Input-Output Equivalence of Unitary and Contractive RNNs

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Background

RNNs:

- Sequence-to-sequence mappings of the form:

$$h^{(k)} = \phi\left(Wh^{(k-1)} + F\,x^{(k)} + b\right),$$
$$y^{(k)} = Ch^{(k)}, \quad h^{(-1)} = h_{-1}.$$

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

Equivalence of RNNs:

- Given Θ_1 and Θ_2:

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

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

Contractive RNNs:

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

$$\|\phi(x) - \phi(y)\| \leq \|x - y\| \quad \text{for all} \quad x, y$$

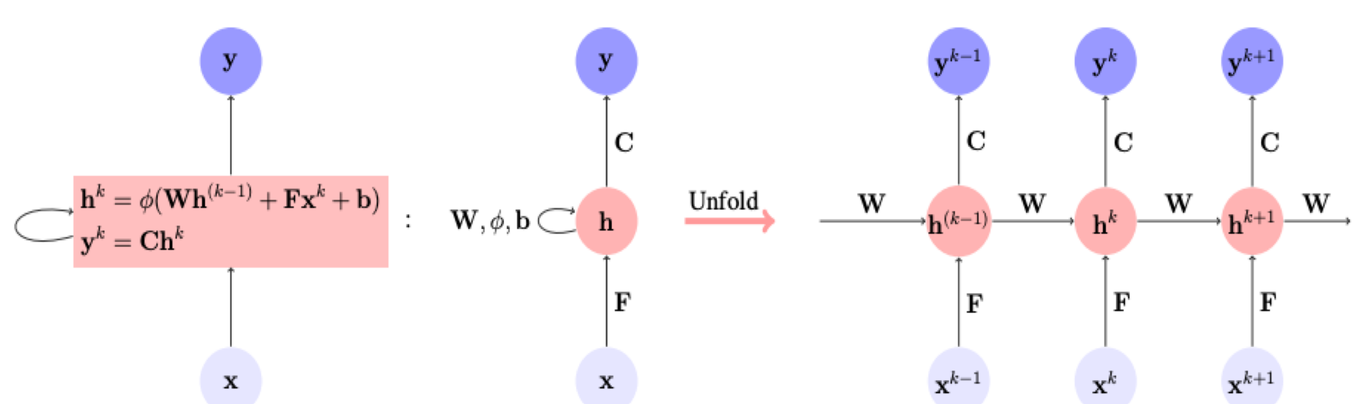

Figure 1: Recurrent neural network (RNN) model

Unitary RNNs (URNN):

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

This work:

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

Main Results

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 and 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

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Main Results

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.

- No exact equivalence even with arbitrary number of states
- Difference due to ReLU zeroing out states

Numerical Simulations

Data Generation:

- Multiple instances of a synthetic RNN with 4 hidden units
- b, F, C matrices ~ iid Gaussian
- Contractive $W_g = I - \epsilon A^T A / \|A\|^2$, A: Gaussian iid
- $\epsilon = 0.01 \to$ slow varying system $\to$ 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×time constant($\frac{1}{\epsilon}$)), test ratio = 0.3

Learning the system:

- Using standard RNNs, URNNs 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 .

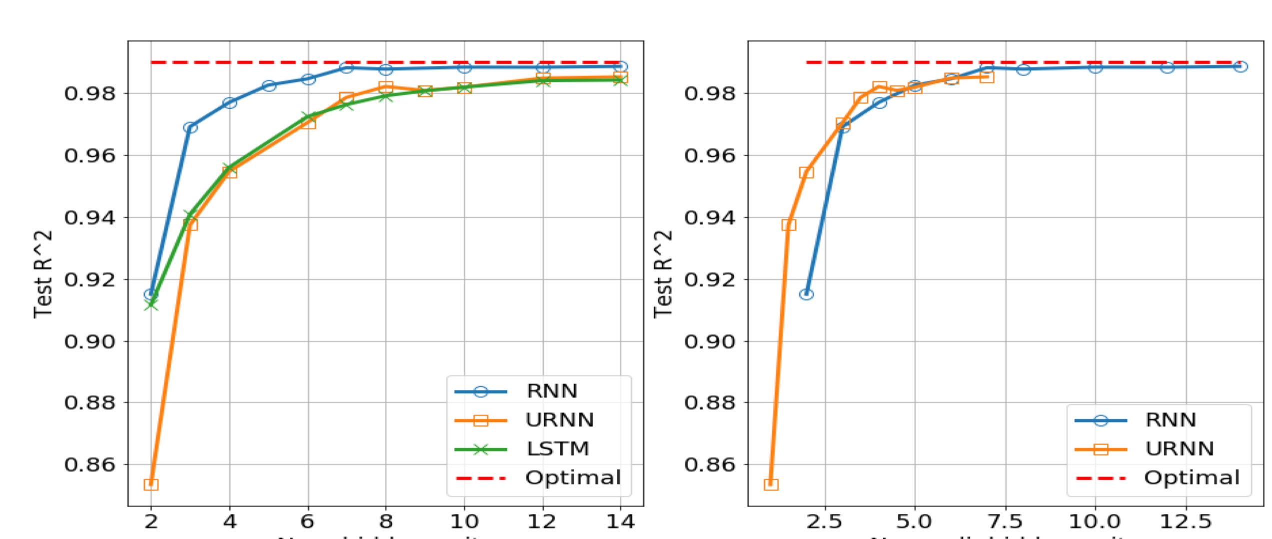


Figure 2: Test R^2 on synthetic data for a Gaussian i.i.d. input and output SNR=20 dB.

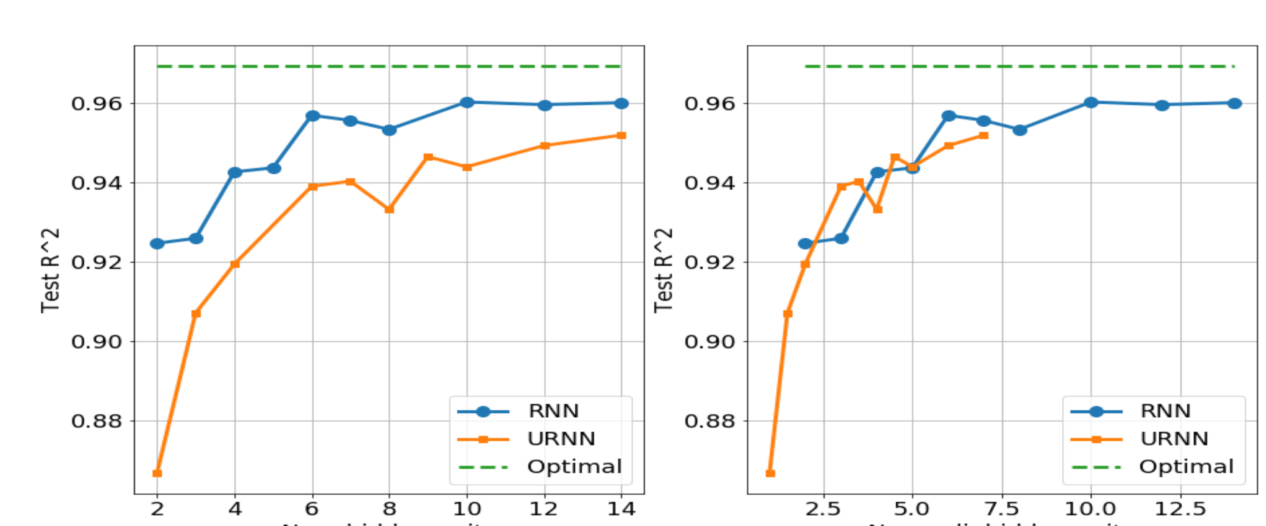
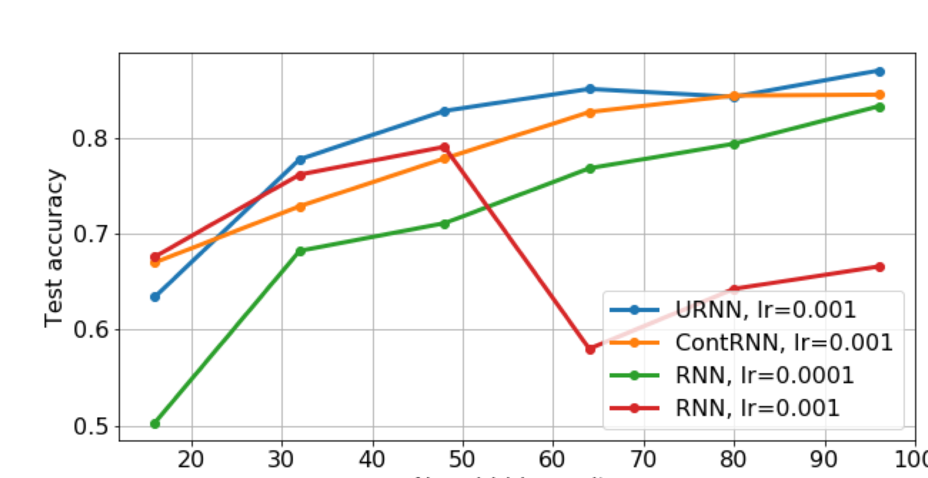


Figure 3: Test R^2 on synthetic data for a Gaussian i.i.d. input and output SNR=15 dB.



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

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