Data assimilation for heterogeneous networks: the consensus set

Timothy D. Sauer[1,*] and Steven J. Schiff[2]

[1]*Department of Mathematical Sciences,*
George Mason University, Fairfax, VA 22030
[2]*Center for Neural Engineering, Departments of Neurosurgery,*
Engineering Science and Mechanics, and Physics,
The Pennsylvania State University, University Park, PA 16802

Abstract

Data assimilation in dynamical networks is intrinsically challenging. A method is introduced for the tracking of heterogeneous networks of oscillators or excitable cells in a nonstationary environment, using a homogeneous model network to expedite the accurate reconstruction of parameters and unobserved variables. An implementation using ensemble Kalman filtering to track the states of the heterogenous network is demonstrated on simulated data and applied to a neural tissue experiment. The approach has broad applicability for the prediction and control of biological and physical networks.

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*Electronic address: `tsauer@gmu.edu`

Data assimilation has grown in importance for the analysis of experiments in physics, in part due to its great success in data-rich, high-dimensional problems. In modern numerical weather prediction, for example, it is common to use advanced filtering and prediction techniques for state estimation and tracking in cases where the experimental data is complicated and high-dimensional [1].

Dynamical networks have become increasingly visible in physical and biological applications. Coupled grids of varying connectivity, often with simple dynamics at each grid node, can lead to interesting nonlinear phenomena, as seen in Josephson junction arrays [2], neuronal networks [3], and a widening array of examples in systems biology [4]. The network structure has been found to be a decisive factor in the resulting dynamics, and is an area of intensive contemporary research [5].

The decentralized nature of networks presents increased difficulty for data assimilation. We propose a novel technique, called the *consensus set method*, that makes tracking and prediction of dynamics possible in a network where the equations of motion are unknown or only partly known, and when the system is only partially observed. After demonstrating the method computationally in heterogeneous model networks of excitable cells, we show the ability of the method to track experimental data from a neural tissue preparation for which no first-principles model exists.

In fact, the main targets of the new technique are networks whose nodal dynamics are poorly described. In such cases, data assimilation may be attempted using models that only qualitatively approximate observed dynamics. Although model parameters and state information determined in this process may have little or no physical significance, the goal of the consensus set method is to capture and track global dynamics despite the lack of system knowledge. In particular, in the following we focus on tracking spiral wave and aperiodic behaviors in networks of excitable cells for prediction and control purposes.

The success of data assimilation is closely linked to the mathematical model for the underlying dynamics of the experiment. State-of-the-art methods such as Ensemble Kalman Filtering (EnKF) normally rely on good models to track the system and update the current system state (called the background in numerical weather prediction). The EnKF [7–12] is routinely used to complete partial state information. More recently, it has been extended to an algorithm for fitting a limited number of parameters as well as reconstructing the system state, in the presence of significant noise levels, sometimes called the dual estimation

problem [13, 14]. The difficulty of fitting increases with the number of parameters needed, due to the rapid increase in data requirements.

Dynamical network models provide an demanding example of data requirements. It is typical for the number of model parameters to proliferate to an unmanageable number, since each element of the network may follow a slightly different local nonlinear dynamical model. Such a situation may overwhelm even the most robust parameter fitting algorithms. Since the model equations cannot be determined accurately, data assimilation applied in this way may be infeasible. We differentiate between two different types of network heterogeneity, calling a network weakly heterogeneous if the individual nodes of the network can be modeled by similar systems with differing parameter settings, and strongly heterogeneous if no such simplification exists. We will show the consensus set method, implemented below in the context of the EnKF, to be useful for tracking and parameter identification in weakly heterogeneous networks undergoing complicated and nonstationary nonlinear dynamics, and in some cases for strongly heterogeneous networks.

First consider the weakly heterogeneous case. Begin with a general dynamical model with k parameters. Assume that several such versions of the model, with different parameter settings, are part of a network, and assume that the resulting dynamics are partially observable. In a moderately large network undergoing nonlinear dynamics, fitting all parameter settings in the network will be infeasible. The idea of the consensus method is to track the weakly heterogeneous network with a *homogeneous* network of identical systems with a single set of k parameters that are fit by the EnKF. The tracking will be inexact, because a heterogeneous network is being tracked by a homogeneous network. However, under the assumption that the heterogeneity is sufficiently weak, we show the ability of the EnKF to determine a consensus set of parameters that enables the homogeneous network to follow the heterogeneous network closely enough for many prediction and control purposes. The goal is not mathematical exactness, but an approximation that is close enough to be useful in an experimental scenario.

In addition to fitting parameters, the EnKF needs to reconstruct the full dynamical states from partial state observations. This reconstruction will also not be perfect, due to the approximation by a homogeneous network. Of course, it would be preferable to fit all parameters of all elements of the heterogeneous system, but in most cases this will be impossible to carry out with partial, or even full, state data, and even in the absence of

observational noise.

We will begin by demonstrating the consensus set method in networks of excitable cells. The Wilson-Cowan equations [15] are designed to model the time evolution of cortical neurons with excitation u and recovery variable a. This system of two differential equations, with a single nonlinearity, supports sustained oscillations. A network of Wilson-Cowan oscillators on an $N \times N$ rectangular grid can carry a wide variety of interesting behavior, including plane and ring waves, spiral waves, and chaotic aperiodic dynamics [16]. The equations at the (i, j) grid point are

$$
\begin{aligned}
\dot{u}_{ij} &= c_{ij1}u_{ij} + c_{ij2}a_{ij} + c_{ij3}\sum_{i'j'}e^{-d}H(u_{i'j'} - c_{ij4}) \\
\dot{a}_{ij} &= c_{ij5}u_{ij} + c_{ij6}a_{ij}
\end{aligned}
\tag{1}
$$

where the sum is taken over all other nodes $i'j'$ in the network, d denotes the distance between grid points ij and $i'j'$, and H denotes the Heaviside function or a smoothed version if a continuous equation is desired [17]. The u variable represents instantaneous excitation, and the a variable represents recovery or adaptation. Biologically meaningful parameters ordinarily require $c_{ij1}, c_{ij2}, c_{ij6} < 0$ and $c_{ij3}, c_{ij5} > 0$.

Each model neuron in the grid follows Wilson-Cowan dynamics with input determined by superthreshold activity of its neighbors. The input is zero unless the variable $u_{i'j'}$ is greater than the threshold c_{ij4}, in which case the neighbor contributes to the input according to its distance in the grid. Initial conditions are used that lead to a sustained nonequilibrium dynamical attractor on the grid. Observing only the u variable with applied noise at the grid points, we attempt to carry out approximate tracking of all u and a variables. To accomplish this, the EnKF will fit unknown parameters in the homogeneous Wilson-Cowan network model.

The Kalman filter uses known linear dynamical equations and observation functions along with observed data to continuously update a Gaussian approximation for the state and its uncertainty. The EnKF accomplishes these goals in the case of nonlinear dynamical equations. At each integration step, system states that are consistent with the current state uncertainty, called sigma points, are chosen. The EnKF consists of integrating the system from the sigma points, estimating mean state values, and then updating the covariance matrix that approximates the state uncertainty. The Kalman gain matrix updates the new most likely state of the system. As pointed out in recent literature [11, 14] the ensemble

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Kalman filter can also be used to fit system parameters from data, introducing the unknown parameters as extra state variables with trivial dynamics. The EnKF with random initial conditions for the parameters will converge to the correct parameters, or in the case of slowly varying parameters, can track them along with the state variables. In recent work [19], we have shown the ability to track a parameter and spatiotemporal variables in homogeneous networks using EnKF in the presence of significant noise.
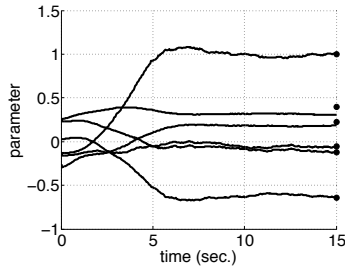

FIG. 1: The six parameters estimated by the EnKF converge over time to consensus values. The network's mean parameter values are denoted by closed circles. Here both the voltage and recovery variables u and a are observed.

In the application of the EnKF to an $N \times N$ network, the state is the dimension $2N^2 + m$ vector composed of the N^2 states u_{ij}, the N^2 states a_{ij}, and the m consensus parameters. The one-step dynamics is the time-T map of the Wilson-Cowan system for some fixed time step T, together with the identity function in the m parameters.

As a first example, we consider a weakly heterogeneous 16×16 network of Wilson-Cowan neurons, where the parameters c_{ijk} are set randomly around the means c_k, where $c_1 = -0.12, c_2 = -0.64, c_3 = 0.22, c_4 = 0.4, c_5 = 1$, and $c_6 = -0.056$. A 10% heterogeneity is used, meaning that for each $k = 1, \ldots, 6$, the 256 coefficients c_{ijk} across the network have standard deviation equal to 10% of the mean c_k. Most random choices of the parameters near these values support chaotic dynamics.

Fig. 1 shows the result of solving for consensus parameters by the EnKF for this network, when the noisy versions of both u_{ij} and a_{ij} are observed. The noise added is 0.4 standard deviations of the clean signal, or 40% noise. Starting from random values, the parameters evolve over 15 s to stable values that roughly approximate the mean values of the c_{ijk}. From the experimental point of view, this is an uninteresting case, since we would like to observe only one voltage u_{ij} at each grid point ij, and consider a_{ij} as a hidden variable to
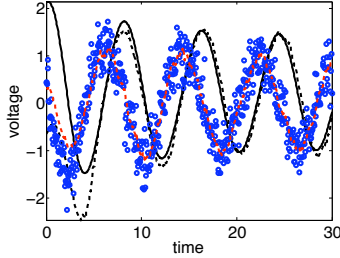
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FIG. 2: The noisy u_{ij} input data (blue points) and the output a_{ij} (black dashed line) from the consensus method at one of the grid points. The solid line is the actual value of a_{ij}, for comparison. The red dashed line is the filtered u_{ij} returned by EnKF.

be reconstructed. To carry out assimilation using only the observed voltages u_{ij} as input, we must address a hidden symmetry of the model (1).

Dual estimation calculations often call for special treatment, because of the interaction of unknown variables and unknown parameters in the model. We next illustrate this problem in the case of the Wilson-Cowan system, and show a general approach that can be applied to directly handle experimental data. Consider the task of determining $a(t)$ and $c_1, \ldots, c_6$ in (1) from the knowledge of $u(t)$ alone (we drop the ij subscripts for simplicity). Any experimental data u that is consistent with $a(t), c_1, c_2, c_3, c_4, c_5, c_6$ is consistent with $a(t)/\gamma, c_1, \gamma c_2, c_3, c_4, c_5/\gamma, c_6$ for arbitrary nonzero γ, meaning that the dual estimation problem is underdetermined. Application of the EnKF directly to this problem results in parameter drift along the manifold of consistent solutions.

To achieve data assimilation in this context, we must force γ to assume a unique value. For example, if c_5 is fixed in the EnKF to the same value as used in generating the input data, then $\gamma = 1$ is forced, and the EnKF will succeed in fitting the remaining 5 parameters. Fig. 2 shows the result of fixing $c_5 = 1$ within the EnKF in the consensus set context. The input data is the same as in Fig. 1 except that only u_{ij} (with added noise) is observed by the EnKF. The five remaining consensus parameters are approximated well, similarly to Fig. 1, in addition to the recovery variables a_{ij}. The variables at a typical ij grid point are shown in Fig. 2, verifying the ability of the method to successfully reconstruct a_{ij}.

In an experimental situation with poor prior knowledge of model dynamics, a correct value for c_5 is too much to assume. We repeat the exercise with a 10% heterogeneous network after changing the mean of parameter c_{ij5} to 0.5, leaving the other parameters as above.
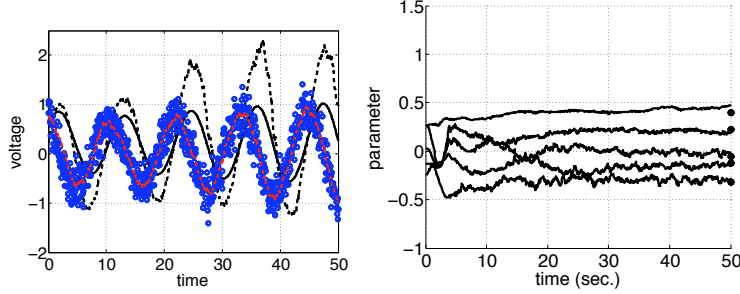
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FIG. 3: (a) The noisy u_{ij} data (blue circles) and the output a_{ij} from the consensus method (dashed line) at one of the grid points. The solid line is the actual value of a_{ij}. The reconstructed a_{ij} is magnified by $1/\gamma = 2$. (b) Consensus parameters from the EnKF. Compared with Fig. 1, c_2 has been replaced by $\gamma c_2 = -0.32$ (lowest trace).

Since the EnKF has c_5 fixed at one, when presented with the u data it will reconstruct the symmetry with $\gamma = 0.5$. As Fig. 3 shows, the result is the same output as in Fig. 2 except for a_{ij} replaced with $a_{ij}/\gamma = 2a_{ij}$, and c_2 replaced by $\gamma c_2 = -0.32$, as expected from the above reasoning. This demonstrates the ability of the consensus set method to reconstruct viable hidden variables together with unknown parameters even in cases of significant model mismatch.

Finally, we are prepared to apply the consensus set method to an experiment first described in [18]. Each element in the model will correspond to the volume of neural tissue imaged with a photodetector after the tissue was saturated with voltage sensitive dye and illuminated. The signal from each photodetector thus represents the local mean field of transmembrane voltage from the ensemble of cells imaged, and is analogous to u in (1). Inhibition was blocked (with bicuculline), and our modelling reflects the lack of synaptic inhibition (a is a recovery variable, reflecting phenomena such as inactivation of sodium channels and potassium membrane repolarization) [17].

A 10×10 grid of voltage-sensitive dye readings were observed as a multidimensional time series. With $c_5 = 3$ held fixed to avoid the symmetry, the consensus parameters converge (in a manner similar to Figs. 1 and 3) to $c_1 = -1.08, c_2 = -2.82, c_3 = 2.01, c_4 = -0.51, c_6 = -0.20$. Note that parameters c_3 and c_5 are positive, as anticipated in biologically reasonable models. Fig. 4 shows the recovery variable a_{ij} created by the EnKF that is sufficiently compatible with the observed signal u_{ij} to allow tracking.
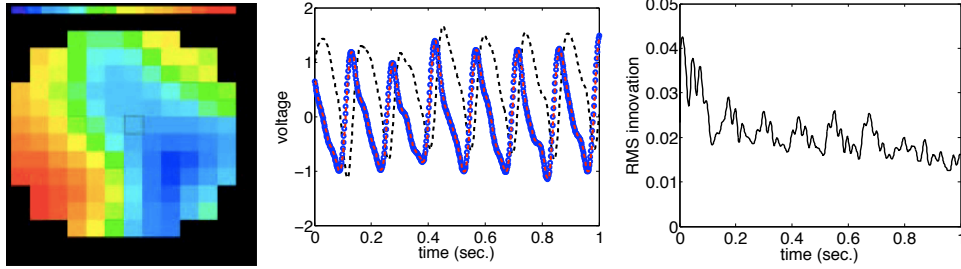
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FIG. 4: (a) Snapshot of the experimental optical intensities u_{ij} from the neural tissue. (b) The u_{ij} (blue trace), the filtered u_{ij} (red trace) and the output a_{ij} from the consensus method (dashed line) at one of the grid points. The reconstructed a_{ij} has no physical significance; it is created by the EnKF to reconstruct a compatible dynamical state in the homogeneous network model. (c) Decrease of the EnKF innovations show stability of the method's convergence.

In a larger sense, reconstructing equivalent dynamics may be more relevant and feasible goals than validating explicit model variables in situations where model inadequacy is severe [20]. Along similar lines, there has been recent work [21] emphasizing the role of dynamical synchronization over model fitting in data assimilation. The method outlined here can be used in conjunction with with localized versions of EnKF [22] designed to address system spatial complexity as well as exploit parallel computation.

We view the consensus set method as a crucial step on the path to the eventual goal of prediction and control of complex dynamical networks, in particular when the individual network nodes are heterogeneous, and in the presence of model uncertainty. Some replacement for parameter fitting is essential for robust data assimilation in the face of model error, and this method, while not completely eliminating the problem of model error, may be a near-optimal choice in such a scenario.

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