2013 European Control Conference (ECC)
July 17-19, 2013, Zürich, Switzerland.

A New Approach to Solving the Inverse Frobenius-Perron Problem*

Xiaokai Nie, Daniel Coca

***Abstract*—This paper proposes a new matrix method to solve the inverse problem for the Frobenius-Perron equation. The method can be used to construct a piecewise linear Markov transformation, which approximates the evolution of an unknown dynamical system, based on a sequence of observed probability density functions generated by the system. This particular nonlinear system identification problem is solved using a three-step approach which involves determining the Markov partition, the matrix representation of the Frobenius-Perron operator and finally the corresponding point transformation. A numerical example is used to demonstrate the applicability of the approach.**

I. Introduction

It is well known that even simple deterministic one-dimensional discrete-time systems can exhibit complex random-like dynamical behaviour. Such systems can be studied in terms of the sequence of probability density functions they generate, rather than point trajectories. In many practical situations, the dynamical system is unknown and the problem is to infer the mathematical description of the system from experimental observations. There are many cases in which individual data point trajectories are not allowed to be recorded but sequences of density functions can be available. Typical examples include phenomena prediction of particle formation in emulsion polymerisation [1], papermaking systems [2], synchronised communication networks [3], biological system [4], cellular uplink load in WCDMA systems [5], etc. A potential new application area is the study of heterogeneity of cell populations using flow cytometry.

The problem of inferring a point transformation $x_{n+1}=S(x_n)$ given probability density functions generated by the system is known as the inverse Frobenius-Perron problem.

The inverse Frobenius-Perron problem (IFPP) for one-dimensional maps has been studied by a number of authors under the assumption that only the invariant density of the unknown system is observed. In [6] an algorithm was developed for reconstructing one-dimensional unimodal maps of dynamical systems with given invariant density. The problem has a unique solution under the certain symmetry assumptions [7]. The problem was also investigated in [8] using graph theoretic methods, for a special class of piecewise constant density functions whose relative minima contains value 0. A differential equation approach was proposed in [9] for specified types of transformations.

Ulam conjectured [10] (the conjecture was proven subsequently by Li [11]) that for one-dimensional systems the Frobenius-Perron operator can be approximated by a Markov transformation defined over a partition of the interval of interest. A method for synthesising the Frobenius-Perron matrix and thus solving the IFPP for semi-Markov transformation was introduced in [12]. An alternative synthesis method based on positive matrix theory was introduced in [3]. The approach can be exploited to synthesise dynamical systems with desired characteristics (Lyapunov exponents, mixing properties) that share the same invariant density [13]. The method can be used to analyse and design communication networks that rely on TCP-like congestion control mechanisms [14]. In [15] the inverse problem is formulated as the problem of stabilizing a target distribution using an open-loop perturbation approach. An optimization approach to finding the elements of the Frobenius-Perron matrix, which may offer a way to characterize the patterns of activity in the olfactory bulb, based on the invariant probability density functions of interspike intervals of receptor firing, was proposed in [4].

All the above methods can be used to construct a map with a given invariant density. In practice however, we are interested to derive a map which describes accurately the dynamical properties of the observed system not just the equilibrium density. Moreover, the matrix-based algorithms proposed so far assume that the Markov partition is known, while in practice this is rarely the case.

This paper proposes a new approach to infer the map, which characterize the observed dynamics. The system identification approach involves, in the first stage, identifying the Markov partition based on the invariant density. This information is then used to design a minimum number of experiments to generate sequences of probability density functions, which provide sufficient information to recover the Frobenius-Perron matrix and ultimately the dynamical system which generated the data.

The paper is organized as follows. In the following section, we give a brief introduction to the Frobenius-Perron operator. The proposed identification method is presented in

*XN gratefully acknowledges financial support from the Department of Automatic Control and Systems Engineering at The University of Sheffield and China Scholarship Council. DC gratefully acknowledges that this work was supported by BBSRC and the Human Frontiers Science Program.

Xiaokai Nie is with the Department of Automatic Control and Systems Engineering, The University of Sheffield, Sheffield S1 3JD, U.K. (e-mail: x.nie@sheffield.ac.uk).

Daniel Coca is with the Department of Automatic Control and Systems Engineering, The University of Sheffield, Sheffield S1 3JD, U.K. (phone: +44 (0)1142225619;e-mail: d.coca@sheffield.ac.uk).

Section III followed by a numerical simulation study in Section IV and conclusions.

II. The Frobenius-Perron Operator

Let $S: I \to I$, $I=[a,b]$ be a non-singular one-dimensional dynamical system capable of generating a density of states

$$x_{n+1} = S(x_n); \qquad n = 0, 1, 2, \ldots \tag{1}$$

Assuming that x_n is a random variable on I having probability density function $f_n \in L^1$ then x_{n+1} is distributed according to the probability density function $f_{n+1} = P_S f_n$ where $P_S : L^1 \to L^1$ given by

$$P_S f_n(x) = \frac{d}{dx}\int_{S^{-1}([a,x])} f_n \, dx \,. \tag{2}$$

is referred to as the Frobenius-Perron operator associated to *S*. A density f^* is said to be invariant under the transformation *S* if $f^* = P_S f^*$.

Let $\Re = \{R_1, R_2, \ldots, R_N\}$ be a partition of *I* into intervals. If *S* is a piecewise monotonic transformation, the Frobenius-Perron operator is given by

$$P_S f_n(x) = \sum_{i=1}^{N} f_n(S_i^{-1}(x)) \left| S'(S_i(x)) \right|^{-1} \chi_{S(R_i)}(x) \,. \tag{3}$$

The focus of the paper is on a special class of piecewise monotonic and expanding transformations for which the invariant density is piecewise constant.

Definition 1. A transformation $S: I \to I$ is said to be Markov with respect to the partition $\Re$ (or $\Re$-Markov) if *S* is monotonic on every interval R_i and $S(R_i)$ is a union of intervals in $\Re$ for $i = 1, 2, \ldots, N$ [12].

The following theorem is proven in [16]:

Theorem 1. If the transformation $S: I \to I$ is piecewise linear with respect to a partition $\Re$ and $\alpha = \inf |S'| > 1$ wherever the derivative exists, then any *S*-invariant density function f^* is piecewise constant on the partition $\Re$.

A richer class of piecewise linear transformations which satisfy the above theorem was introduced in [17]:

Definition 2. A transformation $S: I \to I$ is said to be semi-Markov with respect to the partition $\Re$ (or $\Re$-semi-Markov) if there exist disjoint subintervals $Q_j^{(i)}$ so that $R_i = \bigcup_{j=1}^{k(i)} Q_j^{(i)}$ for $i = 1, 2, \ldots, N$, $S|_{Q_j^{(i)}}$ is monotonic and $S(Q_j^{(i)}) \in \Re$.

III. Identification Algorithm

Here we assume that *S* is an unknown semi-Markov transformation over some unknown partition $\Re$. The aim is to recover *S* (and implicitly the partition) by observing its invariant density as well as the evolution of a number of pre-specified initial density functions under the transformation.

The reconstruction method proposed here involves determining first the partition $\Re$ based on the invariant density function f^* estimated from data.

Since the invariant density function for an $\Re$-semi-Markov is piecewise constant on the partition $\Re = \{R_i\}_{i=1}^{N}$ [17], given θ experimental data points $\{x_i^*\}_{i=1}^{\theta}$ collected in the stationary regime ($f_{n+1} = f^* = P_S f^* = P_S f_n$) the partition $\Re$ can be identified by forming the histogram of the data. Given a sufficiently large number of bins *m*, the height of each bin is given by

$$h_j = \frac{1}{\theta}\sum_{i=1}^{\theta} \chi_{\Delta_j}(x_i^*) \,, \tag{4}$$

where $\Delta_j = \big((j-1)(b-a)/m, j(b-a)/m\big]$, for $j = 1, 2, \ldots, m$, and χ is the characteristic function.

In order to determine an appropriate partition, the absolute value of the gradient of h_j, $l_j = m \cdot |(h_{j+1} - h_j)|$ is computed for $j = 1, 2, \ldots, m-1$, to identify the junctions of the intervals. If $l_j > \varepsilon$, where ε is an empirical value for filtering, then there exists a junction at $(a + j(b-a)/m)$. The number of intervals of the identified partition is given by

$$N = \sum_{j=1}^{m-1} \chi_{\mathbf{R}+}(l_j - \varepsilon) + 1 \,. \tag{5}$$

The identified partition can be written as

$$\Re = \left\{ \underbrace{\big(a, a + d_{j_1}(b-a)/m\big)}_{R_1}, \underbrace{\big(a + d_{j_1}(b-a)/m, a + d_{j_2}(b-a)/m\big)}_{R_2}, \ldots, \underbrace{\big(a + d_{j_{N-1}}(b-a)/m, b\big)}_{R_N} \right\}, \tag{6}$$

where $1 \le d_{j_1} < d_{j_2} < \ldots < d_{j_{N-1}} \le m-1$.

Let $\lambda(R_i)$ denote the length of R_i. Given the identified partition (6), a set of piecewise constant density functions is constructed as follows

$$f_0^i(x) = \sum_{j=1}^{N} w_{ij} \chi_{R_j}(x) \,; \qquad i = 1, 2, \ldots N, \tag{7}$$

where $w_{ij} = 1/\lambda(R_i)$ for $j = i$; and $w_{ij} = 0$ for $j \neq i$.

The vectors f_0^i can be assembled to form the following matrix of probing density functions

$$F_0 = \begin{bmatrix} f_0^1 \\ f_0^2 \\ \vdots \\ f_0^i \\ \vdots \\ f_0^N \end{bmatrix} = \begin{bmatrix} w_{11} & 0 & \cdots & 0 & \cdots & 0 \\ 0 & w_{22} & \cdots & 0 & \cdots & 0 \\ \cdots & \cdots & \ddots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & w_{ii} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \ddots & \cdots \\ 0 & 0 & \cdots & 0 & \cdots & w_{NN} \end{bmatrix}. \quad (8)$$

Each density f_0^i is sampled to generate a set of states

$$X_0^i = \{x_{0,k}^i\}_{k=1}^{\theta}, \qquad i = 1, 2, \ldots, N, \quad (9)$$

which will be used as initial conditions in subsequent probing experiments. The aim is to determine experimentally the set densities f_1^i associated with

$$X_1^i = \{x_{1,k}^i\}_{k=1}^{\theta}, \qquad i = 1, 2, \ldots, N, \quad (10)$$

where $x_{1,k}^i = S(x_{0,k}^i)$.

The density function for X_1^i is given by

$$f_1^i(x) = \sum_{j=1}^{N} v_{ij} \chi_{R_j}(x); \quad i = 1, 2, \ldots N, \quad (11)$$

where $v_{i,j} = \dfrac{1}{\theta} \displaystyle\sum_{k=1}^{\theta} \chi_{R_j}(x_{1,k}^i)$.

Similarly, we can use (11) to construct the following matrix

$$F_1 = \begin{bmatrix} f_1^1 \\ f_1^2 \\ \vdots \\ f_1^i \\ \vdots \\ f_1^N \end{bmatrix} = \begin{bmatrix} v_{11} & v_{12} & \cdots & v_{1j} & \cdots & v_{1N} \\ v_{21} & v_{22} & \cdots & v_{2j} & \cdots & v_{2N} \\ \cdots & \cdots & \ddots & \cdots & \cdots & \cdots \\ v_{i1} & v_{i2} & \cdots & v_{ij} & \cdots & v_{iN} \\ \cdots & \cdots & \cdots & \cdots & \ddots & \cdots \\ v_{N1} & v_{N2} & \cdots & v_{Nj} & \cdots & v_{NN} \end{bmatrix}. \quad (12)$$

In population level studies, for example, this can be achieved by sorting the population into fractions according to the identified partition and then observing the evolution of each fraction over the given sampling period in separate experiments.

The Frobenius-Perron matrix associated with a $\Re$-semi-Markov transformation, $M = (m_{ij})_{1 \le i, j \le N}$ is

$$m_{ij} = \begin{cases} |(S_{Q_k^{(i)}})'|^{-1}, & \text{if } S(Q_k^{(i)}) = R_j; \\ 0, & \text{otherwise.} \end{cases} \quad (13)$$

where $S_{Q_k^{(i)}}$ denotes the restriction of S to $Q_k^{(i)}$.

The relationship between f_0^i and f_1^i can be written as

$$f_1^i = f_0^i \cdot M, \quad (14)$$

where $i = 1, 2, \ldots, N$.

Alternatively, (14) can be written in matrix form as follows

$$F_1 = F_0 \cdot M. \quad (15)$$

Since by design F_0 is non-singular, the Frobenius-Perron matrix M is given by

$$M = (F_0)^{-1} F_1. \quad (16)$$

The identified Frobenius-Perron matrix is used to construct the transformation as illustrated in Fig. 1.

Specifically, given that the derivative of $S_{Q_j^{(i)}}$ is $1/m_{ij}$ the length of $Q_j^{(i)}$ is

$$\lambda(Q_j^{(i)}) = \lambda(R_j) \cdot m_{ij}. \quad (17)$$

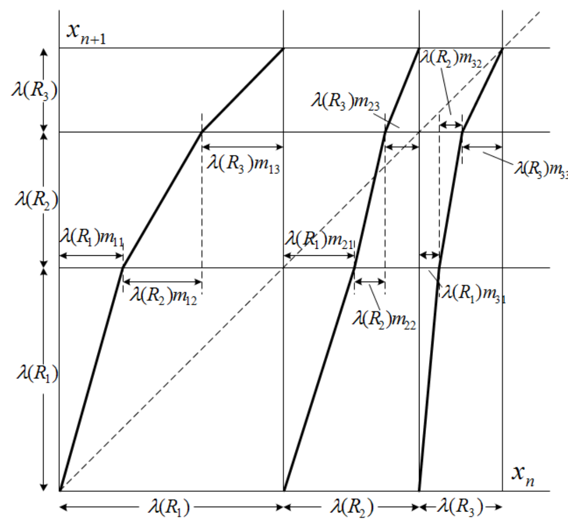

Fig. 1. Construction of 1-D transformation based on the Frobenius-Perron matrix.

So the piecewise linear mapping on $Q_j^{(i)}$ can be expressed as

$$S_{Q_j^{(i)}}(x) = \frac{1}{m_{ij}} \left\{ x - \left[a + \sum_{\alpha=1}^{j-1} \left(\lambda(R_\alpha) \cdot m_{i\alpha} \right) + \sum_{\beta=1}^{i-1} \lambda(R_\beta) \right] \right\} + \sum_{\alpha=1}^{j-1} \lambda(R_\alpha) + a, \quad (18)$$

for $i = 1, 2, \ldots, N$, $j = 1, 2, \ldots, N$.

IV. NUMERICAL SIMULATION EXAMPLE

The applicability of the proposed algorithms is demonstrated using a numerical simulation example. The aim is to reconstruct the piecewise linear transformation defined on $I=[0,1]$, illustrated in Fig. 2, from simulated data.

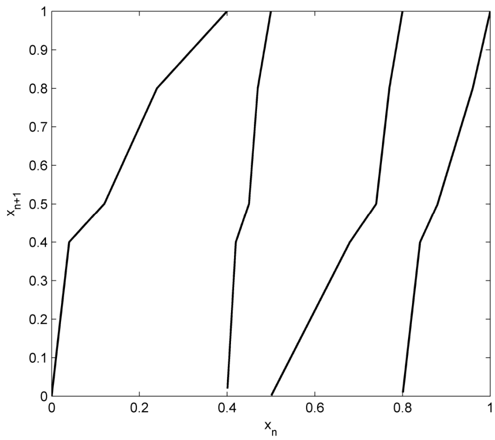

Fig. 2. Original piecewise linear transformation

To obtain the invariant density, 5×10^3 initial states were randomly generated. For each initial state, the map was iterated 20,000 steps. The final states were used to construct the histogram shown in Fig. 3. In this case, the number of bins was set to $m=30$.

The absolute value of the density gradient computed for the resulting histogram is shown in Fig. 4. By setting the empirical threshold value ε to 5, a four-interval partition was identified

$$\Re=\{R_1,R_2,R_3,R_4\}, \tag{19}$$

where R_1=(0, 0.4), R_2=(0.4, 0.5), R_3=(0.5, 0.8), and R_4=(0.8, 1).

Four constant density functions $f_0^i(x)$, i=1,…,4, compactly supported on each interval R_i were constructed and used to generate the distributions, as shown in Fig. 5.

The estimated Frobenius-Perron matrix is as follows

$$M=\begin{bmatrix}0.1010 & 0.7900 & 0.4000 & 0.8040\\ 0.0500 & 0.2980 & 0.0670 & 0.1510\\ 0.4480 & 0.6010 & 0.1020 & 0.1510\\ 0.1000 & 0.4020 & 0.2660 & 0.2000\end{bmatrix}. \tag{20}$$

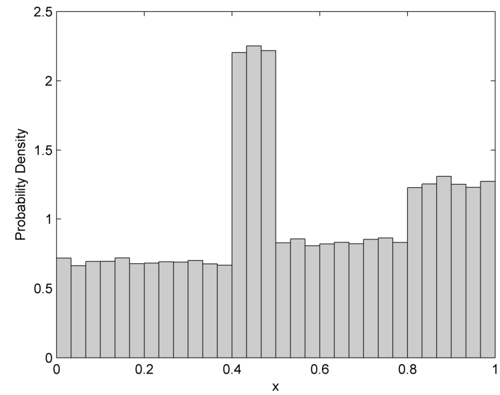

Fig. 3. The invariant density represented by histogram.

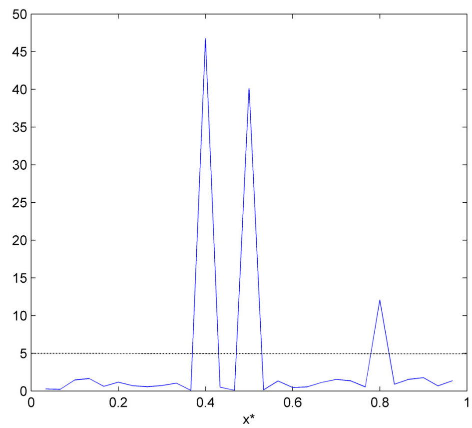

Fig. 4. The modulus of density gradient index

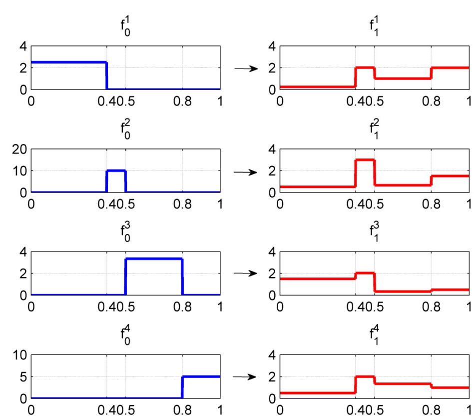

Fig. 5. Mapping of $f_0^i(x)$ into $f_1^i(x)$ for $i=1,2,3,4$.

The estimated Frobenius-Perron matrix M is then used to reconstruct the mapping of the unknown system, as shown in Fig. 6. The relative approximation error between the new density generated by the identified transformation and the one produced by the unknown system from the same initial density can be calculated as

$$\eta(x) = \frac{|f_1'(x) - f_1(x)|}{f_1(x)} \times 100\% , \quad (21)$$

where f_1' is the approximated new density, f_1 is the real new density. The result is shown in Fig. 7.

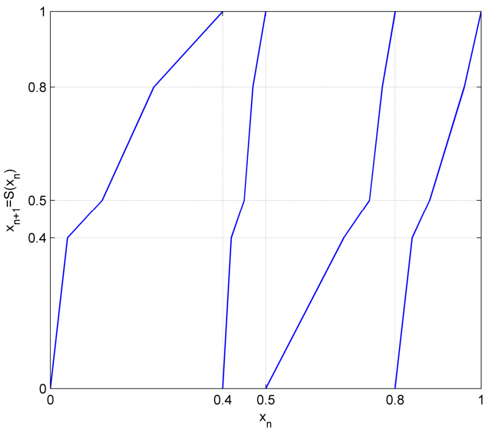

Fig. 6. The identified transformation of the underlying system.

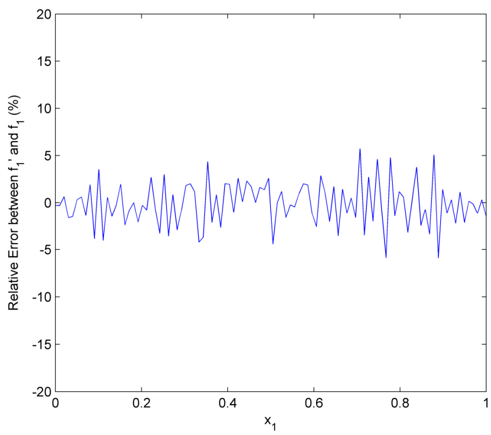

Fig. 7. The relative error between the predicted and real densities. f_0 is set to a uniform probability density function. The densities are calculated with a 100-bin histogram.

V. Conclusion

In many practical situations it is impossible to measure individual trajectories of a dynamical system and the only available information about the system is in the form of density functions. Previous work focused only on deriving a transformation that has a given density function as invariant density. This problem does not have a unique solution so that, while the reconstructed map will have the specified asymptotic dynamics, the inferred model cannot be used to predict the evolution of the system given an arbitrary distribution of initial conditions. Consequently, the model will have limited use for analysis or control.

The method introduced in this paper provides a recipe for designing experiments to probe the system and generate data that can be used to uniquely recover the transformation.

The proposed approach offers a powerful tool to characterize cell population dynamics using flow cytometry. The process of sorting and plating of cell subpopulations followed by re-examination of the resulting colonies, which is routinely used to characterize heterogeneity in cell cultures, mimics the main steps of our algorithm. In this context, the paper provides a method to design the experiment and model the resulting data.

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