Protein Structured Reservoir computing for Spike-based Pattern Recognition

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Abstract—Nowadays we witness a miniaturisation trend in the semiconductor industry backed up by groundbreaking discoveries and designs in nanoscale characterisation and fabrication. To facilitate the trend and produce ever smaller, faster and cheaper computing devices, the size of nanoelectronic devices is now reaching the scale of atoms or molecules — a technical goal undoubtedly demanding for novel devices. Following the trend we explore an unconventional route of implementing a reservoir computing on a single protein molecule and introduce neuromorphic connectivity with a small-world networking property. We have chosen Izhikevich spiking neurons as elementary processors, corresponding to the atoms of verotoxin protein, and its molecule as a ‘hardware’ architecture of the communication networks connecting the processors. We apply on a single readout layer various training methods in a supervised fashion to investigate whether the molecular structured Reservoir Computing (RC) system is capable to deal with machine learning benchmarks. We start with the Remote Supervised Method, based on Spike-Timing-Dependent-Plasticity, and carry on with linear regression and scaled conjugate gradient back-propagation training methods. The RC network is evaluated as a proof-of-concept on the handwritten digit images from the MNIST dataset and demonstrates acceptable classification accuracy in comparison with other similar approaches.

Index Terms—Molecular networks, Reservoir Computing, Liquid State Machine, Izhikevich Model, Remote Supervised Learning, Pattern Recognition.

I. INTRODUCTION

The end of Moore’s law indicates inability of CMOS technology to easily overcome the nanoscale dimensions due to quantum phenomena and, hence, the scaling of conventional transistors beyond gate lengths of 3 nm becomes almost unfeasible. Evolutionary prospects explored in computer science and information technology by imitating the functionality of mechanisms by which biological organisms process information might help us to deal with the scaling problem. The steadily growing disciplines that mainly contribute to the future of technology are Nanotechnology and Machine Learning. In particular, nanotechnology deals mostly with beyond Moore’s law issues proposing tentative solutions, while the field of neuromorphic computing augments the classical computing principles by information processing in a sense of being currently comparable in neuromorphic behaviour to biological neural networks and a relatively recent alternative approach called Reservoir Computing (RC) can be implemented on generic evolved or found Recurrent Neural Networks. More specifically, RC systems are based on the principles of high-dimensional dynamical systems whose behaviour is interpreted as computation and are particularly suited for time varying and multidimensional signal classifications. RC systems are designed in such a way that could transform a set of spike trains or sensory inputs into a spatiotemporal representation where structural feedbacks give rise to temporal memory states in the dynamics of the RC. That collective RC state can be recognised by the readout layer of neurons which can learn to extract (in real time) its current state and past inputs. The key principle of RC systems is that its internal connectivity is kept fixed and the training process occurs only in the readout layer. This strategic design, by maintaining their internal circuitry, overcomes previous implementations of SNNs, due to the SNNs’ lack of simple and efficient machine learning algorithms, and offers a practical training process.

In order to utilise this kind of recursive systems, RC-based approaches traditionally are implemented by creating/generating complex dynamical networks with typically randomised internal network topologies that are capable of creating various spatiotemporal states by which reservoirs store information from past inputs and produce responses which results from the reservoirs “memory” and present inputs. We propose an alternative approach of utilising bio-inspired networks and more specifically molecular assemblies so as to avoid the randomly generated networks that are made with a complex procedures, which sometimes take a long time to be executed and produce acceptable network properties. In this manner, this work attempts to use a real single molecular structure to create the internal connectivity of the RC system paving in a sense the way for alternative usage of real molecules for unconventional computing.

Molecules are nanomaterials fabricated by nature which have several desirable features as molecular networks describing their sub-nanometer scale, their hierarchical structure and smallworld character by their sparse star connectivity. They can also be considered as self-organising networks due to their property of molecular plasticity, as long as their structure is able to be reshaped and to be folded depending on the applied conditions in real-time, as well as the ability to handle molecular dynamics through chemical and spectroscopy mechanisms makes molecules one

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of the most promising novel substrates for physical Reservoir computing [18]. Their small-world character is based on their degree distribution which seems to follow the Poissonian distribution [19], [20], i.e. macro-molecular assemblies have a much smaller number of hubs than the most of self-organised networks. The explanation for this deviation from the scale-free degree distribution lies in the limited restriction to simultaneous binding while atoms may give up their bonds and bind to different local atoms during protein-folding and increasing the small-worldliness while the protein structure becomes progressively compact [17].

This allows us to introduce in this study two kinds of connectivity, the hard and the soft one which are determined by the macro-molecular bonding structure and the local 3D structure accordingly. In this way, we overcome the zero-clustering of the star connectivity consisting of the bonding structure and we provide an enhanced small world effect by scaling up the clustering mean coefficient due to local 3D interactions. Soft connectivity is described by a distance factor which allows the atom to interact with its local surroundings in 3D Euclidean space and it takes values in the scale of Angstrom (Å). The major reason for engaging with soft connectivity is the fact that some attributes of small-world networks are shared on cortical networks [21] which are significantly more clustered but have approximately the same characteristic path length in comparison with random networks [22] which are widely used in Reservoir computing in order to produce its internal recurrent topology as mentioned before [15], [18].

We demonstrate the structure of cell-binding B oligomer of Verotoxin1 molecule (VT-1) produced using X-ray diffraction intensities, with resolution 2.05Å, obtained from E.coli [23] and shown in Fig. 1. We used this molecular conformation as its been also demonstrated as an example with an excitable automata model as well to as to preserve portability with our previous results in terms of Boolean gates realisation via interacting patterns of excitation which shown that higher-dimensional transformations can be illustrated [24].

We propose a novel approach by utilising already existing bio-inspired topologies, in particular molecular conformations, as opposed to randomly generated recurrent artificial topologies and we perform Reservoir Computing on a single molecule introducing the soft connectivity configuration that enables neuromorphic connectivity as it has a significant number of recurrent loops and presents a variety of spatio-temporal states. Non-linear dynamics and high-dimensionality is realised by introducing the Izhikevich neuromorphic model for the spiking neurons considered as elementary neuron-processors and corresponds to the atoms of VT-1 molecule, while their neuromorphic communication relies on the architecture based on both its hard molecular connectivity that is described by its chemical bonds and soft molecular connectivity described by its spatial local arrangement of atoms in euclidean space. We propose an unconventional reservoir computing approach by using this molecular conformation and utilizing its high-dimensional dynamics through the evaluation of a proposed STDP-based (Spike-timing-dependent-plasticity) pattern recognition training algorithm in a supervised fashion on a single output layer of spiking neurons, which is found mainly in echo state networks and not in liquid state machines we use here, in order to investigate its neuromorphic computing potential of dealing with well-known machine learning benchmarks such as solving the MNIST problem.

We describe our approach during the RC setup as well as the calibration of the fine-tuned model parameters took place during the training phase along with the evaluation phase of RC in terms of the MNIST problem. Finally, we discuss our remarks and contributions as we compare it to other similar Reservoir Computing approaches and we give some suggestions for future works.

II. PROPOSED MODEL

VT-1 is a pentamer protein of sixty-nine amino acids for each monomer and is thoroughly studied through its conversion to a non-directed graph whose vertices correspond to the atoms of the molecule and edges correspond to chemical bonds. In this study, the molecular hard connectivity represented by the graph’s topology which has a set of 2,992 nodes and a set of 2,831 edges, respectively. Figure 1 illustrates the molecular hard connectivity of the VT-1 macro-molecule, and the Fig. 3 indicates the sparseness of the hard connectivity (red diagonal area) as long as the degree distribution is limited while the maximum degree observed is four for a few atoms as shown in Fig. 2 (blue distribution).

On the other hand, when we introduce the soft connectivity we get some attractive features like the increased fractal-like connectivity density shown in Fig. 3 (blue area) as well as the right-shifted degree distribution that becomes increasingly evident as Poissonian distribution as the Fig. 2 (orange distribution) indicates. Along with that, the most
intriguing properties of soft connectivity are associated with the clustering coefficient and the average path length of the network. In the case of hard connectivity, it is well-known that proteins are a single chain of amino acids which corresponds to star connectivity due to their bonding structure and have zero-clustering. In contrast, when we include soft connectivity, we notice that we have high clustering as shown in Fig. 4, which represents the local clustering coefficient distribution, and in particular, the average clustering coefficient of the network is $C = 0.69$ and the average path length decrease to $L = 1.88$ which is evident for small-world effect as the inner atoms have more clustering effect in contrast with the outer atoms of the molecule. In this way, we utilise the VT-1 molecular structure integrating on each atom a neuromorphic behaviour. Compared with the SNN approach, which is a general paradigm used in modelling biological neural networks for machine learning purposes, RC are a not-so-general-paradigm; in the latter, the goal is to understand how to ensemble neurons process information. Nevertheless, in both cases, many different neuron models can be considered, in which the information is encoded in temporal distance between the consecutive action potentials. In literature, various neuromorphic behaviours are modelled at different levels of abstraction, ranging from the most biologically realistic Hodgkin-Huxley (HH) model to the simplest and most computationally efficient Leaky Integrate-and-Fire (LIF) model. In our case, we use the Izhikevich neuron model [25], [26] since it offers a good compromise between a biological accuracy and the computational efficiency, as well as it manages to produce several kinds of spike and burst patterns observed in biological neurons by the proper choice of only four variables [27].

The Izhikevich model is described by the following two-dimensional system of differential equations

\[
\begin{align*}
\dot{v}(t) &= 0.04v^2(t) + 5v(t) + 140 - u(t) + I(t) \\
\dot{u}(t) &= a(bv(t) - u(t))
\end{align*}
\]

with after spike resetting

\[
if \quad v(t) \geq 30mV \quad \left\{ \begin{array}{l}
v(t) \rightarrow c \\
u(t) \rightarrow u(t) + d
\end{array} \right.
\]

where $v$ is the membrane potential, $u$ is a recovery variable that contains the dynamics of ions-channels, $I$ represents current stimulation of the neuron and $a$, $b$, $c$ and $d$ are dimensionless.
parameters. Regarding the reset phase, if the membrane potential reaches the firing threshold, then the neuron generates a spike which affects only the adjacent neurons. The variable \( t \) refers to the simulation time that is distinguished in 1 ms. The variable \( s_{i,j} \) denotes the synaptic weight, between the post-synaptic neuron \( i \) and the pre-synaptic neuron \( j \), that varies within the range of \((0,1)\) and creates a specific spike which is multiplied by the \( I_n \), current amplitude to give the appropriate interconnection current value of the order of \( p A \).

This equation represents the sum up of the synapses of the presynaptic neurons that fired together with the addition of an external excitation current \( I_{in}(t) \) to neuron \( i \).

The RC approach can be divided into three parts, the input interface \( W_{in} \), the RC network \( W \) and the readout interface \( W_{out} \) as depicted in Fig. [6]. The input interface concerns the transformation of the input stimulation to time-varying input spike trains or continuous current inputs that can be encoded into spike trains that afterwards excite the RC system. Next, the RC system consists of a 3D structured locally connected network of spiking neurons and is usually randomly created using biologically inspired parameters. In this study we use the molecular connectivity as the RC network and the responses from all neurons are projected to the next output layer where the actual training is performed through supervised learning algorithms to recognise instantaneous spike-based spatio-temporal patterns within the RC.

Figure [5] illustrates the neuromorphic activity of the 28×28 input layer in terms of the membrane potential reflecting on a random input image for an interval of five time-steps of 1 ms each and Fig. [5] shows the response of the molecular-based RC network in terms of the membrane accordingly. We notice that action potentials of the input layer affect significantly the neuromorphic activity on the RC layer at the next time-step.

In the view of avoiding chaotic network dynamics, we introduce two kinds of neurons, with different type of spiking behaviour, the excitatory and inhibitory neurons [29] in the a ratio of excitatory to inhibitory neurons 4:1 as in the mammalian cortex [30]. Assignment of neurons to excitatory or inhibitory types was done in various ways such as to select only oxygen and hydrogen atoms as inhibitory neurons which are about 26% among all atoms of the VT-1 molecule or to randomly select atoms as inhibitory neurons while preserving the ratio 4:1.

The corresponding fitting parameters for both types of neurons have been assigned the values listed in Tab. [I]. For the purpose of avoiding network synchronization each neuron has its own \( a \), \( b \), \( c \) and \( d \) parameters that describe unique neural dynamics.

For the readout mechanism training, we adopted spike-timing-dependent plasticity (STDP) which indicates that if a pre-synaptic neuron \( n_k^{in}(i) \) always fires just before the post-synaptic neuron \( n_j^{o}(i) \) fires suggest that the firings are correlated, then the synaptic weight between them should be increased; otherwise, if a pre-synaptic neuron \( n_k^{in}(i) \) fires just after the post-synaptic neuron \( n_j^{o}(i) \) then the weight should be decreased. The weight adjustment depends on the firing times of the pre- and post-synaptic neurons accordingly [31]. One of the most widely used STDP-based training algorithms, which adapts synaptic weights according to the mechanisms of STDP and anti-STDP is the Remote Supervision Method (ReSuMe) [32], [33].

Two key features of ReSuMe learning are employed: the Remote Supervision and the Learning Window. The remote supervision concerns the usage of a remote “teacher” neuron for each output neuron, or more precisely the use of remote firing times. Regarding this, the synaptic weights depend, not only on the correlation between the firing times of neurons \( n_k^{in}(i) \) and \( n_j^{o}(i) \), but also on the correlation of firing times of neuron \( n_k^{in}(i) \) and remote neuron \( n_j^{d}(i) \). The function called the leaning window determines the correlation between the firings and thus the synaptic weight adjustment.

The ReSuMe learning is executed by the following cost function derivative

$$
\frac{dW_{kl}(t)}{dt} = \eta \left[ S_d(t) - S_{\tau}(t) \right] \left[ 1 + \int_0^{\infty} W(s) S_{in}(t-s) ds \right]
$$

where \( S_d(t), S_{in}(t) \) and \( S_{\tau}(t) \) are the precise desired pre- and post-synaptic spike trains, respectively, the constant \( \eta \) represents the non-Hebbian contribution to the weight changes and the learning rate, while function \( W(s) \) of a time delay \( s = t - t_{in}^{ired} \) between the correlated spikes is known as a learning window. The shapes of \( W(s) \) applied in ReSuMe are similar to the ones used in STDP models and can be represented by the following equation. In this way, over time ReSuMe Learning aims to get the desired and the output spike trains even closer to each other, i.e. to have a simultaneous firings.

$$
W(s) = \begin{cases} 
+ A_+ \cdot e^{-s/\tau_+} & \text{if } s \geq 0 \\
- A_- \cdot e^{s/\tau_-} & \text{if } s < 0
\end{cases}
$$

with amplitudes \( A_+, A_- \geq 0 \) and time constants \( \tau_+, \tau_- > 0 \) of the positive and negative parts of the learning window, respectively [34].

Besides that, multiple linear regression algorithm was used also to train the readout layer for the pattern recognition task as discussed earlier. Concerning the training, in order to utilize the spike-based information the RC system generates, we managed to convert the spikes into a RC state vector \( X \) which represents the whole spiking activity of each neuron to keep the spatio-temporal spiking activity of the RC system and to implement the linear regression training. The RC state vector \( X \) is applied to the readout layer which has sigmoid
Fig. 5. Spatio-temporal representation of the neuromorphic activity in terms of membrane potential (mV) (a) from the $28 \times 28$ Input Layer grid through external stimulation of a random $28 \times 28$ image from the MNIST dataset down-scaled on the range of $(0, 1)$ and (b) from the VT-1 molecular-based RC response over 5 time-steps, 1 ms each, from the Input Layer action potentials.

Fig. 6. Reservoir Computing Model. Adapted from [28].

The readout layer is trained using gradient descent, as described below, in order to minimise the cost function.

Beyond this, we also trained the readout mechanism in Matlab 2018b using Scaled conjugate gradient back-propagation (trainscg) and hence the readout mechanism is not only a layer of ten classifiers but it has hidden neurons.

III. RESULTS

To perform image classification driven by the MNIST handwritten images dataset ReSuMe learning framework is implemented in the molecular-based RC architecture, which is emulated as a Spiking Neural Network and integrated by the appropriately fine-tuned neuromorphic model of Izhikevich. As assumed earlier, the model can produce many spike-based patterns depending on the input by modifying the model parameters. In our case, we aim to reduce the training complexity and in particular to cause the firing of neurons in the shortest possible time interval. Thus, we could provide a rich neuromorphic activity to proceed to readout layer training accordingly in a short period of time. In this fashion, a regular neuromorphic behaviour with the parameters shown in Tab. I for excitatory and inhibitory neurons, which describes different neuromorphic activities, is considered to avoid a chaotic RC activity.

The RC system except the recurrent structure also consists of a single output classifier layer with spiking neurons which have also been integrated by the neuromorphic model of Izhikevich. Since the RC is driven by the handwritten digits from the MNIST dataset, ten spiking readout neurons (labelled 0-9) represents the classified digit value of the input image, schematically illustrated in Fig. 8. This dataset consists of thousands of handwritten images which have $28 \times 28$ pixels in grayscale. To feed the input layer with those current inputs, pixels have been normalised and scaled up to $(0, 1)$ range. The input layer consists of 784 Izhikevich neurons encodes the
Fig. 7. Average confusion matrix of the testing results presenting the obtained classification responses vs. the desired responses over ten presentations of the 10,000 MNIST test dataset. High values on the diagonal indicates correct estimation while at any other point indicates confusion between two digits. (a) STDP approach; (b) Simple Regression approach; (c) Scaled conjugate gradient back-propagation approach using Neural network training toolbox of Matlab 2018b.

Fig. 8. Schematic representation of the raster diagrams of the Input layer consisting of 784 neurons, the RC network consisting of 2922 neurons and the Output layer consisting of 10 classifier neurons observed during a time interval of 200ms after the stimulation of 20 handwritten images from the MNIST dataset for 10 ms learning window each after performing the Resume learning algorithm current input into spike trains that pass through the RC. Fig. 8 illustrates different kinds of spike-based patterns reflecting on each input image stimulating them for a time interval of 10 ms which is called the learning window. The raster diagram represents the exact spike timings of the input layer, the RC network and the output layer response for each image after the training phase for 20 images.

At an early stage, no input layer was used and various neuromorphic settings and input interfaces for the RC system were tested. More specifically, the RC was fed with the pixels of the image in the form of current inputs however due to the size of the RC the entire network could not be fed from the input image and so only 784 nodes stimulated with the input current. Many input interface connection were performed, from the first or the last 784 node sequence of the molecule up to random 784 nodes; however, it was observed that there was no apatio-temporal transformation of the input, i.e. the output was highly correlated with the input, which resulted in fairly low training performance and was rejected. Hence a random input interface to the RC network was used where each neuron received spike-trains from the input layer.

In this case, disordered dynamical behaviour was observed from the RC so the readout layer could not be trained. Consequently, we introduce two kinds of neurons, with a different type of spiking behaviour, the excitatory and inhibitory neurons. In the meantime, although attempts to find the appropriate learning window for each case were made, we kept it low (a few ms) in order to minimize the abrupt dynamical behaviour of the RC which causes divergence on the training performance for long-time learning window.
periods. In this manner, the spike-based readout layer has been trained in a supervised fashion through ReSuMe learning where the synaptic weights are adjusted to minimize the time intervals between the remote and the output spike trains during training where the remote spikes are considered at the end of the learning windows. This means that the ReSuMe learning adjusts the synaptic weights so as to cause the specific output neuron to fire once on the exact timing considered the remote neuron to fire.

For the MNIST recognition task, we have trained the proposed molecular-based RC system with a training dataset consisting of 40,000 handwritten images and evaluate it with 10,000 images testing dataset and we have managed to achieve a satisfactory testing performance of 85.16% through the spike-oriented learning framework called ReSuMe learning.

Beyond that, a multiple linear regression algorithm was used also to train the readout layer for the MNIST recognition task by utilising the Spatio-temporal neuromorphic dynamics the RC system produces and use an RC state vector which consists of the total firings each neuron carried out. In this manner, by using the multiple linear regression a testing performance of 96.83% was achieved. On the other hand, using once again the same RC state vector and applying through the Matlab’s toolbox the scaled conjugate gradient back-propagation we achieved a 98.66% testing accuracy on the handwritten digit images from the MNIST dataset.

IV. CONCLUSIONS AND DISCUSSION

We evaluated a computing potential of a neuromorphic network with architecture based on Verotoxin molecule by using a RC computing approach. This novel approach hybridises computing on a single molecule and classification using neuromorphic models. We demonstrated an unconventional approach by assuming that each atom of a molecule is a neuron and atomic bonds symbolise the synaptic weights between neighbouring neurons. Each neuron produces action potentials by the simple neuron model of Izhikevich and affects both its neighbouring neurons and the output layer. The output layer is trained by various training methods starting with the STDP-based ReSuMe training method, carrying on with the multiple linear regression and at last with the scaled conjugate gradient back-propagation. Despite the fact that we performed the training on a single readout layer we managed to evaluate our proposed network and got a sufficient degree of accuracy.

Despite recent progress of deep SNN on typical benchmarks such as MNIST or CIFAR, there are no similar Reservoir Computing approaches, which are so restricted to the number of synaptic weights, have not reached yet state-of-the-art performances. Said that we proposed a novel approach which uses molecular-based RC network and only a single spike-based readout layer which limits considerably the number of synapses trained and consequently the performance of the proposed RC system. Last but not least, the evidence that we strive to achieve performance on an incompatible dataset, we consider the most stressful case and yet the corresponding results are acceptable.

The small-world effect with the high-clustering attribute of molecular connections classifies them as promising neuromorphic topologies for bio-inspired networks to implement high-dimensional transformations in neuromorphic computing architectures such as RC frameworks. Regarding the bio-inspired molecular ability to alter under different conditions they’re imposed, could lead us to exploit their modification mechanisms or even to utilise the prospect of folding which could occur in real-time and investigate further the utilisation of such single-molecule systems.

As we take inspiration from nature, another promising research field that could potentially be utilized, under the investigation of the mechanisms that underlie the oscillatory behavior of atoms, is the imitation of molecular oscillations using neuromorphic models. This could lead us to other directions like implementing molecular networks for simple or complex digital functionality through oscillatory activity or neuromorphic synchronisation. Regarding simple electronic devices, simple Boolean gates are the best candidates to be illustrated and eventually create other complex electronic circuits.

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