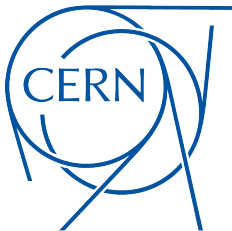
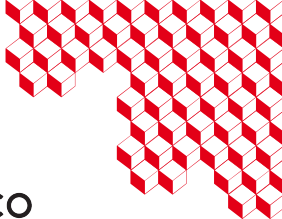




irfu



POLITECNICO  
MILANO 1863



## ESN for DA

Quentin BRUANT, Barbara DALENA (CEA/IRFU)

Future Circular Collider– France/Italy

November 4, 2024



Thanks to the work of M.Casanova (CEA/IRFU-Politecnico), M.Giovanozzi (CERN),  
L.Bonaventura (Politecnico di Milano)

# Table of contents

- 1. Dynamic Aperture (DA)**  
Bonded movement phase-space  
DA and Scaling Law (SL)
- 2. Echo State Network and DA**  
Echo State Network  
Shallow ESN  
Deep ESN
- 3. Results**  
Data splitting  
Hyperparameters





# 1. Dynamic Aperture (DA)

# Table of contents

- 1. Dynamic Aperture (DA)**  
Bonded movement phase-space  
DA and Scaling Law (SL)
2. Echo State Network and DA
3. Results

# Dynamic Aperture

## Bonded movement phase-space

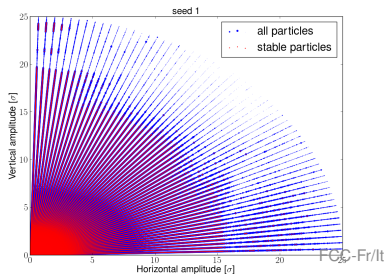
### Bonded movement phase-space region

$$\mathcal{A}(N) = \int \int \int \int \chi(x_1, x_2, p_{x_1}, p_{x_2}) dx_1 dx_2 dp_{x_1} dp_{x_2}$$

$$\chi(x_1, x_2, p_{x_1}, p_{x_2}) = \begin{cases} 1 & \text{if the motion starting at } (x_1, x_2) \\ & \text{with momentum } (p_{x_1}, p_{x_2}) \text{ is bounded after } N \text{ turns} \\ 0 & \text{else} \end{cases}$$

Illustration with  $(p_{x_1}, p_{x_2}) = (0, 0) \Rightarrow$

$$DA = \left( \frac{2\mathcal{A}(N)}{\pi^2} \right)^{\frac{1}{4}}$$



# DA and Scaling Law

## Scaling Law (SL)[1]

$$DA(N) = \frac{b}{\left(\mathcal{B} \ln \frac{N}{N_0}\right)^\kappa}$$

## SL derivative

$$\frac{dDA}{dN}(N) = -\frac{bk}{N} \mathcal{B}^{-k} \ln \left( \frac{N}{N_0} \right)^{-k-1}$$



# 2. Echo State Network and DA

# Table of contents

1. Dynamic Aperture (DA)
- 2. Echo State Network and DA**
  - Echo State Network
  - Shallow ESN
  - Deep ESN
3. Results





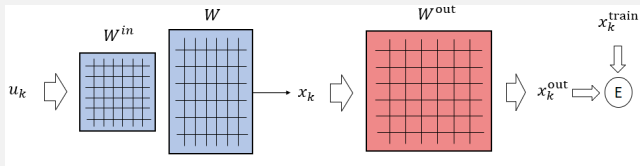


- Recurrent Neural Network (RNN) using the Reservoir Computing approach.
- Fast training
- Usually less prone to over-fit
- Predictive algorithm

Universal approximator of Dynamical Systems [5]

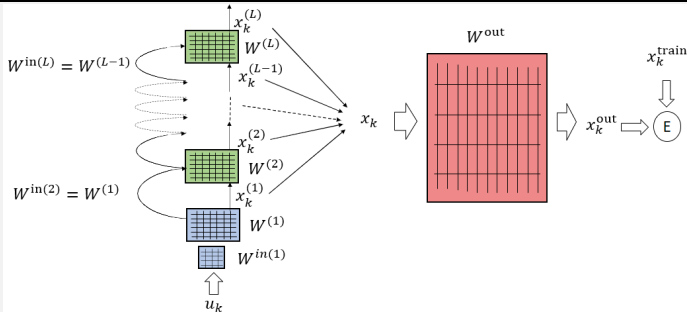
# Shallow ESN

## Shallow ESN



$$x_k = \left(1 - a \frac{\Delta t}{c}\right) x_{k-1} + \frac{\Delta t}{c} f(W^{in} u_k + W x_{k-1}) \quad W^{out} = \operatorname{argmin} \left\{ \frac{1}{M} \sum_{i=0}^M \left( \sum_{k=Bl+1}^{k_{train}} (x_{ik}^{out} - x_{ik}^{train})^2 - \beta \|w_i^{out}\|^2 \right) \right\}$$
$$x_k^{out} = g(W^{out} [x_k; u_k]) \quad W^{out} = X^{train} X^T (X X^T + \beta I)^{-1}$$

# Deep ESN



$$x_k^{(l)} = \left(1 - a \frac{\Delta t}{c}\right) x_{k-1}^{(l)} + \frac{\Delta t}{c} f \left( W^{(l-1)} x_k^{(l-1)} + W^{(l)} x_{k-1} \right), l \geq 1$$

# Echo State Property (ESP)



Echo State Property [4]: assure stability for zero-input case

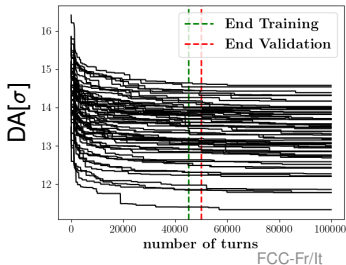
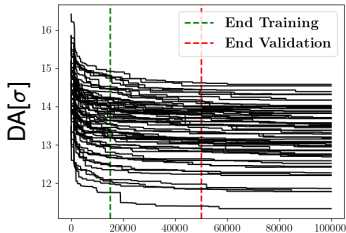
$$\tilde{W} = \frac{\Delta t}{c} |W| + \left(1 - a \frac{\Delta t}{c}\right) I \quad (3)$$

$$\rho(\tilde{W}) < 1 \wedge f : \mathbb{R}^{N_r} \rightarrow \mathbb{R}^{N_r}, x \mapsto \tanh x \quad (4)$$

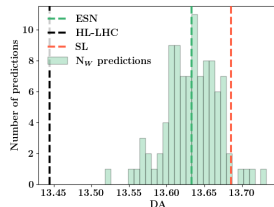
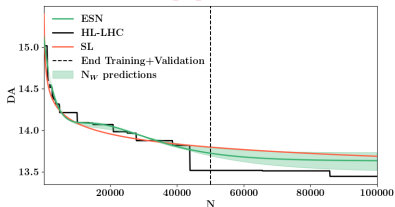
*Sufficient, **not necessary***

# Data set & splitting

- High-Luminosity LHC, simulated
- 60 configurations → 60 distributions in magnetic lattice
- nominal parameters ( $\sqrt{s} = 14$  TeV,  $\beta_{x,y}^* = 15$ cm,  $\epsilon_{x,y} = 3.75$   $\mu$ m)
- DA is shown as normalized to the  $\sigma$  of the beam



# Ensemble approach



## Ensemble approach

- Generate randomly  $N_w$  pair of  $(W_{in}, W)$
- Train and validate all the pairs on the same data set and find a set of hyperparameters minimizing the RRMSE<sup>1</sup> on the validation set for all configurations
- For each configuration, compute the RRMSE w.r.t the data.
- Normalize the prediction on the number  $N_w$  of pairs  $(W_{in}, W)$

1

$$RRMSE^{set}(x^{target}, x_{mean}^{out})[\%] = \frac{100}{N_w} \sum_{i=1}^{N_w} \sqrt{\frac{\sum_{k=1}^{k_{set}} (x_{mean,k}^{out,i} - x_k^{target,i})^2}{\sum_{k=1}^{k_{set}} (x_k^{target,i})^2}}$$



## SL alone

Benchmark. Fit on the training and validation sets

## SL ALL

In use today. SL fitted on all the data set ( $N \approx 1 \times 10^5$ ).

## ESN only

Basic model

ESN trained on the train set, hyperparameters' optimization on the validation and predictions on test set

## SL+ESN

Most evolved model

SL fitted on the training and validation set and on the ESN predictions on the test set



# 3. Results



# Table of contents

1. Dynamic Aperture (DA)

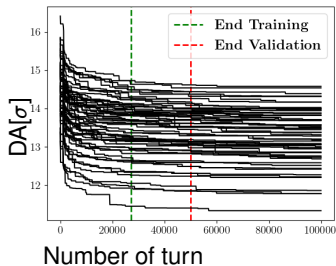
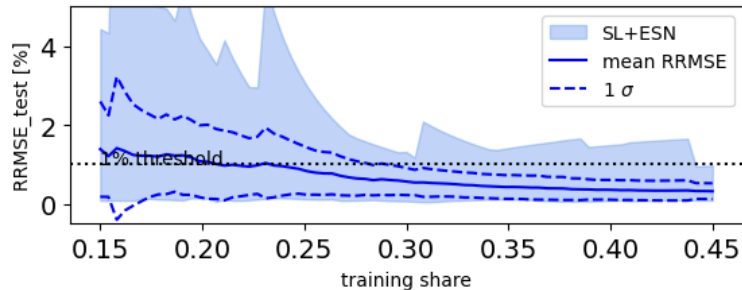
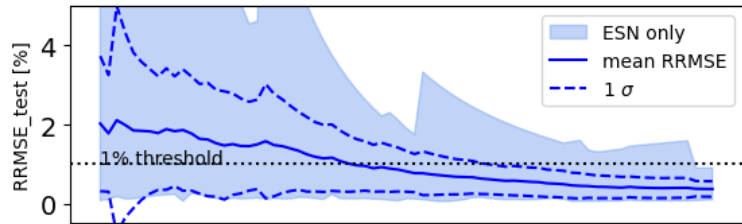
2. Echo State Network and DA

**3. Results**

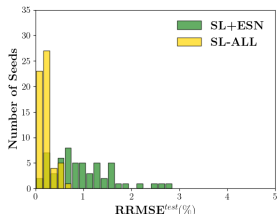
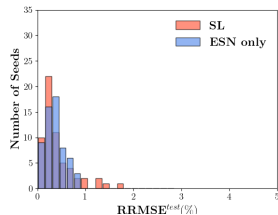
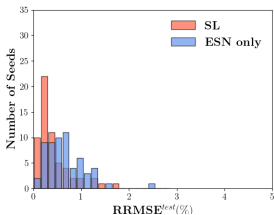
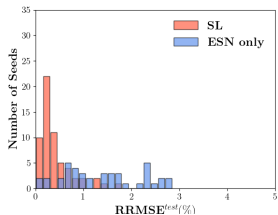
Data splitting

Hyperparameters

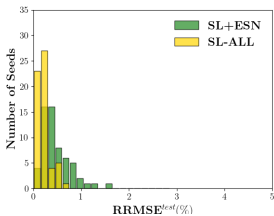
# Evolution of error w.r.t training share



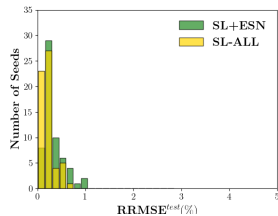
# Model Comparison on Projection



(a) 21%

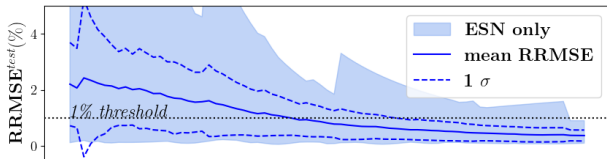


(b) 33%



(c) 45%

# Linking data splitting to SL derivative

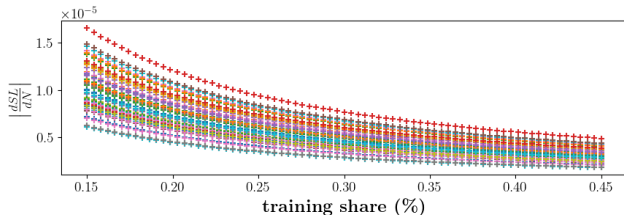


$$\frac{dDA}{dN}(N) = -\frac{bk}{N} \mathcal{B}^{-k} \ln\left(\frac{N}{N_0}\right)^{-k-1}$$

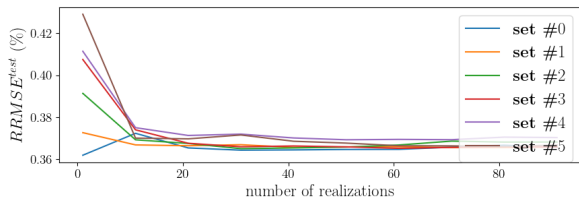
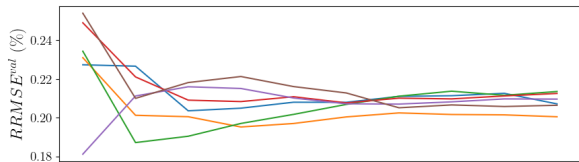
■ the 1% mean RRMSE threshold is achieved around the 30% training mark

■ Matches with  $\left|\frac{dSL}{dN}\right| \approx 5 \times 10^{-6}$

■ Matches with  $\sigma\left(\left|\frac{dSL}{dN}\right|\right) \approx 2 \times 10^{-6}$

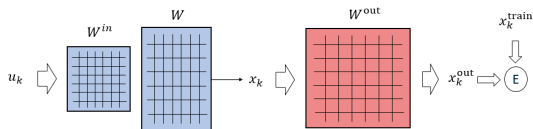


# Random variability control



Parameters: Training share: 45%, Validation: 5%

Most stable value for realizations  $\approx 60$



# Hyperparameters (probabilistic systematic optimization)

Main objective: Use Bayesian Optimization to accelerate the finding of the optimum set of hyperparameters

Tool: hyperopt library

| Set # | $L$ | $N_r$ | $BI$ | dt    | $\beta$ | $\rho$ | Time(s) | $RRMSE_{max}^{test}$ | $RRMSE_{mean}^{test}$ |
|-------|-----|-------|------|-------|---------|--------|---------|----------------------|-----------------------|
| 1     | 2   | 20    | 2    | 0.171 | 1.387   | 1.293  | 14801.7 | 2.261                | 0.925                 |
| 2     | 2   | 15    | 2    | 0.138 | 0.379   | 0.537  | 18039.4 | 1.518                | 0.499                 |
| 3     | 1   | 30    | 2    | 0.111 | 0.618   | 0.298  | 7557.7  | 1.901                | 0.552                 |
| 4     | 1   | 20    | 2    | 0.025 | 1.877   | 1.259  | 6249.9  | 1.336                | 0.449                 |
| 5     | 1   | 10    | 2    | 0.432 | 0.561   | 0.181  | 10438.5 | 2.674                | 1.112                 |

Table: Set of optimized hyperparameters via hyperopt

| $L$ | $N_r$ | $BI$ | dt    | $\beta$ | $\rho$ | $RRMSE_{max}^{test}$ | $RRMSE_{mean}^{test}$ |
|-----|-------|------|-------|---------|--------|----------------------|-----------------------|
| 1   | 20    | 0    | 0.009 | 0.0224  | 0.19   | 0.892                | 0.365                 |

Table: "by-hand" optimized set of parameters

# Conclusion



## Data Splitting

- The main threshold (1% mean RRMSE) is attained with  $\approx 30\%$  training and no great improvement beyond.

## link to SL derivative

- Possible to link Scaling Law derivative to data splitting for automation purposes

## Hyperparameters

- hyperopt library find similar set than "by-hand" optimization, the caveat being its sequential implementation taking too much time for a full automation



## Data Splitting

- Investigate the outlier configurations

## Link to SL derivative

- Try the automation of the splitting based on the 2 parameters described
- Investigate the link to second derivative

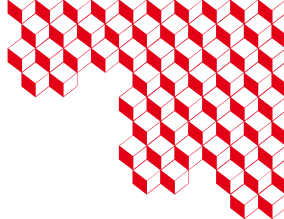
## Hyperparameters

- Working on a custom-made script for a full parallel optimization





irfu



**Thank you !**

**CEA SACLAY**

91 191 Gif-sur-Yvette Cedex  
France

[quentin.bruant@cea.fr](mailto:quentin.bruant@cea.fr)

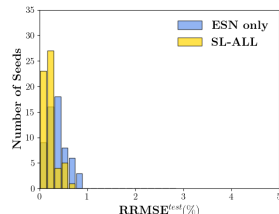
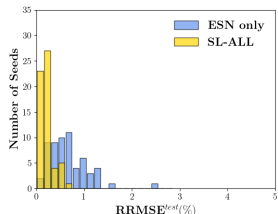
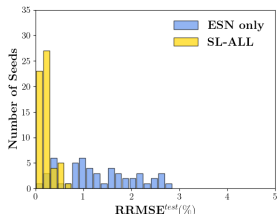
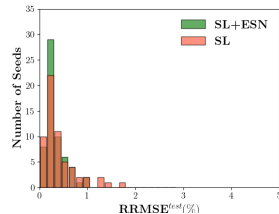
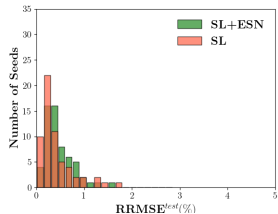
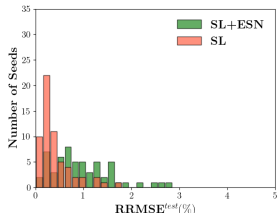
[barbara.dalena@cea.fr](mailto:barbara.dalena@cea.fr)

# References I

- [1] **A. Bazzani et al.** “Advances on the modeling of the time evolution of dynamic aperture of hadron circular accelerators”. In: *Phys. Rev. Accel. Beams* 22 (10 Oct. 2019), p. 104003. DOI: 10.1103/PhysRevAccelBeams.22.104003. URL: <https://link.aps.org/doi/10.1103/PhysRevAccelBeams.22.104003>.
- [2] **J. Bergstra, D. Yamins, and D. D. Cox.** “Making a Science of Model Search: Hyperparameter Optimization in Hundreds of Dimensions for Vision Architectures.”. In: *30th International Conference on Machine Learning (ICML 2013)*. 2013, I-115 to I-23.
- [3] **Eric Brochu, Vlad M. Cora, and Nando de Freitas.** *A Tutorial on Bayesian Optimization of Expensive Cost Functions, with Application to Active User Modeling and Hierarchical Reinforcement Learning*. 2010. arXiv: 1012.2599 [cs.LG].

## References II

- [4] M. Casanova et al. “Ensemble Reservoir Computing for Dynamical Systems: Prediction of Phase-Space Stable Region for Hadron Storage Rings”. In: *The European Physical Journal Plus* 138 (2023). DOI: 10.1140/epjp/s13360-023-04167-y. URL: <https://doi.org/10.1140/epjp/s13360-023-04167-y>.
- [5] Lyudmila Grigoryeva and Juan-Pablo Ortega. *Echo state networks are universal*. 2018. arXiv: 1806.00797 [cs.NE].



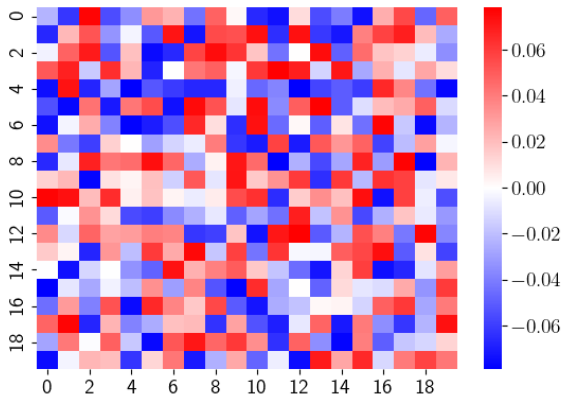


Figure: Reservoir matrix

Use of Tree Parzen Estimator (TPE)[2, 3].

Bayesian Optimization

Main goal:

$$x_{opt} = \arg \min_x f(x)$$

$$P(y|x) \propto P(x|y)P(y)$$

TPE models  $P(x|y)$  and  $P(y)$  by building "probability-density" functions:

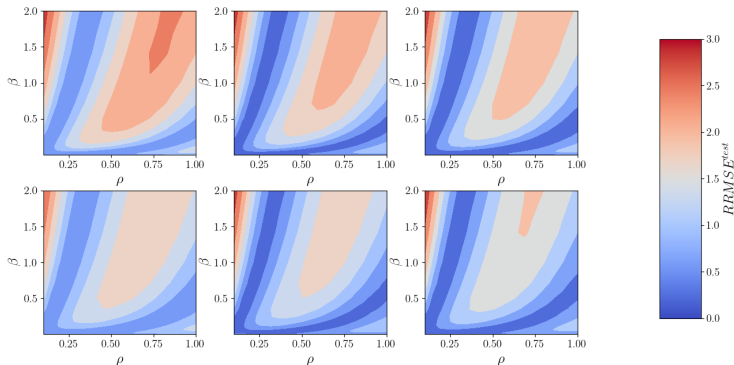
$$P(x|y) = \begin{cases} l(x) & \text{if } y < y^* \\ g(x) & \text{if } y > y^* \end{cases}$$

where  $y^* = \min\{f(x_i), 1 \leq i \leq n\}$  But no specific model for  $P(y)$  is required

# Hyperparameters (mapping)

$$W^{out} = X^{train} X^T (X X^T + \beta I)^{-1}$$

$$\rho = \rho(\tilde{W})$$



Scan of  $(\beta, \rho)$  set of hyperparameters ( $L = 1, N_r=20, BI=0, dt=0.009$ )

From Left to Right, Top to Bottom: Training share: 35%, 37%, 39%, 41%, 43%, 45%