Time-delay reservoir computers: nonlinear stability of functional differential systems and optimal nonlinear information processing capacity. Applications to stochastic nonlinear time series forecasting.

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DarrylFest, July, 2017 1 / 71

Outline

- Machine learning in a nutshell:
 - Discrete vs continuous time
 - Deterministic vs stochastic
- Static problems, neural networks, and approximation theorems
- Oynamic problems and reservoir computing
- Oniversality theorems
 - The control theoretical approach
 - The filter/operators approach
- Time-delay reservoir computers
 - Hardware realizations, scalability, and big data compatibility
 - Models and performance estimations
- Application examples

Machine learning in a nutshell

• We approach to machine learning as an input/output problem.

- Input: it is denoted by the character z. It contains available information for the solution of the problem (historical data, explanatory factors, features of the individuals that need to be classified).
- Output: denoted generically by **y**. Contains the solution of the problem (forecasted data, explained variables, classification results).
- Purely empirical approach not based on first principles but on a training/testing routine.
- We distinguish between static/discrete-time and continuous-time setups and between deterministic and stochastic situations since they lead to very different levels of mathematical complexity.



Examples

- **Deterministic setup**: an explicit functional relation (via a just measurable function) is assumed between input and output.
 - Static/Discrete-time: observables or diagnostics variables in complex physical or noiseless engineering systems (domotics), translators, memory tasks, games.
 - Continuous time: integration or path continuation of (chaotic) differential equations: molecular dynamics, structural mechanics, vibration analysis, space mission design. Autopilot systems, robotics.
- **Stochastic setup**: the input and the output are random variables or processes and only probabilistic dependence is assumed between them.
 - Static/Discrete-time: image classification, speech recognition, time series forecasting, volatility filtering, factor analysis.
 - Continuous time: physiological time series classification, financial bubble detection.

4 / 71

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Setups considered

	Static/Discrete time		Continuous time	
	Deterministic	Stochastic	Deterministic	Stochastic
Characterization of ingredients	$z \in \mathbb{R}^n$ $y \in \mathbb{R}^q$	$egin{aligned} \mathbf{z} \in (L^2(\Omega,\mathcal{F},\mathbb{P}))^n \ \mathbf{y} \in (L^2(\Omega,\mathcal{F},\mathbb{P}))^q \end{aligned}$	$z \in C^\infty([a,b],\mathbb{R}^n) \ y \in C^\infty([a,b],\mathbb{R}^n)$	z and y are \mathbb{R}^n and \mathbb{R}^q -valued processes adapted with respect to a given filtration \mathcal{F}
Problem to be solved	$\mathbf{y} = f(\mathbf{z})$ f measurable	$\mathrm{E}\left[\mathbf{y}\mid\mathbf{z} ight]$	$\mathbf{y}(\cdot) = F(\mathbf{z}(\cdot))$	$\mathrm{E}\left[\mathbf{y}(\cdot)\mid\mathbf{z}(\cdot) ight]$
Object to be	Real/complex	Conditional	Functional/Operator	Stochastic
trained	function	expectation	Causal Filter	Causal Filter
Approach and source of Universality	Approximation theory	(Semi)-parametric statistics Kalman filter	Control theory Stone-Weierstraß	Functional data analysis and Stochastic control theory



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Neural networks



Universality in neural networks and approximation theorems

- Neural networks are implemented as a machine learning device by tuning the weights wⁱ using a gradient descent algorithm (backpropagation) that minimizes the approximation error based on a training set.
- In the deterministic case, the objective is to recover an explicit functional relation between input and output.
- In the absence of noise there is not danger of overfitting.



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- Universality problem: how large is the class of input-output functions that can be generated using feedforward neural networks as in (1)?
- Hilbert's 13th problem on multivariate functions: can any continuous function of three variables be expressed as a composition of finitely many continuous functions of two variables? This question is a generalization of the original problem for algebraic functions posed in the 1900 ICM in Paris and in [Hil27]



The Kolmogorov-Arnold representation theorem and Kolmogorov-Sprecher networks

Theorem (Kolmogorov-Arnold [Kol56, Arn57])

There exist fixed continuous increasing functions $\varphi_{p,q}(x)$ on I = [0,1] such that each continuous function f on I^n can be written as

$$f(x_1,\ldots,x_n) = \sum_{q=1}^{2n+1} g_q\left(\sum_{p=1}^n \varphi_{pq}(x_p)\right)$$

where the g_q are properly chosen continuous functions of one variable.

- This amounts to saying that the only genuinely multivariate function is the sum!
- This is a representation and not an approximation theorem University

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Theorem (Sprecher [Spr65, Spr96, Spr97])

There exist constants λ_p and fixed continuous increasing functions $\varphi_q(x)$ on I = [0, 1] such that each continuous function f on I^n can be written as

$$f(x_1,\ldots,x_n) = \sum_{q=1}^{2n+1} g_q\left(\sum_{p=1}^n \lambda_p \varphi_q(x_p)\right)$$

where the g_q are properly chosen continuous functions of one variable.

- The g_q functions depend on f but not λ_p and φ_q . All the information contained in the multivariable continuous function f is contained in the single variable continuous functions g_q .
- This is not ideal for machine learning applications because we would need to train the g_q functions. It still can be done (see the CMAC in [CG92])

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DarrylFest, July, 2017 11 / 71

The Cybenko and the Hornik et al. theorems

Definition

A squashing function is a map $\psi:\mathbb{R}\to [0,1]$ that is non-decreasing and that

$$\lim_{\lambda o -\infty} \psi(\lambda) = 0$$
 and $\lim_{\lambda o \infty} \psi(\lambda) = 1$

Squashing functions



Approximation of continuous functions

Theorem (Cybenko [Cyb89])

Let ψ be a continuous squashing function. Then, the functions $G_{\psi,N}: I^n \to \mathbb{R}$ of the form

$$G_{\psi,N}(\mathsf{z};\boldsymbol{\theta}) = \left(\sum_{1=1}^{N} w_j^2 \psi\left(\langle \mathsf{w}_j^1, \mathsf{z} \rangle + \theta_j\right)\right), \quad \mathsf{w}_j^1, \mathsf{z} \in \mathbb{R}^n, \mathsf{w}^2 \in \mathbb{R}^N, \theta_j \in \mathbb{R},$$

are dense in $C(I^n)$, that is, given any function $f \in C(I^n)$ and $\epsilon > 0$, there is a sum of this type for which

$$|G_{\psi,N}(\mathbf{z}; \boldsymbol{\theta}) - f(\mathbf{z})| < \epsilon$$
, for all $\mathbf{z} \in I^n$.

• This result proves that any continuous function can be **approximated** using a feedforward neural network with a single hidden layer if we use a given continuous activation function.

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Approximation of measurable functions and functions with finite support

The Hornik, Stinchcombe, and White [HSW89] theorems:

- The previous theorem holds even if the function *f* is only measurable and the activation function is a not necessarily continuous squashing function.
- Functions with finite support can be exactly attained using a feedforward neural network with a single hidden layer if the activation function attains 0 and 1: let {z₁,..., z_k} be a set of distinct points in ℝⁿ and let f : ℝⁿ → ℝ be an arbitrary function, then there exists a feedforward neural network with k neurons in its hidden layer and transfer function G_{ψ,N} such that G_{ψ,N}(z_i; θ) = f(z_i).
- The network can be trained so that it learns not only the function but also its derivatives [HSW90, GW92].

This result has been extended to backpropagation (as opposed output of St. Gallen feedforward) neural networks by Hecht-Nielsen [HN89]

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The Maurey-Jones-Barron Theorem

- Let G be a set of approximating functions: splines with free nodes, trigonometric polynomials with free frequencies, feedforward neural networks.
- The variable basis approximation consists of using the set

$$\operatorname{span}_n G := \left\{ \sum_{i=1}^n w_i g_i \mid w_i \in \mathbb{R}^n, \, g_i \in G \right\}.$$

• When G is a subset of a normed linear space $(X, \|\cdot\|)$, we use the G-variation

$$||f||_{\mathcal{G}} := \inf\{c > 0 \mid f/c \in \operatorname{cl}\operatorname{conv}(\mathcal{G} \cup -\mathcal{G})\}.$$

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Theorem

 $(X, \|\cdot\|)$ a Hilbert space, G a bounded subset and $s_G = \sup_{g \in G} \|g\|$. For every $f \in X$ and every positive integer n

$$||f - \operatorname{span}_n G|| \le \sqrt{\frac{(s_G ||f||_G)^2 - ||f||^2}{n}}$$

- Any function in a ball of radius r in G-variation can be approximated by a neural network with n hidden units computing functions from Gwithin accuracy r/\sqrt{n} .
- This estimate holds for any number of variables: **no curse of dimensionality**.



Implementation

It involves three main issues:

- Choice of an architecture: squashing function, number of layers, number of neurons in each layer, and connectivity between them.
- Estimation of the connectivity weights: a supervised learning approach is taken. Realizations of the input and the output are used to minimize an error function via a gradient descent method. Potential problems:
 - Local minima
 - Flat gradients in deep structures
- Cross validation and regularization: a posteriori verification of the goodness of the architecture choice in the first point regarding:
 - Deterministic case: is this the most economic structure for a prescribed accuracy level in the approximation problem?
 - Stochastic case: are we overfitting?

In both cases the solution is obtained using new architectures selected via cross-validation or pruning techniques (see [KvD03] for references and [SX99, SCHU16] for Lasso related approaches).

Non-linear regressions

The deterministic universal approximation properties of neural networks yield non-parametric estimators for non-linear regression functions. Consider the following heteroscedastic regression model:

$$y_t = f(\mathbf{z}_t) + \varepsilon_t, \ \{\mathbf{z}_t\} \sim \text{IID}(p(\mathbf{z})), \ \varepsilon_t | (\mathbf{z}_t = \mathbf{z}) \sim \text{IID}(0, s_{\varepsilon}^2(\mathbf{z}) < \infty), \ t = 1, \dots, T,$$
(2)

and assume that the functions $f, s_{\varepsilon}^2 : \mathbb{R}^n \to \mathbb{R}$ are continuous and bounded. Notice that hypotheses (2) imply that, in this case,

$$\mathrm{E}\left[y_t|\mathbf{z}_t\right] = f(\mathbf{z}_t).$$

In order to estimate the regression function f, we fit a neural network with a hidden layer and a sufficiently large number N of neurons using two realizations $\{z_1, \ldots, z_T\}$ and $\{y_1, \ldots, y_T\}$ of the input and the output, which yields the following estimator $\hat{\theta}_T$ of the weights vector θ :

$$\widehat{\boldsymbol{\theta}}_{N} = \arg\min_{\boldsymbol{\theta}} \frac{1}{T} \sum_{t=1}^{T} \left\{ y_{t} - G_{\psi,N}(\mathbf{z}_{t};\boldsymbol{\theta}) \right\}^{2}. \qquad (3)$$

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DarrylFest, July, 2017 18 / 71

Under appropriate conditions $\widehat{\theta}_N$ converges in probability for $T \to \infty$ and for a fixed N to the parameter vector θ_N which corresponds to the best approximation of $f(\mathbf{z})$ by a function of type $G_{\psi,N}(\mathbf{z}; \theta)$, that is,

$$\boldsymbol{\theta}_{N} = \underset{\boldsymbol{\theta}}{\operatorname{arg\,min}} = \operatorname{E}[\{f(\mathbf{z}_{t}) - G_{\psi,N}(\mathbf{z}_{t};\boldsymbol{\theta})\}^{2}]. \tag{4}$$

Under somewhat stronger assumptions, it can be shown the asymptotic normality of the estimator $\hat{\theta}_N$ [FN00].

Remark: Many important examples like nonlinear state space models (ARSV for example) do not satisfy the independence hypothesis on the input signal z_t or there is just no function f which makes necessary the use of other tools like the nonlinear Kalman filter.



19 / 71

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Offline and online computing

- Turing machines compute sequentially and offline batches of information. Computations have a beginning and an end.
- Neuronal and "behaving" systems compute online as information arrives (probably desynchronized and with different sampling frequencies) and reuse the result of previous computations



Mathematical formulation of reservoir computing

Reservoir computing is based on three main principles:

• The input signal $\mathbf{z}(t) \in \mathbb{R}^n$ is inserted as the external forcing of the flow $F_t : \mathbb{R}^N \times \mathbb{R}^n \to \mathbb{R}^N$ of a non-autonomous dynamical system (the reservoir):

$$\mathbf{x}(t) = F_t(\mathbf{x}_0, \mathbf{z}(t)). \tag{5}$$

The value $\mathbf{x}(t)$ is the **reservoir state** at time t.

• A static readout $h : \mathbb{R}^N \to \mathbb{R}^q$ is trained in order to obtain the desired output $\mathbf{y}(t)$ out of the input $\mathbf{z}(t)$:

$$\mathbf{y}(t) = h(\mathbf{x}(t)).$$

 Multitasking: different readouts can be trained on the same reservoir output in order to extract different pieces of information about the University of St.Gallen input.

21 / 71

- 3



- Fundamentally new approach to neural computing [Jae01, JH04, MNM02, VSDS07, LJ09]; defining features of RC: the fading-memory, separation, and approximation properties [LJ09]
- Modification of the traditional RNN in which the architecture and the neuron weights of the network are created in advance (for example randomly) and remain unchanged during the training stage
- If readout layer is linear then inference and theoretical performance evaluation becomes possible!!



Reservoir computing and neural processes

- The reservoir computing approach approach resembles neural processes in which sensory inputs (input signals) are pre-processed by the neural microcircuits of a cortical column and then various single neurons (readouts) extract information from it and send it to other brain areas.
- The use of different readouts serves different computational goals. Example: in the case of the visual cortex determine, size, direction of motion, identity of objects.
- The division of information processing between reservoir and readout is very efficient (one processing serves several computational goals) and helps explaining the energy efficiency of the brain.
- Neurophisiology evidence: spike trains coming from different projection neurons from the same cortical column tend to be weakly correlated.

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Universality result for neural circuits [MJS07]

Suppose that we are given an external continuous-time input z(t) and a solution u(t) of a non-autonomous *n*th-order differential equation of the form

$$y^{(n)}(t) = G(y(t), y'(t), y''(t), \dots, y^{(n-1)}(t)) + z(t).$$
 (6)

Then, for any non-autonomous dynamical system of the form

$$\dot{\mathbf{x}}(t) = f(\mathbf{x}(t)) + g(\mathbf{x}(t)) \cdot \mathbf{v}(t), \qquad f, g: \mathbb{R}^n \to \mathbb{R}^n, \tag{7}$$

that has the fading memory property (see below), there exist a feedback $K : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ and a smooth readout $h : \mathbb{R}^n \to \mathbb{R}$ such that any solution y(t) of (6) can be written as $y(t) = h(\mathbf{x}(t))$ with $\mathbf{x}(t)$ the solution of the system

$$\dot{\mathbf{x}}(t) = f(\mathbf{x}(t)) + g(\mathbf{x}(t)) \cdot K(\mathbf{x}(t), z(t) + z_0(t)), \qquad \mathbf{x}(0) = \mathbf{0},$$

with $z_0(t)$ a fixed input that satisfies that $z_0(t) = \mathbf{0}$ for all $t \ge 1$. University of St. Gallen

- The proof of this result is control-theory based.
- The feedback K and the readout h depend only on the function G that characterizes the system that needs to be simulated but not on the external output z(t) that needs to be processed.
- Since these two functions are static, they are ideal targets for learning.
- The function *h* is chosen in many situations to be just linear and training is carried out by solving a simple (regularized) regression problem.
- This result shows that RCs constructed using the solutions of dynamical systems of the form (7) have the computational power of a universal Turing machine when put together with suitable feedback and readout functions. This follows from the fact that every Turing machine can be simulated by systems of equations of the form (6) (see [Bra95, SS94, SS92, Orp97]).
- The dynamical systems (7) include as a particular case the standard systems of nonlinear differential equations that are used to model the dynamics of firing rates in recurrent circuits of neurons.

L. Grigoryeva, J. Henriques, L. Larger, J.-P. Ortega

The operator approach

The filtering/operator point of view [MNM02]

We now use operators $L: C^0(\mathbb{R}^n) \to C^0(\mathbb{R}^N)$ instead of flows F_t like in (5) in order to transform the input signal into the reservoir state curve:

$$L(\mathbf{z}(\cdot)) = \mathbf{x}(\cdot).$$

• Time invariance: Let $U_{t_0}^n$ the time-shift operator for curves in \mathbb{R}^n , that is $U_{t_0}^n(\mathbf{z}(\cdot))(t) = \mathbf{z}(t + t_0)$. The filter L is called time invariant if

$$L \circ U_{t_0}^n = U_{t_0}^N \circ L$$

- Causality: L is causal if $L(\mathbf{z}(\cdot))(t)$ does not depend on z(s) for s > t.
- Fading memory property: L(z(·))(0) can be approximated by the outputs L(u(·))(0) for any other input u that approximates z on a sufficiently long time interval [−T, 0] going back into the pastersity of St.Gallen

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- Equivalently, in order to compute the most significant bits of L(z(·))(0) it is not necessary to know the precise value of the input function z for any time s and it is also not necessary to know anything about the values of z for more than a finite time interval back into the past.
- Fading memory filters are automatically causal.
- The category of time-invariant fading memory filters is large and includes well-known examples like Volterra series; it can actually be shown [BC85, MS00] that any time-invariant fading memory filter can be approximated by a (possibly infinite) Volterra series.
- Separation property: a class \mathcal{L} of filters has the separation property if for any two inputs z and u such that $z(s) \neq u(s)$, for some $s \leq t$, there exists $L \in \mathcal{L}$ such that $L(z)(t) \neq L(u)(t)$.



Universality theorem [MM04]

Theorem

Let F be an arbitrary time-invariant filter that satisfies the fading memory property. Assume the availability of a space of fading memory filters \mathcal{L} that satisfies the pointwise separation property. Then, for any chosen accuracy, there exists $m \in \mathbb{N}$, filters L_1, \ldots, L_m in the space \mathcal{L} , and a readout function $h : \mathbb{R}^m \to \mathbb{R}$ such that F can be approximated by the composition $h \circ (B_1, \ldots, B_m)$.



Observations

• Examples

- Dynamic networks [MS00]: feedforward neural networks with time-varying weights.
- Synaptic dynamical models by Tsodyks, Pawelzik, and Markram [TPM98].
- Remarkable consequence: for a large variety of classes \mathcal{L} of basis filters (such as delay lines, linear filters, dynamic synapses, or circuits with fading memory) the pointwise separation property, in combination with sufficiently "flexible" readout maps, endows the resulting RC with universal computational power in the giant class of filters \mathcal{F} that are time-invariant and have fading memory.
- Fading memory filters only generate fading memory filters. Not the case using the neural circuit approach. Major computational jump.
- Proof goes via the Stone-Weierstrass theorem.



29 / 71

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Time-delay reservoir computers

TDRs are based on the interaction of the discrete input signal $z(t) \in \mathbb{R}$ with the solution space of a TDDE of the form

$$\dot{x}(t) = -x(t) + f(x(t-\tau), I(t), \theta), \tag{8}$$

where f is a nonlinear smooth function (**nonlinear kernel**), $\theta \in \mathbb{R}^{K}$ is the parameter vector, $\tau > 0$ is the **delay**, $x(t) \in \mathbb{R}$, and $I(t) \in \mathbb{R}$ is obtained via temporal multiplexing of the input signal z(t) over the delay period.

The choice of nonlinear kernel f is determined by the physical implementation; consider two parametric sets of kernels:

• Mackey-Glass [MG77]: $f(x, I, \theta) = \frac{\eta(x+\gamma I)}{1+(x+\gamma I)^p}$, $\theta = (\eta, \gamma, p)$

• Ikeda [Ike79]: $f(x, I, \theta) = \eta \sin^2 (x + \gamma I + \phi)$, $\theta = (\eta, \gamma, \phi)$ Used in the RC electronic [ASV⁺11] and optoelectronic [LSB⁺12] realizations.

30 / 71

Discrete time model of TDR

Consider the Euler time-discretization of (8) with integration step $d := \tau/N$:

$$(x(t) - x(t - d))/d = -x(t) + f(x(t - \tau), I(t), \theta).$$
(9)

Define neuron layers $\mathbf{x}(t)$ and input layers $\mathbf{I}(t) := C\mathbf{z}(t) \in \mathbb{R}^N$ by setting

$$x_i(t) := x(t\tau - (N-i)d), \quad l_i(t) := l(t\tau - (N-i)d), \quad i \in \{1, \ldots, N\}, \quad t \in \mathbb{Z},$$

where $x_i(t)$ is the *i*th neuron value of the *t*th layer of the reservoir. Then the solutions of (9) are given by

$$x_i(t) := e^{-\xi} x_{i-1}(t) + (1 - e^{-\xi}) f(x_i(t-1), l_i(t), \theta), \ x_0(t) := x_N(t-1), \ \xi := \log(1+d),$$

A smooth map $F : \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R}^K \to \mathbb{R}^N$ specifies the neuron values as a recursion via

$$\mathbf{x}(t) = F(\mathbf{x}(t-1), \mathbf{I}(t), \boldsymbol{\theta}), \tag{10}$$

where F is constructed out of the nonlinear kernel map f; F is referred to as the **reservoir map**.

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Input and output modules

Input: Take a multi-dimensional time series $\mathbf{z}(t) \in \mathbb{R}^n$ as the input signal. For each *t* define $\mathbf{I}(t) := C\mathbf{z}(t) \in \mathbb{R}^N$, where $C \in \mathbb{M}_{N,n}$ is the so called **input mask** that takes care of the dimensional and temporal multiplexing.

Output: Let the training be carried out with a **teaching signal** $\mathbf{y}(t) \in \mathbb{R}^n$ that is used to construct a readout W_{out} out of the solution of the ridge regression:

$$W_{\text{out}} := \operatorname*{arg\,min}_{W \in \mathbb{M}_{N,n}} \left(\sum_{t=1}^{T^*} \| W^\top \cdot \mathbf{x}(t) - \mathbf{y}(t) \|^2 + \lambda \| W \|_{\text{Frob}}^2 \right), \qquad (11)$$

whose solution is

$$W_{\text{out}} = (XX^{T} + \lambda \mathbb{I}_{N})^{-1} XY, \qquad (12)$$

where $X \in \mathbb{M}_{N,T^*}$ is the reservoir output given by $X_{i,j} := x_i(j)$ and $Y \in \mathbb{M}_{T^*,n}$ is the teaching matrix containing the vectors $\mathbf{y}(t)$, $t \in \{1, \ldots, T^*\}$, organized by rows, $\lambda \in \mathbb{R}$ is a regularization parameter (usually obtained via cross-validation).

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Physical implementation: reservoir computing (RC) devices

- A major feature of the RC is the possibility of constructing physical realizations of reservoirs instead of simulating them using a computer
- Chaotic dynamical systems can be used to construct reservoirs that exhibit the RC features: in [ASV⁺11] using chaotic electronic oscillators or using optoelectronic devices like in [LSB⁺12]





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Information processing using a single dynamical node as complex system

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Parallel photonic information processing at gigabyte per second data rates using transient states

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Experimental demonstration of reservoir computing on a silicon photonics chip

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Time-delay reservoir computers

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Universality vs performance optimization

Universality is a reassuring feature but in practice there are architecture restrictions on the:

- Basis filters available
- Functional form of the readout

It is hence important to be able to evaluate RC performance for a given architecture and a given task so that it can be optimized by tuning the available parameters in the setup.

We do so in what follows in the setup of TDRs so that we can test the robustness of a given setup with respect to modifications in the task and the parameters.



Optimal performance: stability and unimodality



Behavior of the reservoir performance in a quadratic memory task as a function of the \bar{c} and var(c). The top panels show how the performance degrades very quickly as soon as \bar{c} and var(c) separate from zero. The bottom panels depict the reservoir performance as a function of the various output means and variances. We have indicated with red markers the cases in which the reservoir visits the stability basin of a contiguous stable equilibrium tencer showing allen how unimodality is associated to optimal performance.

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Stability analysis

Theorem (Grigoryeva, Henriques, Larger, JPO, 2015)

Let x_0 be an equilibrium of the reservoir time-delay differential equation in autonomous regime, that is, when I(t) = 0, and suppose that there exists $\varepsilon > 0$ and $k_{\varepsilon} \in \mathbb{R}$ such that one of the following conditions holds

(i)
$$f(x + x_0, 0, \theta) \le k_{\varepsilon} x + x_0$$
 for all $x \in (-\varepsilon, \varepsilon)$
(ii) $\frac{f(x + x_0, 0, \theta) - x_0}{x} \le k_{\varepsilon}$ for all $x \in (-\varepsilon, \varepsilon)$.

If $|k_{\varepsilon}| < 1$ then x_0 is asymptotically stable. If $|k_{\varepsilon}| \leq 1$ then x_0 is stable.

Corollary (Grigoryeva, Henriques, Larger, JPO, 2015)

Let x_0 be an equilibrium of the reservoir TDDE and suppose that the nonlinear reservoir kernel function f is continuously differentiable at x_0 . If $|\partial_x f(x_0, 0, \theta)| < 1$ (respectively, $|\partial_x f(x_0, 0, \theta)| \leq 1$), then x_0 is asymptotically stable (respectively, stable).

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Corollary (Stability of the equilibria of the Ikeda TDDE; Grigoryeva, Henriques, Larger, JPO, 2015)

Consider the reservoir TDDE in autonomous regime based on the Ikeda kernel,

$$f(x,0,\theta) = \eta \sin^2(x+\phi). \tag{13}$$

The Ikeda nonlinear TDDE exhibits two families of equilibria:

- (i) The trivial solution $x_0 = 0$ for any $\eta \in \mathbb{R}$ and $\phi = \pi n$, $n \in \mathbb{Z}$. The equilibium $x_0 = 0$ is asymptotically stable for any $\eta \in \mathbb{R}$.
- (ii) The non-trivial equilibria x_0 are obtained as solutions of the equation $x_0 = \eta \sin^2(x_0 + \phi)$, for any $\eta \in \mathbb{R}$ and $\phi \neq \pi n$, $n \in \mathbb{Z}$. These equilibria are asymptotically stable (respectively, stable) if

$$|\sin(2x_0+2\phi)| < rac{1}{|\eta|}$$
 (respectively, $|\sin(2x_0+2\phi)| \leq rac{1}{|\eta|}$).

When $|\eta| < 1$ (respectively, $|\eta| \le 1$), there exists only one non-trivial equilibrium that is always asymptotically stable (respectively, stable).

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Stability of the TDR: discrete time approximation

Proposition (Grigoryeva, Henriques, Larger, JPO, 2015)

The point $x_0 \in \mathbb{R}$ is an equilibrium of the reservoir time-delay differential equation in autonomous regime, that is when I(t) = 0, if and only if the vector $\mathbf{x}_0 := x_0 \mathbf{i}_N$ is a fixed point of the N-dimensional discretized nonlinear time-delay reservoir

$$\dot{\mathbf{x}}(t) = F(\mathbf{x}(t-1), \mathbf{I}(t), \boldsymbol{\theta})$$
(15)

in autonomous regime, that is, when $\mathbf{I}(t) = \mathbf{0}_N$.

Theorem (Grigoryeva, Henriques, Larger, JPO, 2015)

Let $\mathbf{x}_0 = x_0 \mathbf{i}_N$ be a fixed point of the N-dimensional recursion $\mathbf{x}(t) = F(\mathbf{x}(t-1), \mathbf{l}(t), \boldsymbol{\theta})$ in autonomous regime. Then, $\mathbf{x}_0 \in \mathbb{R}^N$ is asymptotically stable (respectively stable) if $|\partial_x f(x_0, 0, \boldsymbol{\theta})| < 1$ (respectively, $|\partial_x f(x_0, 0, \boldsymbol{\theta})| \leq 1$).

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The approximating model and nonlinear memory capacity

Consider a stable equilibrium $x_0 \in \mathbb{R}$ of the autonomous system associated to (8) or, equivalently, a stable fixed point $\mathbf{x}_0 := (x_0, \dots, x_0)^\top \in \mathbb{R}^N$ of (10). We construct the approximation of (10) by using its linearization at \mathbf{x}_0 with respect to the delayed self-feedback and its *R*th-order Taylor expansion with respect to its dependence on the signal injection:

$$\mathbf{x}(t) = F(\mathbf{x}_0, \mathbf{0}_N, \theta) + A(\mathbf{x}_0, \theta)(\mathbf{x}(t-1) - \mathbf{x}_0) + \varepsilon(t),$$
(16)

where $A(\mathbf{x}_0, \boldsymbol{\theta}) := D_{\mathbf{x}}F(\mathbf{x}_0, \mathbf{0}_N, \boldsymbol{\theta})$ and $\varepsilon(t)$ is given by:

$$arepsilon(t) = (1 - e^{-\xi}) \left(q_R \left(z(t), c_1 \right), \ldots, q_R \left(z(t), c_1, \ldots, c_N \right) \right)^{\top},$$

with

$$q_{R}(z(t), c_{1}, \dots, c_{r}) := \sum_{i=1}^{R} \frac{z(t)^{i}}{i!} (\partial_{I}^{(i)} f)(x_{0}, 0, \theta) \sum_{j=1}^{r} e^{-(r-j)\xi} c_{j}^{i},$$

and $(\partial_{I}^{(i)} f)(x_{0}, 0, \theta)$ the *i*th order partial derivative of the nonlinear kernel *f* with respect to $I(t)$ evaluated at $(x_{0}, 0, \theta)$.

Let the input signal be $\{z(t)\}_{t\in\mathbb{Z}} \sim \operatorname{IID}(0, \sigma_z^2)$, then $\{\mathbf{I}(t)\}_{t\in\mathbb{Z}} \sim \operatorname{IID}(\mathbf{0}_N, \Sigma_I)$, with $\Sigma_I := \sigma_z^2 \mathbf{c}^\top \mathbf{c}$, and $\{\varepsilon(t)\}_{t\in\mathbb{Z}} \sim \operatorname{IID}(\boldsymbol{\mu}_{\varepsilon}, \Sigma_{\varepsilon})$ with

$$oldsymbol{\mu}_{arepsilon} = (1-e^{-arepsilon}) \left(oldsymbol{q}_{R} \left(\mu_{z}, oldsymbol{c}_{1}
ight), \ldots, oldsymbol{q}_{R} \left(\mu_{z}, oldsymbol{c}_{1}, \ldots, oldsymbol{c}_{N}
ight)
ight)^{ op},$$

where $\mu_z^i := \mathrm{E}\left[z(t)^i\right]$ and $\Sigma_{\varepsilon} := \mathrm{E}\left[(\varepsilon(t) - \mu_{\varepsilon})(\varepsilon(t) - \mu_{\varepsilon})^{\top}\right] \in \mathbb{S}_N$ with the entries given by:

$$\begin{split} (\Sigma_{\varepsilon})_{ij} = & (1 - e^{-\xi})^2 ((q_R(\cdot, c_1, \ldots, c_i) \cdot q_R(\cdot, c_1, \ldots, c_j))(\mu_z) \\ & - q_R(\mu_z, c_1, \ldots, c_i) q_R(\mu_z, c_1, \ldots, c_j)), \ i, j = 1, \ldots, N. \end{split}$$

The process (16) is a VAR(1) model

$$\mathbf{x}(t) - \boldsymbol{\mu}_{\mathbf{x}} = A(\mathbf{x}_0, \boldsymbol{\theta})(\mathbf{x}(t-1) - \boldsymbol{\mu}_{\mathbf{x}}) + (\varepsilon(t) - \boldsymbol{\mu}_{\varepsilon})$$
(17)

with $\mu_x = (I_N - A(\mathbf{x}_0, \theta))^{-1} (F(\mathbf{x}_0, \mathbf{0}_N, \theta) - A(\mathbf{x}_0, \theta)\mathbf{x}_0 + \mu_{\varepsilon})$ and an autocovariance function $\Gamma(k) := \mathbb{E}\left[(\mathbf{x}(t) - \mu_x) (\mathbf{x}(t-k) - \mu_x)^{\top} \right]$, $k \in \mathbb{Z}$, recursively determined by the Yule-Walker equations [Lüt05]:

$$\operatorname{vec}(\Gamma(0)) = (\mathbb{I}_{N^2} - A(\mathbf{x}_0, \boldsymbol{\theta}) \otimes A(\mathbf{x}_0, \boldsymbol{\theta}))^{-1} \operatorname{vec}(\boldsymbol{\Sigma}_{\varepsilon}),$$

$$\Gamma(k) = A(\mathbf{x}_0, \boldsymbol{\theta}) \Gamma(k-1), \ \Gamma(-k) = \Gamma(k)^{\top}.$$

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The nonlinear memory capacity estimations

A *h*-lag memory task is determined by a function $H : \mathbb{R}^{h+1} \to \mathbb{R}$ (in general nonlinear) that is used to generate $y(t) := H(z(t), z(t-1), \ldots, z(t-h)) \in \mathbb{R}$ out of the reservoir input $\{z(t)\}_{t \in \mathbb{Z}}$.

Recall, that the optimal linear readout \mathbf{W}_{out} adapted to the memory task H is given by the solution of a ridge (or Tikhonov [Tik43]) linear regression problem

$$(\mathbf{W}_{\text{out}}, \boldsymbol{a}_{\text{out}}) := \operatorname*{arg\,min}_{\mathbf{W} \in \mathbb{R}^{N}, \boldsymbol{a} \in \mathbb{R}} \left(\mathrm{E}\left[(\mathbf{W}^{\top} \cdot \mathbf{x}(t) + \boldsymbol{a} - \boldsymbol{y}(t))^{2} \right] + \lambda \|\mathbf{W}\|^{2} \right).$$
(18)

Using the fact that $\{\mathbf{x}(t)\}_{t\in\mathbb{Z}}$ is the unique stationary solution of VAR(1) approximating system (17) for the TDR (17) obtain

$$\mathbf{W}_{\text{out}} = (\Gamma(0) + \lambda \mathbb{I}_N)^{-1} \text{Cov}(y(t), \mathbf{x}(t)),$$
(19)

$$\boldsymbol{a}_{\text{out}} = \mathbf{E}\left[\boldsymbol{y}(t)\right] - \mathbf{W}_{\text{out}}^{\top} \boldsymbol{\mu}_{\boldsymbol{x}}, \tag{20}$$

where μ_x , $\Gamma(0) \in \mathbb{S}_N$ are provided in (17), and $\operatorname{Cov}(y(t), \mathbf{x}(t))$ is a vector in \mathbb{R}^N that has to be determined for every specific memory task H.

The error committed by the reservoir when using the optimal readout is

$$\begin{split} \mathrm{MSE}_{H} &= \mathrm{var}\left(y(t)\right) - \mathrm{Cov}(y(t), \mathbf{x}(t))^{\top} (\Gamma(0) + \lambda \mathbb{I}_{N})^{-1} (\Gamma(0) + 2\lambda \mathbb{I}_{N}) \\ &\times (\Gamma(0) + \lambda \mathbb{I}_{N})^{-1} \mathrm{Cov}(y(t), \mathbf{x}(t)). \end{split}$$

Using the VAR(1) approximating model (17) of RC, the corresponding H-memory capacity is

$$C_{H}(\boldsymbol{\theta}, \mathbf{c}, \lambda) = \operatorname{Cov}(\boldsymbol{y}(t), \mathbf{x}(t))^{\top} (\boldsymbol{\Gamma}(0) + \lambda \mathbb{I}_{N})^{-1} (\boldsymbol{\Gamma}(0) + 2\lambda \mathbb{I}_{N})$$
(21)

$$\times (\Gamma(0) + \lambda \mathbb{I}_N)^{-1} \operatorname{Cov}(y(t), \mathbf{x}(t)) / \operatorname{var}(y(t)).$$
(22)

Additionally,

$$0 \leq C_H(\boldsymbol{\theta}, \mathbf{c}, \lambda) \leq 1.$$

Once a specific reservoir and task H have been fixed, the capacity function $C_H(\theta, \mathbf{c}, \lambda)$ can be explicitly written down and it can hence be used to find reservoir parameters θ_{opt} and an input mask \mathbf{c}_{opt} that maximize it, by solving the optimization problem

$$(\boldsymbol{\theta}_{\mathrm{opt}}, \mathbf{c}_{\mathrm{opt}}) := \underset{\boldsymbol{\theta} \in \mathbb{R}^{K}, \mathbf{c} \in \mathbb{R}^{N}}{\operatorname{arg\,max}} C_{H}(\boldsymbol{\theta}, \mathbf{c}, \lambda).$$
(23)

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Optimal nonlinear capacity

The *h*-lag quadratic memory task. Take a quadratic task function of the form $H(\mathbf{z}^{h}(t)) := \mathbf{z}^{h}(t)^{\top} Q \mathbf{z}^{h}(t)$, for some symmetric h + 1-dimensional matrix Q. In this case $\operatorname{var}(y(t)) = (\mu_{z}^{4} - \sigma_{z}^{4}) \sum_{i=1}^{h+1} Q_{ii}^{2} + 4\sigma_{z}^{4} \sum_{i=1}^{h+1} \sum_{j>i}^{h+1} Q_{ij}^{2}$, and

$$\begin{aligned} \operatorname{Cov}(y(t), x_i(t)) &= (1 - e^{-\xi}) \sum_{j=1}^{h+1} \sum_{r=1}^{N} Q_{jj}(A^{j-1})_{ir} \\ &\times (s_R(\mu_z, c_1, \dots, c_r) - \sigma_z^2 q_R(\mu_z, c_1, \dots, c_r)), \end{aligned}$$

where the polynomial s_R on the variable x is defined as $s_R(x, c_1, \ldots, c_r) := x^2 \cdot q_R(x, c_1, \ldots, c_r)$.



46 / 71

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Error exhibited by a TDR computer with a Mackey-Glass kernel in a 3-lag quadratic memory task as a function of the separation between neurons d and the parameter γ , respectively. The points in the surfaces of the middle and right panels are the result of Monte Carlo evaluations of the NMSE exhibited by the discrete and continuous time TDRs, respectively. The left panel was constructed modeling the reservoir with an approximating VAR(1) model. University of St.Gallen



Error exhibited by a TDR computer with a Mackey-Glass kernel in a 6-lag quadratic memory task as a function of the separation between neurons d and the parameter η . The points in the surfaces of the middle and right panels are the result of Monte Carlo evaluations of the NMSE exhibited by the discrete and continuous time TDRs, respectively. The left panel verify of St.Gallen constructed modeling the reservoir with an approximating VAR(1) model.

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Optimal nonlinear information processing capacity in delay-based reservoir computers

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49 / 71

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Other applications of the reservoir model

• Evaluation of the finite sample training and testing errors: Given a reservoir output X of size T, the total mean square reservoir training error conditional on X and for any teaching signal Y, is given by

$$\begin{split} \mathrm{MSE}_{\mathrm{total},\lambda} \mid X &= \mathrm{trace}\left(\Sigma\right) \\ &+ \frac{1}{T} \mathrm{trace}[\mathrm{trace}\left(\Sigma\right) \left(R_{\lambda} \mathcal{X} A \mathcal{X}^{\top} \left(R_{\lambda} \mathcal{X} \mathcal{X}^{\top} - 2 \mathbb{I}_{N+1} \right) \right) \\ &+ \lambda^{2} T^{2} R_{\lambda} \mathcal{W} \mathcal{W}^{\top} R_{\lambda} \mathcal{X} \mathcal{X}^{\top}], \end{split}$$

where *N* is the number of neurons of the reservoir, $\mathcal{X} = (\mathbf{i}_T || X^\top)^\top$, and $\mathcal{W} := (\mathbf{a} || W^\top)^\top$ with $W := \Gamma(0)^{-1} \text{Cov}(\mathbf{x}(t), \mathbf{y}(t))$ and $\mathbf{a} := \boldsymbol{\mu}_y - W^\top \boldsymbol{\mu}_x$. Finally, $R_\lambda := (\mathcal{X} A \mathcal{X}^\top + \lambda T \mathbb{I}_{N+1})^{-1}$ and $\boldsymbol{\Sigma} := \text{Cov}(\mathbf{y}(t), \mathbf{y}(t)) - W^\top \Gamma(0) W$.

L. Grigoryeva, J. Henriques, L. Larger, J.-P. Ortega

- The RC defining features: Consider the reservoir model driven by the real valued and non-necessarily stationary input signal {z(t)}_{t∈ℤ}.
 - (i) Let $\mathbf{c} \in \mathbb{R}^N$ be an input mask and $\mathbf{I}(t) := \mathbf{c}z(t)$ the corresponding input forcing. Let

$$F_{I}^{R}(\mathbf{I}(t),\mathbf{x}_{0},\boldsymbol{\theta}) := \sum_{i=1}^{R} \frac{1}{i!} D_{\mathbf{I}}^{(i)} F(\mathbf{x}_{0},\mathbf{0}_{N},\boldsymbol{\theta}) \overbrace{\mathbf{I}(t) \otimes \cdots \otimes \mathbf{I}(t)}^{i \text{ factors}}$$

Assume that one of the following conditions holds:

(a) The map $F_l^R(\cdot, \mathbf{x}_0, \theta) : \mathbb{R}^N \to \mathbb{R}^N$ is injective. (b) The input signal is bounded.

If $A(\mathbf{x}_0, \boldsymbol{\theta}) := D_{\mathbf{x}}F(\mathbf{x}_0, \mathbf{0}_N, \boldsymbol{\theta})$ has no zero eigenvalues, then the reservoir model satisfies the separation property.

(ii) The input signal $\{z(t)\}_{t\in\mathbb{Z}}$ is strictly stationary with finite automoments up to order 2R and that it is bounded and the linear map $A(\mathbf{x}_0, \theta)$ is such that $||A(\mathbf{x}_0, \theta)|| < 1$, then the reservoir model satisfies the uniform fading memory property.

Application examples: usual benchmarks and early applications

- RC has outperformed well-established methods of nonlinear system identification, prediction, and classification (see [LJ09] for a review):
 - Prediction of chaotic dynamics (three orders of magnitude accuracy improvement [JH04])
 - Nonlinear wireless channel equalization (two orders of magnitude improvement [JH04])
 - Japanese Vowel benchmark (zero test error rate, previous best: 1.8% [JLPS07])
 - Financial forecasting (winner of the international forecasting competition $\mathsf{NN32}^1)$
 - Isolated spoken digits recognition (improvement of word error rate on benchmark from 0.6% of previous best system to 0.2% and further to 0% test error in more recent works [JLPS07, ASV⁺11, LSB⁺12, PDS⁺12, BSMF13])
 - NARMA model identification task [AP00, RT11].

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52 / 71

¹http://www.neural-forecasting-competition.com/NN3/index.htm < >>

L. Grigoryeva, J. Henriques, L. Larger, J.-P. Ortega

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Application examples: classification

- Deep RC networks outperform all state-of-the-art techniques in the written digit classification using the MNIST corpus [JDD⁺15]. RC halves the error exhibited by deep neural network committees and the results are robust with respect to the presence of various noises.
- A similar architecture [TJSM10] has shown performances comparable to state-of-the-art technology in the phoneme recognition problem based on the TIMIT corpus with a competitive training effort.
- Hi-Res EEG signals: monitoring of epileptic seizures in animals [BSVS09, BVvM⁺11, BVN⁺13, NDK11] and in the discrimination of the emotion valence in humans [KHBG15].
- Electrocardiogram signals (ECGs) [LS13].
- Fuel cell diagnostics [Hugo]



53 / 71

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Application examples: forecasting

- Industrial production time series [WSS08, WS10]
- Great Lakes water level in [Cou10]
- Short-term forecasting of wind speed [FLdA⁺08]
- Water inflow forecasting [SOP+07]
- Short-term electric consumption [DS12] and temperature [DOS13]
- Telephone calls load [BSU+15]
- Short-term stock price prediction [LYS09] with applications to intelligent stock trading systems [LYS11]



Application examples: volatility forecasting

• TDRs have been shown in [GHLO14] to outperform standard multivariate parametric models in the modeling of realized financial volatility and correlations.



Average realized volatility forecasting performance using RC and VEC(1,1) models estimated via maximum likelihood (MLE). The sMSFE reported is obtained with the estimated parametric models. All the TDRs considered have been generated using the nonlinear Macked Glassicker are ballen with p = 2.

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Stochastic nonlinear time series forecasting using time-delay reservoir computers: Performance and universality

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56 / 71

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A final example: volatility filtering

The standard ARSV model is given by the prescription

$$\begin{cases} y_t = \mu + \sigma_t \epsilon_t, & \{\epsilon_t\} \sim \text{IID}(0, 1) \\ b_t = \gamma + \phi b_{t-1} + w_t, & \{w_t\} \sim \text{IID}(0, \sigma_w^2) \end{cases}$$
(24)

where $b_t := \log(\sigma_t^2)$, $\gamma \in \mathbb{R}$, $\phi \in (-1, 1)$. Assume that $\{\epsilon_t\}$ and $\{w_t\}$ are uncorrelated (can be relaxed to account for the leverage effects and assymetric behaviour of stock prices). Observations:

- the process {σ_t} is a non-traded stochastic latent variable that, unlike in GARCH-like models [Eng82, Bol86] is not a predictable process that can be written as a function of previous returns and volatilities;
- the unique stationary returns process induced by (24) provided that $\phi \in (-1, 1)$ is a WN (no autocorrelation) with finite moments of arbitrary order.

- 3

57 / 71

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ARSV: estimation and filtering techniques

References on the model: Taylor [Tay86, Tay05]

- Bayesian approach: Jacquier et al. [JPR94], many others.
- Non-Bayesian approaches:
 - Harvey et al. [HRS94], Ruiz [Rui94] suggested a QML estimator based on the Kalman filter
 - Meyer et al. [MFB03] and Shimada and Tsukuda [ST05] use approximated linear filtering methods based on Laplace approximation to produce a MLE
 - h-likelihood estimation approach of Castillo and Lee [dCL08], [LWLdC11] based on treating the ARSV models as a GLM with varying random effects



58 / 71

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Performance comparison



L. Grigoryeva, J. Henriques, L. Larger, J.-P. Ortega

Time-delay reservoir computers

- Kalman testing error: 100.63%
- *h*-likelihood testing error: 82.50%
- Reservoir testing error (5 nodes, Ikeda kernel, optimized parameters): 73.88%
- No restrictions on the model prescription or on the innovations character



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62 / 71

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65 / 71

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Image: A matrix and a matrix

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