BOOLEAN KALMAN FILTER WITH CORRELATED OBSERVATION NOISE

Levi D. McClenny, Mahdi Imani, Ulisses M. Braga-Neto

Texas A&M University, Department of Electrical and Computer Engineering, TX, USA

ABSTRACT

This paper is concerned with optimal estimation of the state of a Boolean dynamical systems observed through correlated noisy Boolean measurements. The optimal Minimum Mean-Square Error (MMSE) state estimator for general Partially-Observed Boolean Dynamical Systems (POBDS) can be computed via the Boolean Kalman Filter (BKF). However, thus far in the literature only the case of white observation noise has been considered. In this paper, we develop the optimal MMSE filter for a class of POBDS with correlated Boolean measurements. The performance of the proposed method is subsequently investigated using the p53-MDM2 negative feedback loop genetic network model.

Index Terms— Optimal MMSE State Estimator, Correlated Measurements, Partially-Observed Boolean Dynamical Systems, Boolean Kalman Filter.

1. INTRODUCTION

The Partially-Observed Boolean Dynamical System (POBDS) model is a special class of Hidden Markov Model (HMM) that is comprised of Boolean state variables. Instances of POBDS occur in fields such as genomics [1], robotics [2], digital communication systems [3], etc. Several tools for POBDS have been developed recently, such as the optimal filter and smoother based on the minimum mean square error (MMSE) criterion, called the Boolean Kalman Filter (BKF) [4] and Boolean Kalman Smoother (BKS) [5], respectively. In addition, adaptive filter, network inference, fault detection and control algorithms for POBDS were introduced in [6–10]. Furthermore, the software tool "BoolFilter" [11] is available for estimation and inference of partially-observed Boolean dynamical systems.

The existing BKF algorithm relies on the fact that the observation noise is white. However, this assumption might be violated in various applications in which the measurements are correlated in time [12, 13]. In this paper, we address the problem of optimal state estimator for POBDS with correlated observations by considering an equivalent state space model containing only uncorrelated noise. We also discuss an instance of POBDS as a model of gene regulatory networks, and assess performance of the filter using the p53-MDM2 negative feedback loop Boolean network.

2. PARTIALLY-OBSERVED BOOLEAN DYNAMICAL SYSTEMS WITH CORRELATED BOOLEAN MEASUREMENTS

Deterministic Boolean network models are unable to cope with uncertainty in state transition due to system noise and the effect of unmodeled variables. Stochastic models have been proposed to overcome this difficulty, including Random Boolean Networks [1], Boolean Networks with perturbation (BNp) [14], and Probabilistic Boolean Networks (PBN) [15]. All of these models, however, assume that the Boolean states of the system are directly observed, thus they are not directly applicable to *partially-observed* dynamical systems. The partially-observed Boolean dynamical systems (POBDS) model was proposed in [4] to deal with the aforementioned difficulties, and an algorithm for optimal minimum meansquare error (MMSE) state estimation in this model was proposed, called the Boolean Kalman Filter.

However, the BKF algorithm given in [4], and further studied in [6–10, 16, 17], relies on independence of the observation noise at distinct time points. In this section, we introduce a special class of POBDS with correlated noisy Boolean measurements, and in the next section, introduce an equivalent POBDS containing only uncorrelated noise, which can then be solved optimally by the BKF.

2.1. State Model

We assume that the system is described by a *state process* $\{\mathbf{X}_k; k = 0, 1, ...\}$, where $\mathbf{X}_k \in \{0, 1\}^d$ is a Boolean vector of size *d*. The state evolution is thus specified by the following discrete-time nonlinear signal model:

$$\mathbf{X}_{k} = \mathbf{f} \left(\mathbf{X}_{k-1}, \mathbf{u}_{k} \right) \oplus \mathbf{n}_{k}, \qquad (1)$$

for k = 1, 2, ..., where $\mathbf{u}_k \in \{0, 1\}^d$ is the input at time $k, \mathbf{f} : \{0, 1\}^{2d} \rightarrow \{0, 1\}^d$ is a *network function*, $\{\mathbf{n}_k; k = 1, 2, ...\}$ is a state noise process with $\mathbf{n}_k \in \{0, 1\}^d$, and " \oplus " indicates

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component-wise modulo-2 addition. The noise is white in the sense that it is independent; i.e., \mathbf{n}_k and \mathbf{n}_l are independent for $k \neq l$. In addition, the noise process is assumed to be independent of the state process.

2.2. Observation Model

In most real-world applications, the system state is only partially observable and distortion can be introduced in the observations by sensor noise. Let $\{\mathbf{Y}_k; k = 1, 2, ...\}$ be the observation process. We assume in this paper that \mathbf{Y}_k is a binarized version of the (typically) continuous measured data. Due to sensor noise, \mathbf{Y}_k is an imperfect copy of \mathbf{X}_k , as given by the following equation:

$$\mathbf{Y}_k = \mathbf{h}(\mathbf{X}_k, \mathbf{v}_k) = \mathbf{X}_k \oplus \mathbf{v}_k, \qquad (2)$$

where $\mathbf{v}_k \in \{0, 1\}^d$ is the error noise at time step k. We assume here that the observation process is correlated, so that \mathbf{v}_k is correlated to \mathbf{v}_{k-1} . In this paper we assume the following correlation structure, which is reminiscent of the AR(1) noise in linear filtering:

$$\mathbf{v}_k = I_{\beta_k < \rho} \, \mathbf{v}_{k-1} \, \oplus \, \mathbf{r}_k \,, \tag{3}$$

where $\mathbf{r}_k \in \{0, 1\}^d$ such that \mathbf{r}_k is independent of \mathbf{r}_l for $k \neq l$, $I_{\beta_k < \rho}$ is an indicator function which returns 1 if $\beta_k < \rho$ and 0 otherwise, with $\beta_k \sim$ Uniform [0, 1], while $0 \leq \rho \leq 1$ is a fixed value denoting the amount of dependency between \mathbf{v}_k and \mathbf{v}_{k-1} . Notice that a ρ value close to 0 or 1 denotes low and high correlation, respectively. In the next section, the optimal MMSE estimator for this signal model will be discussed.

3. MMSE FILTER FOR CORRELATED NOISE

To be able to find the optimal MMSE state estimator for the signal model proposed in (1)-(3) with correlated Boolean measurements, we define an equivalent state space model by augmenting state X_k with the noise value v_k and writing

$$\begin{bmatrix} \mathbf{X}_k \\ \mathbf{v}_k \end{bmatrix} = \begin{bmatrix} \mathbf{f}(\mathbf{X}_{k-1}, \mathbf{u}_k) \\ I_{\beta_k < \rho} \mathbf{v}_{k-1} \end{bmatrix} \oplus \begin{bmatrix} \mathbf{n}_k \\ \mathbf{r}_k \end{bmatrix}, \quad (4)$$
$$\mathbf{Y}_k = \mathbf{X}_k \oplus \mathbf{v}_k$$

If we define $\mathbf{Z}_k = (\mathbf{X}_k, \mathbf{v}_k)$ and $\mathbf{w}_k = (\mathbf{n}_k, \mathbf{r}_k)$, then the previous model can be put in the form

$$\mathbf{Z}_{k} = \mathbf{f}'(\mathbf{Z}_{k-1}, \mathbf{u}_{k}) \oplus \mathbf{w}_{k},$$

$$\mathbf{Y}_{k} = \mathbf{h}'(\mathbf{Z}_{k})$$
(5)

for the appropriate functions \mathbf{f}' and \mathbf{h}' , as can be readily verified. The new state variable \mathbf{Z}_k contains 2d variables and 2^{2d} unique states $\{\mathbf{z}^1, \mathbf{z}^2, ..., \mathbf{z}^{2d}\}$. The optimal MMSE estimator for state-space model (5) can be found using the original

BKF algorithm in [4]. We will briefly describe the procedure below.

Define the state conditional state probability distribution vectors $\Pi_{k|k}$ and $\Pi_{k|k-1}$ by

$$\boldsymbol{\Pi}_{k|k}(i) = P\left(\mathbf{Z}_{k} = \mathbf{z}^{i} \mid \mathbf{Y}_{1:k}\right),
\boldsymbol{\Pi}_{k|k-1}(i) = P\left(\mathbf{Z}_{k} = \mathbf{z}^{i} \mid \mathbf{Y}_{1:k-1}\right),$$
(6)

for $i = 1, ..., 2^{2d}$, and k = 1, 2, ... We also define $P(\mathbf{X}_k = \mathbf{x}^i)$ to be the initial (prior) distribution of the states \mathbf{x}^i at time zero. At time k = 0 there are no measurements, so $\mathbf{v}_k = \mathbf{0}$. Therefore, the initial state distribution is given by:

$$\mathbf{\Pi}_{0|0}(i) = P(\mathbf{Z}_0 = \mathbf{z}^i) = \begin{cases} P(\mathbf{X}_0 = \mathbf{x}^i), & \text{if } \mathbf{v}_k = \mathbf{0}, \\ 0, & \text{Otherwise,} \end{cases}$$
(7)

for $i = 1, ..., 2^{2d}$. The *prediction matrix* M_k of size $2^{2d} \times 2^{2d}$ which is the transition matrix of the augmented state Markov chain, can be defined as:

$$(M_k)_{ij} = P(\mathbf{Z}_k = \mathbf{z}^i \mid \mathbf{Z}_{k-1} = \mathbf{z}^j), \qquad (8)$$

for $i, j = 1, ..., 2^d$. For simplicity, we will assume a noise distribution where the noise vectors \mathbf{n}_k and \mathbf{r}_k have i.i.d. components (the general non-i.i.d. case can be similarly handled, at the expense of introducing more parameters), with $P(\mathbf{n}_k(i) = 1) = p$ and $P(\mathbf{r}_k(i) = 1) = q$, for i = 1, ..., d. Parameters 0 < p, q < 1/2 correspond to the amount of "perturbation" to the Boolean state and measurement processes, respectively — the cases p = 1/2 or q = 1/2 corresponding to maximum uncertainty. In this case, the prediction matrix M_k in (8) can be rewritten as:

$$(M_{k})_{ij} = P\left(\mathbf{n}_{k} = \mathbf{f}(\mathbf{x}^{j}, \mathbf{u}_{k}) \oplus \mathbf{x}^{i}\right) P\left(\mathbf{r}_{k} = I_{\beta_{k} < \rho} \mathbf{v}^{j} \oplus \mathbf{v}^{i}\right)$$
$$= p^{\|\mathbf{x}^{i} \oplus \mathbf{f}(\mathbf{x}^{j}, \mathbf{u}_{k})\|_{1}} (1-p)^{d-\|\mathbf{x}^{i} \oplus \mathbf{f}(\mathbf{x}^{j}, \mathbf{u}_{k})\|_{1}}$$
$$\times \left[\rho q^{\|\mathbf{v}^{i} \oplus \mathbf{v}^{j}\|_{1}} (1-q)^{d-\|\mathbf{v}^{i} \oplus \mathbf{v}^{j}\|_{1}} + (1-\rho) q^{\|\mathbf{v}^{i}\|_{1}} (1-q)^{d-\|\mathbf{v}^{i}\|_{1}}\right],$$

$$(9)$$

for $i, j = 1, ..., 2^{2d}$, where $||\mathbf{v}||_1 = \sum_{i=1}^d \mathbf{v}(i)$ for a vector \mathbf{v} of size d.

Additionally, given a value of the observation vector $\mathbf{Y}_k = \mathbf{y}_k$ at time k, the update matrix $T_k(\mathbf{y}_k)$ of size $2^{2d} \times 2^{2d}$ is a diagonal matrix, with diagonal elements:

$$(T_k(\mathbf{y}_k))_{ii} = P(\mathbf{Y}_k = \mathbf{y}_k | \mathbf{Z}_k = \mathbf{z}^i)$$

$$= \begin{cases} 1, & \text{if } \mathbf{x}^i \oplus \mathbf{v}^i = \mathbf{y}_k, \\ 0, & \text{otherwise,} \end{cases}$$
(10)

for $i = 1, ..., 2^{2d}$.

The optimal MMSE filtering problem given observations $\mathbf{Y}_{1:k} = (\mathbf{Y}_1, \dots, \mathbf{Y}_k)$ consists of finding an estimator $\hat{\mathbf{Z}}_k = h(\mathbf{Y}_{1:k})$ of the state \mathbf{Z}_k that minimizes the conditional mean-square error (MSE):

$$MSE(\mathbf{Y}_{1:k}) = E\left[\|\hat{\mathbf{Z}}_k - \mathbf{Z}_k\|^2 | \mathbf{Y}_{1:k} \right]$$
(11)

at each value of $\mathbf{Y}_{1:k}$ (such that it also minimizes the frequentist expected MSE over all possible realizations of $\mathbf{Y}_{1:k}$) up to the current time k, for k = 1, 2, ...

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, ..., d, $\mathbf{v}^c \in \{0,1\}^d$ via $\mathbf{v}^c(i) = 1 - \mathbf{v}(i)$, for i = 1, ..., d; where $I_{\mathbf{v}(i)>1/2}$ returns 1 if $\mathbf{v}(i) > 1/2$ and 0 otherwise. The optimal MMSE estimator at time step k, $\hat{\mathbf{Z}}_k$ is given by [4,6]

$$\hat{\mathbf{Z}}_{k} = \overline{E\left[\mathbf{Z}_{k} \mid \mathbf{Y}_{1:k}\right]}, \qquad (12)$$

with optimal filtering MMSE

$$MSE^{*}(\mathbf{Y}_{1:k}) = \left\| \min\left\{ E\left[\mathbf{Z}_{k} \mid \mathbf{Y}_{1:k} \right], E\left[\mathbf{Z}_{k} \mid \mathbf{Y}_{1:k} \right]^{c} \right\} \right\|_{1},$$
(13)

where the minimum is computed by component.

Define the matrix A of size $2d \times 2^{2d}$ via $A = [\mathbf{z}^1 \cdots \mathbf{z}^{2^{2d}}]$, which contains all possible Boolean states of the system. Both (12) and (13) require the computation of $E[\mathbf{Z}_k | \mathbf{Y}_{1:k}]$. This can be obtained as

$$E[\mathbf{Z}_k \mid \mathbf{Y}_{1:k}] = A \mathbf{\Pi}_{k|k}, \qquad (14)$$

where $\Pi_{k|k}$ is defined in (6). It is clear that $\Pi_{k|k}$ can be obtained based on the following Bayesian recursion:

$$\begin{aligned} \mathbf{\Pi}_{k|k}(i) &= P(\mathbf{Z}_{k} = \mathbf{z}^{i} \mid \mathbf{Y}_{1:k}) \\ &= \frac{p(\mathbf{Y}_{k} \mid \mathbf{Z}_{k} = \mathbf{z}^{i}) P(\mathbf{Z}_{k} = \mathbf{z}^{i} \mid \mathbf{Y}_{1:k-1})}{P(\mathbf{Y}_{k} \mid \mathbf{Y}_{1:k-1})} \\ &= \frac{(T_{k}(\mathbf{Y}_{k}))_{ii} \mathbf{\Pi}_{k|k-1}(i)}{\|T_{k}(\mathbf{Y}_{k}) \mathbf{\Pi}_{k|k-1}\|_{1}}, \end{aligned}$$
(15)

so that $\Pi_{k|k} = T_k(\mathbf{Y}_k) \Pi_{k|k-1} / ||T_k(\mathbf{Y}_k) \Pi_{k|k-1}||_1$, where $\Pi_{k|k-1}$ and $T_k(\mathbf{Y}_k)$ are defined in (6) and (10), respectively. On the other hand,

$$\boldsymbol{\Pi}_{k|k-1}(i) = P(\mathbf{Z}_{k} = \mathbf{z}^{i} | \mathbf{Y}_{1:k-1})
= \sum_{j=1}^{2^{d}} P(\mathbf{Z}_{k} = \mathbf{z}^{i} | \mathbf{Z}_{k-1} = \mathbf{z}^{j}) P(\mathbf{Z}_{k-1} = \mathbf{z}^{j} | \mathbf{Y}_{1:k-1})
= \sum_{j=1}^{2^{d}} (M_{k})_{ij} \boldsymbol{\Pi}_{k-1|k-1}(j)$$
(16)

so that $\Pi_{k|k-1} = M_k \Pi_{k-1|k-1}$, where M_k is defined in (8).

Equations (14)-(16) lead to a fully recursive procedure for computation of the optimal MMSE estimate of the Boolean

states along with the optimal MMSE estimate of measurement noise at each time point. The complete procedure is summarized in Algorithm 1. The computation is "on-line", in the sense that at each new time point, the computation does not need to be restarted from the beginning, but can be efficiently updated.

Algorithm 1 Boolean Kalman Filter with Correlated Boolean Measurements

1: Initialization:

• Create 2^{2d} Boolean states,

$$\{\mathbf{z}^1 = (\mathbf{x}^1, \mathbf{v}^1), \dots, \mathbf{z}^{2^{2d}} = (\mathbf{x}^d, \mathbf{v}^d)\}$$

• Let:

$$\mathbf{\Pi}_{0|0}(i) = P(\mathbf{Z}_0 = \mathbf{z}^i) = \begin{cases} P(\mathbf{X}_0 = \mathbf{x}^i), & \text{if } \mathbf{v}^i = 0, \\ 0, & \text{otherwise.} \end{cases}$$

For k = 1, 2, ..., do:

2: Prediction:
$$\Pi_{k|k-1} = M_k \Pi_{k-1|k-1}$$

- 3: Update: $\boldsymbol{\beta}_k = T_k(\mathbf{Y}_k) \boldsymbol{\Pi}_{k|k-1}$
- 4: Filtered Distribution Vector:

$$\mathbf{\Pi}_{k|k} = \boldsymbol{\beta}_k / ||\boldsymbol{\beta}_k||_1$$

5: MMSE Estimator Computation:

$$\hat{\mathbf{Z}}_k = \overline{A \mathbf{\Pi}_{k|k}}$$

with optimal conditional MSE

$$MSE(\mathbf{Y}_1,\ldots,\mathbf{Y}_k) = \|\min\{A\mathbf{\Pi}_{k|k}, (A\mathbf{\Pi}_{k|k})^c\}\|_1.$$

4. NUMERICAL EXPERIMENT

In this section, we conduct a numerical experiment using a Boolean network based on the well-known pathway for the p53-MDM2 negative feedback loop [20]. The genetic regulatory network consists of four genes: *ATM*, *p53*, *Wip1*, and *MDM2*, as well as an input, "dna_dsb," which indicates the presence of DNA double strand breaks. The pathway diagram for this network is presented in Fig 1.

The network function **f** in (1) is obtained from this path diagram as follows. Let $\mathbf{f} = (f_1, \ldots, f_d)$, where each component $f_i : 2 \times \{0, 1\}^d \rightarrow \{0, 1\}$. We let

$$f_i(\mathbf{x}, \mathbf{u}) = \begin{cases} 1, & \sum_{j=1}^d a_{ij} \mathbf{x}(j) + \mathbf{u}(i) > 0, \\ 0, & \sum_{j=1}^d a_{ij} \mathbf{x}(j) + \mathbf{u}(i) \le 0, \end{cases}$$
(17)

where $a_{ij} = +1$ if there is positive regulation (activation) from gene j to gene i; $a_{ij} = -1$ if there is negative regulation (in-



Fig. 1: Activation/repression pathway diagram for the p53-MDM2 negative feedback loop Boolean network.

hibition) from gene j to gene i; and $a_{ij} = 0$ if gene j is not an input to gene i.

The average rates of correct state estimation over 500 iterations obtained by applying the original BKF algorithm assuming uncorrelated noise and by the BKF with correlated noise on a time series of length 100 are presented in Table 1. It can be seen that as ρ increases, the BKF begins to perform poorly while the correlated BKF performs well (or better, at a minimum) in all conditions.

In addition, we observe a higher performance of the proposed correlated BKF in the presence of small measurement and process noises and no stress condition (dna_dsb = 0). The reason for this phenomenon is that the system with active DNA damage has cyclic attractors, as opposed to a singleton attractor for a "no stress' condition, making the estimation process more difficult for the case where dna_dsb = 1.

Table 1: Average performance of the BKF assuming uncorrelated noise and the BKF for correlated noise.

			$dna_dsb = 0$		$dna_dsb = 1$	
p	q	ρ	BKF	Correlated BKF	BKF	Correlated BKF
0.01	0.01	0.1	0.94	0.96	0.93	0.94
		0.5	0.87	0.96	0.86	0.94
		1.0	0.22	0.96	0.21	0.93
	0.1	0.1	0.91	0.92	0.82	0.84
		0.5	0.87	0.92	0.77	0.82
		1.0	0.57	0.91	0.54	0.83
0.1	0.01	0.1	0.89	0.90	0.85	0.86
		0.5	0.83	0.89	0.80	0.86
		1.0	0.26	0.89	0.21	0.86
	0.1	0.1	0.62	0.64	0.53	0.56
		0.5	0.53	0.64	0.49	0.56
		1.0	0.15	0.63	0.10	0.54

Figure 2 shows the original and estimated state trajecto-

ries for a single time series of length 100, $\rho = 1$, dna_dsb = 0, p = 0.01, and q = 0.05. It is clear that better estimation is achieved for all genes using the correlated BKF in comparison to the BKF.



Fig. 2: Original and estimated gene activities.

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