

Input-Output Equivalence of Unitary and Contractive RNNs



Melikasadat Emami, Mojtaba Sahraee-Ardakan, Alyson K. Fletcher University of California, Los Angeles

Sundeep Rangan New York University

Background

RNNs:

• Sequence-to-sequence mappings of the form:

$$h^{(k)} = \phi (Wh^{(k-1)} + Fx^{(k)} + b),$$

$$y^{(k)} = Ch^{(k)}, \quad h^{(-1)} = h_{-1}.$$

- Parameters: $\Theta = (W, F, B C, h_{-1})$
- Input-output mapping: $y = G(x, \Theta)$

Equivalence of RNNs:

• Given Θ_1 and Θ_2 :

$$G(x, \Theta_1) = G(x, \Theta_2)$$
 for all $x = (x^{(0)}, ..., x^{(T-1)})$

- Internal states may be different
- Does not imply that parameters are identical
- Example: invertible *T*, identity activation
- $W \to TWT^{-1}$, $C \to CT^{-1}$, $F \to TF$, $h_{-1} \to Th_{-1}$

Contractive RNNs:

- $||W|| \coloneqq \max_{h \neq 0} \frac{||Wh||_2}{||h||_2}$
- Contractive: ||W|| < 1, non-expansive: $||W|| \le 1$.
- Non expansive activation function:

$$\|\phi(x) - \phi(y)\| \le \|x - y\|$$
 for all x, y

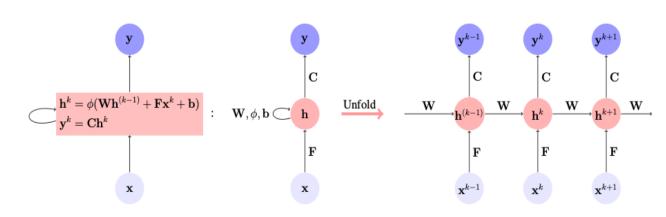


Figure 1: Recurrent neural network (RNN) model

Unitary RNNs (URNN):

- $W^HW = WW^H = I$
- Overcome the vanishing/exploding gradient problem
- Improve the stability of the network

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Main Results

This work:

- Characterizes how restrictive the unitary constraint is on an RNN.
- Compares input-output mappings achievable by URNNs and RNNs

Equivalence Results for RNNs with ReLU Activations:

Theorem 1: Given any contractive RNN with n hidden states, bounded input, and ReLU activations, there exists a URNN with at most 2n hidden states with the identical input-output mapping.

- No loss in modeling with URNNs compared to RNNs
- Cost: two-fold increase in state dimension Proof idea:
- Construct a URNN with 2n states
- Match the first n states with the original RNN
- Last n states are zero

Theorem 2: For every positive n, there exists a contractive RNN with ReLU activations and state dimension n such that every equivalent URNN has at least 2n states.

- Converse result for Theorem 1
- 2n achievability is tight

Equivalence Results for RNNs with Sigmoid Activations:

Theorem 3: There exists a contractive RNN with sigmoid activations such that there is no URNN with any finite number of states that exactly matches the input-output mapping.

- Difference in equivalence for smooth and non-smooth activations
- No exact equivalence even with arbitrary number of states

Synthetic Data Generation

- Multiple instances of a synthetic RNN with 4 hidden units
- F, C, b matrices ~ iid Gaussian
- Contractive $W_q = I \epsilon A^T A / \|A\|^2$, A: Gaussian iid
- $\epsilon = 0.01 \rightarrow \text{slow varying system} \rightarrow \text{long term dependencies}$
- Biases adjusted to ensure hidden states are on 60% of the time
- Additive output noise with SNR= 15, 20 dB
- Each trial: T= 1000 i.e. $(10 \times \text{time constant}(\frac{1}{\epsilon}))$, test ratio = 0.3

Numerical Simulation

Learning the system:

- Standard RNNs, URNNs, LSTMs with [2,4,6,8,10,12,14] hidden units
- MSE loss, batch-size = 10, learning-rate = 0.01
- Averaged over 30 realization of original contractive system
- Unitary constraint: projection on unitary space using SVD

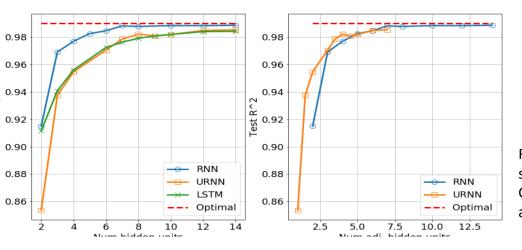


Figure 2: Test \mathbb{R}^2 on synthetic data for a Gaussian i.i.d. input and output SNR=20 dB.

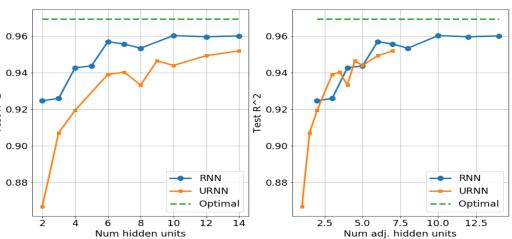


Figure 3: Test R^2 on synthetic data for a Gaussian i.i.d. input and output SNR=15 dB

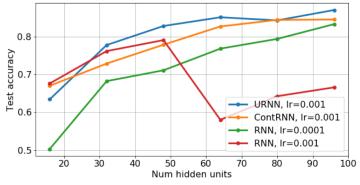


Figure4: Accuracy on Permuted MNIST task for various models trained with RMSProp, validation-based early termination.

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