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On Useful Redundancy in Dynamic Inverse Problems Related Optimization

Mazen Alamir*

* University of Grenoble
Gipsa-Lab, Control Systems Dept., Sysco-Group,
Rue de la Houille Blanche, Domaine Universitaire, ST Martin d'Hères,
France (Tel: +33 4-76-82-63-26), (e-mail: mazen.alamir@inpg.fr)
Website: http://www.lag.ensieg.ipg.fr/alamir

Abstract: In this paper, it is pointed-out that inverse problems arising in nonlinear control systems design such as state reconstruction and/or parameter estimation are naturally redundant. It is also shown that this redundancy can be used to enhance avoiding singularity heuristics. Some related algorithms are discussed and illustrated on a simple example of chemical reactors. These algorithms can be added to any optimization algorithm in order to enforce the singularity avoidance capabilities.

Keywords: Nonlinear Systems; Moving-Horizon Observers; Inverse Problems; Singularities Avoidance; Nonconvex Optimization

1. INTRODUCTION

Chemical and biological processes are generally characterized by highly nonlinear dynamics that involve badly known parameters. They also suffer from the lack of sensors making the use of state observers mandatory.

While many analytic observer design methods are conceptually available for nonlinear systems (Gauthier et al. [1992], Slotine et al. [1987]), the need for structural properties that have to be satisfied by the system model tremendously reduces the class of systems to which analytic observers can be applied.

On the contrary, optimization-based observers (Michalska and Mayne [1995]) that reconstruct the state by minimizing output prediction error related cost are particularly suitable as they enable complex modeling as well as state constraint handling. More precisely, given a nonlinear model of the general form:

$$x(t) = X(t, t_0, x_0) \in \mathbb{R}^n \quad ; \quad y = h(x) \in \mathbb{R}^m \tag{1}$$

these observers more or less look for the global minimum, say $z_{opt}(t)$, of the cost function defined at instant t by:

$$J_0(z, t, y_{t-T}^t) = \int_{t-T}^t ||Y(\tau, t - T, z) - y(\tau)||_Q^2 d\tau$$
(2)

in order to produce an estimation $z_{opt}(t)$ of the past state x(t-T). This estimation is then used to obtain the estimation of the state at instant t according to:

$$\hat{x}(t) := X(t, t - T, z_{opt}(t))$$

Note that by the very definition of observability, $z_{opt}(t)$ is the unique global minimum of $J_0(\cdot,t,y_{t-T}^t)$. Moreover, one clearly has in the absence of modeling errors and measurement noise:

$$J_0(z_{opt}(t), t, y_{t-T}^t) = 0$$

One of the major issues is therefore to ensure the global convergence of the iterates when solving the underlined optimization problem:

$$\min_{z \in \mathcal{Z}} J_0(z, t, y_{t-T}^t)$$

where \mathcal{Z} denotes the admissible set of states. This paper suggests a heuristic that may be useful in avoiding incidental singularities that an optimizer may encounter. More precisely, the starting point of the present work is to recognize that

The global optimum one is looking for is very particular since it is shared by an infinite number of cost functions!

Indeed, $z_{opt}(t)$ is the unique global minimum for any cost function of the following form:

$$J_i(z, t, y_{t-T}^t) := \int_{t-T}^t \Phi_i(\tau) \cdot \Psi_i(\epsilon_y(\tau, z, t)) d\tau \qquad (3)$$

where $\epsilon_y(\tau,z,t) := Y(\tau,t-T,z) - y(\tau)$ is the output prediction error at instant τ , Ψ_i is any continuous positive definite function defined on \mathbb{R}^m while Φ_i is any scalar positive function. The classical cost function (2) is obtained by the obvious choices: $\Phi_0(\cdot) \equiv 1$ and $\Psi_0(\cdot) \equiv \|\cdot\|_Q^2$.

Based on the above discussion, it comes out clearly that one must be able to do *something more* than just using standard optimization schemes as if the optimization problem was uniquely given once for all. This is the aim of the

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present paper.

It is worth mentioning that a preliminary and quite particular version of the ideas proposed in this paper has been successfully applied to the robust state estimation of monomers concentrations in terpolymerization reactors Alamir et al. [2006]. This paper gives a general conceptual framework that is motivated by that success.

The remainder of the paper is organized as follows: first, in section 2, the general framework of redundant optimization problems is set-up and sufficient conditions for useful redundancy are given together with a dedicated algorithm. The application of the general framework to safely-redundant state-observers related problems is also discussed. In section 3, the framework is illustrated through a bio-reactor while a parallel version of the algorithm is proposed in section 4.

2. GENERAL FRAMEWORK FOR REDUNDANT OPTIMIZATION PROBLEMS

Consider a constrained optimization problem defined on \mathbb{R}^n by:

$$\mathcal{P}_0$$
 : $\min_{z \in \mathcal{Z}} J_0(z)$; $\mathcal{Z} \subset \mathbb{R}^n$

where J_0 is a positive cost function admitting the global minimum z_{opt} and probably other local minima.

Consider also an optimizer that uses some iteration S:

$$z^{(i+1)} = \mathcal{S}(z^{(i)}, J_0(\cdot))$$

in order to find the solution z_{opt} of \mathcal{P}_0 . r successive iterations of \mathcal{S} lead to the multi-steps updating map that is denoted hereafter by $\mathcal{S}^{(r)}$, namely:

$$z^{(i+r)} = \mathcal{S}^{(r)}(z^{(i)}, J_0)$$

The sequence of values that is *induced* by the successive iterations starting from some initial guess $z^{(0)}$, namely

$$\left\{\mathcal{S}^{(r)}(z^{(0)},J_0)\right\}_{r\in\mathbb{N}}$$

is called hereafter, the $(z^{(0)}, J_0)$ -solver path as it depends on both the initial guess and the cost function J_0 being used. Note that under convexity condition one may expect the following asymptotic property to hold

(under convexity)
$$\lim_{r \to \infty} S^{(r)}(z^{(0)}, J_0) = z_{opt}$$

while in the general case, the solver path may be trapped by some local minima of J_0 . The redundancy invoked in the introduction is to be used to avoid such situations. For this, consider the following definition:

Definition 1. The optimization problem \mathcal{P}_0 is called *N*-safely redundant if and only if the following conditions hold

- (1) There exists a finite sequence of N cost functions J_i defined on \mathbb{R}^n that admits z_{opt} as a global minimum.
- (2) There exists a solver S and a finite integer $r^* \in \mathbb{N}$ such that the following inequality

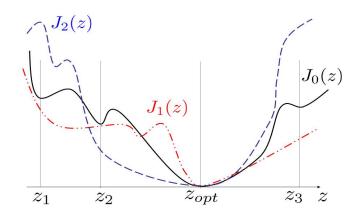


Fig. 1. Typical scheme for a 2-safely redundant optimization problem defined by the cost function J_0 . J_0 (in black-solid line) admits one global minimum z_{opt} and 3 local minima z_1 , z_2 and z_3 . However, the singularities z_1 and z_3 can be crossed following the (z_1, J_1) and the (z_3, J_2) -solver pathes respectively while the singularity z_2 can be crossed following the (z_2, J_3) -solver path.

$$\Delta(z) := \min_{i \in \{1, \dots, N\}} \left[J_0(\mathcal{S}^{(r^*)}(z, J_i)) - \gamma J_0(z) \right] \le 0$$
(4)

holds for some $\gamma \in [0,1[$ and all $z \in \mathcal{Z}$. Moreover:

$$\mathcal{S}^{(r^*)}(z, J_{1^*}) \in \mathcal{Z} \tag{5}$$

where 1^* is the optimal argument of the minimization invoked in (4)

Note that conditions (4) and (5) simply state that regardless the current iterate z, there exists at least one of the (z, J_i) -path solvers that leads to a decrease in the value of the original cost J_0 and this after at most r^* iterations. Figure 1 shows a schematic view of a 2-safely redundant optimization problem in which J_0 admits 4 local minima (including the global minimum).

Definition 1 suggests the algorithm depicted on figure 2 that can be better understood through the following comments:

Step 0

The initial guess is set to z and the iteration index σ is set to 0.

Step 1

This loop is the main loop that ends as soon as the current iterate $z^{(\sigma)}$ corresponds to a sufficiently small value of J_0 .

Step 1.1

When the logical variable again is true, a new solver path has to be tried based on the next element in the sequence of cost functions $\{J_i\}_{i=1}^N$ as the preceding one failed to decrease J_0 . This is checked in **Step 1.2.2** where again is updated.

Step 1.2

As long as again is true AND there is remaining solver pathes to be explored $(i \leq N)$, the next solver path is explored by performing r^* steps of the optimizer iterations

Algorithm A_1

0. Initialization $z^{(0)}$ initial guess, $\sigma \leftarrow 0$ 1. while $(J_0(z^{(\sigma)}) > \varepsilon)$ do **1.1** $i \leftarrow 1$; again $\leftarrow true$ 1.2 while (again & $i \leq N$) do 1.2.1 $\xi^{(\sigma,i)} \leftarrow \mathcal{S}^{r^*}(z^{(\sigma)},J_i)$ 1.2.2 $again \leftarrow \left(J_0(\xi^{(\sigma,i)}) > \gamma J_0(z^{(\sigma)})\right)$ 1.2.3 If again then $i \leftarrow i+1$ 1.2.4 Else $\sigma \leftarrow \sigma+1, z^{(\sigma)} \leftarrow \xi^{(\sigma,i)}$ End while

End while

Fig. 2. The algorithm that enables redundancy to be exploited for N-safe redundant optimization problems.

(Step 1.2.1) and again is updated accordingly (Step 1.2.2). If significant decrease is achieved then again becomes false and Step 1.2.4 is fired leading to the update of $z^{(\sigma+1)}$ and the iteration index σ and a new iteration is started. Otherwise, the next cost function corresponding solver path is visited by incrementing i (Step 1.2.3).

It goes without saying that by the very definition of Nsafe redundancy, the above algorithm leads to a globally convergent iterations despite possible local minima of J_0 . This is formally stated in the following proposition:

Proposition 1. If the optimization problem is safely redundant then the algorithm A_1 stops with the iterate $z^{(\sigma)}$ that satisfies the following property:

$$J_0(z^{(\sigma)}) \le \varepsilon$$

Consequently, if $\varepsilon = 0$ is used, the sequence $z^{(\sigma)}$ globally asymptotically converges to the unique global minimum z^{opt} .

Proof By definition of N-safe redundancy expressed in condition (4), each time the loop of step 1.2 is visited, there is an index 1 that makes the logical variable again false since

$$J_0(\xi^{(\sigma,1)}) \le \gamma J_0(z^{(\sigma)}) \tag{6}$$

leading to the updating step 1.2.4:

$$z^{(\sigma+1)} = \xi^{(\sigma,1)} \tag{7}$$

Based on (6)-(7), one obtains the following discrete dynamic

$$J_0(z^{(\sigma+1)}) \le \gamma J_0(z^{(\sigma)}) \tag{8}$$

which clearly ends the proof.

2.1 Application to the state estimation related problem

As mentioned in the introduction of this paper, the sequence of cost functions $\{J_i\}_{i=1}^N$ may be obtained in the case of the state estimation related problem using the definition (3) by choosing sequences of functions $\{\Phi_i\}_{i=1}^N$ and $\{\Psi_i\}_{i=1}^N$. To be specific, let us make the following choice

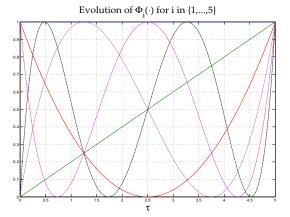


Fig. 3. Plots of the time non uniform weighting functions Φ_i given by (9)-(11) for the first 5 values of i when the observation horizon is taken equal to T=5.

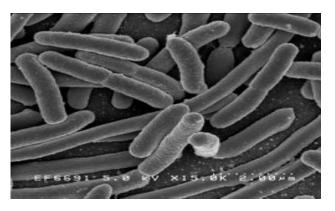


Fig. 4. Escherichia coli under 15000 magnification factor

$$\Psi_i(y) = y^T y$$
 ; $\Phi_i(\tau) = \frac{1}{2} \left[T_i (\frac{2\tau}{T} - 1) + 1 \right]$ (9)

where for $i \in \{1, ..., N\}$, T_i stands for the *i*th Tchebychev polynomials of the first kind, namely:

$$T_0(x) = 1$$
 ; $T_1(x) = x$ (10)

$$T_{i+1}(x) = 2xT_i(x) - T_{i-1}(x)$$
(11)

Note that $\Phi_i(\cdot)$ are simply shifted versions of the Tchebychev polynomials $T_i(\cdot)$ that takes arguments in [0,T] and values in [0, 1] so that they can be used as time non uniform weighting of the output prediction error. Figure 3 shows the plots of the function Φ_i for $i \in \{1, ... 5\}$.

3. ILLUSTRATIVE EXAMPLES

In order to illustrate the above ideas on a concrete example, let us consider the dynamical model of recombinant Escherichia Coli strain (Nardi et al. [2006], Lee and Ramirez [1992], Cha et al. [2000]). This model is a mass balance model describing the pure recombinant microbial batch culture of E. Coli strain X growing on the limiting substrate glycerol S while yielding a final intracellular product β -galactosidase protein P:

parameter	Values	Units
μ_m	0.49	h^{-1}
k_s	0.06	g/l
k_p	0.047	g/l
k_d	0.005	g/l
k_m	0.21	h^{-1}
k_l	0.03	g/h
y_s	0.75	g cell / g glycerol
y_p	0.32	g protein/ β -galactosidase
y_l	17.6	U/β -galactosidase

Table 1. Identified parameters for the dynamic model (12)-(15) according to (Nardi et al. [2006])

$$\dot{X} = \mu(S)X - k_d \exp(-\frac{k_p}{P})X \tag{12}$$

$$\dot{S} = -y_s \mu X - k_m X \tag{13}$$

$$\dot{P} = y_p \mu(S) \frac{I}{I + k_I} X - k_d \exp(-\frac{k_p}{P}) P \tag{14}$$

where μ is the growth rate that is modeled using classical Monod-type relation:

$$\mu(S) = \frac{\mu_m S}{k_s + S}$$

in which μ_m is the maximum specific growth rate for the cell growth in (h^{-1}) . k_s is the half saturation constant. k_p and k_d are constants involved in the Arrhenius-type death kinetic that depends on P. k_m is a maintenance rate that describes the energy required for normal upkeep and repair. y_s , y_l [used in the measurement equation (15) below] and y_p are identified yield coefficients. I stands for the arabinose inducer that is assumed to be constant (no degradation).

The output measurement is the light produced by the bioluminescence that is linked to the state variables by the following expression:

$$L = y_l \cdot \mu(S) \frac{I}{I + k_l} XP \tag{15}$$

In the recent work (Nardi et al. [2006]), the parameters of the above model have been identified and the resulting model has been experimentally validated using Micro-Fermentor testbed. The resulting set of values are given on table 1.

Now consider the optimization problem that arises when the real state of the system at instant t-T, namely x(t-T) is given by:

$$x(t-T) = (0.08, 2, 0.1)$$
; $T = 10$

and let us examine the evolution of the corresponding cost functions $J_i(\cdot,t,y_{t-T}^t)$ given by (3) in which the Tchebychev polynomials are used according to (9). These cost functions depend on the three dimensional unknown vector z which makes cumbersome a visual exploration. Nevertheless, such exhaustive exploration is not necessary to illustrate the redundancy issue. For this, let us fix z_2 and z_3 to their true values, namely $z_2 = x_2(t-T)$ and $z_3 = x_3(t-T)$ and see how the cost functions J_i evolve when the first coordinate z_1 spans the admissible set [0,0.1]. Figure 5 shows the evolutions of the cost functions

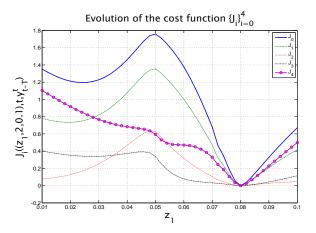


Fig. 5. Evolution of the cost function $J_i(\cdot,t,y^t_{t-T})$ when z spans the admissible region $[0,0.1] \times \{x_2(t-T)\} \times \{x_3(t-T)\}$ where x(t-T) = (0.08,2,0.1) and T=10. Note how the local minimum situated around $z_1=0.025$ for the classically used cost J_0 is not shared by the cost function J_4 suggesting that the underlying optimization problem shows 4-safe-redundancy property w.r.t the sequence of cost functions $\{J_i\}_{i=1}^4$.

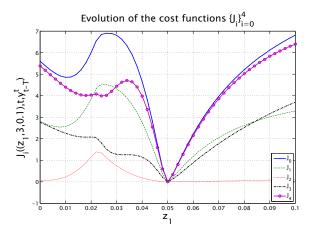


Fig. 6. Evolution of the cost function $J_i(\cdot,t,y_{t-T}^t)$ when z spans the admissible region $[0,0.1] \times \{x_2(t-T)\} \times \{x_3(t-T)\}$ where x(t-T) = (0.05,3,0.1) and T = 15. Note how the local minimum situated around $z_1 = 0.01$ for the classically used cost J_0 is not shared by the cost function J_4 or J_3 . Note also that J_4 shows local minimum near $z_1 = 0.025$ that is not shared by J_3 . Again, algorithm A_1 would clearly be of great interest in crossing the singularities.

$$J_i(\begin{pmatrix} z_1 \\ x_2(t-T) \\ x_3(t-T) \end{pmatrix}, t, y_{t-T}^t) \quad ; \quad i \in \{0, \dots, 4\}$$

as functions of z_1 . From this figure, it can be easily inferred that for i=0 (nominal classically used cost function), the cost function shows a local minimum around $z_1=0.025$. Local minima also exist for i=2,3. However, for i=4, there is no such singularity in the same region and the cost function is such that the application of algorithm A_1 enables the singularity to be safely crossed.

Figure 6 shows the same features when the past state x(t-T) and the observation horizon T are given by:

$$x(t-T) = (0.05, 3, 0.1)$$
; $T = 15$

In this situation, note that J_4 has now 2 local minima (near $z_1 = 0.018$ and 0.024 respectively) that are not shared by J_3 . On the other hand J_3 presents an almost stationary curve between when $z_1 \in [0.03, 0.038]$ that can be efficiently crossed following the J_2 -solver path. This clearly shows the cooperative character of the sequence $\{J_i\}_{i=0}^N$ in exploring the admissible domain towards the unique shared global minimum. This is especially true when using receding horizon observers are used where the position of the local minima is continuously moving together with the index of the good solver path to be temporarily followed as suggested in algorithm A_1 .

4. PARALLEL VERSION OF ALGORITHM A_1

An interesting feature of Algorithm A_1 described above is the possibility to use parallel computation architecture. Indeed, **Step 1.2.1** that amounts to explore the $(z^{(\sigma)}, J_i)$ -path solver for successive values of i (until a decrease in J_0 occurs) and starting from the same initial state $z^{(\sigma)}$ can be executed using parallel computations, each dedicated to one value of the index i. As soon as one of the path solvers

$$\left\{ \left(z^{(\sigma)}, J_i \right) \right\}_{i=0}^N$$

realizes a significant decrease in the original cost function J_0 as guaranteed by assumption (4), the corresponding processor sends an interruption signal to all of the other processors in order to update $z^{(\sigma)}$ and to start a new cycle of parallel computing.

Figure 7 shows a Petri nets representation of the parallel version of algorithm A_1 in the case N=3. Recall that a Patri net is a collection of places (denoted by P) and transitions (denoted by T). A place represents a configuration that is active when a mark is inside it. The mark exists the place as soon as the condition associated to an output transition is true (we then say that the transition is fired). A mark enters a place as soon as an input transition is fired. Using these definitions, the Petri Net representing the evolution of the parallel version of algorithm A_1 and depicted on figure 7 can be interpreted as follows:

- Place P_0 At the initial time, the only mark of the Petri net is placed in P_0 . This means that the algorithm initializes the variable $z^{(\sigma)}$. In the future, this place corresponds also to the updating mode after one of the transitions T_{i2} is fired as explained below.
- Transition T₀: This transition is fired as soon as the initialization/updating step is completed.
- Places P_i : As soon as transition T_0 is fired, each place P_i , i = 1, ..., N has one mark meaning that all the N processors are working in parallel to perform one iteration in the exploration of the $(z^{(\sigma)}, J_i)$ -solver

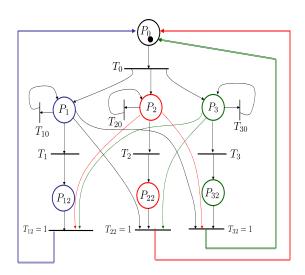


Fig. 7. Petri net representation of the parallel implementation of the singularity avoidance algorithm A_1 in the case where N=3. P_0 is the initialization/updating place, places P_i 's represent several processors working in parallel to explore the different path solvers associates to J_i 's, $i=1,\ldots,N$. Transitions T_{i0} 's correspond to the end of one step in the path solvers exploration. A mark reaches the place P_{i2} as soon as the corresponding path solver encounter a decrease in the original cost function J_0 . This enhance a global interruption of all the processors task and update the value of the current best solution $z^{(\sigma)}$.

pathes. This amounts to compute one step of the iteration:

$$\xi^{j_i,(\sigma,i)} = \mathcal{S}\left(\xi^{j_i-1,(\sigma,i)}, J_i\right) \quad \xi^{0,(\sigma,i)} = z^{(\sigma)} \quad (16)$$

where the assignment $j_i = 0$ is applied as soon as the places P_i is reached.

- Transition T_{i0}: This transition is fired when the following two conditions are satisfied:
 - (1) The computation of the step (16) is achieved
 - (2) The following inequality holds:

$$J_0(\xi^{j_i,(\sigma,i)}) > \gamma J_0(z^{(\sigma)}) \tag{17}$$

that is, no significant decrease in J_0 is obtained after the last step taken on the $(z^{(\sigma)},J_i)$ -solver path.

Once the transition T_{i0} is fired, the mark returns to P_i and the processor i computes another step in the iteration (16)

• Transitions T_i : This transition is fired as soon as the processor i finds an iterate $\xi^{j_i,(\sigma,i)}$ that achieves a decrease in J_0 , namely:

$$J_0(\xi^{j_i,(\sigma,i)}) \le \gamma J_0(z^{(\sigma)}) \tag{18}$$

Note that according to the very definition of N-safe redundancy, one of the transitions T_i is necessarily fired after at most r^* iterations. This means that one of the places P_{i2} necessarily receives a mark.

• Place Pi2: Note that according to the above discussion, it is easy to understand that the places P_{i2} are mutually exclusive since if 1* is the first processor that encounters condition (18), the mark transits from place P_{1*} to place P_{1*2} and since the transition T_{1*2} is unconditional $(T_{i2} = 1 \text{ means that the transition})$ T_{i2} is fired as soon as a mark is available in the place P_{i2}), the mark moves from all the places

$$\left\{P_j\right\}_{j\neq 1^*}$$

 $\left\{P_{j}\right\}_{j\neq 1^{*}}$ to the updating place P_{0} bypassing the places $\left\{P_{j2}\right\}_{j\neq 1^{*}}$. This clearly corresponds to an interruption fired by the processor 1^* . At P_0 , the following updating rule is applied:

$$z^{(\sigma)} \leftarrow \xi^{j_{1^*},(\sigma,{\scriptscriptstyle 1}^*)}$$

which clearly leads to the following convergence condition:

$$J_0(z^{(\sigma^+)}) \le \gamma J_0(z^{(\sigma)}) \tag{19}$$

In addition to the fact that computation of the solver pathes are done in parallel, the main difference between the sequential and the parallelized version of algorithm A_1 is that all the explorations are stopped as soon as an improvement is found which means which means that the unfruitful pathes are never completely explored.

5. DISCUSSION

- It is worth underlying that the two versions of algorithm A_1 proposed in this paper provide tools for singularities avoidance that can be used regardless the optimization technique that underlines the solver \mathcal{S} . No matter whether the solver implements a gradient approach, an SQP method or even non smooth technique such as the simplex iteration. In particular, the above layer can be added to the gradient-based differential version of moving horizon observer proposed in Alamir [1999] where the integration of the observer differential equation (written for a given cost function J_i) can be used to explore the path solver $(z^{(\sigma)}, J_i)$.
- It is important to strengthen that the singularities avoidance technique proposed here is not a multiple initial guess technique. Indeed, the later amounts to modify the starting point of a given solver from one trial to another. In algorithm A_1 , $z^{(\sigma)}$ is kept constant as index i changes. More precisely, the current guess is maintained and IT IS THE PROBLEM THAT CHANGES!. This is made possible only because of the very particular feature (N-safe redundancy) of the optimization problem that is related to nonlinear state estimation issue.
- The presentation in this paper focusses on the state estimation problem. However, it is straightforward that under appropriate identifiability conditions, the concept of N-safe redundancy can be extended to the problem of parameter identification and/or simultaneous state and parameters estimation.
- The last remark clearly applies also to the problem of robust state estimation where some uncertainty

profile $w(\cdot)$ needs to be estimated together with the state vector. This clearly assume that some finite dimensional temporal parametrization of $w(\cdot)$ is used that faithfully contains the actual unknown behavior as a possible instantiation. In this case, even non regular temporal parametrization of the form

$$w(\cdot) = \mathcal{W}(\cdot, p_w) \quad ; \quad p_w \in \mathbb{P} \subset \mathbb{R}^{n_p}$$

can be used in the context of hybrid systems. In this case, the overall framework would apply on the extended unknown state:

$$\bar{x} := \begin{pmatrix} x \\ p_w \end{pmatrix} \in \mathbb{R}^n \times \mathbb{P} \quad ; \quad \dot{p}_w = 0$$
 (20)

6. CONCLUSION & FUTURE WORK

In this paper, the concept of N-safe redundant optimization problem is introduced and its potential efficiency in the context of dynamic nonlinear inverse problems is illustrated through a realistic state estimation example. Corresponding algorithms are also proposed that can be incorporated to any existing iterative scheme that may be used to solve the corresponding optimization problem. Concrete implementation and wide numerical investigations are now under study in order to clearly quantify the benefit from such scheme in crossing singularities.

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