

Overview of mathematical properties of Echo State Networks

Luca Bonaventura



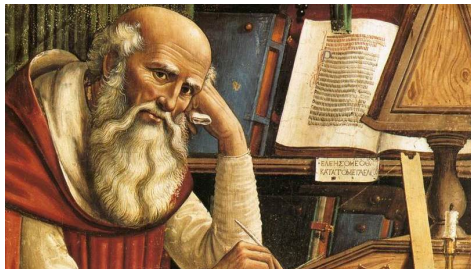
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Paris-Saclay, 7.6.22



REFLECTIONS OF A FORMER NEURAL NETWORK SKEPTIC



Overview



- Review of the main concepts and definitions in **Reservoir Computing** and more specifically **Echo State Networks**



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- Review of some **key mathematical properties** that justify a **wide range of applications**



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- Perspective on the **forthcoming developments** and applications of RC



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- Review of some **key mathematical properties** that justify a **wide range of applications**
- Perspective on the **forthcoming developments** and applications of RC
- Some **motivations** for the choice of ESN as **ML tool for particle beam design**



Acknowledgements and references



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- Some **key references and sources** for this presentation:
 - I. Daubechies**, R. DeVore, S. Foucart et al, [Nonlinear Approximation and \(Deep\) ReLU Networks](#), Constructive Approximation, 55, 127--172, 2022
 - M. Lukosevicius and **H. Jaeger**, [Reservoir computing approaches to recurrent neural network training](#). Computer Science Review, 3, 127--149, 2009
 - A.Hart and J. Hook and J. Dawes, [Embedding and approximation theorems for echo state networks](#), Neural Networks 128, 234--247, 2020



Geophysical Research Letters

RESEARCH LETTER

10.1029/2020GL087776

Key Points:

- A low-resolution, global, reservoir computing-based machine learning (ML) model can forecast the atmospheric state
- The training of the ML model is computationally efficient on a massively parallel computer
- Compared to a numerical

A Machine Learning-Based Global Atmospheric Forecast Model

Troy Arcomano¹, Istvan Szunyogh¹, Jaideep Pathak², Alexander Wikner², Brian R. Hunt³, and Edward Ott⁴

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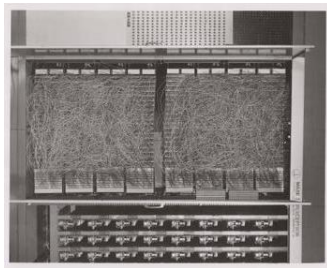
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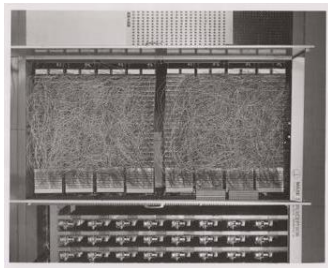
- RC is starting to solve **large scale, real life problems** that entail the simulation of an underlying **large dynamical system**
- RC is **not the only ML approach** that can do so, but it seems to be the **cheapest and easiest to train**



(Artificial) Neural Networks



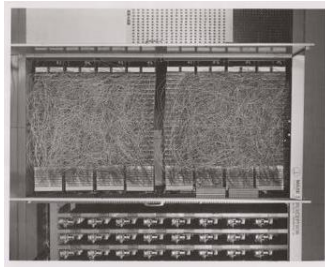
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- At the beginning was the **perceptron**: built **as physical device** in the 1950s, analyzed **mathematically** in the 1960s



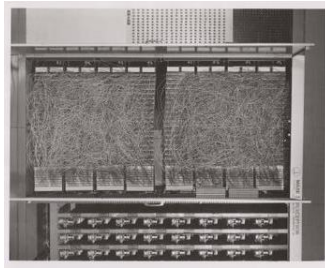
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- Example of network **without hidden layers**: **unable** to approximate **arbitrary input-output** relationships
- Networks with **one or more hidden layers** were first investigated systematically in the 1980s



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High degree polynomials are **computationally unstable**, low degree polynomials are **insufficient** to approximate **globally complicated functions** (indeed scientific computing uses **local polynomial approximations**)



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Fourier series suffer from the **Gibbs phenomenon**



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I. Daubechies et al 2022



Feedforward vs Recurrent NN



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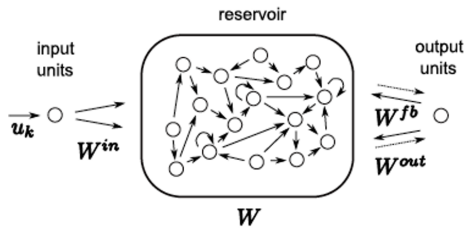


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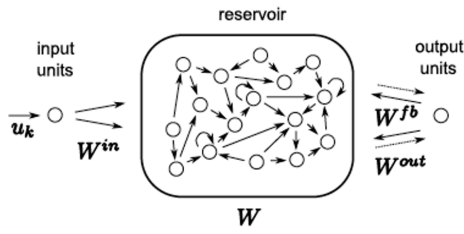
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Reservoir computing



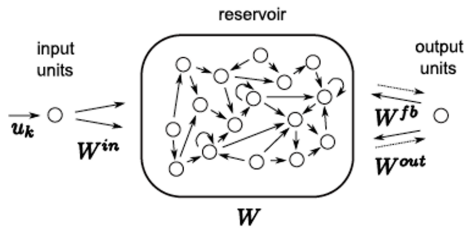
Reservoir computing



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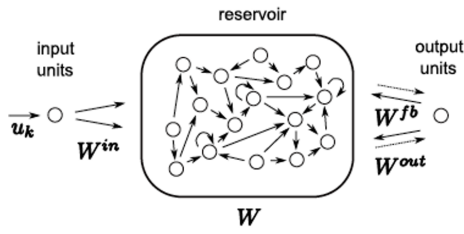
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- No **backpropagation** is necessary
- Training is performed only by (usually) **linear regression** to compute **weights** used to project the reservoir state onto the **output state**



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- **Echo System Networks** (Jaeger): use **simpler neuron models** with randomly generated network connectivity
- ESN found to be easier to implement and **sufficient** for **chaotic system prediction** (Jaeger and Haas, 2004)...but **never say never**...



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- RC approaches based on **directed** networks are **universal approximators** of dynamical systems: Funahashi and Nakamura 1993, Gonon and Ortega, 2020, **Hart, Hook and Dawes, 2020**
- **Physical RC** devices are feasible, often with **photonic** devices:

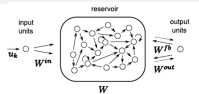
K. Nakajima, [Physical reservoir computing|an introductory perspective](#), *Japanese Journal of Applied Physics* 59,060501, 2020

Van der Sande et al., [Advances in photonic reservoir computing](#), *Nanophotonics*, 6, 561--576, 2017



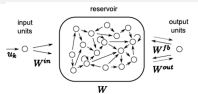
Formal ESN definition in discrete time

$$\begin{aligned}x_{k+1} &= f(Wx_k + W^{in}u_{k+1} + W^{fb}x_k^{out}) \\x_{k+1}^{out} &= g(W^{out}[x_{k+1}; u_{k+1}])\end{aligned}$$



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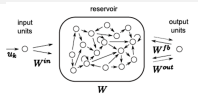


- States $x_k \in \mathbb{R}^N$ **internal state**, $u_k \in \mathbb{R}^K$ **input state**, $x_k^{out} \in \mathbb{R}^L$ **output state**, with $N \gg K, L$, at each **discrete time** $k \in \mathbb{Z}$



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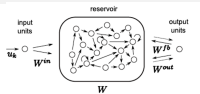


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- Matrices: $W \in \mathcal{M}_N(\mathbb{R})$ **internal weights** (reservoir), $W^{in} \in \mathcal{M}_{N \times K}(\mathbb{R})$ **input**, $W^{fb} \in \mathcal{M}_{N \times L}(\mathbb{R})$ **feedback**, $W^{out} \in \mathcal{M}_{L \times (N+K)}(\mathbb{R})$ **output**



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- Functions: $f: \mathbb{R}^N \rightarrow \mathbb{R}^N$, **componentwise sigmoid**, $g: \mathbb{R}^L \rightarrow \mathbb{R}^L$, **componentwise sigmoid or identity**



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- An infinite sequence of states $y_k \quad k \leq 0$ is **compatible** with a given input sequence $u_k \quad k \leq 0$ if
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- **ESP**: Given a network such that x_k, u_k belong to compact sets, it has the **Echo State Property** wrt the input sequence $u_k \quad k \leq 0$ if **all sequences compatible with $u_k \quad k \leq 0$ coincide**



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- ESP guarantees that the ESN future evolution is **uniquely determined by the input**



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- More **subtle and complex** conditions on the **internal weight matrix**, discussed in **Yildiz, Jaeger and Kiebel, 2012**
- In practice, entries of W are **rescaled with maximum eigenvalue** to guarantee ESP



Other important possible features



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- **Leaky neurons:** introduce parameter $a \in [0, 1]$ and define

$$x_{k+1} = (1 - a)x_k + af(Wx_k + W^{in}u_{k+1})$$

Corresponds to **low pass filtering** of the response to the input: **smaller a** implies **slower reservoir response**



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- Combine **multiple** reservoirs with different time scales:
Long Short Term Memory (LSTM)



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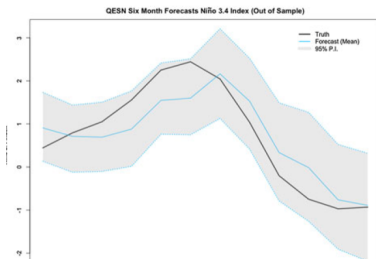
P.L. McDermott, C.K. Winkle, [An ensemble quadratic echo state network for nonlinear spatio-temporal forecasting](#), STAT, 6, 315-330, 2017



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- Having a naturally and **trivially parallelizable** approach to predict **probability distributions** of quantities of interest does not seem such a bad idea
- Furthermore, scrapping the network may imply also losing all the **super-approximation** properties: **do we really want that?**



The future is hybrid

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RESEARCH ARTICLE
10.1029/2021MS002712

Special Section:
Machine learning application to
Earth system modeling

Key Points:

- A hybrid model incorporating machine learning produces more

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Troy Arcomano¹ , Istvan Szunyogh¹ , Alexander Wikner², Jaideep Pathak³, Brian R. Hunt⁴, and Edward Ott^{1,5}

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- No need to waste time **learning what you already know**



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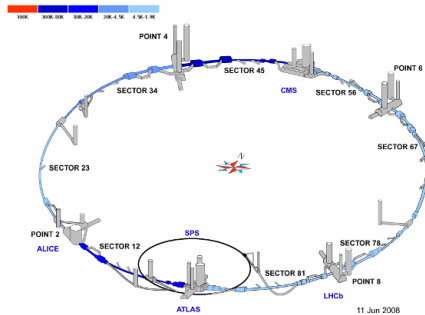
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- Use RC (and, more generally, ANN) predictions to **complement and integrate** more conventional, equation based models
- No need to waste time **learning what you already know**
- Possible bottom line: classical approximation methods (polynomials etc.) **do it better** for **smooth functions/larger scales**, while data based methods for **irregular functions/fine, turbulent scales**



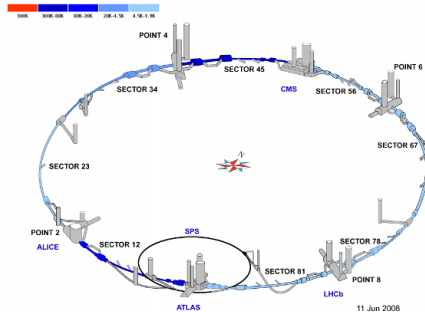
What are we doing with RC?



ML emulation of particle beam evolution in **particle accelerators**, such as the **Large Hadron Collider**



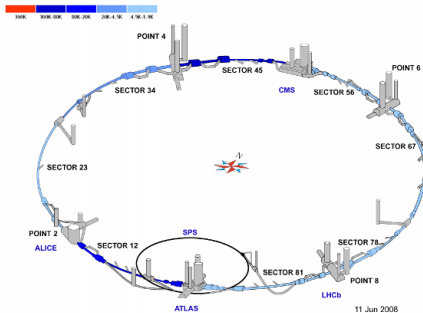
What are we doing with RC?



Particle beam modelling mostly relies on simulation of a **small Hamiltonian** system, whose trajectories must be simulated for a **very long time: $O(10^9)$ turns or more**: direct simulation is **expensive**



What are we doing with RC?



An approach based on a combination of **cheaper emulators** and **asymptotic scaling laws** looks promising (see **next talk!**)

