Machine Learning for Forecasting and Data Assimilation

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Partially funded by ARO, DARPA, and LTS
Machine Learning

- Machine-learning algorithms are trained with data to perform a particular task, such as classification.

- Starting from generic input-output equations, training means choosing parameter values that minimize the difference between the actual outputs and the desired outputs ("supervised" learning).

- In most applications, the task is static; training data is a set of input-output pairs.

- Reservoir computing is a type of machine learning well suited to dynamic tasks, mapping an input time series to an output time series.
Forecasting and Attractor Reconstruction

- We seek to use reservoir computing to create an ad hoc forecast model, based only on a finite-time sample (training data) from a dynamical system.

- We are interested in two tasks for our forecast model:
  - Forecast "weather": Predict future measurements (only feasible in short-term for chaotic systems).
  - Learn "climate": Reproduce long-term properties of a chaotic attractor, such as Lyapunov exponents.
Reservoir Computing

- A **reservoir** is a driven dynamical system whose internal parameters are not adjusted to fit the training data; only a linear post-processor is trained.

- **Train** the reservoir by driving it with an input time series $u(t)$ and fitting a linear function of the reservoir state $r(t)$ to a desired output time series $v(t)$.

- This approach was proposed as Echo State Networks (Jaeger 2001) and Liquid State Machines (Maass, Natschlaeger, Markram 2002); see [http://www.scholarpedia.org/article/Echo_state_network](http://www.scholarpedia.org/article/Echo_state_network)

- A reservoir can be a (super-fast) hardware device.
Reservoir During Training

reservoir state $r(t)$

Matrices $W_{in}$ and $M$ are chosen randomly in advance.
Continuous-Time Jaeger ESN

- **Listen:** \[ \beta \frac{dr}{dt} = -r(t) + \tanh[Mr(t) + W_{in}u(t) + c] \]
  
  (in software, solve with Euler time step $\tau$).

- We choose $M$ and $W_{in}$ at random, scaling $M$ to have spectral radius close to 1 and scaling $W_{in}$ so that $W_{in}u$ is of order 1.

- We choose $\beta$ commensurate with the input time scale and we listen for $0 \leq t \leq T$, where $T$ is the duration of the training time series $u(t)$.

- **Fit:** Find the matrix $W_{out}$ such that $\hat{v}(t) = W_{out}r(t)$ least-squares minimizes the residuals $\hat{v}(t) - v(t)$ for $0 \leq t \leq T$. 


Inference Task (DA w/o Model)

- Suppose that we can inexpensively measure some state variables of a dynamical system, but other variables of interest are difficult to measure.

- Let $u(t)$ consist of state variables that can be measured for all time, and $v(t)$ consists of state variables that are only measured for $0 \leq t \leq T$.

- After training, we continue to evolve the listening equation for $t \geq T$, attempting to infer $v(t)$ from $u(t)$.

- The estimated value of $v(t)$ is $\hat{v}(t) = W_{out} r(t)$. 
Example: Lorenz System

• We ran the Lorenz system with time step $\tau = 0.05$:
  \[
  \frac{dx}{dt} = 10(y - x), \quad \frac{dy}{dt} = x(28 - z) - y, \quad \frac{dz}{dt} = xy + 8z/3.
  \]

• For training, we used $u(t) = [x(t)]$ and $v(t) = [y(t), z(t)]^T$.

• We trained a 400-node reservoir (meaning that the dimension of $r(t)$ is 400) for training time $T = 200$.

• Details are in (Lu et al., Chaos, 2017).
Inferring Lorenz $y(t)$ and $z(t)$ from $x(t)$
Forecasting with Feedback

• Suppose training data is sampled at time interval $\tau$, but we want to forecast farther than $\tau$ into the future.

• One option is to train with lead time $n\tau$ [that is, set $v(t) = u(t + n\tau)$] for the value(s) of $n$ of interest.

• We’ve gotten better results by training with lead time $\tau$ and iterating the trained time-$\tau$ forecast $n$ times.

• We train with desired output $v(t) = u(t + \tau)$ and then forecast with $u(t)$ replaced with $\hat{u}(t)$.

• This feedback approach (Jaeger & Haas 2004) can be used with other machine-learning methods.
Forecast Model for $t > T$

Predict:

$$\beta \frac{dr}{dt} = -r(t) + \tanh[Mr(t) + W_{in}\hat{u}(t)]$$

$$\hat{u}(t) = W_{out}r(t - \tau)$$
Lorenz system: Actual and Predicted $z(t)$
Actual and Predicted Attractors
Poincaré Section of Successive $z(t)$ Maxima

$z_{n+1}^{\text{max}}$ vs $z_n^{\text{max}}$

Actual vs Predicted
Questions Raised

• How can a reservoir “learn” these dynamics? Is there an approximate copy of the Lorenz attractor in the high-dimensional $r(t)$ system that we chose independently of the training data?

• No – the feedback term in our forecast model depends on the matrix $W_{out}$ determined from training.

• We have found an approximation to the Lorenz system in a family parametrized by $W_{out}$, which has more than 1000 entries.

• But how is it feasible to find appropriate parameter values in practice? Partial theory to follow.
Theoretical Framework

• During training/listening, the reservoir and its input form a “skew product” or “drive-response” system:

  • Input Dynamics (Drive): \( u(t + \tau) = f[u(t)] \)

  • Listening (Response): \( r(t + \tau) = g[r(t), u(t)] \)

• Assume that \( f \) and \( g \) are continuous on Euclidean spaces, that \( f \) is invertible, and that \( u \) lies in a compact attracting set \( A \).

• If \( g \) is uniformly contracting w.r.t. \( r \), then as \( t \to \infty \), the reservoir state \( r(t) \) becomes independent of its initial state (roughly, Jaeger’s “echo state property”).
Generalized Synchronization

• Furthermore, we get generalized synchronization: there is a continuous function $\phi$ on $A$ such that $r(t) - \phi(u(t)) \to 0$ as $t \to \infty$ [short proof in (Stark 1997)].

• Asymptotically, the reservoir state $r(t)$ is a function of the current input $u(t)$ only, not the entire history of $u$. However, we don’t know the function $\phi$ in practice.

• Uniform contraction can be guaranteed by choice of $g$, but strong contraction may inhibit extraction of $u$ from $r$ [extreme case: if $g$ is identically 0, then so is $r$].
Inverting the Synchronization Function

- If $r$ is much higher-dimensional than the attractor $A$, then embedding theory (Sauer-Yorke-Casdagli 1991) suggests that $\phi$ is likely to be one-to-one on $A$.

- If so, the inverse of $\phi$ on the set $\phi(A)$ can be extended to $r$-space in many ways.

- **Fitting**: In training, we attempt to find a linear function $W_{out}$ that approximately inverts $\phi$ on $\phi(A)$:

  $$u(t) \approx W_{out}r(t) \approx W_{out}\phi(u(t)).$$

- This does not require $\phi$ to be approximately linear. It requires only that we can approximate the nonlinear function $\phi^{-1}$ on a low-dimensional set by a linear function on a high-dimensional space.
Attractor Reconstruction and Stability

- If training is successful, then our forecast model
  \[ r(t + \tau) = g[r(t), W_{out}r(t)] \] (1)
  approximates [on \( \phi(A) \)] the idealized model
  \[ r(t + \tau) = g[r(t), \phi^{-1}(r(t))] \]. (2)

- Generalized synchronization implies that system (2) is conjugate to true dynamics \( u(t + \tau) = f(u(t)) \) on \( A \).

- To reproduce the climate of \( A \) in practice, we need system (1) to approximate an extension of system (2) that makes \( \phi(A) \) attracting.

- More “theory” in (Lu et al., Chaos 2018).
Kuramoto-Sivashinsky PDE

• We tested our methods on the spatiotemporally chaotic KS system

\[ u_t = -uu_x - u_{xx} - u_{xxxx} \]

with periodic boundary condition \( u(x + L, t) = u(x, t) \).

• With system size \( L = 60 \), we trained a 9000-node reservoir for time \( T = 20000 \) to predict the (numerical) KS solution.

• The largest Lyapunov exponent is \( \Lambda_{max} \approx 0.1 \), so we trained for roughly 2000 Lyapunov times.

• Details are in (Pathak et al., Chaos 2017).
Kuramoto-Sivashinsky Forecast

Top: “Truth”  Middle: Reservoir  Bottom: Error

\[ \mathcal{X} \]

\[ \Lambda_{\text{max}} t \]
Estimation of Lyapunov Exponents

Actual exponents

Reservoir exponents
Hybrid Forecasting

- Suppose we have an imperfect knowledge-based forecast model for a physical system.

- A hybrid method uses machine learning to improve (rather than replace) the model.

- We train by feeding the same input to the model and the reservoir, and optimize a linear combination of the model output and the reservoir output.

- We tested on the KS system with $L = 35$, using an imperfect model that replaces $u_{xx}$ with $(1 + \varepsilon)u_{xx}$.

- Details in (Pathak et al., Chaos 2018).
Hybrid Architecture

Knowledge-Based Model

\[ M \]

Input: \[ u(t) \]

\[ W_{in} \]

Reservoir

\[ W_{out} \]

Output: \[ \hat{u}(t + \Delta t) \]
Forecast Errors: 8000 nodes, $\epsilon = 0.01$

Top: Model  
Middle: Reservoir  
Bottom: Hybrid

Lyapunov times
Forecast Errors: 500 nodes, $\varepsilon = 0.1$
Parallel Reservoir Architecture

• We developed a method for forecasting high-dimensional, spatially extended systems with multiple reservoirs that can process in parallel (Pathak et al., PRL 2018).

• Each reservoir forecasts on a local region based on input from its own and neighboring regions.
Preliminary Results with a GCM

- We are currently developing with T. Arcomano and I. Szunyogh (Texas A&M) a parallel hybrid code for the SPEEDY model (Molteni 2003) from ICTP.

- Model grid is T30 ($96 \times 48$) with 8 vertical levels.

- We interpolated the ERA5 reanalysis (ECMWF) to the SPEEDY grid for training and verification data.

- Preliminary results are from a parallel-only code (no hybrid yet) using 9 years of hourly data for training.

- We added noise to the reservoir input during training to improve stability.
Parallel Regions on SPEEDY Grid

Red: Input Region  Blue: Output Region
Comparison with Persistence Forecast

Global RMSE
Model level 4 Temperature

- Parallel Reservoir
- ERA Persistence

Normalized RMSE vs Forecast Hour
48-hour Machine-Learning Forecast

500 hPa Temperature Reservoir Prediction
Forecast Hour 48
72-hour Machine-Learning Forecast
24-hour Forecasts: Tropics

Tropical Temperature RMSE
Forecast Hour 24

- ERA Persistence
- Parallel Reservoir
- SPEEDY

RMSE (Kelvin)

hPa
24-hour Forecasts: NH

NH Temperature RMSE
Forecast Hour 24

- ERA Persistence
- Parallel Reservoir
- SPEEDY
Further directions

• We are developing and testing various approaches to combine our hybrid method with data assimilation.

• Training directly on observations rather than on reanalysis is a challenge.

• One goal is to perform adaptive (“online”) training of the machine-learning component as part of the data assimilation cycle.

• Our colleagues Dan Gauthier (Ohio State) and Dan Lathrop (Maryland) are using FPGAs and ASICs to create hardware reservoirs that are vastly faster than software implementations.
Concluding Remarks

- Reservoir forecasting with a feedback loop is relatively simple to implement and capable of learning the dynamics behind chaotic time series from a modest amount of training data.

- Hybrid approach uses machine learning to improve (not replace) an imperfect knowledge-based model.

- Parallel method scales to high-dimensional spatiotemporal systems by considering only local interactions.

- Simplified training relative to other machine-learning methods makes reservoir computing attractive for hardware implementations.
Data from Magnetohydrodynamic Experiment

- Dan Lathrop’s lab at U.Md. has a 3-meter diameter rotating sphere filled with liquid sodium, with an internal counter-rotating sphere and an externally applied magnetic field.

- We attempted to predict time series data from 33 sensors, 31 of which are on the outer sphere.

- The duration of the training data was about 150 rotations of the sphere.
Prediction of Experimental Data