Network Topology Estimation through Synchronization: A Case Study on Quantum Dot CNN

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***Abstract*— The reconstruction of the links among coupled dynamical systems can be handled in many ways. One of them is through synchronization, building a system composed by a "mirror" network and by evolution equations for the links of interest, in such a way that the two networks will synchronize if and only if the links are correctly estimated. A procedure based on this idea to estimate the topology of a network of interacting objects when the state variables are known is already present in literature, and here it is extended to systems ruled by implicit differential equations, to better suit some actual cases arising, in particular, in electric and electronic systems. The developed method is applied to a case of practical interest: the test of connections in a nanoscale device, introduced in the literature as "quantum dot cellular neural network", which can be easily produced in a self-assembled way. The whole iter has some steps sensitive to errors which can lead to a final device where the links among the "dots" are different from the desired ones. Our interest is in applying the method to detect such bad links.**

I. Introduction

A system of interacting agents, like neurons, lasers, people or computers, can be efficiently modeled by a network having a node, or cell, for each agent and a link for each connection. If the agents evolve according to some differential equations, the whole system evolution is then ruled by a set of coupled differential equations, where the links of the network account for the coupling among the agents. The real world provides lots of examples of complex networks [1], [2]. A great part of research on complex networks has focused on how the topological properties of the network influence the dynamics of the cells and of the whole system [3]–[5]. Another important issue which is interesting to study is how to infer information on the topology of the network and the state of the cells from observations, and how to use it to control the network. Our work is related to this aspect. In [6], the authors proposed a technique, based on synchronization, to estimate the topology of a network of coupled dynamical systems observing the time evolution of the cells. The method was applied to different kinds of systems, like neurons [7] and phase oscillators [8]. One of the basic assumptions of the paper is that the differential system accounting for the evolution of the cells is in normal form.

However, some interesting systems, as, for example, networks of quantum dots [9]–[12] do not satisfy this assumption. These networks, formed by nanoelectronic components, possess interesting computational features, in fact they produce associative memory effects, perform 2D image processing and solve NP-complete combinatorial optimization problems.

The aim of this work is to extend the technique proposed in [6] to networks which do not admit a description of the evolution of the cells with differential systems in normal form. As a practical example, quantum dot cellular neural networks are considered [13].

At first, in Section II, the original method is succinctly described. Then, in Section III, the device taken into consideration as a practical application is introduced, with an overview of the problem under study. In Section IV our developments are explained and in Section V are illustrated by an example. Conclusions (Section VI) and acknowledgement close the paper.

II. Preliminaries

In this Section, the method proposed in [6] is summarized. A network composed of n 1D cells is considered, so that the dynamical evolution on the network is given by:

$$\dot{x}_i = f_i(x_i) + \sum_{j \in V} A_{ij} h_j(x_j) \tag{1}$$

where $i \in V := \{1, 2, \dots, n\}$, $x_i \in \mathbb{R}$ is the state of node i, $f_i : \mathbb{R} \to \mathbb{R}$ describes the evolution of node i when uncoupled and $h_j : \mathbb{R} \to \mathbb{R}$ is the output from node j, which is seen by node i weighted with the term A_{ij}. The matrix $\boldsymbol{A} = \{A_{ij}\}$ has then $A_{ij} \neq 0$ if and only if there is a link between node j and node i and $A_{ij} = 0$ otherwise. We assume that the maps f_i and h_i are Lipschitzian uniformly in $i \in V$, *i.e.* there exist positive constants L_f, L_h such that

$$|f_i(\nu) - f_i(\xi)| \leq L_f |\nu - \xi|, \quad \forall i \in V \tag{2}$$

and

$$|h_i(\nu) - h_i(\xi)| \leq L_h|\nu - \xi|, \quad \forall i \in V. \tag{3}$$

Moreover, we assume that the states x_i can be experimentally measured (are observable), for all $i \in V$. The proposed method uses these observations to find the topology of the network connections, more precisely to estimate the elements of the matrix $\boldsymbol{A}$. The main idea is to consider a new system of n cells, described by the state variable $y_i(t)$, whose evolution is ruled by equations similar to (1), but with a matrix $\boldsymbol{B}(t)$ instead of $\boldsymbol{A}$. This matrix can change in time according to functions linked to the differences $y_i - x_i$. By letting $\boldsymbol{x} = [x_1, \ldots, x_n]^T$ and $\boldsymbol{y} = [y_1, \ldots, y_n]^T$, under some mild mathematical conditions one can design control signals $u_i(\boldsymbol{x}, \boldsymbol{y})$, such that the following system can track the topology of the network:

$$\begin{cases} \dot{x}_i &= f_i(x_i) + \sum_{j \in V} A_{ij} h_j(x_j) \\ \dot{y}_i &= f_i(y_i) + \sum_{j \in V} B_{ij} h_j(y_j) + \Delta_i(\mathbf{y}, B_{ij}, t) + u_i \\ \dot{B}_{ij} &= -\gamma_{ij} h_j(y_j)(y_i - x_i), \end{cases} \tag{4}$$

where γ_{ij} are positive constants, Δ_i represents some unknown nonlinear functions (such as disturbances and modeling errors) and $i, j \in V$. It has been proved in [6] that, as $t \to +\infty$ we have $B_{ij} \to A_{ij}$ for all $i, j \in V$. The proof is based on the Lyapunov function

$$2\Omega(t) = \sum_i e_i^2 + \sum_i \sum_j (1/\gamma_{ij})(B_{ij} - A_{ij})^2, \tag{5}$$

where $e_i = y_i - x_i$ for each $i \in V$. The time derivative of $\Omega(t)$ is showed to be non-positive and to reach the value zero only when $\boldsymbol{x} = \boldsymbol{y}$ and $\boldsymbol{A} = \boldsymbol{B}$.

III. Quantum Dot CNN

The quantum dot architecture proposed in [9]–[12] is a 2-D locally interconnected architecture analogous to a cellular neural network (CNN) [14].

The active elements in the architecture are the "quantum dots," which are electrically coupled to their nearest neighbors and interfaced with a nonohmic substrate (exhibiting a negative differential resistance). The procedure to build this kind of devices is described in [9]–[12] and is based on evaporation, electrodeposition and controlled etching in a self-assembled fashion.

In Figure 1 the circuit model of the dots and the nonlinear function representing the interaction between each dot and the nonohmic substrate are depicted. The circuit model for the coupling between two neighbors is shown in Figure 2, and Figure 3 gives a very schematic picture of the network considered.

Using Kirchhoff's current law, the evolution of the voltage v_i of the i-th of the n dots can be described by

$$C_{si}\dot{v}_i = I_{Bi} - J_{si} + \sum_{j \neq i} J_{ij}, \tag{6}$$

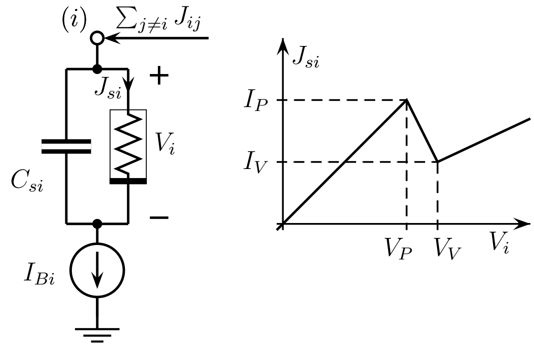

Fig. 1. Equivalent circuit of a dot and nonlinear characteristic of the nonhomic substrate

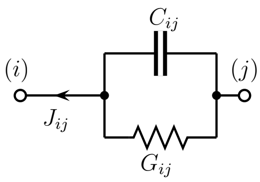

Fig. 2. Equivalent circuit of the coupling between dot i and dot j

where I_{Bi} is the bias current for dot i, C_{si} is the dot-to-substrate capacitance, J_{si} is the current which comes to node i from the semiconductor wire underlying the dot, and J_{ij} is the current from dots j to dot i, which can be a linear or a non linear functions of the difference between dot potentials (Figure 2).

Assuming a linear capacity-resistance model for the dot-to-dot coupling, we get this version of (6)

$$\left(C_{si} + \sum_{j \neq i}^{n} C_{ij} \right) \dot{v}_i = I_{Bi} - J_{si} + \\ + \sum_{j \neq i}^{n} \big(G_{ij}(v_j - v_i) + C_{ij}\dot{v}_j \big), \tag{7}$$

where C_{ij} and G_{ij} are, respectively, the capacitance and conductance between dot i and dot j (Figure 2). The local connectivity eliminates a lot of the interconnection problem, but the whole process has some steps sensitive to manufacturing errors, and the scale does not allow an easy checking of whether a contact between two dots really exists or not. We are then interested in developing a method which uses the time evolution of the dot potentials starting from an unknown initial state in order to obtain information regarding the connections of the grid. This could be a practical application of the method developed in [6], but with some caveats.

IV. Estimation with synchronization

In this case we are not dealing with general coupling functions as in [6], but there is a coupling on the derivative side too, a fact which creates both theoretical and, especially, computational difficulties. A naïve approach could consist in

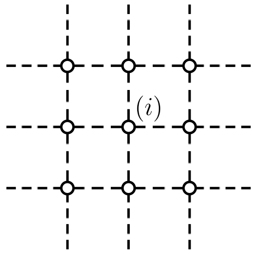

Fig. 3. Network schematization

inverting the capacity matrix $\boldsymbol{C} = \{C_{ij}\}$, in order to have a normal form system and to be able to apply the method described in [6]. This solution has some negative aspects, since it involves a numerically tough operation like the inversion of a matrix. Moreover, if the matrices $\boldsymbol{C}$ and $\boldsymbol{G} = \{G_{ij}\}$ are sparse or have some regular structure to be exploited to simplify the problem, as in the real case taken into consideration, after the inversion this is generally not true anymore. We are then interested in estimating the network of connections working with implicit differential equations. Following [9] and the simulations performed therein, we can assume some restrictions to the general form. We can suppose the matrices $\boldsymbol{C}$ and $\boldsymbol{G}$ to be both proportional to the same matrix $\boldsymbol{A}$, so that $\boldsymbol{C} = c\boldsymbol{A}$ and $\boldsymbol{G} = g\boldsymbol{A}$. This is strictly related to the physics of the system: as the capacity-resistance model accounts for the coupling made by electrodeposition and etching of a semiconductor and a metal in the self-assembly procedure, we can reasonably think that if the process went wrong and some couplings did not exist, then both the resistance part and the capacity part are missing. By the same reasoning, we can suppose that the coupling is bidirectional and so we suppose the matrix $\boldsymbol{A}$ to be symmetric. Moreover, we have $A_{ii} = 0$ and we suppose the bias current I_{Bi} to be constant and the dot-to-substrate capacitances C_{si} to be equal for each i. After normalization on the quantity C_{si}, the system (7) can then be rewritten in the form

$$\dot{x}_i + \sum_{j=1}^{n} A_{ij}\big(c(\dot{x}_i - \dot{x}_j) + g(x_i - x_j)\big) - f(x_i) = 0 \tag{8}$$

for each $i \in V$. Here $f(x_i)$ accounts for the bias current I_{Bi} and for the current J_{si} coming from the substrate. Our task is to estimate the unknown entries of $\boldsymbol{A}$.

Referring to (8), we can consider the following system,

$$\begin{cases} \dot{x}_i + \sum_{j=1}^{n} A_{ij}\big[c(\dot{x}_i - \dot{x}_j) + g(x_i - x_j)\big] - f(x_i) = 0 \\ \dot{y}_i + \sum_{j=1}^{n} B_{ij}\big[c(\dot{y}_i - \dot{y}_j) + g(y_i - y_j)\big] - f(y_i) - u_i = 0 \\ \dot{B}_{\ell k} + \xi_{\ell k}\big[g(y_k - y_\ell) + c(\dot{y}_k - \dot{y}_\ell)\big](y_\ell - x_\ell) = 0 \end{cases} \tag{9}$$

where $B_{\ell k}$ are the estimates of the unknown connections we want to reconstruct and u_i are control functions to be specified. Note that some practical considerations could suggest that not all the entries in $\boldsymbol{A}$ are actually unknown, so we have used different indices ℓ, k, instead of i, j, for the elements of $\boldsymbol{B}$ which really have to track the connections. In the other cases, we simply put $B_{ij} = A_{ij}$ and $\dot{B}_{ij} = 0$. If the function f is Lipschitz with constant L, then it is possible to choose control functions $u_i(\boldsymbol{x}, \boldsymbol{y})$ such that the system (9) will track the topology of the network, or, in other words, $B_{\ell k} \to A_{\ell k}$ as $t \to +\infty$. To show this, let $e_i = y_i - x_i$ and consider the function

$$\begin{aligned} 2\Omega(t) = \sum_{i=1}^{n} e_i^2 + \sum_{i=1}^{n}\sum_{j=1}^{n} \frac{(B_{ij} - A_{ij})^2}{\xi_{ij}} + \\ + c\sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}\frac{(e_i - e_j)^2}{2}. \end{aligned} \tag{10}$$

It follows that

$$\begin{aligned} \dot{\Omega} = \sum_i e_i \dot{e}_i + \sum_i\sum_j \frac{(B_{ij} - A_{ij})\dot{B}_{ij}}{\xi_{ij}} \\ - \frac{c}{2}\sum_i\sum_j A_{ij}(e_i - e_j)(\dot{e}_j - \dot{e}_i) = \\ = \sum_i e_i \left(f(y_i) - f(x_i) + g\sum_j A_{ij}(e_j - e_i) + u_i \right). \end{aligned} \tag{11}$$

With

$$\bar{k} = ||\boldsymbol{A}||_1 = \max_{i \in V} \left\{ \sum_j |A_{ij}| \right\} \tag{12}$$

and taking control functions of the form

$$u_i = -Ke_i \quad i \in V \tag{13}$$

we have,

$$\begin{aligned} \dot{\Omega} = \sum_i e_i\big(f(y_i) - f(x_i)\big) - K\sum_i e_i^2 + \\ + g\sum_i e_i \sum_j A_{ij}e_j - g\sum_i e_i^2 \sum_j A_{ij} \leq \\ \leq \sum_i |e_i|\big|f(y_i) - f(x_i)\big| - K\sum_i e_i^2 + g\sum_i\sum_j A_{ij}e_ie_j \leq \\ \leq \sum_i |e_i|L|e_i| - K\sum_i e_i^2 + \frac{g}{2}\sum_i\sum_j A_{ij}(e_i^2 + e_j^2) \leq \\ \leq L\sum_i e_i^2 - K\sum_i e_i^2 + \frac{g\bar{k}}{2}\sum_i e_i^2 + \frac{g}{2}\sum_j e_j^2 \sum_i A_{ij} \leq \\ \leq L\sum_i e_i^2 - K\sum_i e_i^2 + \frac{g\bar{k}}{2}\sum_i e_i^2 + \frac{g\bar{k}}{2}\sum_j e_j^2 \leq \\ \leq \big(L - K + \bar{k}g\big)\sum_i e_i^2. \end{aligned} \tag{14}$$

We are generally able to give an upper bound to the value $\bar{k}$, by some physical considerations. Then, choosing $K > L +$

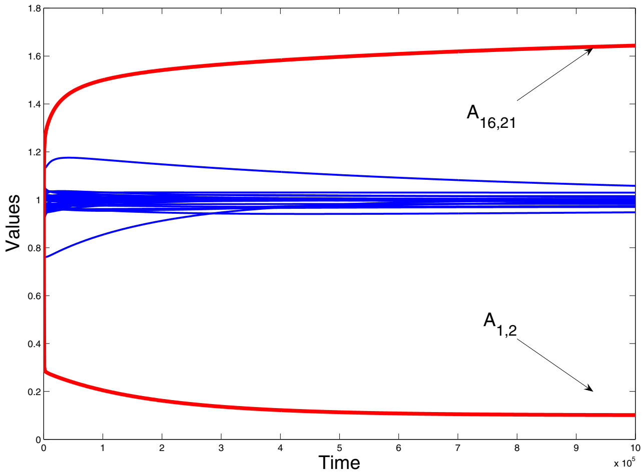

Fig. 4. Time evolution of connection estimates.

$\bar{k}g$, we have that $\dot{\Omega} \leq 0$. This means that the estimate error exponentially decreases, so

$$y_i(t) \to x_i(t) \quad \forall i \in V \tag{15}$$

and for all ℓ, k of interest

$$B_{\ell k}(t) \to A_{\ell k}, \tag{16}$$

as long as we can state that $\sum_{i=1}^{n} e_i^2 = 0$ if and only if $B_{ij} = A_{ij}$ for all $i, j = 1, \dots, n$. To obtain this condition, which actually means that the system $x_1, \dots, x_n$ has not to converge too rapidly to an equilibrium point, we have to permanently excite the system in some way - [15], [16]-, for example by connecting sinusoidal current generators to some of the dots. To test the feasibility of this method, a numerical integration of the system (9) has been performed. The choice of the routine needs particular attention, as the differential equations to be integrated are implicit.

V. Example

We have simulated a regular grid of 5×5 dots, with all the connections equal to 1, *i.e* correct, except for two. The first of them is the connection between dot 1 and dot 2, supposed smaller than the others, $A_{1,2} = 0.1$, and the second one, the connection between dot 16 and dot 21, bigger, $A_{16,21} = 1.7$. Five sinusoidal generators with different phase and amplitude are used to permanently excite the system, connected to the four corner dots and to the central one. The evolution of the estimates of the unknown elements of $\boldsymbol{A}$ is depicted in Figure 4. It is clearly visible that the method recognizes the values of the right connections and correctly estimates those of the two wrong ones. Interesting further developments of this method could be a theoretical and numerical analysis of performances when only a reduced number of states x_i can be observed and its use for monitoring the evolution of time dependent connections, for example to detect on-line damages in power grids [17].

VI. Conclusion

In [6], the authors proposed a technique, based on synchronization, to estimate the topology of a network of coupled dynamical systems observing the time evolution of the cells. In this work we have extended that method to the case when the coupling is among the derivatives too and applied the resulting tool to an actual problem: the estimation of links in a quantum dot CNN [9]. A numerical simulation has been performed to test the method. The theory developed can be used for other cases when there is a coupling among the derivatives of the state of the cells to be estimated, a situation which often arises in electrical and electronic applications [17].

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