Machine Learning for Forecasting and Data Assimilation

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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.

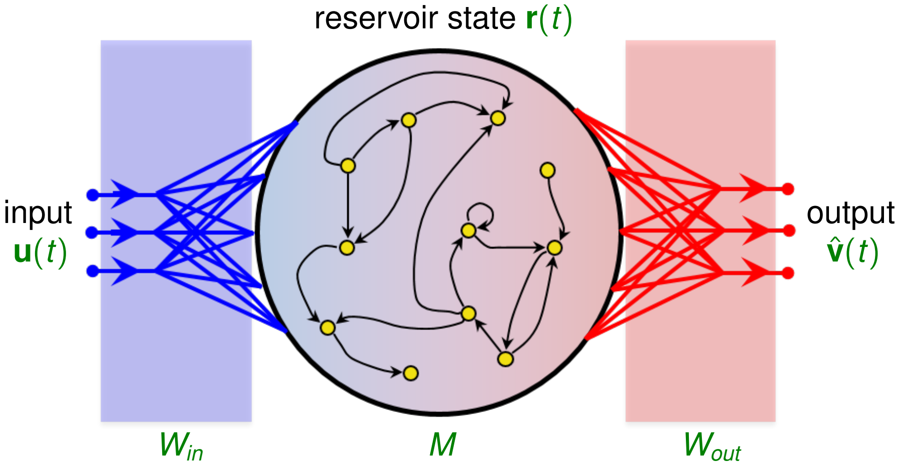
Forecasting and Attractor Reconstruction

- 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 $\mathbf{u}(t)$ and fitting a linear function of the reservoir state $\mathbf{r}(t)$ to a desired output time series $\mathbf{v}(t)$.
- 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`
- A reservoir can be a (super-fast) hardware device.

Reservoir During Training



Matrices W_{in} and M are chosen randomly in advance

Continuous-Time Jaeger ESN

- Listen: $\beta d\mathbf{r}/dt = -\mathbf{r}(t) + \tanh[M\mathbf{r}(t) + W_{in}\mathbf{u}(t) + \mathbf{c}]$ (in software, solve with Euler time step τ).
- We choose M and W_{in} at random, scaling M to have spectral radius close to 1 and scaling W_{in} so that $W_{in}\mathbf{u}$ is of order 1.
- We choose β 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 $\mathbf{u}(t)$.
- Fit: Find the matrix W_{out} such that $\hat{\mathbf{v}}(t) = W_{out}\mathbf{r}(t)$ least-squares minimizes the residuals $\hat{\mathbf{v}}(t) - \mathbf{v}(t)$ 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 $\mathbf{u}(t)$ consist of state variables that can be measured for all time, and $\mathbf{v}(t)$ 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 $\mathbf{v}(t)$ from $\mathbf{u}(t)$.
- The estimated value of $\mathbf{v}(t)$ is $\hat{\mathbf{v}}(t) = W_{out}\mathbf{r}(t)$.

Example: Lorenz System

- We ran the Lorenz system with time step $\tau = 0.05$:

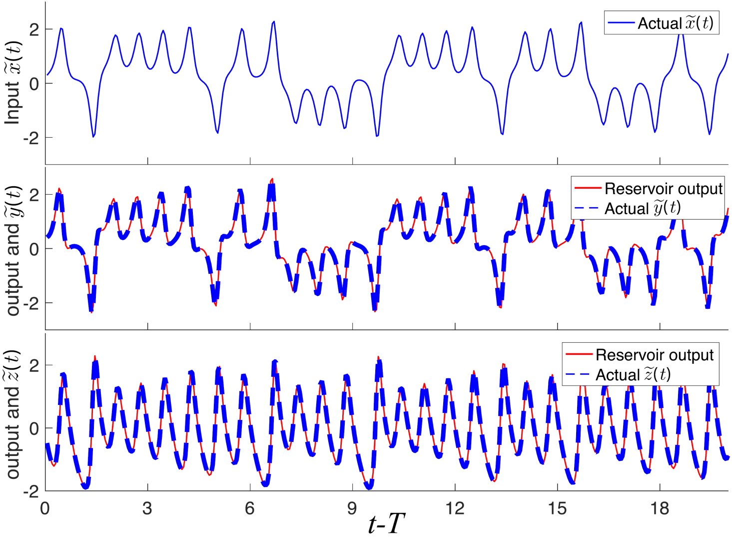
$$\frac{dx}{dt} = 10(y-x), \quad \frac{dy}{dt} = x(28-z)-y, \quad \frac{dz}{dt} = xy+8z/3.$$

- For training, we used $\mathbf{u}(t) = [x(t)]$ and $\mathbf{v}(t) = [y(t), z(t)]^T$.

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

- Details are in (Lu et al., Chaos, 2017).

Inferring Lorenz $y(t)$ and $z(t)$ from $x(t)$



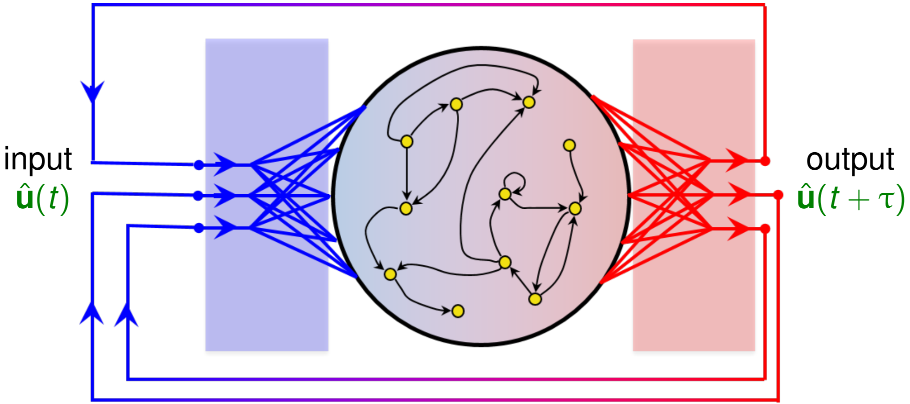
Forecasting with Feedback

- Suppose training data is sampled at time interval τ, but we want to forecast farther than τ into the future.
- One option is to train with lead time $n\tau$ [that is, set $\mathbf{v}(t) = \mathbf{u}(t + n\tau)$] for the value(s) of n of interest.
- We've gotten better results by training with lead time τ and iterating the trained time-τ forecast n times.
- We train with desired output $\mathbf{v}(t) = \mathbf{u}(t + \tau)$ and then forecast with $\mathbf{u}(t)$ replaced with $\hat{\mathbf{u}}(t)$.
- This feedback approach (Jaeger & Haas 2004) can be used with other machine-learning methods.

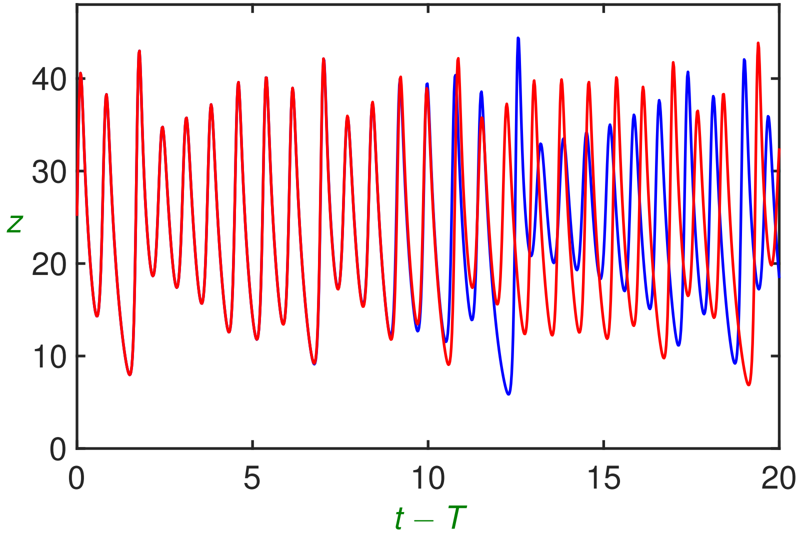
Forecast Model for $t > T$

Predict: $\beta\, dr/dt = -\mathbf{r}(t) + \tanh[M\mathbf{r}(t) + W_{in}\hat{\mathbf{u}}(t)]$

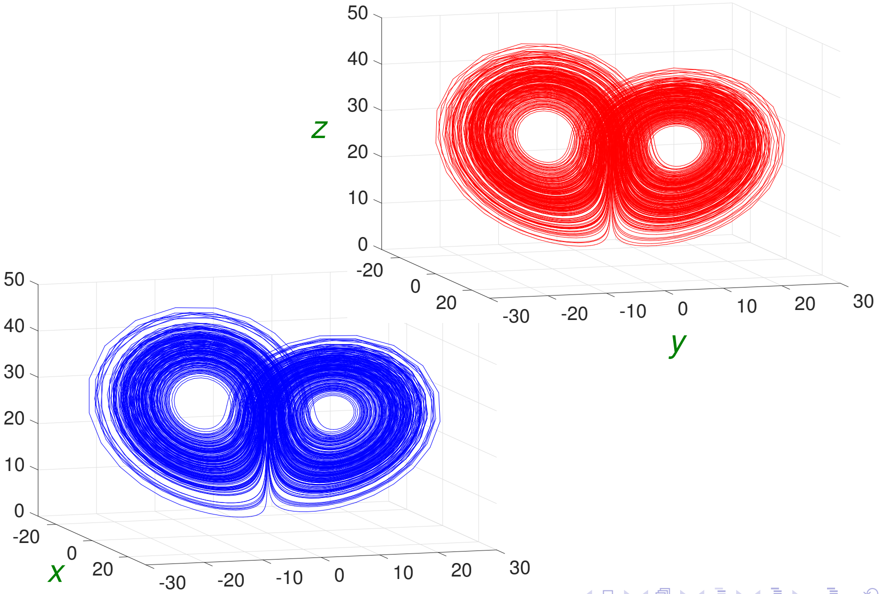
$$\hat{\mathbf{u}}(t) = W_{out}\mathbf{r}(t - \tau)$$



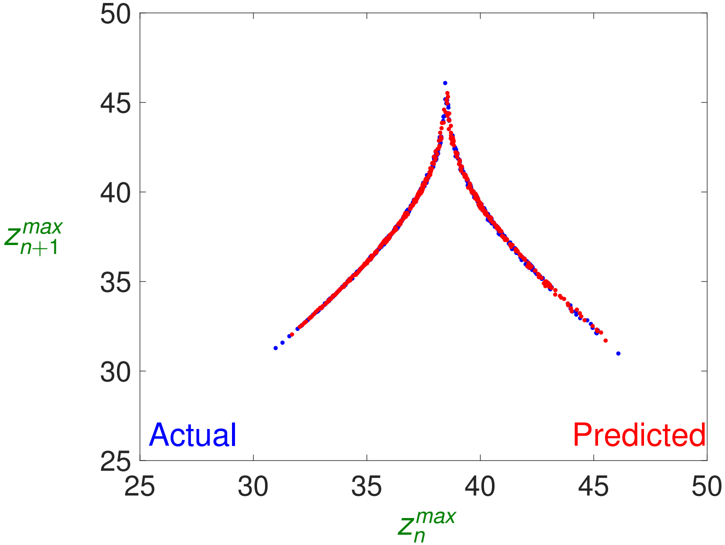
Lorenz system: Actual and Predicted $z(t)$



Actual and Predicted Attractors



Poincaré Section of Successive $z(t)$ Maxima



Questions Raised

- How can a reservoir "learn" these dynamics? Is there an approximate copy of the Lorenz attractor in the high-dimensional $\mathbf{r}(t)$ 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): $\mathbf{u}(t+\tau) = \mathbf{f}[\mathbf{u}(t)]$
- Listening (Response): $\mathbf{r}(t+\tau) = \mathbf{g}[\mathbf{r}(t), \mathbf{u}(t)]$
- Assume that $\mathbf{f}$ and $\mathbf{g}$ are continuous on Euclidean spaces, that $\mathbf{f}$ is invertible, and that $\mathbf{u}$ lies in a compact attracting set A.
- If $\mathbf{g}$ is uniformly contracting w.r.t. $\mathbf{r}$, then as $t \to \infty$, the reservoir state $\mathbf{r}(t)$ becomes independent of its initial state (roughly, Jaeger's "echo state property").

Generalized Synchronization

- Furthermore, we get generalized synchronization: there is a continuous function ϕ on A such that $\mathbf{r}(t) - \phi(\mathbf{u}(t)) \to 0$ as $t \to \infty$ [short proof in (Stark 1997)].
- Asymptotically, the reservoir state $\mathbf{r}(t)$ is a function of the current input $\mathbf{u}(t)$ only, not the entire history of $\mathbf{u}$. However, we don't know the function ϕ in practice.
- Uniform contraction can be guaranteed by choice of $\mathbf{g}$, but strong contraction may inhibit extraction of $\mathbf{u}$ from $\mathbf{r}$ [extreme case: if $\mathbf{g}$ is identically 0, then so is $\mathbf{r}$].

Inverting the Synchronization Function

- If $\mathbf{r}$ is much higher-dimensional than the attractor A, then embedding theory (Sauer-Yorke-Casdagli 1991) suggests that ϕ is likely to be one-to-one on A.
- If so, the inverse of ϕ on the set $\phi(A)$ can be extended to $\mathbf{r}$-space in many ways.
- Fitting: In training, we attempt to find a linear function W_{out} that approximately inverts ϕ on $\phi(A)$:

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

- This does not require ϕ to be approximately linear. It requires only that we can approximate the nonlinear function ϕ^{-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
$$\mathbf{r}(t+\tau) = \mathbf{g}[\mathbf{r}(t), W_{out}\mathbf{r}(t)] \qquad (1)$$
approximates [on $\phi(A)$] the idealized model
$$\mathbf{r}(t+\tau) = \mathbf{g}[\mathbf{r}(t), \phi^{-1}(\mathbf{r}(t))]. \qquad (2)$$
- Generalized synchronization implies that system (2) is conjugate to true dynamics $\mathbf{u}(t+\tau) = \mathbf{f}(\mathbf{u}(t))$ 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 $u(x + L, t) = u(x, t)$.

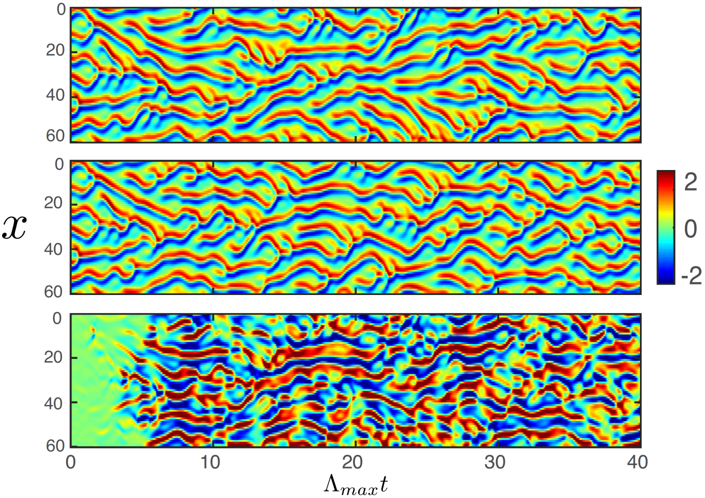
- With system size $L = 60$, we trained a 9000-node reservoir for time $T = 20000$ to predict the (numerical) KS solution.

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

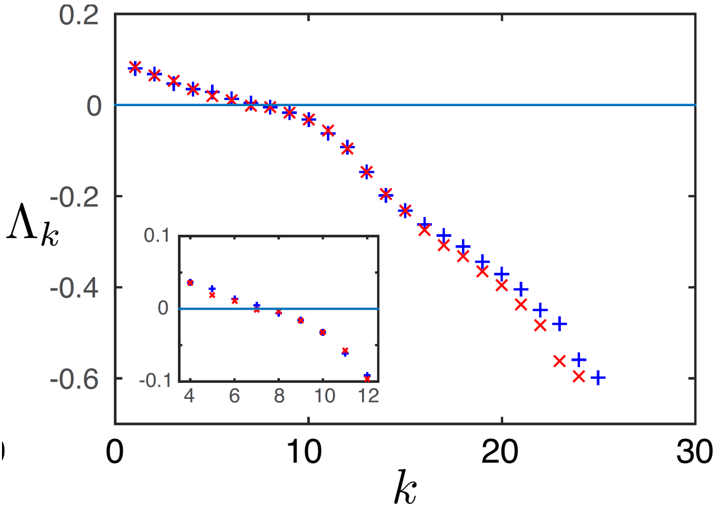
- Details are in (Pathak et al., Chaos 2017).

Kuramoto-Sivashinsky Forecast

Top: “Truth” Middle: Reservoir Bottom: Error



Estimation of Lyapunov Exponents



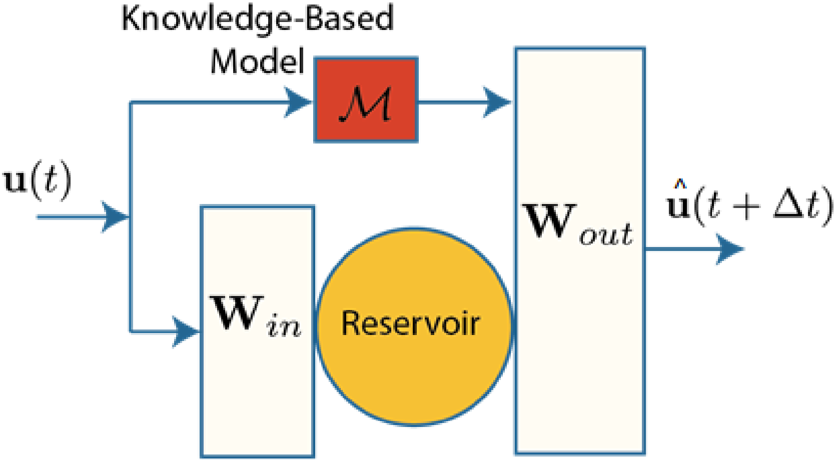
Actual exponents

Reservoir exponents

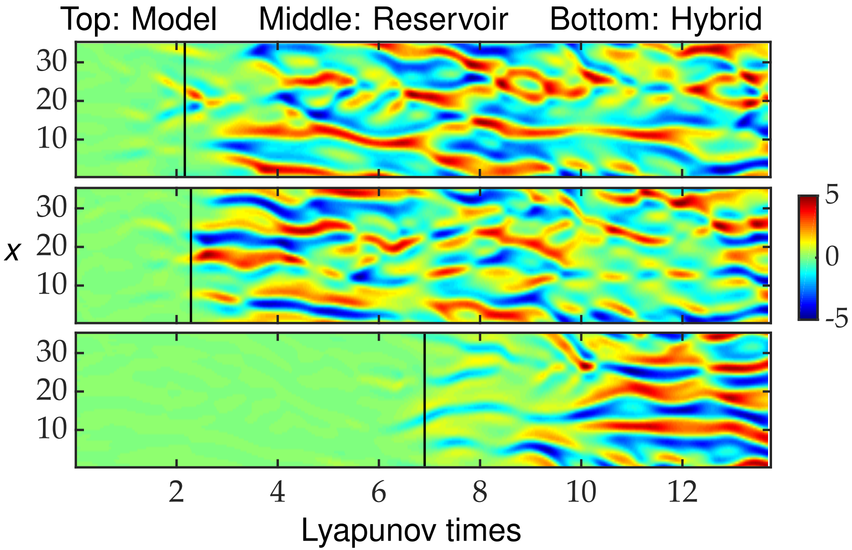
Hybrid Forecasting

- 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).

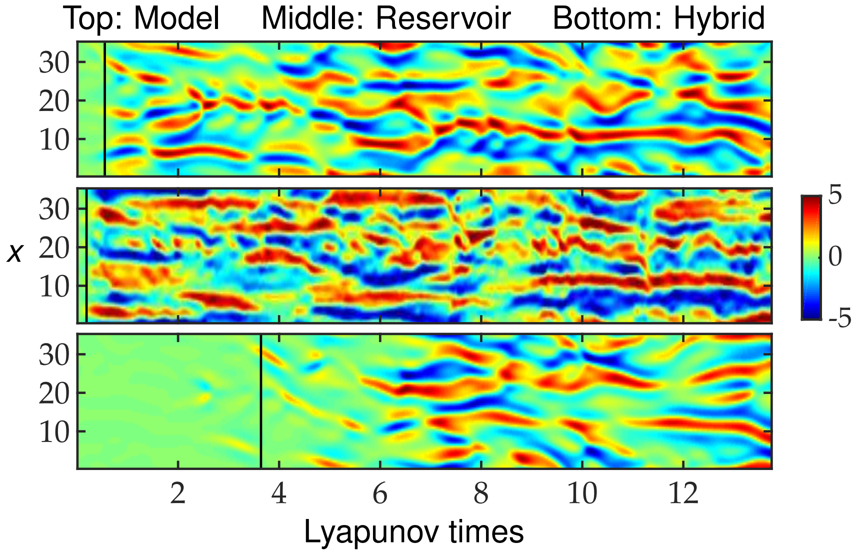
Hybrid Architecture



Forecast Errors: 8000 nodes, $\varepsilon = 0.01$



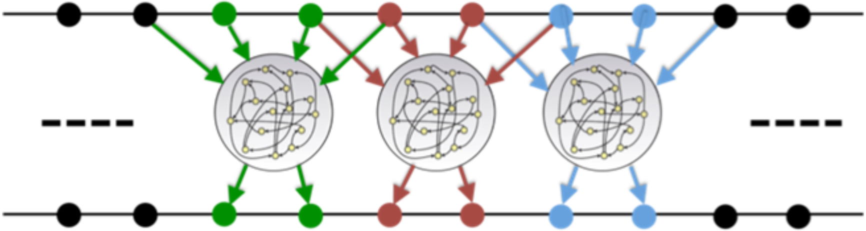
Forecast Errors: 500 nodes, $\varepsilon = 0.1$



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).

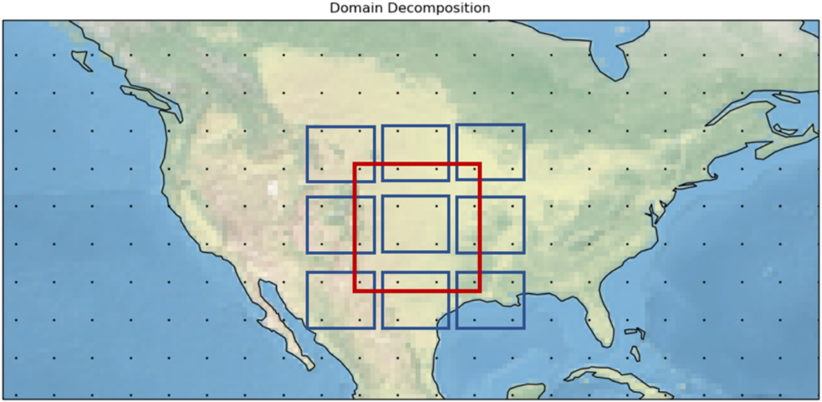
- Each reservoir forecasts on a local region based on input from its own and neighboring regions.



Preliminary Results with a GCM

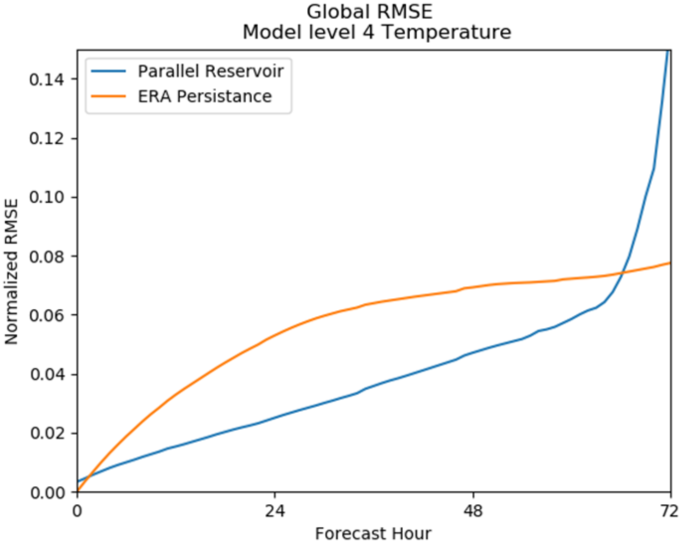
- We are currently developing with T. Arcomano and I. Szunyogh (Texas A&M) a parallel hybrid code for the SPEEDY model (Molteni 2003) from ICTP.
- Model grid is T30 (96×48) with 8 vertical levels.
- We interpolated the ERA5 reanalysis (ECMWF) to the SPEEDY grid for training and verification data.
- Preliminary 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

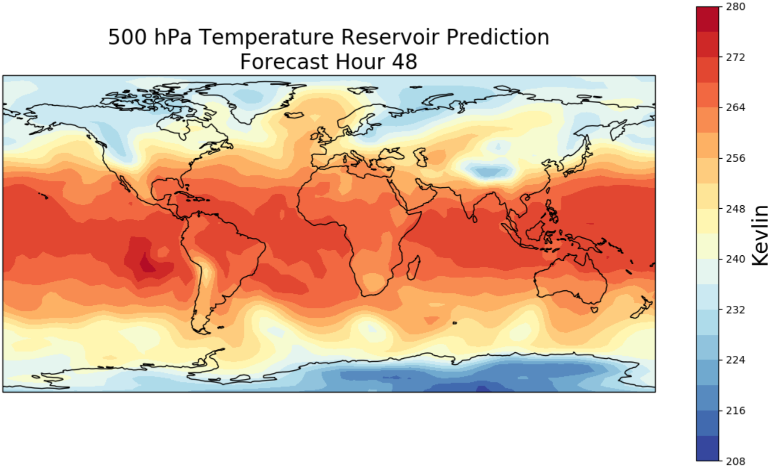


Red: Input Region Blue: Output Region

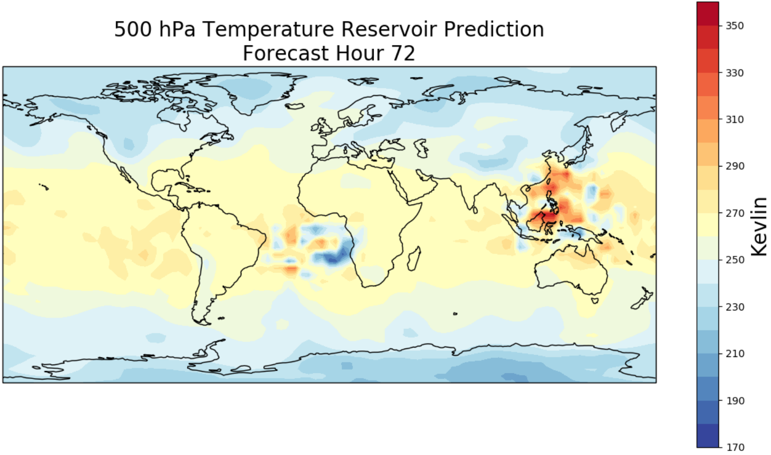
Comparison with Persistence Forecast



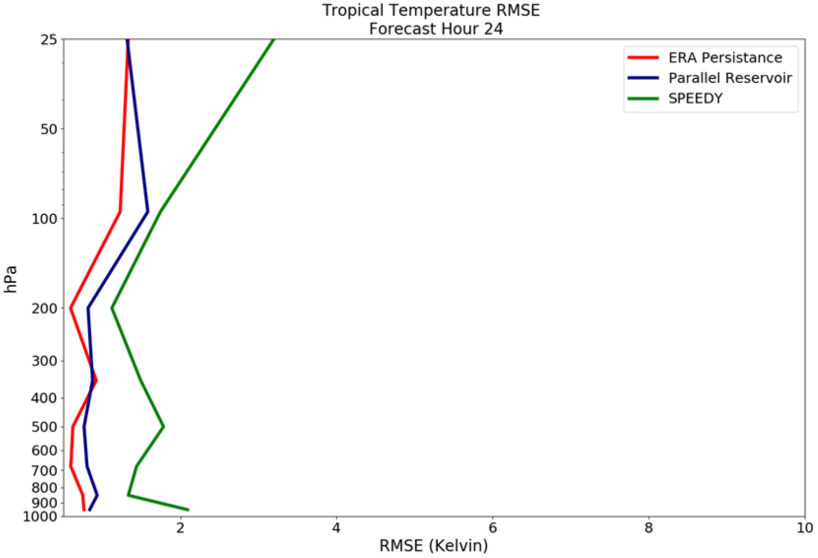
48-hour Machine-Learning Forecast



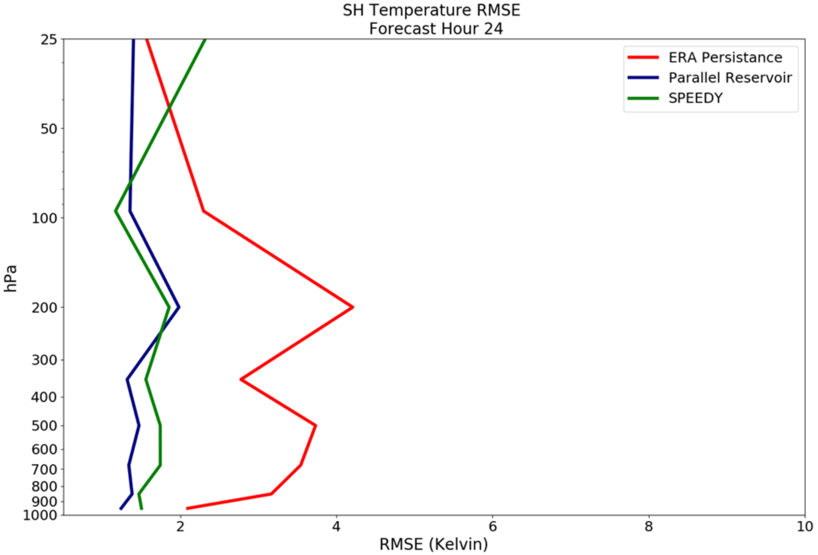
72-hour Machine-Learning Forecast



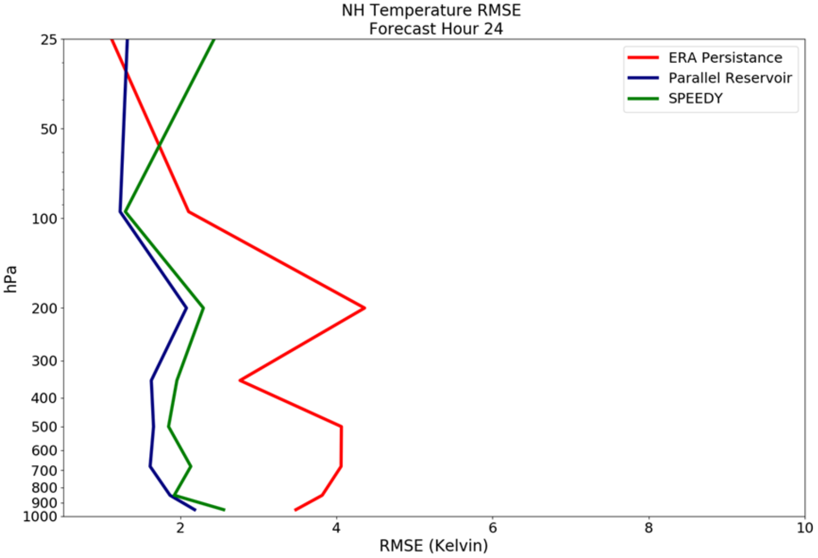
24-hour Forecasts: Tropics



24-hour Forecasts: SH



24-hour Forecasts: NH



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