

# Utilizing hidden Markov processes as a new tool for experimental physics

Ido Kanter, Aviad Frydman and Asaf Ater

*Minerva center and the Department of Physics, Bar Ilan University, Ramat-Gan 52900, Israel*

A hidden Markov process is a well known concept in information theory and is used for a vast range of applications such as speech recognition and error correction. We bridge between two disciplines, experimental physics and advanced algorithms, and propose to use a physically oriented hidden Markov process as a new tool for analyzing experimental data. This tool enables one to extract valuable information on physical parameters of complex systems. We demonstrate the usefulness of this technique on low dimensional electronic systems which exhibit time dependent resistance noise. This method is expected to become a standard technique in experimental physics.

In a typical scenario of experimental physics, the experiment is designed to detect a desired set of physical parameters. The resultant physical data often consists of time-dependent measurements and includes time series data. It has been long recognized that stochastic and non-stochastic noise may provide important insight to the physics of the system and the processes responsible for the data [1].

The description of complex systems suffers from the limitations of both theoretical and experimental tools. On one hand, the many-body system in many cases is too complicated to be solved using existing analytical tools. On the other hand, the experimental results do not necessarily provide enough information to identify the sources and the amplitudes of the possible noises, and the physical interpretation of the outcome data stream is in question. Hence, the emergence of a new analysis of experimental physical data is of a great interest. We suggest a new technique for analyzing experimental physical data. The new tool is a physically oriented Baum-Welch (BW) algorithm [2] for the analysis of Hidden Markov Process (HMP). We bridge between two disciplines, experimental physics and advanced algorithms, to create a new way to study experimental findings.

A Markov model is a finite state machine that changes state once every time unit. The manner in which the state transitions occur is probabilistic and is governed by a state-transition matrix,  $M$ . If, in a Markov model, the state sequence that produced the observation sequence is not known deterministically, then the Markov process is called a HMP. Thus, HMPs are double embedded stochastic processes.

To exemplify a HMP in the realm of physical systems, let us assume that a snapshot is taken from a simulation of a 1D Ising model with nearest neighbor interactions and temperature  $T$ . The snapshot consists of a sequence of  $\pm 1$  elements. The observed snapshot is that of the pure Ising model simulation with additional random independently flipped spins from 1 to  $-1$  (from  $-1$  to 1) with a given probability  $f_+$  ( $f_-$ ). An observer knows only that the physical system is 1D Ising with nearest neighbor interactions, but he does not know the coupling strength,  $J$ , nor does he know  $f_{\pm}$ . Hence, it is very dif-

ficult to identify how many of the spin flips are due to a usual thermal fluctuations and how many are a result of other unknown processes. The observed sequence can be seen as a result of a HMP. The elements of the HMP include the following ingredients, where the numbers in the parenthesis stands for the above Ising case: the number of the states in the model  $q(2)$ , the Markov transition matrix  $M q \times q(2 \times 2)$ , the observation sequence transition distribution  $N q \times q(f_{\pm})$ , the initial state distribution of the first element  $\pi$  (a vector of rank  $q(2)$ ) and an observed sequence of length  $L$ . The aim of the BW algorithm is to accurately estimate  $M$ ,  $N$  and  $\pi$  from the observation of the sequence  $L$ . In our toy model, the 1D Ising system, the physical question is to estimate the coupling strength  $J$  and the flipping rate  $f_{\pm}$  from the observation of the distorted snapshot.

An attempt to solve the above problem in its direct way is computationally infeasible even for relatively small values of  $q$  and  $L$  (for instance, for  $q = 5$  and  $L = 100$ ,  $10^{72}$  operations are required to accurately estimate  $N$  and  $M[2]$ ). A more efficient procedure to solve this task is the BW algorithm which is based on forward-backward procedures for the estimation of the transition probabilities of the two stochastic processes [2]. The key point of the BW algorithm is a recursive calculation of the transition probabilities from the left/right direction of each element in the sequence. For each such element there are only finite number,  $q$ , possible states independent of the length of the sequence  $L$ .

This approach is different than the typical scenario of the study of physical systems which is based on the following chart flow: *System's Hamiltonian*  $\rightarrow$  *free energy*  $\rightarrow$  *macroscopic physical properties*. Here we suggest the *reversed paradigm*. We start from the experimental data and by utilizing the BW algorithm we try to reveal the relevant physical properties: *Experimental data*  $\rightarrow$  *algorithm*  $\rightarrow$  *relevant physical properties and processes*.

As a test case for the analysis we concentrate on mesoscopic (low-dimensional electronic) systems (for reviews see [1, 3, 4]). Many low dimensional systems are characterized by large time-dependent fluctuations of the electronic transport properties due to the fact that a relatively small number of conductance modes govern the

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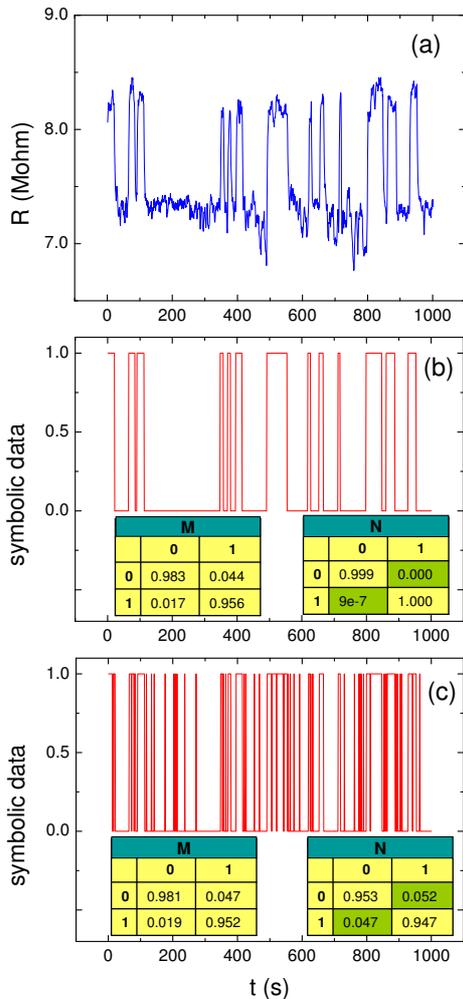


FIG. 1: Resistance as a function of time,  $R(t)$ , taken at  $T=4.2K$ , of a narrow  $InO_x$  strongly disordered wire prepared by step edge technique [5]. The wire dimensions are  $5\mu m$  long,  $50nm$  wide and  $30nm$  thickness. Panel (a) shows the real data and panel (b) shows the clipped symbolic sequence with the transition matrices of the BW analysis for the Markov (M) and the noise (N). Panel (c) depicts the symbolic sequence with artificially added 5% noise. Note that the relevant elements in matrix N detect this induced noise.

transport. A typical example is shown in Fig. 1a which depicts the time dependent resistance of a strongly disordered narrow wire. The conductance exhibits large time dependent variations which take the form of switching between different values. A natural interpretation of such data is the existence of two major conductance modes between which the conduction electrons switch due to thermal fluctuations (also known as a "telegraph noise"). In order to check this assumption we first generate a symbolic sequence that consists of two levels denoted as 0/1, by clipping the sequence around 7.8 (see Fig 1b). Next we run the BW procedure on the clipped sequence. The outcome of the BW algorithm consists of the following two transition matrices. The first one represents the tran-

sition probability due to the predicted Markov process between the current state of the sequence (0 or 1) and the proceeding one. Hence we end up with a  $2 \times 2$  matrix denoted by M, where  $M(i, j)$  stands for the transition probability from  $j$  to  $i$ . The second matrix stands for the frequency of unexpected transitions which are a result of a hidden process, known as the noise matrix, N. The two matrices are shown in Fig. 1b. The interpretation of the two matrices is as follows. The elements of the matrix M stand for known physical properties, in our case barrier heights and the degeneracy of the levels, while matrix N provides information about the unknown physical processes, which can be a result of external fields, thermal drifts, time dependent processes etc.

In Fig. 1b the off-diagonal (highlighted) elements of matrix N are practically zero, indicating that the sequence is generated by a simple Markov process. The pure Markov process, *without noise*, represents the fact that the main process behind these data results from a simple Two Level System (TLS), related to the two dominant conductance modes. The energy levels are denoted by  $E_0 = 0$  and  $E_1$ , and the barrier from  $1 \rightarrow 0$  ( $0 \rightarrow 1$ ) is denoted by  $\Delta$  ( $E_1 + \Delta$ ). The off-diagonal elements,  $M(1, 0)$  and  $M(0, 1)$ , are equal to  $\exp(-\beta(\Delta + E_1))$  and  $\exp(-\beta E_1)$ , respectively. From the values of these off-diagonal elements one can derive  $\Delta$  and  $E_1$ . In our case  $\Delta = 2.6meV$  and  $E_1 = 1.14meV$ .

In order to check the reliability of the analysis we introduce *artificial* random noise by flipping bits in the symbolic sequence from  $0 \rightarrow 1$  or from  $1 \rightarrow 0$  with probability  $f$ . The data of Fig. 1b with additional 5% of such noise and the two relevant matrices are presented in Fig. 1c. The results of the BW algorithm show that indeed the noise is revealed by the algorithm, while *the Markov matrix is only slightly affected*. We repeated this analysis for several data streams, some having much larger length, and obtained similar results. It is important to note that by eye-balling the data it is impossible to deduce that one of these symbolic data sets is generated by a simple Markov process while the other includes a hidden process. Moreover, it would be hard to guess that the origin of these two sequences is the same Markov process. This demonstrates the potential ability of the algorithm to provide better insight into the relevant physical processes governing the behavior of this many-body system.

Another example of the usefulness of the analysis procedure can be seen in Fig. 2. Here we show the data sequence of a metallic Ni wire. In this case the data appears to be much noisier than that of Fig. 1 and a physical interpretation based on a TLS scenario is less obvious. The experimentalist might regard this as useless physical data. The BW analysis, on the other hand, reveals that this sequence is also generated by a pure Markov process. The reason why this data might appear as random noise is due to the fact that in this case  $E_1 = 0meV$  and  $\Delta = 1.1meV$ . Hence, the barrier is less than a half of

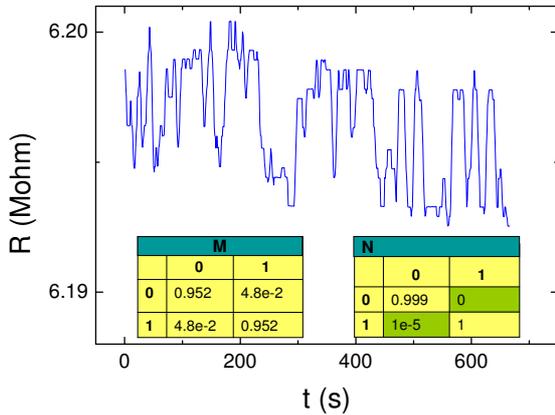


FIG. 2:  $R(t)$  at  $T=4.2K$  of a narrow Ni wire having dimensions of  $50\mu m$  by  $50nm$  by  $30nm$ . The data were clipped at 6.197, however, the resulting matrices were insensitive to the precise clipping value

that of Fig. 1, and the two levels are degenerate resulting in frequent transitions [6]. This example illustrates the ability of the procedure to extract physical meaning to experimental results which might appear worthless.

In the previous examples we did not deal with physical systems where a HMP was inherent to the system (practically zero off-diagonal elements of N). We now provide an example for such a scenario. Fig. 3 depicts the time dependent resistance of a dilute 2D granular Ni sample, while sweeping a magnetic field back and forth between 2 and -2 Tesla. Application of an external field on such samples causes sharp resistance changes at specific magnetic fields [8] which are superimposed on the usual time dependent resistance sequence. In the current sample these changes occur at fields of  $-0.255$ ,  $-0.86$ ,  $0.97$  and  $0.266 T$ . Though the origin of these switches is not fully understood they are very reproducible and do not originate from random telegraph noise. The noise matrix, N, obtained from the BW procedure, reveals considerable noise, illustrated by the ratios  $N(0,1)/M(0,1)$  and  $N(1,0)/M(1,0)$  which can exceed 0.2. This means that a non-negligible fraction of the transitions does not arise from a simple Markovian process (TLS). We note that in the absence of a magnetic field, the measured data generates Markov matrices with practically zero noise [9]. Similar results were obtained when allowing samples, that generate pure Markov matrices, to drift in temperature from  $4K$  to  $300K$ . Clearly, the procedure is able to detect non-Markovian perturbations to the physical systems.

The above examples illustrate the existence of three different regimes, characterized by the typical ratio,  $R$ , between the off-diagonal elements of N and M  $\{N(i,j)/M(i,j)\}$  [10]. In the first regime,  $R$  is practically zero as exemplified in Fig. 1b. In this case the physical generator of the sequence is well defined. In the second regime (as in Fig. 3)  $R$  is smaller than 1 but

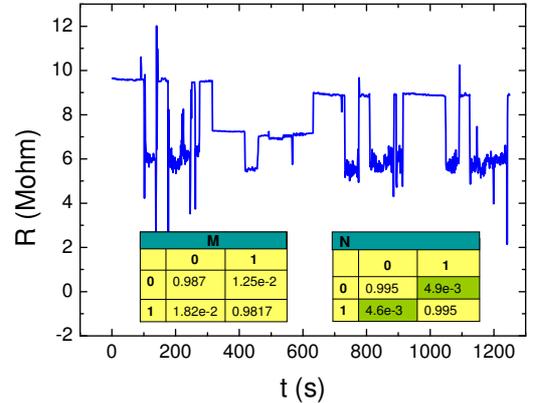


FIG. 3: Resistance as a function of time of a granular Ni film on the verge of electric percolation prepared by quench condensation [7]. The geometry of the sample is a monolayer of grains with lateral dimensions of  $200nm * 200nm$  and the average grain size is  $10nm$ . The measurements were performed while sweeping a magnetic field back and forth between  $H = 2T$  and  $H = -2T$ . The data was clipped at 7.9.

finite. The conclusion should be that the sequence is generated by a well defined Markov process, however, some unknown processes are present and slightly influence the data. In the third regime  $R \sim 1$  (as in Fig. 1c). This should be taken as a red alert for the experimentalist indicating that the assumption that the data is generated from a simple process is problematic, since most of the information is an outcome of unknown physical processes.

In the above examples we demonstrated the effectiveness of the analysis of HMPs in interpreting experimental data for a number of simple mesoscopic systems. This idea can be extended to much broader fields of application, hence we turn to a more general discussion of the basic concepts of this bridging.

Looking more carefully at Fig. 3 one might ask himself whether it would not be more appropriate to treat the data as being a result of 3 levels or perhaps even more, in which case the physical interpretation of the experimental data would change. This leads to a more general question of how to map the experimental data to a symbolic sequence. The main two issues are the following: (a) What is the most appropriate vocabulary size to describe the system, i.e. to how many levels should one clip the data? (b) For a given vocabulary size, what are the preferred clipping thresholds? Let us first exemplify this issue by studying the data of Fig. 1a. Assume that the vocabulary size is two (consisting of 0/1) and let us clip the data at 9 or 6. It is clear that the clipped sequence consists of only zeros or only ones, respectively. Such a sequence does not provide any insight about the physical processes (see green boxes in Fig. 4). The obvious reaction of an experimentalist to such an analysis is that this unintelligent clipping suppresses all important changes in the data. This is indeed the answer of information theory, since the information stored in the clipped data is zero. Hence the threshold should be chosen between the two

levels. Practically, we suggest to use one of the known clustering methods to fit the data to two Gaussians (or, for a general case, a distribution function for each level) representing the energy levels (centers and broadening) [11]. The clipping is thus determined by assigning each data point to the most probable Gaussian source.

Choosing the appropriate vocabulary size is less trivial. If prior physical knowledge exists, it should be used to select the correct number of levels. If such prior knowledge is not available one has to select the vocabulary size that would maximize the total entropy of the HMP,  $S_{HMP}(M, N)$  [12]. One can convince himself that such a maximum exists by regarding the following limiting cases. Consider again the data of Fig. 1a and let us clip the data to an infinite number of levels (practically,  $L$  levels as the number of data points). In such a limiting scenario, the Markov transition matrix consists of a single one in each column and zeros elsewhere. This analysis is useless since each point represents a switch, and the important physical switches are not visible. More precisely, the entropy of the generated sequence from the Markov process is zero, and represents only the sequence itself. Also choosing only one symbolic level results in zero entropy. Hence, it can be expected that there is an intermediate vocabulary size which maximizes the entropy, while providing a stationary solution for the HMP. For instance, a similar HMP solution should be obtained for the first/last half of the sequence. Note that it is probable that the entropy has a number of maxima or even a plateau rather than a unique maximal value. For instance, in the data of Fig. 1a one can easily convince himself that choosing three or four levels (and the appropriate thresholds between 7.3 and 8) results in a similar entropy value, since the additional levels are redundant. Practically, for finite sequences and the experimental errors one has to define a sensible tolerance for the entropy and a plateau is naturally obtained. In such a case it makes sense to choose the minimal number of level within the plateau of maximal entropy.

The complete suggested scheme of the data analysis is thus the following: Acquire the data sequence and assume a logical number of levels. Determine the clipping thresholds by clustering the data. Then, apply the BW procedure on the clipped sequence, obtain the relevant matrices and estimate the entropy of the HMP,  $S_{HMP}(M, N)$ . Repeat this procedure for different vocabulary sizes and choose the vocabulary size that generates the maximal Hidden Markov entropy provided that it represents a stationary solution. The general prescription of the analysis procedure is illustrated in Fig. 4.

Finally we note that the usefulness of the above-mentioned procedure can be generalized to more complex physical systems and in particular, systems with more than two levels and different sources for generating switches which manifest themselves as HMPs. Such an analysis would require a more comprehensive com-

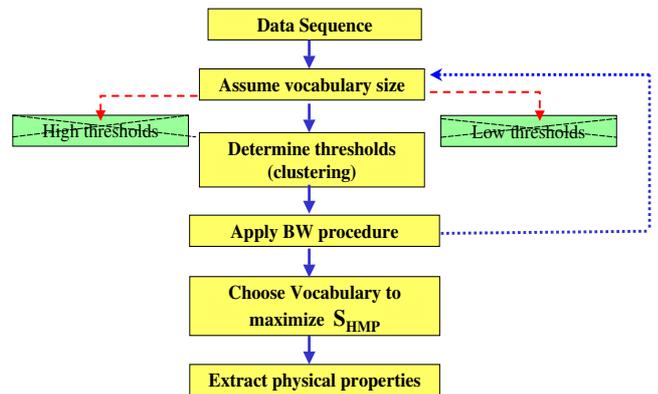


FIG. 4: A schematic diagram of the analysis process.

putational algorithm in order to optimize the physical requirements taking into account careful choice of thresholds and vocabulary sizes. This tool can be applied to other physical phenomena, such as shot-noise, radioactive decay, fluctuations in optic emission experiments etc, and is expected to become a standard technique in experimental physics.

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  - [9] Furthermore, applying the BW procedure on sequences with similar  $L$ , generated from the Markov matrix,  $M$ , always reveals practically zero noise.
  - [10] In cases where the ratio between off-diagonal elements of matrices  $M$  and  $N$ , significantly varies, one can define  $R$  as the ratio between the entropy of the Markov process,  $-\sum_j P_j \sum_i M(i, j) \log(M(i, j))$ , and the entropy of the noise,  $-\sum_j P_j \sum_i N(i, j) \log(N(i, j))$ , where  $\{P_i\}$  is the stationary solution of the Markov process.
  - [11] For simple examples see R.O. Duda and P.E. Hart, *Pattern Classification and Scene Analysis* (Wiley, NY, 1992).
  - [12] One can calculate the upper and the lower bounds for  $S_{HMP}$ , for any finite size segment of a sequence, see for instance, T.M. Cover and J.A. Thomas, *Elements of Information Theory* (Wiley, NY, 1991).