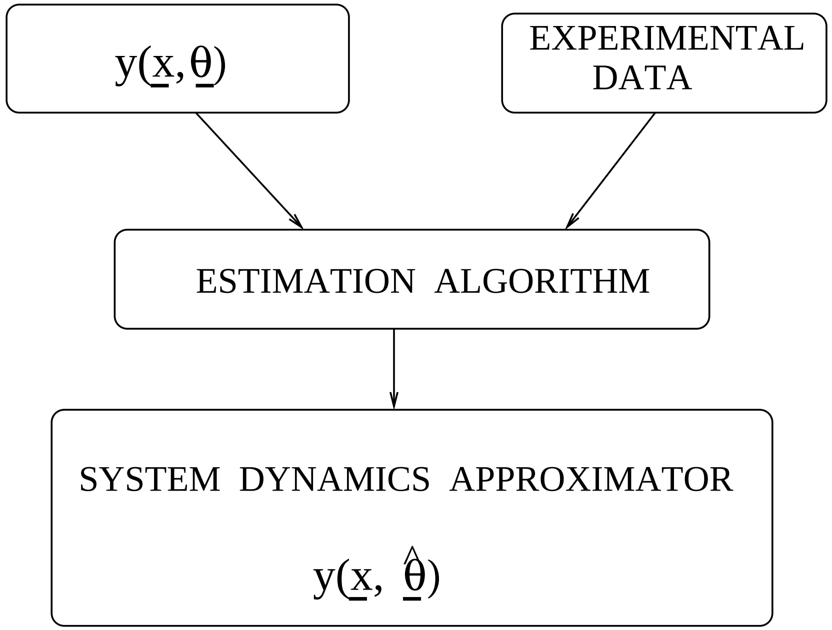


0	$\longrightarrow$	Zero
$(0, Th^*)$	$\longrightarrow$	Low
Th^*	$\longrightarrow$	Medium
(Th^*, inf)	$\longrightarrow$	High

0	$\longrightarrow$	Zero
$(0, ThPP^*)$	$\longrightarrow$	Low
$ThPP^*$	$\longrightarrow$	Medium
$(ThPP^*, inf)$	$\longrightarrow$	High

t=T5: IF Th_t is Low AND $ThPP_t$ is Medium THEN $ThPP_{t+1}$ is Low

Parameter Estimation



Estimation algorithms:

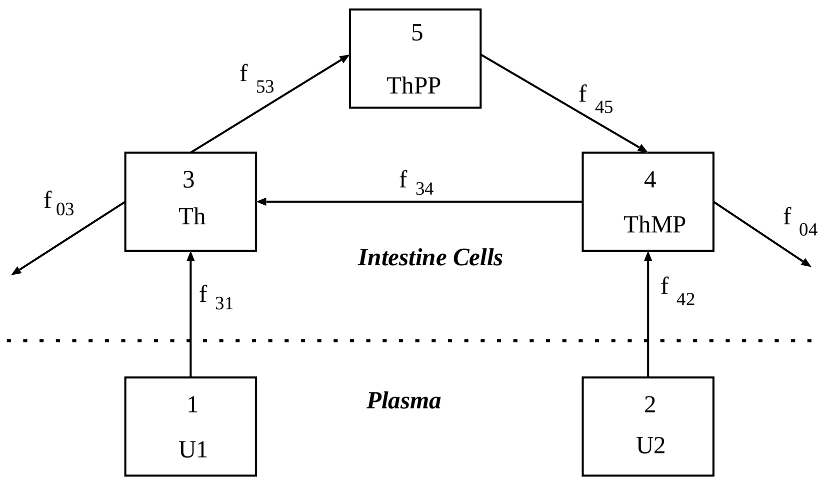
- back–propagation
- linear least squares

Application to medical domains

- one-step ahead predictor of the Blood Glucose Level dynamics in diabetic patients in response to insulin therapy and meals assumption
- simulator of the kinetics of Thiamine and its phosphoesters in the cells of the intestine tissue

A model of Thiamine Kinetics

A model of the intracellular distribution of Thiamine is very useful to describe syndromes with Thiamine deficiency (e.g. severe liver diseases)

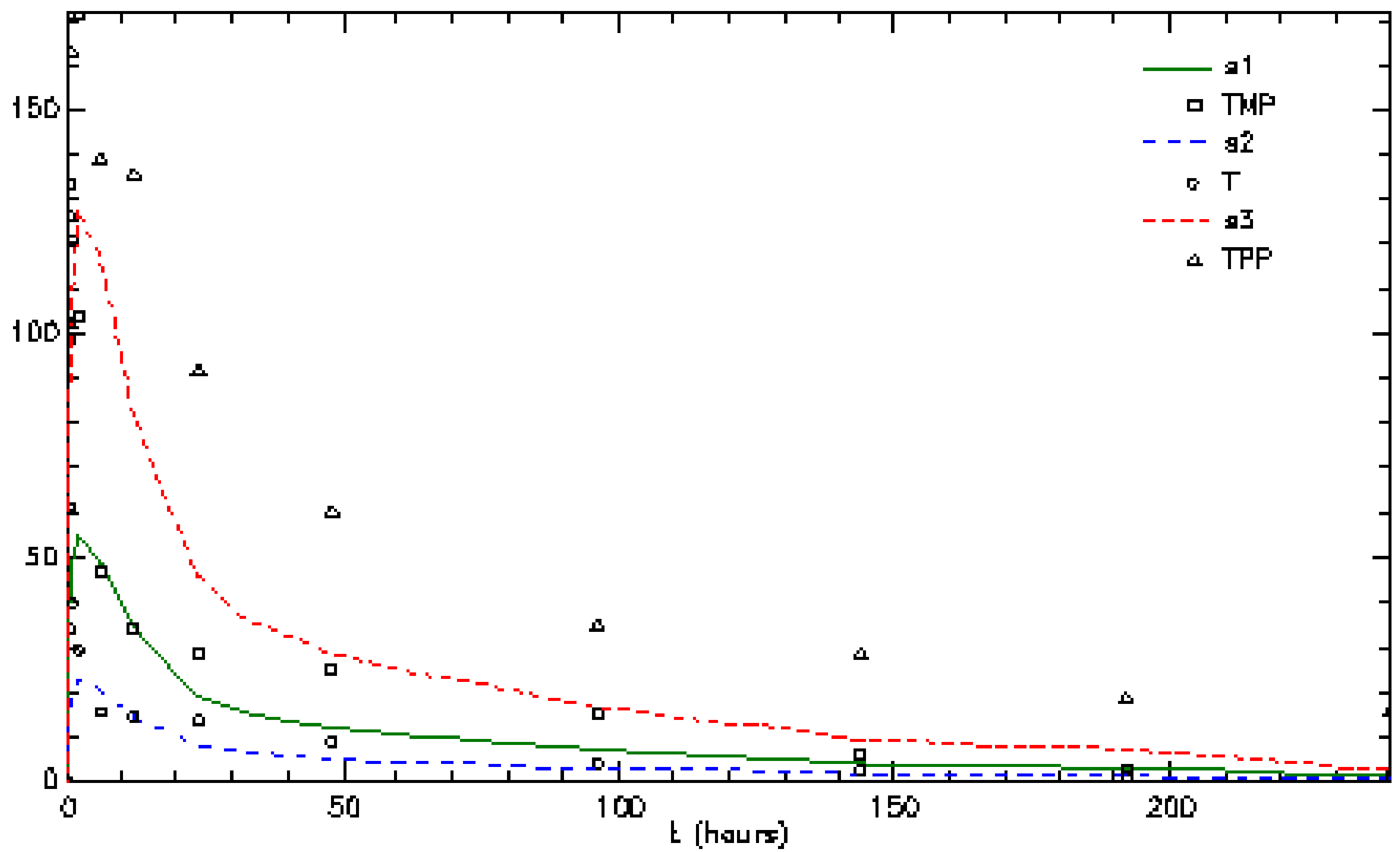


Modeling Problems:

- modeling through ODE is hampered by identification problems
- the chemical reactions are nonlinear
- the linearity assumption, considered in the literature, is completely inadequate
- poor data set

Structural Identification results - SAAM

Although, under the linearity assumption, the *a priori* identifiability is satis-fied, identification results are unsuccesful



The black-box model

$$
\begin{aligned}
Th_{t+1} &= f_1(Th_t, ThMP_t, U_{1t}) \\
ThPP_{t+1} &= f_2(ThPP_t, Th_t) \\
ThMP_{t+1} &= f_3(ThMP_t, ThPP_t, U_{2t}
\end{aligned}
$$

- 3 decoupled subsystems
- 3 QSIM models

1. Th : $\boxed{\dot{Th} = S^+(u_1) + M^+(ThMP) - M^+(Th)}$
2. ThPP: $\boxed{\dot{ThPP} = M^+(Th) - M^+(ThPP)}$
3. ThMP: $\boxed{\dot{ThMP} = S^+(u_2) + M^+(ThPP) - M^+(ThMP)}$

Simulation

- Simulation of a tracer experiment
  - The chemical reactions of one form into another are modeled as triangular shaped functions, the absortions from plasma as saturable functions of the input signals
  - at $t = 0, \; qmag(x_i) = 0$, x_i system variables
- generated behaviors

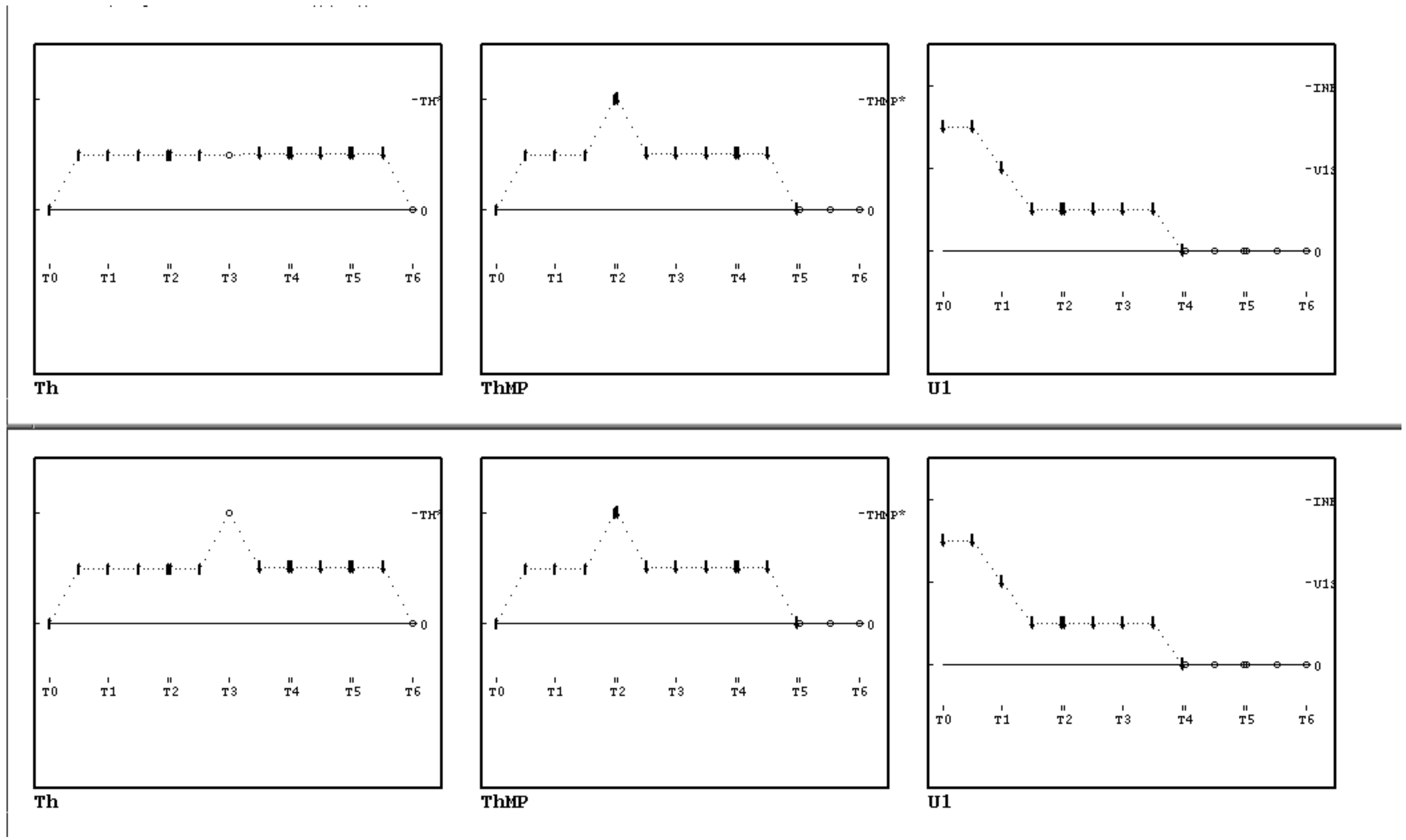
Subsystem	# QQB's	# AQB's
1	20	2
2	6	6
3	42	7

QQB: Quiescent qualitative behavior

AQB: Admissible qualitative behavior

QSIM outcomes

Thiamine subsystem



- 16 out of 20 behaviors are filtered out for inconsistency with the condition: $u_1(t^*) < u_s$, $t^* : Th(t^*) = maxTh$
- aggregation procedures have identified 2 different behaviors

Mapping between Q_L and Q_F

Variables	Q_L	Q_F		
			$\hat{x}$ (nCi/g)	σ (nCi/g)
x_1	0	Low	0	13
	(0 Th^*)	Medium	30	13
	Th^*	High	60	13
x_2	0	Low	5	30
	(0 $ThPP^*$)	Medium	80	30
	$ThPP^*$	High	165	35
x_3	0	Low	0	22
	(0 $ThMP^*$)	Medium	50	20
	$ThMP^*$	High	130	44
u_1	0	Low	20	400
	(0 $U1S$)	Medium	1000	400
	$U1S$	High	2000	400
	$(U1S\ inf)$	Very High	3000	400
u_2	0	Low	70	140
	(0 $U2S$)	Medium	330	70
	$U2S$	High	470	50
	$(U2S\ inf)$	Very High	600	60

Generated Rules

Thiamine subsystem: 11 rules

1. "If Th_t is L and $ThMP_t$ is L and U_1t is V-H then Th_{t+1} is L"
2. "If Th_t is L and $ThMP_t$ is L and U_1t is V-H then Th_{t+1} is Th_{t+1} M"
3. "If Th_t is M and $ThMP_t$ is M and U_1t is V-H then is M"
4. "If Th_t is M and $ThMP_t$ is M and U_1t is H then Th_{t+1} is M"
5. "If Th_t is M and $ThMP_t$ is M and U_1t is M thenTh_{t+1} is M"
6. "If Th_t is M and $ThMP_t$ is H and U_1t is M then Th_{t+1} is M"
7. "If Th_t is M and $ThMP_t$ is M and U_1t is L then Th_{t+1} is M"
8. "If Th_t is M and $ThMP_t$ is L and U_1t is L then Th_{t+1} is M"
9. "If Th_t is M and $ThMP_t$ is L and U_1t is L then Th_{t+1} is L"
10. "If Th_t is M and $ThMP_t$ is M and U_1t is M then Th_{t+1} is H"
11. "If Th_t is H and $ThMP_t$ is M and U_1t is M then Th_{t+1} is M"

THPP subsystem: 9 rules
ThMP subsystem: 12 rules

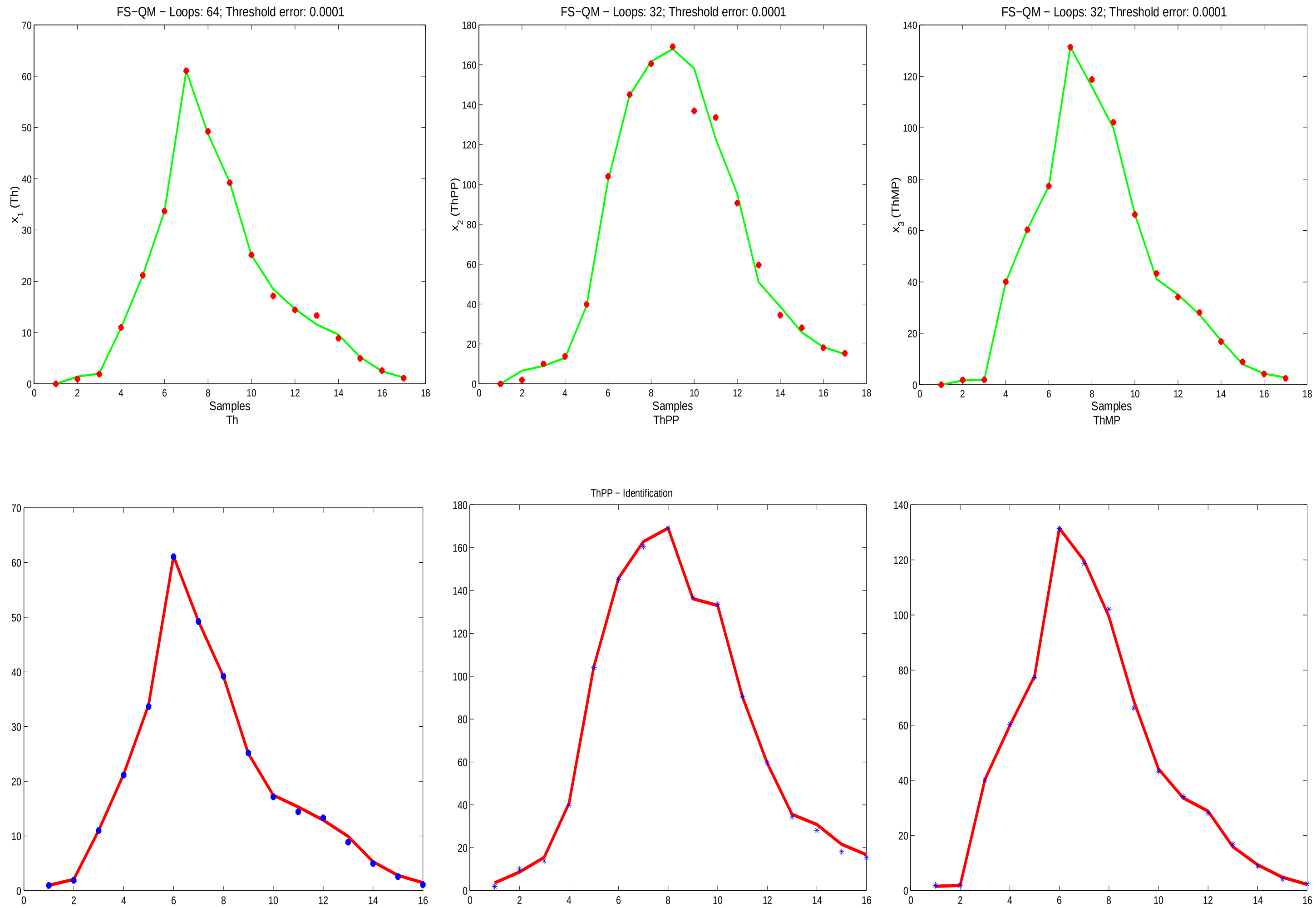
An approximator for simulation

The overall scheme consists of three phases:

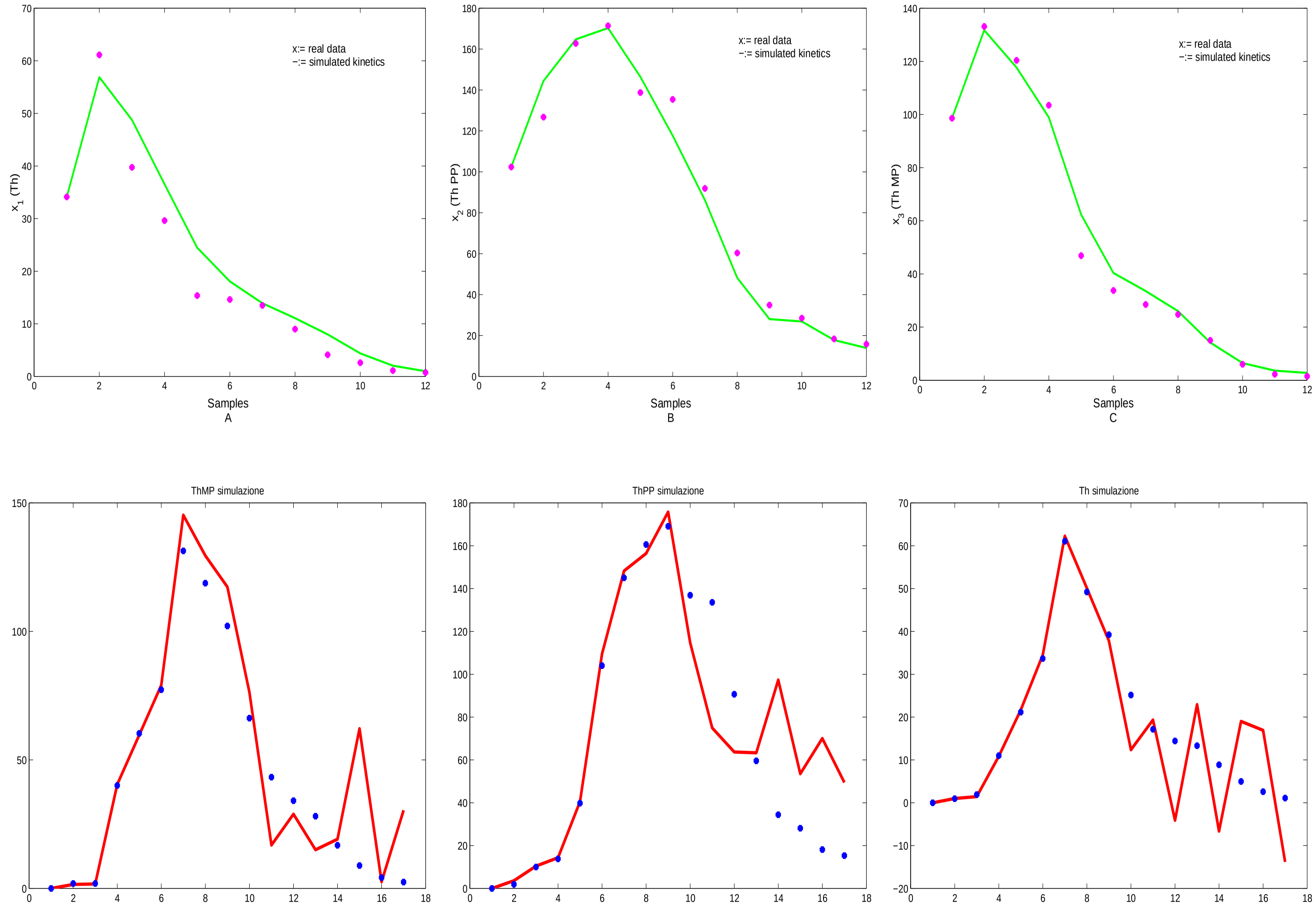
1. identification phase: find each $\tilde{f}_i$
   - *Observed data*: response of a group of rats to an intravenous bolus of radioactive Th observed for 240 h and sampled with non-uniform time intervals
2. validation phase: test each $\tilde{f}_i$
   - *Validation data*: a new data set of data collected in an independent experiment
3. simulation phase: test each $\tilde{f}_i$ in a parallel scheme where only the current inputs to the whole system are measured data
   - *Validation data*: as at step 2

Identification results

Our method (FS-QM); a data-driven black–box approach (FNN)



Forecasting results



Remarks

- Identification phase
  - Comparable performance also in terms of number of loops
- FS-QM performs quite well both in the validation and simulation phase
- FNN is not even able to simulate the same data used for identification

Open Problems

- Mathematical formalization: range of validity and applicability
- Choice of proper membership function shapes to improve the capability to express prior knowledge
- Mapping of the sampling time set into the qualitative time set
- Methods for dealing with hybrid models
- Experimentation of other parameter estimation procedures

Conclusive remarks

Traditional black-box approches to SI does benefit from the integration with QR

Integrated frameworks:

- allow us to identify systems for which a poor data set is available
- allow us to properly initialize both the identifier scheme and the guess of parameter values
- guarantee better efficiency and robustness

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