Cross-Attractor Transformations: A Novel Machine Learning Framework to Minimize Forecast Error in the Presence of Model Bias

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Abstract

Imperfect models are often used for forecasting and state estimation of complex dynamical systems, typically by mapping a reference initial state into model phase space, making a forecast, and then mapping back to the reference space. In many cases these mappings are implicit, and forecast errors thus reflect a combination of model forecast errors and mapping errors. Techniques to infer parameterizations and parameters to reduce model bias have been the subject of intense scrutiny; however, we lack a general framework for discovering optimal mappings between system and model attractors. Here we propose a novel Machine Learning paradigm for inferring cross-attractor transformations (CATs) that minimize forecast error. CATs are pairs of transformations from the phase space of a reference system to the phase space of a model and vice versa that serve as a bridge between the attractors of a true system and an imperfect model. A computationally efficient analog approximation to tangent linear and adjoint models is developed to enable efficient stochastic gradient descent algorithms to train CAT parameters. Neural networks constructed with a custom analog-adjoint layer permit specification of affine transformations as well as more general nonlinear transformations.

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Introduction

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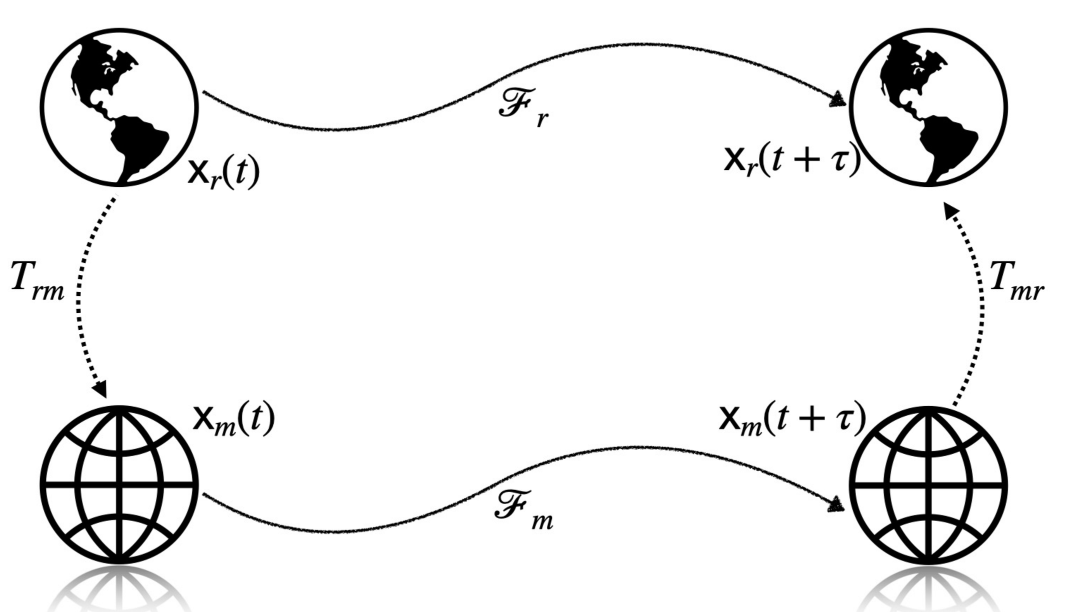
Here we propose a novel Machine Learning paradigm for inferring cross-attractor transformations (CATs) that minimize forecast error. CATs are pairs of transformations from the phase space of a reference system to the phase space of a model and vice versa that serve as a bridge between the attractors of a true system and an imperfect model. A computationally efficient analog approximation to tangent linear and adjoint models is developed to enable efficient stochastic gradient descent algorithms to train CAT parameters. Neural networks constructed with a custom analog-adjoint layer permit specification of affine transformations as well as more general nonlinear transformations.

Theory and Methods

Consider two dynamical systems, reference and model, denoted by r and m, respectively. Their states, x_r and x_m, belong to Hilbert spaces V_r and V_m, respectively, with propagation maps $\mathcal{F}_r : V_r \to V_r$ and $\mathcal{F}_m : V_m \to V_m$. We seek two maps T_{rm} (reference to model) and T_{mr} (model to reference) such that

$$[T_{mr} \circ \mathcal{F}_m \circ T_{rm}](x_r) \approx \mathcal{F}_r\,(x_r).$$



A schematic diagram of CATs (τ: forecast lead time)

An obvious loss function for the training of T-map parameters is:

$$\left\| x_r(t+\tau) - [T_{mr} \circ \mathcal{F}_m \circ T_{rm}]\big(x_r(t)\big) \right\|^2$$

However, for optimization, differentiation through the model dynamical system $\mathcal{F}_m$ is required, which is generally infeasible. Therefore, an analog approximation of $\mathcal{F}_m$ was considered with a carefully designed tangent linear model.

Training methodology:

- Consider catalogs (datasets) of the two dynamical systems, composed of pairs of states separated by a lag τ (denoted by + and -), i.e.,

$$\mathcal{C}_r = \{(x_{r,i}^-, x_{r,i}^+)\}_{i=1}^{N_r}\,, \qquad \mathcal{C}_m = \{(x_{m,j}^-, x_{m,j}^+)\}_{j=1}^{N_m}.$$

- To compute the forecast of any state x_m in V_m, we first express it as a linear combination of its N nearest neighbors (or, analogs), i.e

$$x_m = c_1\, x_{m,j_1}^- + \cdots + c_N\, x_{m,j_N}^-\,,$$

  where $\{j_1, j_2, \ldots, j_N\} \subset \{1,2,\ldots,N_m\}$ are nearest neighbors' indices. This can be expressed as,

$$c = (\boldsymbol{A}^T \boldsymbol{A})^{-1}\, \boldsymbol{A}^T\, x_m\,,$$

  where $\boldsymbol{A} = [x_{m,\,j_1}^-, x_{m,\,j_2}^-, \ldots, x_{m,\,j_N}^-]$, $c = [c_1, c_2, \ldots, c_N]$

- Then use analog forecasting ($\hat{F}$) to advance the state as

$$\hat{F}(x_m) = \boldsymbol{B}\, c = \boldsymbol{B}\,(\boldsymbol{A}^T \boldsymbol{A})^{-1}\, \boldsymbol{A}^T x_m\,,$$

  where $\boldsymbol{B} = [x_{m,j_1}^+, x_{m,j_2}^+, \ldots, x_{m,j_N}^+]$. Here, $\boldsymbol{A}$ and $\boldsymbol{B}$ are piecewise-constant functions of x_m, and thus $d\hat{\boldsymbol{F}}(x_m)/dx_m = \boldsymbol{B}\,(\boldsymbol{A}^T \boldsymbol{A})^{-1}\, \boldsymbol{A}^T$. This allows computing gradient of the loss function.

- A multilayer Neural Network (NN) is used to optimize T_{rm} and T_{mr} with a custom analog forecast layer in the middle; this layer also uses a custom gradient, as calculated above. NN input: $x_{r,i}^-$, NN output: $x_{r,i}^+$.

Post training, the original model dynamical system $\mathcal{F}_m$ can be used to produce forecasts instead of the analogs. However, only analog results are shown here.

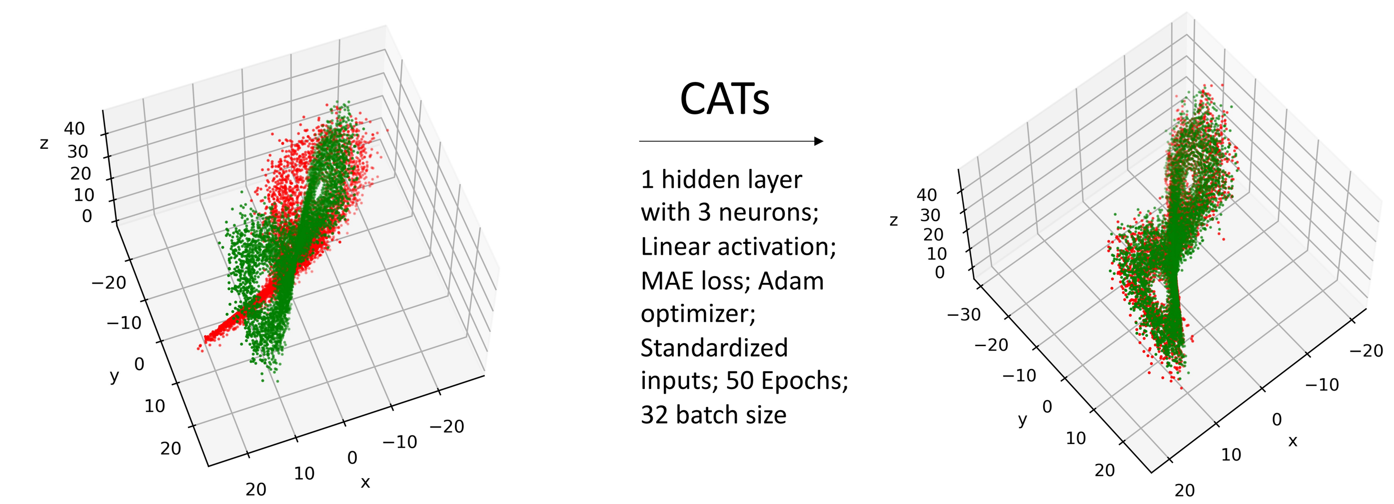
Results

Testbed: Lorenz'63 (L63) butterfly system

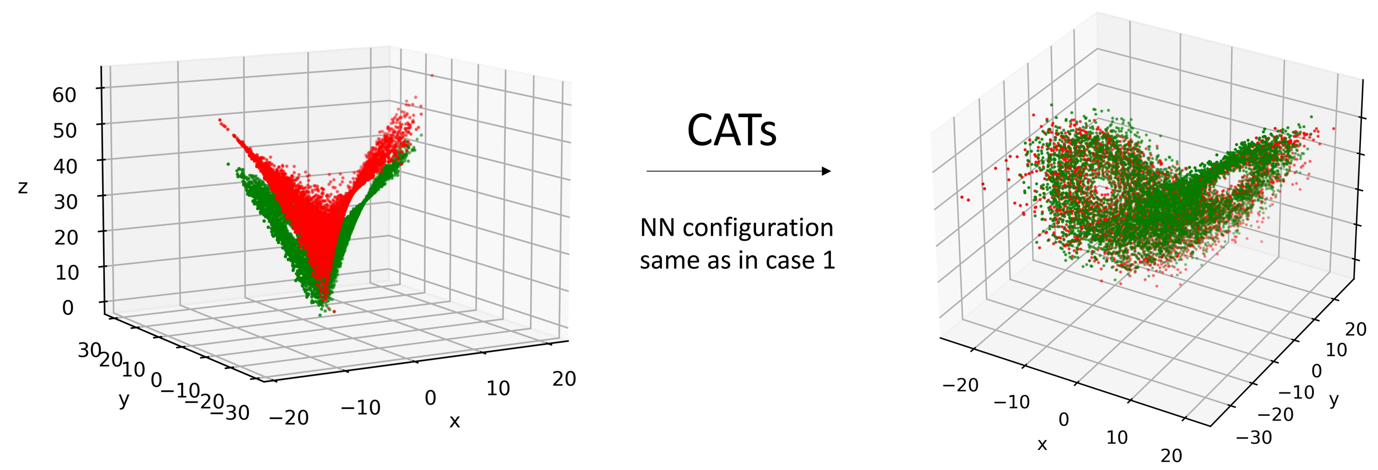
$$\frac{dx}{dt} = \sigma(y - x);\ \frac{dy}{dt} = x(\rho - z) - y;\ \frac{dz}{dt} = xy\ - \beta z$$

Reference: L63 with the parameter values $\sigma = 10, \rho = 28, \beta = 8/3$.
Model Forecast: L63 with different levels of errors. Four cases are considered.

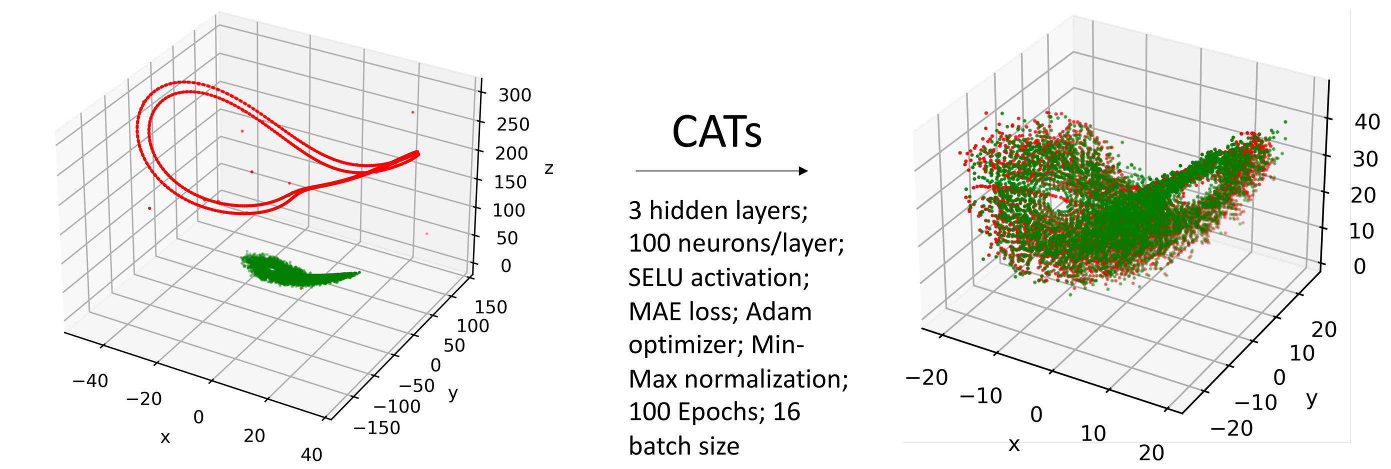
Case 1: L63 with x and y interchanged, i.e., $x \to y$ and $y \to x$. This is a simple affine transformation. Note that T_{rm} & T_{mr} are known analytically in this case.



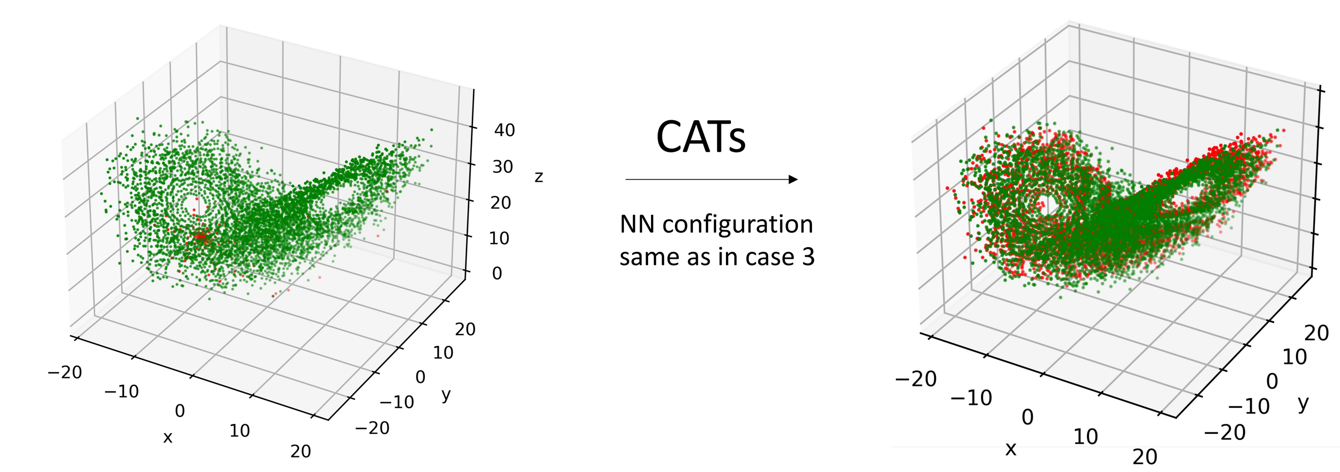
Case 2: L63 with $\sigma = 7.5,\ \rho = 35,\ \beta = 1.9$. This shifts the attractors along the z axis.



Case 3: L63 with $\sigma = 10,\ \rho = 220,\ \beta = 8/3$. The Lorenz two-attractor system converts to to a simple 3D orbit.



Case 4: L63 with $\sigma = 12.25,\ \rho = 19,\ \beta = 3.3$. The Lorenz system collapses to an equilibrium state.



Conclusions and Discussion

- CATs can skillfully map different phase space attractors of the Lorenz'63 system using minimally complex NNs.
- The current results are for $\tau = 1$, but a short study using higher lead times produced similar quality results.
- Testing on Lorenz'96 is in progress and will be followed by testing on multi-layered quasi-geostrophic ocean dynamics with different vertical levels.
- However, CATs can be generalized much further to, e.g., high-res vs low-res systems, coupled vs atmosphere-/ocean-only models.
- One significant downside of the current CATs implementation is the dependency on analog forecasting, which carries errors by definition.