

Recent advances in efficient learning of recurrent networks

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Abstract. Recurrent neural networks (RNNs) carry the promise of implementing efficient and biologically plausible signal processing. They both are optimally suited for a wide area of applications when dealing with spatiotemporal data or causalities and provide explanation of cognitive phenomena of the human brain. Recently, a few new fundamental paradigms connected to RNNs have been developed which allow insights into their potential for information processing. They also pave the way towards new efficient training algorithms which overcome the well-known problem of long-term dependencies. This tutorial gives an overview of this recent developments in efficient, biologically plausible recurrent information processing.

1 Introduction

Recurrent neural networks (RNNs), in particular Hopfield networks, were among the models which led to a renaissance of neural network research in the 90th after the rapid decrease of interest in neural network research caused by the exact mathematical proof of the limitations of the simple perceptron and extensions thereof by Minsky and Papert in the 70th. Convincing properties of the Hopfield model include biological plausibility as associative memory, exact mathematical treatment of the capacities and dynamics in terms of an underlying cost function and associated stable states, and the possibility to apply the model to classical problems, such as the traveling salesperson problem.

Since then, a variety of very different recurrent neural networks with different dynamics and application areas has emerged. The models include partially recurrent systems such as discrete and continuous time models for time series prediction, simulation of dynamical systems, and processing of language. Fully recurrent models such as Boltzmann machines and associative memories, models involving only local or restricted recurrence such as long short term memory networks or locally recurrent, globally feedforward networks, recurrent models which resemble classical filters, or recurrent systems aimed for an explanation of biological recurrent networks such as the neocortex have also been developed.

When investigating these models, the key issues remain widely the same: the biological plausibility of recurrent systems and their connected dynamic phenomena, the exact mathematical characterization of the network dynamics, and applicability to relevant problems. While the mathematical treatment of recurrent networks of various form has reached a matured state in some respects, the applicability to classical problems and training of recurrent networks still faces severe problems. Practitioners therefore often prefer a simple feedforward modeling over the in theory much more powerful recurrent treatment of problems involving temporal or spatial dependencies.

We will argue in this overview that new developments in the context of recurrent models, in particular a matured characterization of stability of recurrent systems, new biologically plausible training modes, and network models such as reservoir computing have lead to a state of the art where these problems may be overcome.

2 Applications

One of the most general formulations of the dynamics of recurrent networks is given by the simple formula

$$y(t+1) = f(x(t), y(t), o(t)), \quad o(t+1) = g(y(t))$$

in discrete time or

$$\dot{y} \sim f(x, y, o), \quad \dot{o} \sim g(y)$$

in continuous time with inputs x , hidden states y , outputs o , and nonlinear activation functions f and g . These formulas can be used to model different dynamics: on the one hand the most common usage of RNNs is short or long term prediction of time series, when only a fixed time horizon is predicted based on given inputs and an initial state. On the other hand, they model also approximation of global fixed points when the system is driven up to convergence based on a given initial state or, more generally, generation of patterns when the system is driven towards an autonomously generated periodic, quasi-periodic, or more complex (possibly chaotic) attractor.

Correspondingly, recent applications of recurrent networks can be found in a variety of different areas. One of the classical application scenarios of RNNs is the prediction of time series and classification of temporal patterns [16, 47] such as the prediction of the stock market [68], of electricity load [10], the modeling of natural phenomena such as sandbars or wind speed [100, 6, 5], the classification of birdsongs [59], speech or speaker recognition [60, 34], event detection in robotics [2], or the modeling of speech and grammar [18, 32]. When a RNN is put into a loop with the system nonlinear control can be achieved. This is one of the most popular application areas of RNNs, accompanied by a vast literature concerning control designs which fulfill certain important properties such as stability or optimality [83, 76, 104, 46, 155, 130, 128]. Applications in this context reach from the control of industrial and technical systems [110, 104, 62] up to robotics [154, 53]. When referring to stable states of RNNs or their long term dynamics in the form of associative memories, RNNs can be used to solve complex dynamic tasks such as classical problems including the traveling salesperson problem [134, 125], Boolean factor analysis [33], or object segmentation in images [90, 144]. Further, RNNs can be used to directly model biological counterparts such as biological networks; successful inference of gene regulatory networks by means of RNNs has been presented e.g. in [70, 149].

3 Cost function optimization

The original Hopfield network uses the RNN dynamics to retrieve stable states associated to initial conditions of a given network the their respective basins of attraction. One of the achievements of Hopfield was the explicit formulation of a corresponding cost function which is optimized by the network dynamics. This

principle lies behind a variety of general design rules of RNNs to solve complex dynamical tasks. One of the early applications which are still investigated is given by solutions for the traveling salesperson problem [134, 125]. More general approaches design RNNs to solve general linear or quadratic optimization problems [50, 4, 23, 79, 80, 82] possibly with constraints [36, 146] which can be used e.g. for the distributed training of support vector machines [105]. Counterparts in continuous space concern various variational problems (linear/nonlinear, possibly with constraints) [147, 49, 145, 48]. Due to its biological plausibility, another very popular function designed by means of fully recurrent RNNs is the winner takes all function and generalizations thereof such as the k-WTA function, as investigated e.g. in [81, 15, 115]. Apart from applications e.g. for the rapid parallel retrieval of data from huge databases, these models are relevant to explain parts of the functionality of biological systems.

4 Stability

The attractors of an associative memory are the stable states of the underlying dynamics. The notion of stability, however, concerns a much richer mathematical terrain, as pioneered e.g. in the approaches [131, 128] for RNNs. While stable states or stable attractors constitute the essential solutions of associative memories and RNNs used for optimization purpose, stability constitutes a key property for RNNs used for control tasks. Thereby, different mathematical notions of stability exist, often global exponential stability (as strongest and, therefore, most desirable property) is proved, but weaker conditions are also investigated, including new notions of stability such as e.g. investigated in [22].

Much research has been done to find easy to test conditions for stability of RNNs with adaptive parameters (weights and delays) and different activation functions (assuming additional properties such as boundedness or differentiability, if necessary). Often, standard techniques from stability theory are applied such as Lyapunov functions, and, mostly, conditions in the form of linear matrix inequalities are derived, which can be tested in practice, see e.g. the articles [160, 121, 111, 126, 161, 156, 86, 123, 21, 78, 77, 1, 103, 158, 84, 157, 17, 73, 75, 130, 128] for stability properties under different conditions. Some approaches deal with the stabilization of RNNs [103, 122] e.g. by inducing appropriate noise into the system. Moreover, apart from stability conditions, analysis of the number of stable states or periodic attractors and the corresponding basins of attraction is of interest [86, 148, 74]. This knowledge is very relevant to design reliable learning algorithms for fully recurrent networks acting as associative memory, on the one hand, and RNNs used for control, on the other hand. Further, the dynamic properties of RNNs as manifested in their stable states are of relevance to fully understand RNNs which model biological systems.

5 Mathematical analysis

Closely related to stability analysis is the analysis of the dynamics of RNNs. This extends classical stability analysis e.g. considering conditions for multi-periodicity [162, 159] and an exact investigation of the dynamical properties of RNNs under different conditions. It is well known that the full spectrum of dynamic behavior can be observed already in very small networks. While small

systems (e.g. three neurons) can still be analyzed analytically [35, 9, 44], the situation becomes more and more complex for larger networks. Correspondingly, approximations [72] or a more global analysis become necessary. For large (random) models, the effect of the network topology on important properties can provide such measurement [106], e.g. the ability of random networks to solve benchmark pattern recognition tasks [31], the effect of the topology on the synchronizability of such systems [19], or the capacity of such systems depending on topology and form of neurons [69, 138]. The approach [40] successfully derives a mapping of meta-parameters of RNNs derived similar to Google's PageRank to the resulting dynamics.

These findings are interesting for the design of training algorithms or the design of network blocks which can act e.g. as pattern generator. Further, when investigating biologically plausible models such as e.g. linear threshold circuits [133] or spiking networks [3], the findings can help to correctly interpret the function of biological systems. Very interesting results have also been found in the frame of language learning, where the state space reveals insights into the underlying recursive process [20, 135].

6 Biologically inspired models

The mathematical analysis of RNNs serves different purposes: on the one hand, it helps to design efficient training algorithms, on the other hand, it allows insight into the principles underlying RNNs. Thereby, the design and analysis of models which mirror important properties of biological systems is of particular relevance to the understanding of biological RNNs and, eventually, the mechanisms underlying the human brain. Research which investigates biological aspects of RNNs can be classified into different categories: Some approaches model biologically plausible RNNs at a very abstract level and try to understand fundamental properties of such network architectures. As an example, the approach [36] models large random RNNs and investigates synchronization in such systems, since synchronization can frequently be observed in biological systems and it might play an important role in information coding. Similarly, the article [66] investigates correlations which occur in large networks. The approach [96] also deals with the encoding of temporal stimuli in biologically plausible RNNs. Biologically relevant networks architectures including RNNs with lateral inhibition, circuits of leaky integrate and fire neurons, and systems of spiking neurons are investigated in [89, 114, 92, 67], and relevant properties such as mean firing rate and dynamical characteristics are systematically described. Further, some work deals with simplified descriptions and models such as e.g. [102], which presents a general possibility to substitute RNN synapses with mixed sign by biologically more plausible models involving only one sign, or [150] which describes connections of biological RNNs to classical Kalman filters. Interesting further properties concern the role of noise in biological systems, including the tolerance of stable oscillatory patterns to noise [13], or even potential beneficial effects of response noise to better account for general synaptic noise [8].

Other approaches deal directly with a specific biological system or biological effect and devise simple models which can explain such findings and, eventually, lead to a better understanding of potential underlying mechanisms. This includes, for example, RNN models of the hippocampus [71], of cerebellar learning [48], the visual cortex or retina [139, 98, 65], mirror neurons [24], as well as RNN

models which mimic specific effects such as retrospective and prospective recall activity [63], visual aftereffects and illusory contour formation [28, 91], pattern generation of the locomotor system [51], the emergence of dendritic stimulus selectivity [93] or modeling of eye saccades [97]. These models are partially highly specific and this field is closely connected to biological research and new developments and techniques in neurosciences. It targets at complementing the theoretical models by experimental data.

Several particularly interesting research directions deal with the understanding and modeling of biologically plausible and effective training mechanisms implemented in biological networks. One very active and particularly promising field of research concerns biological explanations of reinforcement learning processes in the brain, as presented e.g. in [107, 45, 116]. Reinforcement learning can bridge the gap between fully unsupervised paradigms, which can be well explained by different biologically plausible unsupervised models developed already at a very early stage in neural network research e.g. by Kohonen and von der Malsburg (recent work on unsupervised organization in RNN can be found in [38]), and supervised learning, which often relies on biologically not very plausible mathematical terms such as gradients and higher order derivatives.

7 New training paradigms

One of the merits of a deeper mathematical analysis of RNNs is the beneficial effect on efficient and robust training algorithms. As an example, conditions for RNN stability can be directly put as constraints to RNN learning applied to control tasks. Traditionally, RNN training mostly takes place according to one of two different paradigms: extensions of Hebbian learning for fully recurrent auto-associative memory RNNs, and gradient based approaches for classical supervised tasks in the frame of time series modeling and prediction. For the computation of gradients, either backpropagation through time (BPTT) or real time recurrent learning (RTRL) is commonly used, constituting efficient ways to compute the gradients (and, if necessary, also higher derivatives) in a forward-backward or purely forward way. However, it has been observed very early that gradient based training faces the problem of long-term dependencies, i.e. numerically stable backpropagation of error signals over long periods of time is hardly possible. Correspondingly, a large variety of modifications has been proposed, but still no widely accepted efficient training model exists in this framework.

Research on RNN training separates into diverse approaches to tackle this fundamental problem: some work deals with a better numerical realization of basic RTRL and BPTT training, including e.g. adaptive learning rates and a combination of BPTT and RTRL [127, 85, 153, 25] as well as extensions of these classical paradigms to more general models such as complex valued or spiking neurons [136]. As an alternative training paradigm, extended Kalman filter training is frequently used for RNN training, showing good results depending on the underlying task at hand [26, 109, 37, 108]. Further, formulations of RNN training as a reinforcement problem become more and more common to overcome the problem of temporal credit assignment. However, these methods often suffer from very long training times [39, 132, 52]. Alternative optimization methods are offered by classical meta-heuristics which are adapted to RNN parameter optimization such as evolutionary algorithms or particle swarm optimization [83, 149, 117]. Some approaches try to avoid the problem of vanishing gradients

by designing the architecture appropriately, e.g. restricting recurrence basically to linear neurons as done in long short term memory and extensions thereof [117].

If prior knowledge about the task is available, knowledge based modeling can shape the search space towards efficient solutions. One common framework is offered by neuro-fuzzy systems such as e.g. classical Mamdani or Takagi-Sugeno controllers put into the architecture of an appropriate RNN [95, 61]. Efficiency can also be gained by means of a decomposition of the learning task using e.g. mixture of experts [95, 64] or incremental approaches [99]. As an alternative to neuro-fuzzy systems, the close link of RNNs to the dynamics of classical finite automata has been observed already very early and methods to put known automata rules into a RNN before training have been proposed. The inverse process, extraction of finite automata from RNNs, is also approximately possible (since RNNs are more powerful than finite automata, this is necessary an approximation), and can lead to much better long term behavior and generalization than the original RNN [54].

Despite these promising approaches no efficient learning algorithm for RNNs which is universally accepted exists by now, and also the underlying theory which guarantees the principled learnability of RNNs e.g. in the classical sense of probably approximate learnability is far from understood [41, 94].

8 Reservoir computing

One of the fundamental new paradigms and possible breakthroughs in RNN learning is offered by the principle of reservoir computing, which has been introduced simultaneously in several RNN models and corresponding learning algorithms, in particular in echo state networks (ESN) [55] and liquid state machines (LSM) [88]. Later it was shown under the notion backpropagation decorrelation (BD) that a reservoir with online learning naturally arises by simplification of a rigid error function minimization approach [129]. Basically, this type RNN learning rules rely on a usually fixed recurrent network often termed “dynamic reservoir” or just “reservoir”, which displays a rich but untrained dynamics, and a simply trainable readout. This mostly consists of only one linear layer and can therefore be trained analytically using e.g. the standard pseudo-inverse of the reservoir activations or using standard online schemes like least mean squares. LSM, ESN, and BD originally differed in the exact form of the reservoirs and learning rules, but these techniques are now generally referred to as Reservoir Computing (RC) systems [143]. Recent theoretical work [118] even further brought the theoretical work on ESNs and LSMs closer together. Interestingly, these models are not only very fast to train, but they are also biologically relevant, since training can be restricted to direct Hebb training of the readout instead of a mathematically complicated gradient training of the recurrent reservoir. The overall structure and learning method is very similar to models of the cerebellum, a connection which has been explored to some detail in [152].

Surprisingly, these models show excellent learning behavior depending on the task at hand (see e.g. [57]). It has been shown that they constitute universal approximators of relevant functions such as filters with fading memory. However, their full potential regarding practical applications as well as ways to best design the reservoir for a given task have not yet been fully understood.

Recent research in reservoir computing concerns, on the one hand, appli-

cations and benchmark comparisons to test the applicability of these ideas to different areas. This includes applications for language modeling [137], control [141], and time series modeling [142], for example. Optimal training of reservoir networks constitutes a further active field of research, whereby this concerns both, the adaptation of the readout as well as an optimum design of the recurrent reservoir (an overview can be found in [87]). While the readout relies on supervised paradigms including, for example, support vector machines [124] or logistic regression [29], the reservoir is created based on general principles or using only very slow adaptation. Promising approaches propose to modify the connections such that the states are Gaussian distributed [120] or Laplacian distributed [12], to use highly clustered connectivity as present e.g. in scale-free networks [27], to enlarge the reservoir capacity by means of leaky integrators [58], or to include stability issues into reservoir adaptation such that maximum decorrelation is achieved together with robustness [130]. Note that, while adapting the reservoir, its stability should always be guaranteed, which can be guaranteed by classical conditions of stability theory as presented e.g. in [130, 14].

While RC is usually applied to spatio-temporal or sequential input, in recent work, the use of RC on static or semi-static data has also been researched [30, 113]. In this case the reservoir acts as a primal-space kernel which is intrinsically regularized by the stable dynamics of the recurrent network. In this context, it is of particular interest that a reservoir based architecture can allow online learning of static mappings, while data are presented in temporal correlation [112]. This is a very typical task in robotics applications, where data are generated and evaluated along trajectories such that previously only local models with their limited generalization capabilities could be used.

An important recent trend is the research on hierarchical reservoir systems. One of the disadvantages of RC systems is that they have trouble coping with spatiotemporal data where the relevant information spans a large frequency range (such as in speech: ranging from sound features over phonemes to words). A first solution is presented in [56], where a hierarchical RC system is presented where the layered readout is trained using backpropagation. A fundamental work in this direction recently showed that such a hierarchically organized recurrent architecture can emerge also under a classical BPTT training scheme when using different time scales [151].

Interestingly, reservoir models constitute efficient biologically plausible models which also allow a very efficient realization in hardware as demonstrated e.g. in the approach [119] or even as a novel computing approach in photonics [140]. Although their practical applicability and optimal training is still a matter of recent research, they constitute one of the most promising RNN models of recent years to bridge the gap between biologically plausible models and efficient learning systems with non-trivial applications.

9 New models

Apart from reservoir models, quite a few other new RNN models have been proposed in recent years to fill the gap of spatiotemporal pattern processing using connectionist systems. Mostly, these new models can be put into the frame of classical RNNs as characterized by the standard dynamic equations above. However, a few models have been proposed which add fundamental new principles to recurrent processing rather than only a minor extension of known

models. As already mentioned, based on the principle of full recurrence and cost function optimization, RNNs can solve difficult optimization tasks. One particularly interesting model is offered by the competitive layer model which can be used as an efficient and trainable RNN for perceptual grouping, thus automatically solving non-trivial tasks in image processing [144] and automatic segmentation of task demonstrations in imitation learning [101].

Partially recurrent networks are driven by the input sequence and can thus be used for time series prediction and modeling. This principle has been generalized to more complex recursive structures, in particular tree and graph structures: so-called recursive neural networks constitute well-established models for the processing of trees, thus they can be used to bridge the gap between symbolic data and connectionist processing, since trees naturally encode formulas and symbolic terms. These models have recently been generalized to graph structures including acyclic and even cyclic graphs, thus opening the way towards efficient and fault tolerant machine learning techniques on general graphs [43, 11].

One further active and emerging field of research is the unsupervised training of recursive systems, where very diverse architectures which mirror different principles and capacities exist [42, 7].

10 Conclusions

One of the next big challenges in machine learning will be the processing of temporal or sequential data. In many application areas such speech recognition, robot control, forecasting, language understanding, etc. the current approaches seem to asymptote to a level of performance well below what humans can achieve. RNNs form a very compelling candidate for solving this conundrum: the model has strong connections to biological systems, it has extensively been theoretically studied, and owing to the recent advances in learning methods, can be efficiently and robustly trained. The next hurdle is devising architectures and techniques that can cope with vast and noisy application domains where information present in a wide temporal range needs to be integrated. Online and incremental learning in real time will get even more important for adaptive technology like interacting robots or speech processing devices. A further issue concerns data with different intrinsic timescales as e.g. found in robotics, where controller and planning levels contribute differently to movement, which can be tackled by hierarchies of systems or more complex recurrent networks displaying different timescales as well. As discussed, to all of these problems first pioneering work is just starting and can now rely on a large variety of promising approaches.

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