Optimal Finite-Horizon Sensor Selection for Boolean Kalman Filter

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***Abstract*—Partially-observed Boolean dynamical systems (POBDS) are large and complex dynamical systems capable of being monitored through various sensors. However, time, storage, and economical constraints may impede the use of all sensors for estimation purposes. Thus, developing a procedure for selecting a subset of sensors is essential. The optimal minimum mean-square error (MMSE) POBDS state estimator is the Boolean Kalman Filter (BKF) and Smoother (BKS). Naturally, the performance of these estimators strongly depends on the choice of sensors. Given a finite subsets of sensors, for a POBDS with a finite observation space, we introduce the optimal procedure to select the best subset which leads to the smallest expected mean-square error (MSE) of the BKF over a finite horizon. The performance of the proposed sensor selection methodology is demonstrated by numerical experiments with a p53-MDM2 negative-feedback loop gene regulatory network observed through Bernoulli noise.**

***Index Terms*—Optimal Finite-Horizon Sensor Selection, Partially-Observed Boolean Dynamical Systems, Boolean Kalman Filter, Gene Regulatory Networks.**

I. Introduction

Partially-observed Boolean dynamical systems (POBDS) [1], [2] offer a rich framework for estimation and prediction in fields as varied as genomics [3], robotics [4], and digital communications [5], and more. The optimal recursive minimum mean-square error (MMSE) POBDS state estimators are the Boolean Kalman Filter (BKF) [2] and Smoother (BKS) [6]. Several other tools have been developed for the POBDS model in recent years, such as particle filters for state and parameter estimation [7], schemes for simultaneous state and parameter estimation [1], optimal filter with correlated observation noise [8], network inference [9], and control [10]–[13]. Most of these tools are freely available through an open-source R package called "BoolFilter" [14], [15].

POBDSs can be monitored through various sensors that carry information about different parts of the system with various degrees of uncertainty. However, the number of sensors is often limited either by economical constraints (hardware costs), or the availability of physical or storage space [16]. While the BKF is the optimal MMSE POBDS state estimator, its performance strongly depends on the choice of sensors. Therefore, selecting the appropriate subset of sensors before starting the estimation process is crucial.

Sensor selection is widely discussed in the literature for both linear [17]–[19] and nonlinear dynamical systems [16], [20], [21]. These methods use various objective functions such as the Chernoff and Kullback-Leibler distances [22], information gain [23], and estimation error [24]. However, due to the derivativeless nature of the Boolean state equation in a POBDS, none of the mentioned sensor selection methods are directly applicable here.

This paper introduces an optimal methodology for selecting the best sensor to minimize the expected mean-square error (MSE) of a BKF with finite measurement space over a finite-horizon. Performance is investigated using a Boolean network model of the p53-MDM2 negative feedback loop network observed through Bernoulli noise.

II. Partially-Observed Boolean Dynamical Systems

We assume that the system is described by a *state process* $\{\mathbf{X}_r; r=0,1,\dots,T\}$, for a finite horizon T, where $\mathbf{X}_r \in \{0,1\}^d$ is a Boolean vector of size d. The states are assumed to be updated at each discrete time through the following Boolean signal model:

$$\mathbf{X}_r = \mathbf{f}(\mathbf{X}_{r-1}, \mathbf{u}_r) \oplus \mathbf{n}_r\,, \tag{1}$$

for $r=1,\dots,T$. Here, $\mathbf{u}_r \in \{0,1\}^d$ is an input at time r which is assumed to be deterministic and known, $\mathbf{n}_r \in \{0,1\}^d$ is Boolean transition noise at time r, "$\oplus$" indicates component-wise modulo-2 addition, and $\mathbf{f}$ is the *network function*.

The states are observed indirectly through the *observation process* $\{\mathbf{Y}_r; r=1,\dots,T\}$. In this paper, we assume a simple additive-noise Boolean observation model:

$$\mathbf{Y}_r = \mathbf{X}_r \oplus \mathbf{v}_r\,, \tag{2}$$

for $r=1,\dots,T$, where $\mathbf{v}_r \in \{0,1\}^d$ is Boolean observation noise at time r. Hence, $\mathbf{Y}_r \in \{0,1\}^d$ is a Boolean observation vector at time r. Both noise processes $\{\mathbf{n}_r; r=1,\dots,T\}$ and $\{\mathbf{v}_r; r=1,\dots,T\}$ are assumed to be "white" in the sense that the noises at distinct time points are independent. It is also assumed that the noise processes are independent from each other and from the initial state $\mathbf{X}_0$; their distribution is otherwise arbitrary.

The *optimal filtering* problem consists of, given observations $\mathbf{Y}_{1:r} = (\mathbf{Y}_1, \dots, \mathbf{Y}_r)$, for $r \le T$, finding an estimator $\hat{\mathbf{X}}^{\mathrm{MS}}_{r|r}$ of the state $\mathbf{X}_r$ that minimizes the conditional mean-square error (MSE):

$$\mathrm{MSE}(\hat{\mathbf{X}}_{r|r} \mid \mathbf{Y}_{1:r}) = E\left[||\hat{\mathbf{X}}_{r|r} - \mathbf{X}_r||^2 \mid \mathbf{Y}_{1:r} \right], \quad (3)$$

where $||\mathbf{v}||^2 = \sum_{i=1}^d \mathbf{v}(i)^2$ is the square of the L_2 norm of vector $\mathbf{v}$. Clearly, for Boolean vectors, $||\mathbf{v}||^2 = ||\mathbf{v}||_1 = \sum_{i=1}^d |\mathbf{v}(i)|$ is the L_1 norm of $\mathbf{v}$.

We present next a recursive algorithm to compute $\hat{\mathbf{X}}^{\mathrm{MS}}_{r|r}$, known as the Boolean Kalman Filter (BKF) [2], [13]. Define the conditional probability distribution vectors:

$$\begin{aligned} \mathbf{\Pi}_{r|r}(i) &= P\left(\mathbf{X}_r = \mathbf{x}^i \mid \mathbf{Y}_{1:r}\right), \\ \mathbf{\Pi}_{r|r-1}(i) &= P\left(\mathbf{X}_r = \mathbf{x}^i \mid \mathbf{Y}_{1:r-1}\right), \end{aligned} \quad (4)$$

for $i = 1, \dots, 2^d$, and $r = 1, \dots$. Notice that $\mathbf{\Pi}_{0|0}$ is the initial (prior) distribution of the states at time zero.

Let M_r be the *transition matrix* of the Markov chain defined by the state model, specified by:

$$\begin{aligned} (M_r)_{ij} &= P(\mathbf{X}_r = \mathbf{x}^i \mid \mathbf{X}_{r-1} = \mathbf{x}^j) \\ &= P\left(\mathbf{n}_r = \mathbf{f}(\mathbf{x}^j, \mathbf{u}_r) \oplus \mathbf{x}^i\right), \end{aligned} \quad (5)$$

for $i, j = 1, \dots, 2^d$. Additionally, given a value of the observation vector $\mathbf{Y}_r$ at time r, the *update matrix* $T_r(\mathbf{Y}_r)$ of size $2^d \times 2^d$ is a diagonal matrix defined by:

$$(T_r(\mathbf{Y}_r))_{ii} = P\left(\mathbf{Y}_r \mid \mathbf{X}_r = \mathbf{x}^i\right), \quad (6)$$

for $i = 1, \dots, 2^d$.

Finally, let $A = [\mathbf{x}^1 \cdots \mathbf{x}^{2^d}]$ be a $d \times 2^d$ matrix with all possible state vectors as columns. In addition, for a vector $\mathbf{v}$ of size d, define $\overline{\mathbf{v}} \in \{0,1\}^d$ via $\overline{\mathbf{v}}(i) = I_{\mathbf{v}(i) > 1/2}$ for $i = 1, \dots, d$, and $\mathbf{v}^c \in \{0,1\}^d$ via $\mathbf{v}^c(i) = 1 - \mathbf{v}(i)$, for $i = 1, \dots, d$; where $I_{\mathbf{v}(i) > 1/2}$ returns 1 if $\mathbf{v}(i) > 1/2$ and 0 otherwise.

The full procedure of the BKF is presented in Algorithm 1.

Algorithm 1 Boolean Kalman Filter

1: Initialization: $(\mathbf{\Pi}_{0|0})_i = P\left(\mathbf{X}_0 = \mathbf{x}^i\right)$, for $i = 1, \dots, 2^d$.

For $r = 1, \dots, T$, do:

2: Prediction: $\mathbf{\Pi}_{r|r-1} = M_r \, \mathbf{\Pi}_{k-1|k-1}$

3: Update: $\boldsymbol{\beta}_r = T_r(\mathbf{Y}_r) \, \mathbf{\Pi}_{r|r-1}$

4: Filtered Distribution Vector:

$$\mathbf{\Pi}_{r|r} = \boldsymbol{\beta}_r / ||\boldsymbol{\beta}_r||_1$$

5: MMSE Estimator Computation:

$$\hat{\mathbf{X}}^{\mathrm{MS}}_{r|r} = \overline{A\mathbf{\Pi}_{r|r}}$$

6: Optimal Conditional MSE:

$$\mathrm{MSE}(\hat{\mathbf{X}}^{\mathrm{MS}}_{r|r} \mid \mathbf{Y}_{1:r}) = ||\min\{A\mathbf{\Pi}_{r|r}, (A\mathbf{\Pi}_{r|r})^c\}||_1$$

III. Finite-Horizon Sensor Selection

Suppose that one would like to select among M available *sensors*, where each sensor is a fixed vector function of the observation vector $\mathbf{Y}_r$. In this paper, we consider a simple case where each sensor corresponds to a different subset of the measurements in $\mathbf{Y}_r$, but linear and nonlinear combinations of all or a subset of the measurements may be considered as well. Hence, we have M sensors $\mathbf{Y}^m = \{\mathbf{y}^{m,1}, \dots, \mathbf{y}^{m,|\mathbf{Y}^m|}\}$, for $m = 1, \dots, M$, which are different subsets of the available observation vector $\mathbf{Y}$. The value obtained by the mth sensor at time r is:

$$\mathbf{Y}^m_r = \mathbf{X}^m_r \oplus \mathbf{v}^m_r, \quad (7)$$

where $\mathbf{X}^m_r$ and $\mathbf{v}^m_r$ are the corresponding subsets of the state $\mathbf{X}_r$ and observation noise $\mathbf{v}_r$ at time r. The goal is to select a sensor, *before* the start of the filtering process, to use over the entire interval $r = 1, \dots, T$ while achieving the best possible performance, as defined below. The problem of scheduling different sensors at different times will be considered in future work.

Let $\mathcal{O}^m_r$ be the space of observation sequences $\mathbf{Y}^m_{1:r}$ provided by the mth sensor up to time r. Note that in the setting assumed in this paper, $\mathcal{O}^m_r$ is finite, with $|\mathcal{O}^m_r| = 2^{|\mathbf{Y}^m| \times r}$. Let $\mathcal{X}^m_{r|r}$ be the set of all estimators of $\mathbf{X}_r$ based on observations $\mathbf{Y}^m_{1:r} \in \mathcal{O}^m_r$, for $m = 1, \dots, M$. Before execution, we do not know the specific realization $\mathbf{Y}^m_{1:r}$ for any of the sensors. Therefore, we consider the *expected* MSE and define the optimal estimator:

$$\hat{\mathbf{X}}^{m,\mathrm{MS}}_{r|r} = \underset{\hat{\mathbf{X}}_{r|r} \in \mathcal{X}^m_{r|r}}{\operatorname{argmin}} \; E[\mathrm{MSE}(\hat{\mathbf{X}}_{r|r} \mid \mathbf{Y}^m_{1:r})]. \quad (8)$$

We then select the sensor that achieves the best average expected MSE over the interval $r = 1, \dots, T$:

$$m^* = \underset{m=1,\dots,M}{\operatorname{argmin}} \; \frac{1}{T} \sum_{r=1}^{T} E[\mathrm{MSE}(\hat{\mathbf{X}}^{m,\mathrm{MS}}_{r|r} \mid \mathbf{Y}^m_{1:r})]. \quad (9)$$

From Algorithm 1, we have that:

$$\begin{aligned} & E[\mathrm{MSE}(\hat{\mathbf{X}}^{m,\mathrm{MS}}_{r|r} \mid \mathbf{Y}^m_{1:r})] \\ & \quad = E[||\min\{A\mathbf{\Pi}^m_{r|r}, (A\mathbf{\Pi}^m_{r|r})^c\}||_1] \\ & \quad = \sum_{\mathbf{Y}^m_{1:r} \in \mathcal{O}^m_r} P(\mathbf{Y}^m_{1:r}) \, ||\min\{A\mathbf{\Pi}^m_{r|r}, (A\mathbf{\Pi}^m_{r|r})^c\}||_1 . \end{aligned} \quad (10)$$

Calculating $E[\mathrm{MSE}(\hat{\mathbf{X}}^{m,\mathrm{MS}}_{r|r} \mid \mathbf{Y}^m_{1:r})]$ exactly thus requires, in principle, the computation of the conditional MSE given all possible sequences of measurements. Since the observation space $\mathcal{O}^m_r$ is finite, this computation is possible, as described next, provided that the sensor dimensionalities $|\mathbf{Y}_m|$ and horizon T are small enough. Approximations for the case of large sensor dimensionalities and long horizons will be dealt with in future work.

Given that $\mathbf{\Pi}_{0|0}$ is the initial distribution vector, the posterior distribution at time 1 associated to measurement $\mathbf{y}^{m,j}$ can be computed using the Bayes' rule as:

$$\Pi^{m,j}_{1|1} = P(\mathbf{X}_1 \mid \mathbf{Y}^m_1 = \mathbf{y}^{m,j}) = \frac{T_1(\mathbf{y}^{m,j}) \, M_1 \, \mathbf{\Pi}_{0|0}}{||T_1(\mathbf{y}^{m,j}) \, M_1 \, \mathbf{\Pi}_{0|0}||_1}, \quad (11)$$

for $j = 1, ..., 2^{|\mathbf{Y}^m|}$. (Notice that there is no superscript "m" over $\mathbf{X}_1$.) The probability of observing $\mathbf{y}^{m,j}$ at time step 1 can be computed as follows:

$$\mathbf{w}_1^{m,j} = P(\mathbf{Y}_1 = \mathbf{y}^{m,j} \mid \mathbf{\Pi}_{0|0}) = ||T_1(\mathbf{y}^{m,j})\, M_1\, \mathbf{\Pi}_{0|0}||_1\,, \tag{12}$$

for $j = 1, ..., 2^{|\mathbf{Y}^m|}$. This process can be continued recursively to compute all needed probabilities, as illustrated in Figure 1.

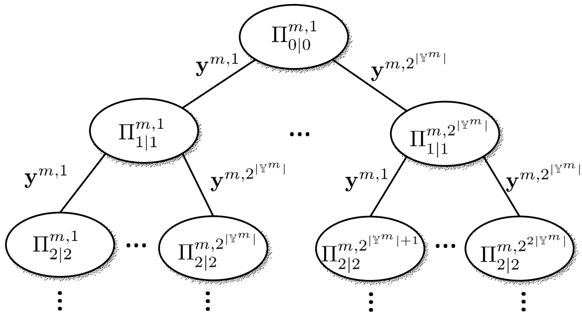

Fig. 1: Posterior distribution tree for mth sensor.

The entire process of finite-horizon sensor selection for the BKF is presented in Algorithm 2.

Algorithm 2 Optimal Finite-Horizon Sensor Selection for the BKF

1: Posterior Distributions Computation:

For $m \in \{1, ..., M\}$, do:

– Initialization: $\Pi_{0|0}^{m,1} = \mathbf{\Pi}_{0|0}$, $\mathbf{w}_0^{m,1} = 1$.

For $r = 1, ..., k$, do:

For $i = 1, ..., 2^{|\mathbf{Y}^m|(r-1)}$, do:

– $\Pi_{r|r-1}^{m,i} = M_r\, \Pi_{r-1|r-1}^{m,i}$.

For $j = 1, ..., 2^{|\mathbf{Y}^m|}$, do:

– $\Pi_{r|r}^{m,(i-1)2^{|\mathbf{Y}^m|}+j} = \dfrac{T_r(\mathbf{y}^{m,j})\, \Pi_{r|r-1}^{m,i}}{||T_r(\mathbf{y}^{m,j})\, \Pi_{r|r-1}^{m,i}||_1}$.

– $\mathbf{w}_r^{m,(i-1)2^{|\mathbf{Y}^m|}+j} = \{\mathbf{w}_{r-1}^{m,i} ||T_r(\mathbf{y}^{m,j})\, \Pi_{r|r-1}^{m,i}||_1\}$.

2: The Optimal Selected Sensor:

$$m^* = \underset{m \in \{1,...,M\}}{\operatorname{argmin}} \sum_{r=1}^{k} \sum_{i=1}^{2^{|\mathbf{Y}^m|r}} \mathbf{w}_r^{m,i} || \min\{A\Pi_{r|r}^{m,i}, (A\Pi_{r|r}^{m,i})^c\}||_1$$

IV. Numerical Experiments

In this section, we describe an application of our methodology to Boolean gene regulatory networks observed through noisy measurements. We base our experiments on the well-known *p53-MDM2* negative-feedback gene regulatory network [25]. The pathway diagram for this network is presented in Fig. 2. The *p53* gene codes for the tumor suppressor protein p53 in humans, and its activation plays a critical role in cellular responses to various stress signals that might cause genome instability. The gene regulatory network consists of four genes: *ATM*, *p53*, *Wip1*, and *MDM2*, and the input "dna_dsb", which indicates the presence of DNA double strand breaks. The Boolean function is represented by the following logic functions:

$$\begin{aligned}
\text{ATM}_k &= \overline{\text{WIP1}_{k-1}} \;\textit{AND}\; \text{dna_dsb} \\
\text{p53}_k &= \text{ATM}_{k-1} \;\textit{AND}\; \overline{\text{WIP1}_{k-1}} \;\textit{AND}\; \overline{\text{MDM2}_{k-1}} \\
\text{WIP1}_k &= \text{p53}_{k-1} \\
\text{MDM2}_k &= \Big(\overline{\text{ATM}_{k-1}} \;\textit{AND}\; (\text{p53}_{k-1} \;\textit{OR}\; \text{WIP1}_{k-1})\Big) \\
&\qquad \textit{OR}\; \big(\text{p53}_{k-1} \;\textit{AND}\; \text{WIP1}_{k-1}\big)
\end{aligned}$$

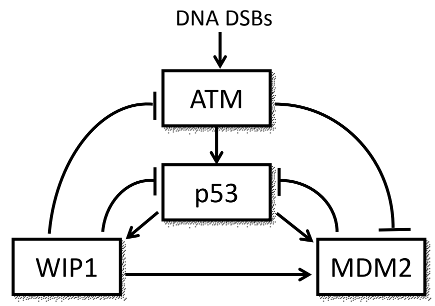

Fig. 2: Activation/repression pathway diagram of the P53-MDM2 negative feedback loop Boolean network.

The process noise is assumed to have independent components distributed as Bernoulli, with intensity p, so that all genes are perturbed with a small probability. We assume the states are observed through i.i.d. Bernoulli noise with parameter q the same for all genes. Four sensors are assumed in this numerical experiment ($M = 4$), in which each sensor consists of the noisy observation of one of the genes in the network.

The average expected optimal MSE of the BKF over a time horizon 10 for various sensors are presented in Table I. The average expected optimal MSE is larger for larger observation noise. Furthermore, one can also see that the average expected error is larger in the case of an active dna_dsb input in comparison to an inactive one. This can be explained by the attractor structure of the p53-MDM2 Boolean network in the presence and absence of external input, in which the system has a singleton and cyclic attractor in the absence and presence of DNA damage, respectively. For more information, see [13].

The optimal sensor is specified by bold numbers in Table 1. One can see that in the case of an inactive dna_dsb input, MDM2 is the best choice in all cases. With an active dna_dsb input, either ATM, p53 or Wip1 sensors are the best choices, depending on the parameters of the system. For example, the choices of optimal sensor in the case of small process and observation noise are different for two initial distribution vectors. The similar trend can be seen in the case of large measurement noise. From the results of Table I, one can clearly understand the importance of the sensor selection process, and its dependency on the initial distribution, the values of noise and input to the system.

TABLE I: Optimal Finite-Horizon Sensor Selection Results for Horizon $T = 10$.

			No stress (dna_dsb = 0)				DNA damage (dna_dsb = 1)			
q	p	Initial Distribution	ATM	p53	Wip1	Mdm2	ATM	p53	Wip1	Mdm2
0.05	0.01	$[\frac{1}{16}, ..., \frac{1}{16}]^T$	0.2750741	0.2638027	0.1656234	**0.1068837**	1.474933	1.495893	**1.443079**	1.733152
		$[0, ..., 1]^T$	0.3759515	0.3700666	0.336286	**0.2862778**	**1.557895**	1.564755	1.569989	1.709767
	0.1	$[\frac{1}{16}, ..., \frac{1}{16}]^T$	0.7762779	0.7450073	0.5673365	**0.4586170**	**1.218192**	1.371414	1.25308	1.480116
		$[0, ..., 1]^T$	0.8456097	0.8206338	0.6542587	**0.5223727**	**1.261300**	1.395272	1.284143	1.431346
0.15	0.01	$[\frac{1}{16}, ..., \frac{1}{16}]^T$	0.2763222	0.2666612	0.187685	**0.1429032**	1.582349	1.546739	**1.520243**	1.767097
		$[0, ..., 1]^T$	0.3771996	0.3721163	0.3515226	**0.3258301**	1.682476	**1.650215**	1.658933	1.753322
	0.1	$[\frac{1}{16}, ..., \frac{1}{16}]^T$	0.7896947	0.7643199	0.6193023	**0.5399353**	1.351779	1.420585	**1.342386**	1.528136
		$[0, ..., 1]^T$	0.8590265	0.8387905	0.7193224	**0.6283275**	1.388158	1.443909	**1.383008**	1.509838

The effect of the length of horizon on the choice of optimal sensor is investigated next. The parameters used are $\mathbf{\Pi}_{0|0} = [0, ..., 1]^T$, $p = 0.01$, $q = 0.05$ and dna_dsb = 1. The average expected MSE over time-horizon of the optimal filter for different choices of sensors and various time-horizons is presented in Fig. 3. As it is clear in Fig. 3, for time-horizons 1, 6-8, 11-13 and 15, observing the Wip1 gene will result in the minimum expected MSE of the BKF, for time steps 2 and 3, Mdm2 has the lowest expected optimal MSE, and for the intervals 4-5, 9-10 and 14 the best sensor is ATM. This emphasizes the difficulty and importance of the sensor selection procedure.

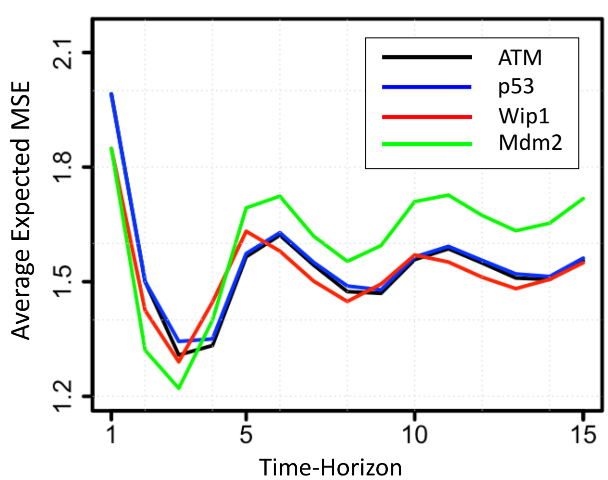

Fig. 3: Average expected optimal MSE for different choices of sensors and time-horizons.

V. Conclusion

We developed an optimal finite-horizon sensor selection procedure for state estimation for POBDS models with a finite observation space. The sensor selected by the developed method is guaranteed to yield the minimum expected mean-square error (MSE) for the optimal filter. Performance was investigated using a model of the p53-MDM2 negative feedback loop network. Future work will include the use of more complex sensor models and approximations for large sensor dimensionality and long time horizons.

Acknowledgment

The authors acknowledge the support of the National Science Foundation, through NSF award CCF-1320884.

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