CRNN: current state and future improvements

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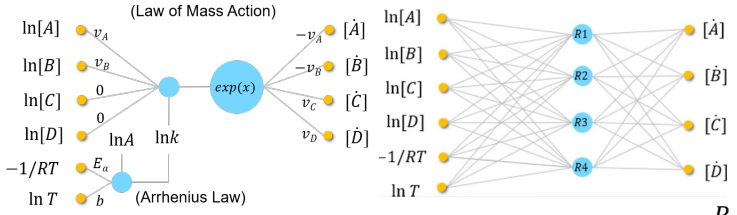
Introduction

$$\nu_A A + \nu_B B \rightarrow \nu_C C + \nu_D D$$



$$r = k[A]^{\nu_A}[B]^{\nu_B}[C]^0[D]^0 \qquad Ln\,(k) = \ln(A) + b\ln(T) - \frac{R}{T}$$

$$r = \exp(ln(k) + \nu_A \ln([A]) + \nu_B \ln([B]) + 0\ln([C]) + 0\ln([D]))$$

Methodology

Data Generated From

2A	→	B
B	→	C
C	→	D
B + D	→	E

Error Functions

$$\mathrm{E(W)} = \min_{p \in \mathcal{P}(4, W_{CRNN})} MSE(K_{GT}, W_{CRNN}(p))$$

$$\mathrm{E(K)} = \min_{p \in \mathcal{P}(4, K_{CRNN})} MSE(K_{GT}, K_{CRNN}(p))$$

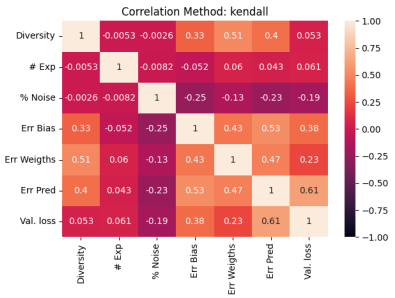
$$\mathrm{E(P)} = \mathrm{MSE}(Y_{GT}, Y_{CRNN})$$

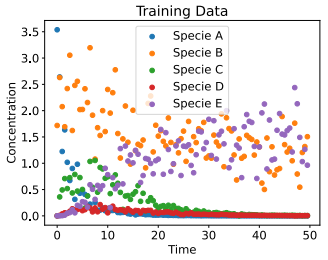
Test CRNN - Varying Training Set Creation

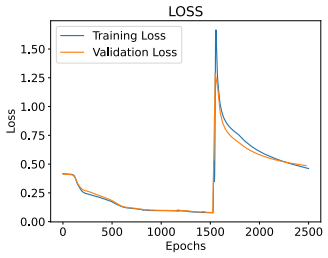
- # Exps → [20,…, 1500]
- Δ Initial Condition → [1, …, 15]
- Noise → [0, …, 40%]

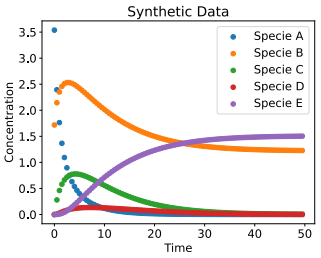
} 392 Tests ~ 82 hours

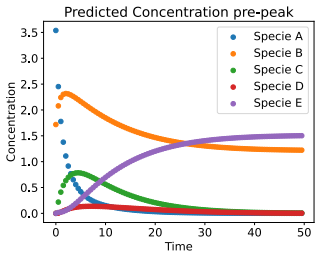
Results

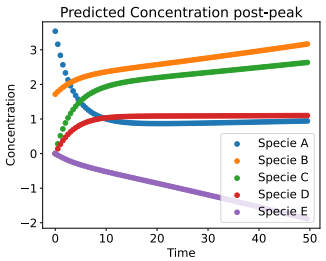












0.1B + 0.9C → 0.6A + 0.1D + 0.4E
0.7A + 0.1B + 0.1E → 0.5C + 0.1D
2.9A + 0.1D → 1.4B + 0.1C + 0.2E
0.9B + 0.9D → 0.4C + 0.5E

0.6C + 0.1E → 0.6A + 0.2B + 0.4D
1.1A + 0.1E → 0.2B + 0.9C + 0.4D
2.6A + 0.5D + 0.3E → 0.9B + 0.2C
0.5B + 1.1D → 0.2A + 0.4C

Summary

Tests demonstrated that CRNN:

- Robust to noisy data
- Does not require many data
- Able to reconstruct the original model

CRNN & Vanishing Gradient

- Gradient descent gets "lost"
- Optimal prediction does not guarantee a correspondance with the original model

Ongoing Work

Constraint the model to:

- Mass conservation

$$Loss_{TOT} = \alpha\, Loss_{Prediction} + (1 - \alpha)\, Loss_{Mass}$$

Additional Test Regarding

- Increasing number of species and reactions
- Application on H_2 mechanism

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