Faculty of Science

Echo State Networks and Anomaly Detection in Simulation Data

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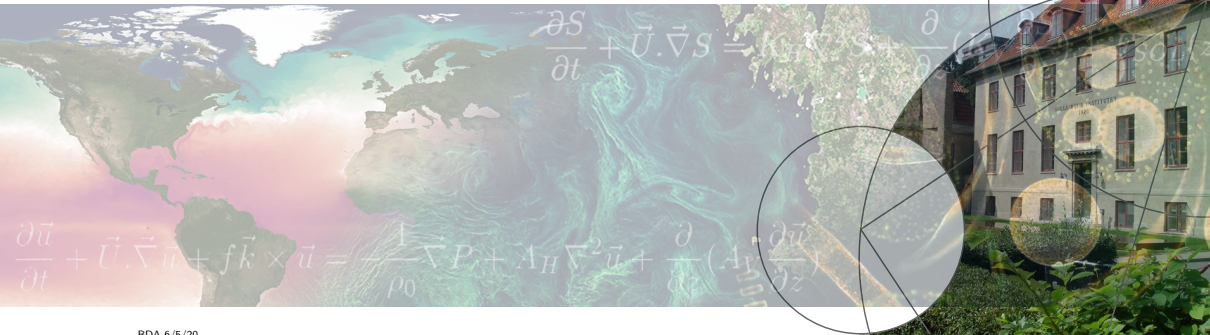
Niels Bohr Institute, University of Copenhagen



The Trouble with RNN

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Difficulties in Training RNN

RNN are extremely versatile, but the high expressiveness comes at cost.

Under the right definition, RNN are:
Turing complete $\implies$ universal ($\implies$ training uncomputable).

In practice:
Restricted but very large expressiveness, with expensive but (usually) computable training.

Difficulties in Training RNN

Back-Propagation Through Time (BPTT) unrolls recurrent network graph (like unrolling a loop in a computer program), yielding static but very deep network.

Two problems arise:

1. Optimizing becomes extremely resource intensive
2. ...and can fail completely (due to e.g. vanishing gradients, bifurcations in the state space).

What are state space bifurcations?

Consider an RNN with just a single variable:

$$x_{t+1} = \tanh(wx_t + b)$$

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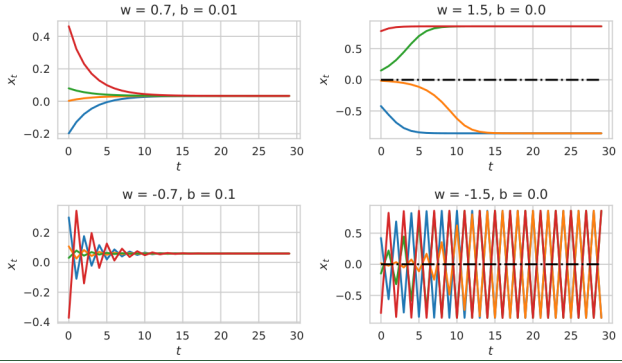
Stable and unstable fixed-points (attractors and repellers):



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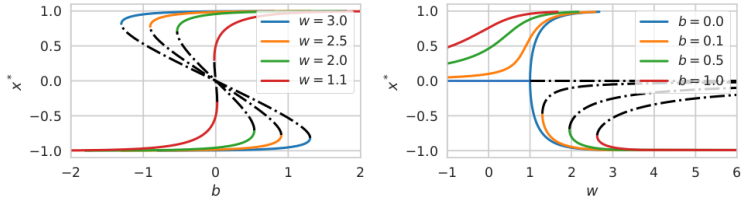
Bifurcations happen when attractors split into two (or more):



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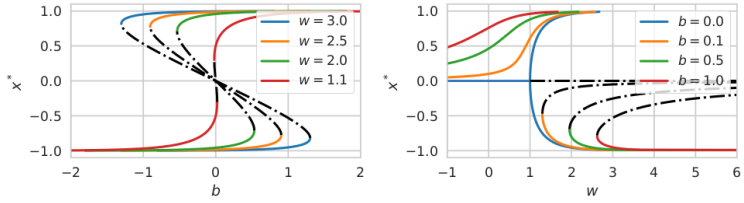


Resulting huge gradients can destroy hundreds of learning steps in a single iteration.

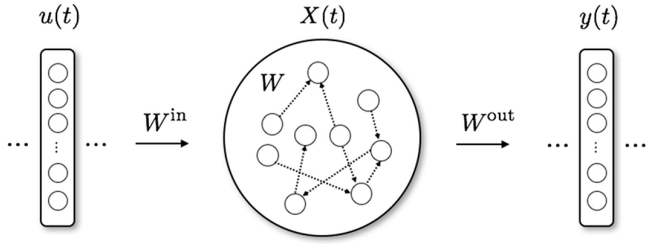
Echo State Networks

Comparison between LSTM and ESN

ESN are *much* weaker than general RNN, and weaker than LSTM, but are simple, extremely fast to train, and most importantly: stable.

	RNN	LSTM	ESN
Expressive Power	∞	Very strong	Medium
Vanishing Gradients	Yes	No	No
Many local minima	Yes	Yes	No
Training Bifurcations	Yes	Yes	No
Convergence can fail	Yes	Yes	Nothing to Converge
Training time	∞	Very Slow	Very Fast

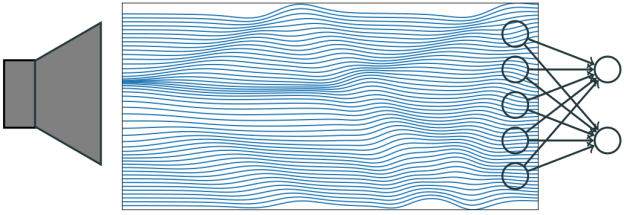
How is it Done?



$$\vec{x}_{t+1} = \varphi\left(\mathbf{W}^{\text{in}}\vec{u}_t + \mathbf{W}\vec{x}_t\right)$$
$$\vec{y}_{t+1} = \psi\left(\mathbf{W}^{\text{out}}\vec{x}_{t+1}\right)$$

Only output matrix $\mathbf{W}^{\text{out}}$ is trained. If ψ is identity, training is just solving a least-squares problem!

An ESN Metaphor: Pattern Recognition in a Bucket



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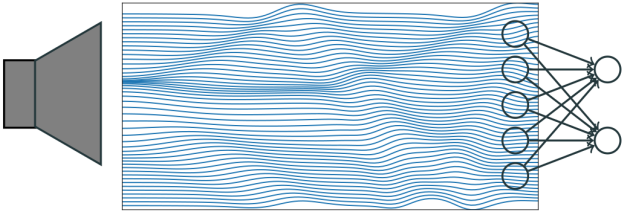

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Hidden matrix $\mathbf{W}$ must be sparse, but connected:

1. Sparsity provides "locality" condition: Every hidden variable gets a "neighbourhood" of its neighbours, from which information can gradually propagate.
2. Connectedness makes sure that information eventually reaches everywhere.
3. Bonus: Sparsity makes matrix-vector multiplication $\mathcal{O}(n)$ instead of $\mathcal{O}(n^2)$.

The *eigenvalues* of the hidden matrix **W** control how memory attenuates.

In particular, we need to scale **W** to have a desired *spectral radius* $\rho(\mathbf{W}) \simeq 1$, so that it neither **explodes** ($\rho \gg 1$) or **dies out** ($\rho \ll 1$).

In the "waves in a bucket" metaphor, ρ is like the viscosity of the fluid.

Performance

The main selling point of ESN is how efficiently they can be trained:

Instead of gradient descent (heavy, can fail to converge), training is a single deterministic least-squares calculation.

The predictions are: $\mathbf{y}_t = \mathbf{W}^{\text{out}}\mathbf{x}_t$, where $\mathbf{x}$ is the input concatenated with the current state.

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This can be optimized in a single step by solving the $N_{\text{hidden}} \times N_{\text{out}}$ least-squares problem

$$\mathbf{W}^{\text{out}} = \arg\min_{\mathbf{W}} \|\mathbf{W}\mathbf{X} - \mathbf{D}\|^2 + \beta^2 \|\mathbf{W}\|^2$$

This is so fast, that we can do online training!

An Example: A Chaotic Time Sequence

Mackey-Glass sequence:

$$\frac{\partial y(t)}{\partial t} = \beta \frac{y(t-\tau)}{1+y^n(t-\tau)} - \gamma y(t)$$

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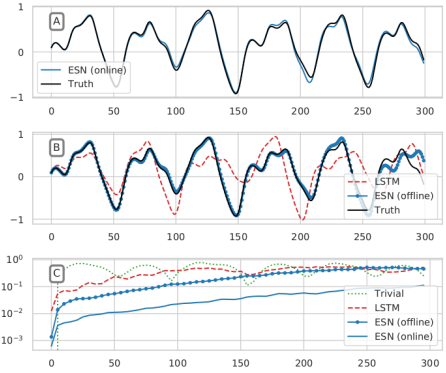

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Anomaly Detection

Anomaly Detection

Once we have an RNN that can "understand" a sequence well enough to predict it somewhat reliably, we can use it to automatically discover when it starts behaving strange.

Knowing that something weird is going on, even a little bit in advance, can save lives and resources...

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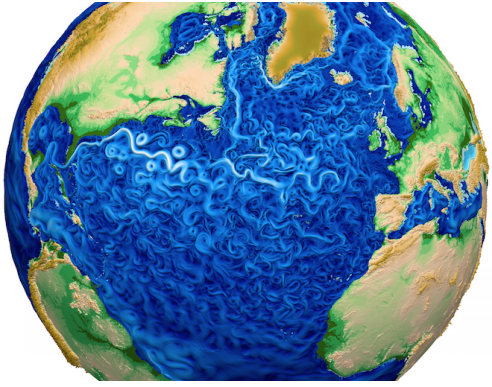
Knowing that something weird is going on, even a little bit in advance, can save lives and resources... everywhere!

E.g.: Detecting failure in nuclear reactors, engine break down, weather event, etc. before they happen.

Anomaly Detection in Climate Simulations

We'll look at discovering weird phenomena in *climate simulation data*:



Challenge:

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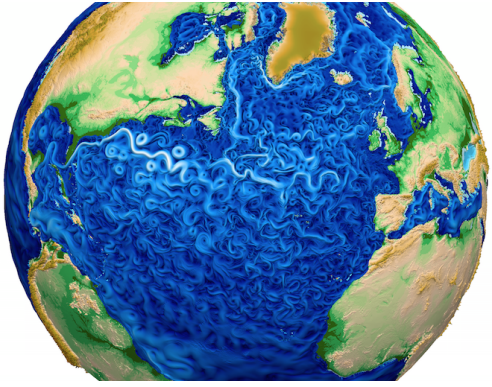

Challenge: Enormous data sets, gigabytes per time step, terabytes in total.

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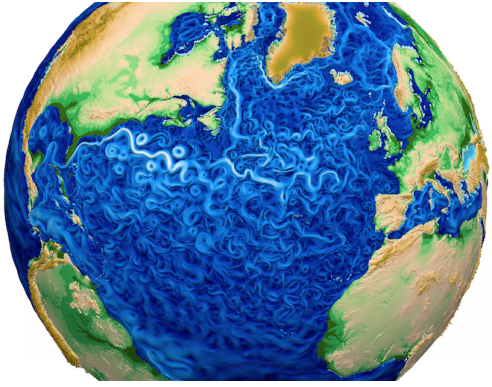


Challenge: Enormous data sets, gigabytes per time step, terabytes in total.
High-dimensional; ESN only really work for 1D sequences.

Anomaly Detection from Predictions

Idea: Given a good method for prediction, we quantify normal behaviour as *how well we were able to predict it*.

Choose a window size T at the same scale as the anomalies we wish to discover. To evaluate the *normality* of step t, start at $t - T/2$, and predict T steps, until $t + T/2$.

Now compare $y_{t-T/2}, \ldots, y_{t+T/2}$ to the real data. The integral of the error is used to calculate a *normality score*. If the error suddenly becomes much bigger than usual, we may have discovered an *anomaly*.

Example in 1D: Mackey-Glass

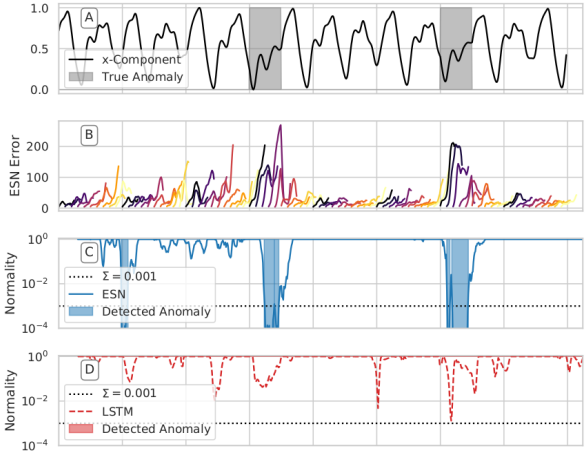
We use the chaotic equation from before

$$\frac{\partial y(t)}{\partial t} = \beta \frac{y(t-\tau)}{1+y^n(t-\tau)} - \gamma y(t)$$

and train on 2000 steps with $\gamma = 0.10$.
In the anomaly-detection phase, we change γ to 0.13 for 50 steps at random steps.

Result:

The difference is imperceptible to humans, but we catch both instances with our ESN predictor.



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Extending ESN to Finite-Difference Simulations

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Finite-difference simulations are:

1. Simulation of fields with values on a regular grid, similar to *images*.
2. Generally smooth or close to it: few, localized discontinuities, if any.
3. Spatially and temporally correlated: guided by differential equations that determine value from neighbours in time and space.

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Let's exploit this structure!

Extending ESN to Finite-Difference Simulations

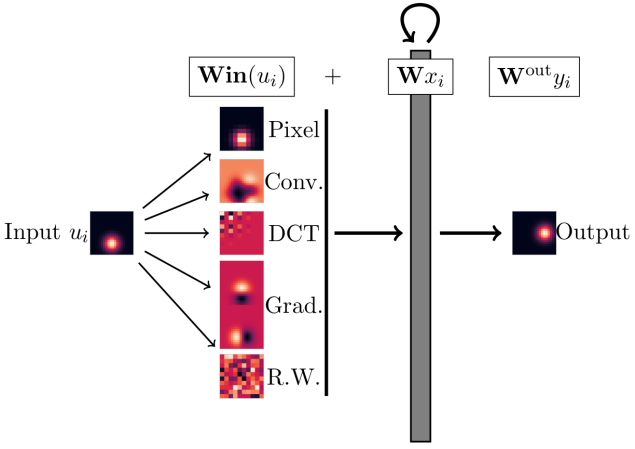
Recall: In standard ESN, we need to map input to a much higher-dimensional hidden space, where the recurrence happens.

This map, $\mathbf{W}^{\text{in}}$ is uniformly random, and throws away all information about spatial and temporal locality, and other interdependence between variables. Let's not do that!

Idea: Replace random map with one that preserve meaningful features.

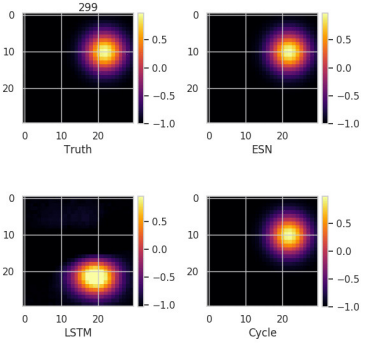
Extending ESN to Finite-Difference Simulations

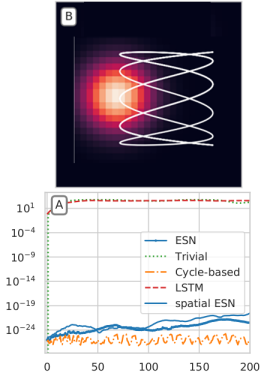
We stack convolutions, derivatives, cosine transform. Other useful maps could be divergence, curl, turbulence, etc.



Video of Blob in Periodic Lissajous Pattern

$$(x, y) = (cos(\alpha t), sin(\beta t))$$

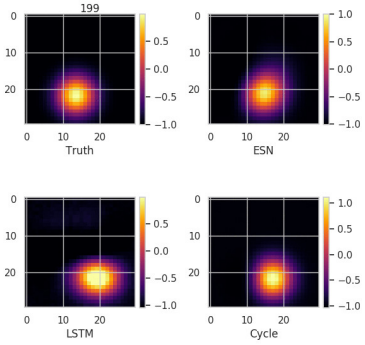


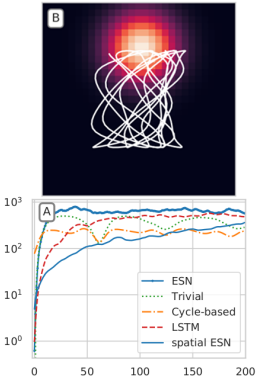


Trained on 2000 steps, predicting 300 into the future.

Video of Blob in Chaotic Mackey-Glass Pattern

$$(x, y) = (\text{mackey}(t), sin(t))$$





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Finding Anomalies in Ocean Simulation Data

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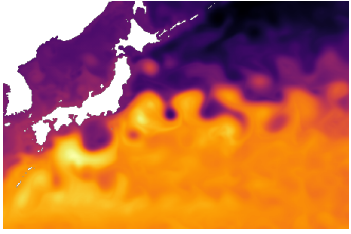
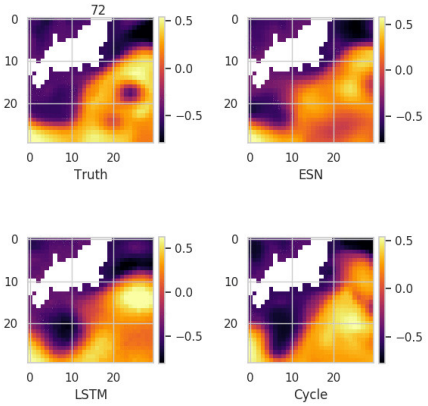
We trained on 10 years of simulation data, and then evaluated normality through 5 years. For each step, we predicted a year into the future, and calculated a normality score from the total error during the period.

The goal was to automatically discover a known ocean phenomenon: The Kuroshio (“Black Tide”).



Kuroshio Ocean Current off the Coast of Japan



Trained on first 10 years of 5-day means (730 steps), predict one year (73 steps) into the future for 5 remaining years (365 times).

Localizing an anomaly in space

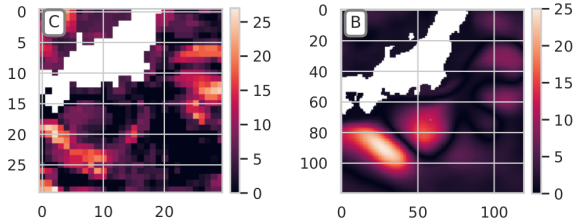
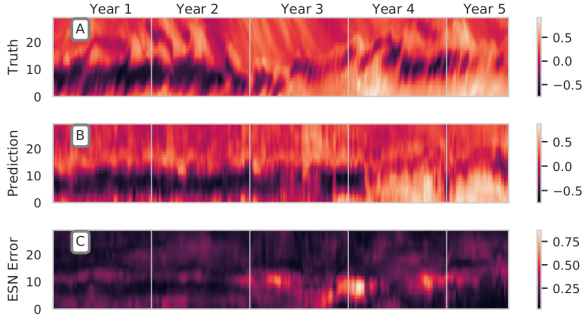


Figure: Left: a “heat map” of low normality scores, accumulated over the 5 year prediction period. Right: Known localization if the Kuroshio phenomenon.

Localizing an anomaly in time



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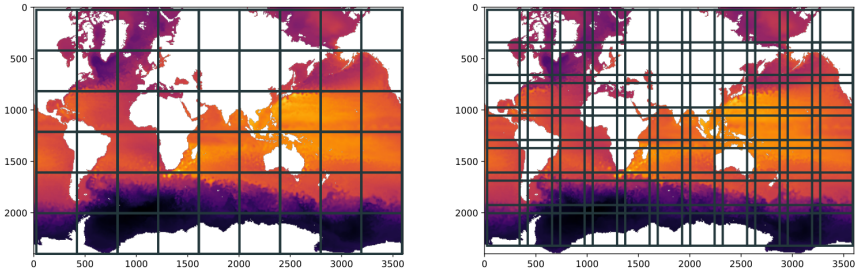
The Next Stage

Scour the (simulated) Seven Seas for new oceanographic phenomena!



Needs new development that allows us to scale up the methods to the world.
Possible MSc project!