Physics-reinforced Deep Learning for Fast Chemical Sensing

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I. Motivation

- Newly deployed chemical sensors can take a long time to saturate (due to slow chemical processes).
- Task : Predict future sensor readings (at saturation) given initial readings

Why combine physics and deep learning ?

- Physics models cannot predict accurate transients
  ⇒ need deep learning models
- DL methods require large amounts of data, and may learn spurious patterns in data
  ⇒ need physics models

II. Physics Model for Nitrate Sensors

Compact Physics Model

$$\boldsymbol{V_{linear}}(t) = \frac{\mathrm{kT}}{\mathrm{q}} \cdot \ln\left(D \cdot \frac{t}{t_0}\right)(t < t_c) \rightarrow \boldsymbol{V_{linear}}(t) = B \cdot \ln(A \cdot t)\,(t < t_c)$$

$$\boldsymbol{V_{sat}} = \frac{kT}{q} \ln\left(C_1 \frac{n_0 h^2}{\kappa}\right) + \mathrm{C}_2 \quad (t > t_c) \rightarrow \quad \boldsymbol{V_{sat}} \quad = C \quad (t > t_c)$$

$$V_{ana}(t) = \frac{V_{linear}(t)}{\left(1 + \left(\frac{V_{linear}(t)}{V_{sat}}\right)^{\beta}\right)^{\frac{1}{\beta}}}$$

III. Neural Network Architecture

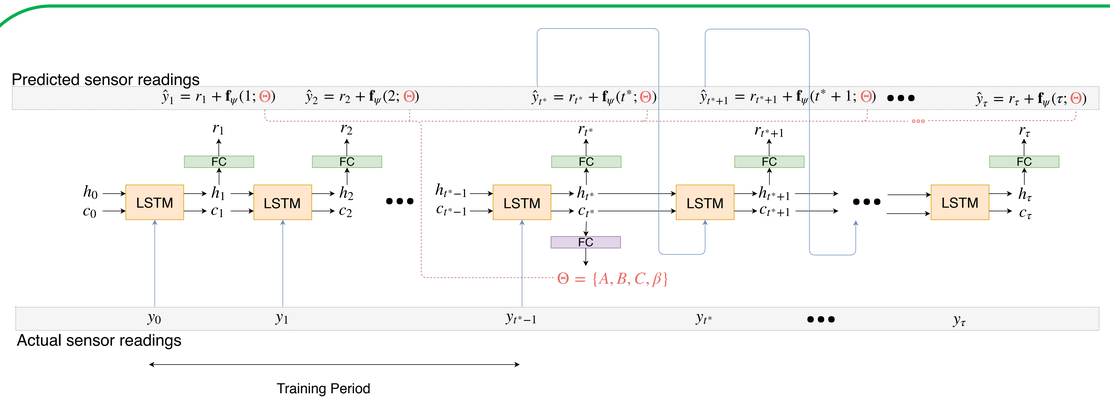

Figure 1: Proposed architecture for dynamic sequence prediction (sensor readings) with the help of an LSTM and a physics model, f_ψ.

- Predict physics parameters at time t^* (initial training period).
- Compute physics predictions and residuals.
- NN residuals r_t decay with time t; use only Physics model at saturation
- Horizon τ sampled using Russian Roulette technique.
- Allows for variable length sequences

IV. Results

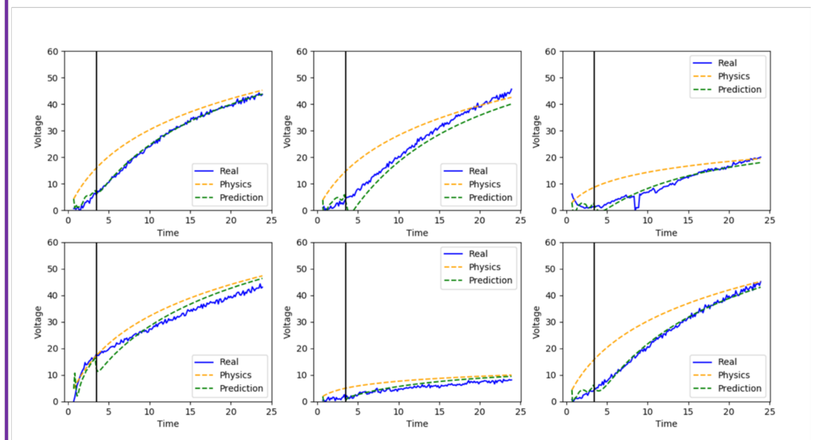

Figure 2: Nitrate sensors in solution (31 Jul - 07 Sep). Black vertical line denotes the training period. Proposed model predicts the physics parameters and adjusts the predictions for the transients.

Methods	RMSE
LSTM ($\tau = 10$)	181.5
LSTM-Physics ($\tau = 10$)	136.9
LSTM-Physics-RR (E[τ] = 10)	80.3

Table 1: Nitrate sensors in solution (31 Jul - 07 Sep). Root Mean Square Error (RMSE) for the all the methods (averaged over 5 runs).

Collaborators:

V. Impact of Our Research

- Our work can help engineering disciplines in **adding physics to deep learning** models
- Accurately predicted future sensor readings using just few initial hours of readings
- Employed a theoretically correct sampling technique for a practical data collection procedure.