Chemical Reaction Network Implementation of Logic Gates and Neural Networks Using a Molecular Exchange Mechanism

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Introduction

- Synthetic biological circuits enable programmable cellular behaviors with applications in disease diagnostics, therapeutics, and tissue engineering.
- These circuits must demonstrate a high degree of reproducibility for their various use cases, while also being able to absorb different forms of perturbations.
- This work proposes the Molecular Exchange Mechanism (MEM) for constructing logic gates and a winner-take-all (WTA) network for pattern recognition.
- Our MEM-based circuits exhibit improved reproducibility across multiple benchmark datasets, offering a promising design for molecular computing.

Methodology

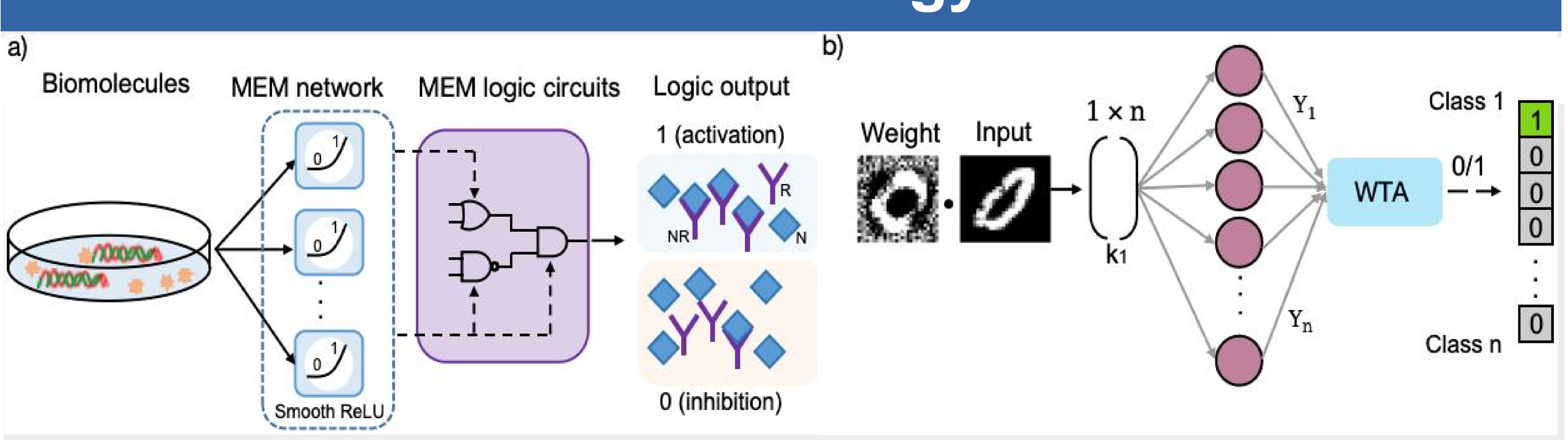


Figure 1: a) General construction of logic gate circuits using MEM from aqueous inputs. b) The winner-take-all circuit implementation for pattern recognition. Here, an example is shown using the MNIST dataset.

- **Biomolecular Logic Gates:**
  - We build biomolecular logic gates (AND, OR, XOR) by tuning the parameters of the MEM perceptron networks.
  - We also create inverted gates (NAND, NOR, XNOR) by swapping roles of the species NR and the species NE.
  - Each gate shows soft boundaries due to smooth-ReLU activation, which we hypothesize to contribute to enhancing reproducibility and controlling perturbations.
- **Biomolecular Winner-Take-All (WTA) Network:**
  - We construct a biomolecular single layer neural network with one MEM perceptron node per class.
  - We train the WTA network via stochastic gradient descent and compare test accuracies with similar networks using previously built biomolecular perceptrons such as molecular sequestration.
  - The formation rate of the decision-making species NR is the dot product of inputs & weights for each node and the node with highest NR concentration is the "winner".

Results

Logic Gate Implementation

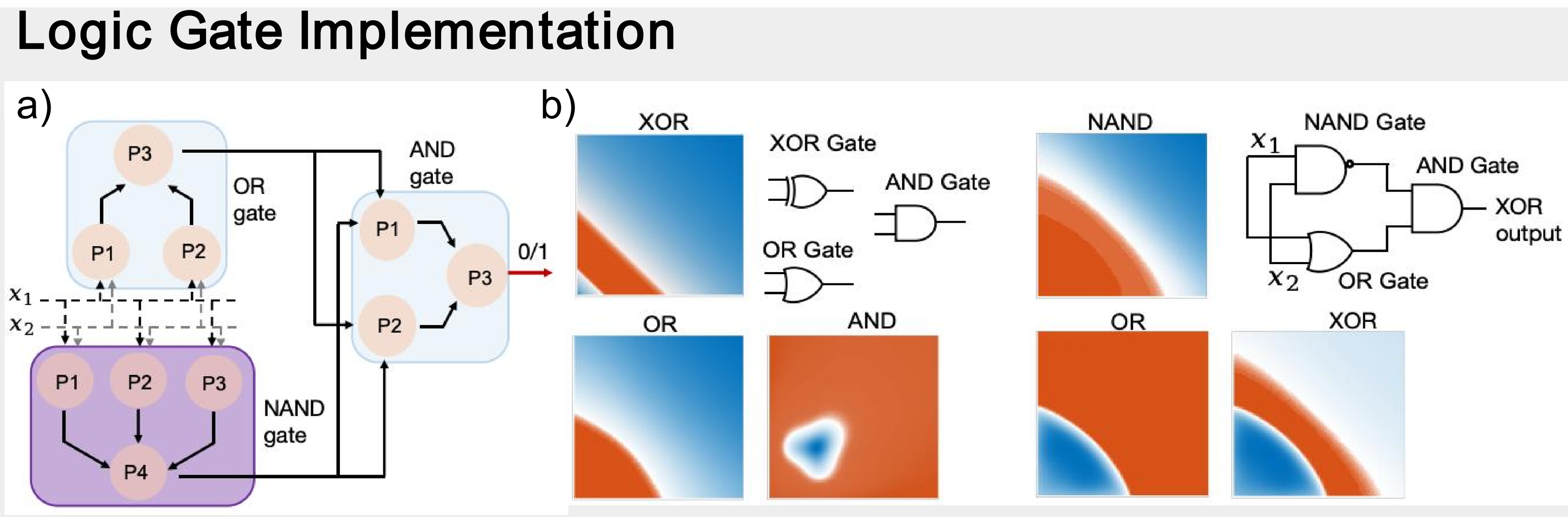
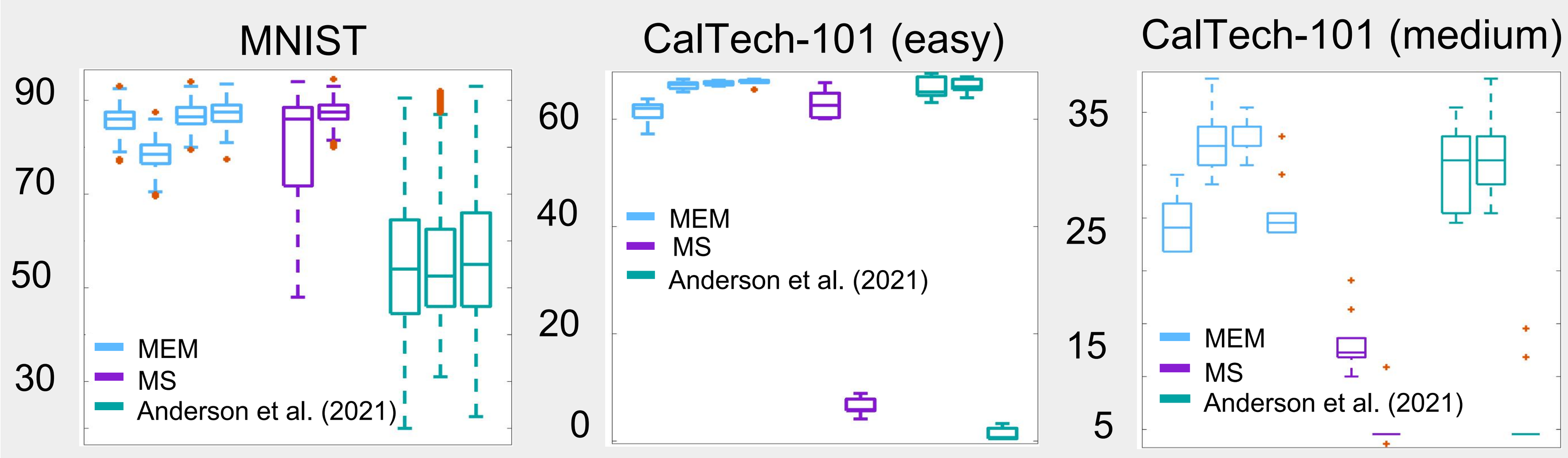


Figure 2: a) The schematic diagram showing the internal structure of each logic gate design used to construct the XOR gate. All logic gates are designed in a similar way having two layers, where the first layer generates individual decision boundaries and the output layer node combines those boundaries to form the desired logic gate output using specifically tuned weights. b) Different logic outputs obtained by tuning the weights of the MEM perceptrons in the respective logic gate circuits.

Results

Reproducibilty



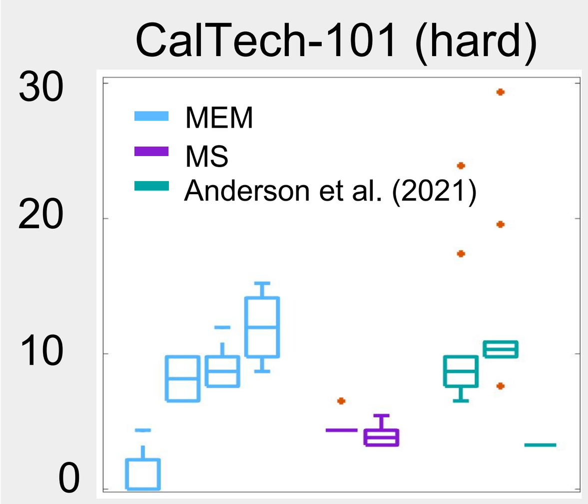


Figure 3: Box plots showing test accuracy variation of the MEM-based WTA network, molecular sequestration-based (MS) WTA network, and a WTA network designed using the chemical reaction network in Anderson et al. (2021). Models were evaluated on the MNIST and three subsets (easy, medium, hard) of the CalTech101 Silhouettes dataset, defined by MLP classification difficulty. Each model was run 10 times with different learning rates with different learning rates; standard deviation of test accuracy was used to assess reproducibility.

Model	η	Mean test accuracy			
		MNIST	EASY	MEDIUM	HARD
MEM	0.01	0.7835±0.0296	0.6163 ±0.0199	0.2455 ±0.0291	0.0185 ±0.0162
MS	0.01	0.8070±0.1114	0.0638±0.0148	0.0573±0.0275	0.0391±0.0076
Anderson et al. 2021	0.01	0.5493±0.1517	0.6627±0.0122	0.3073±0.0378	0.1283±0.0662

Table 1: The performance of MEM over the other models corresponding to the box plots in Fig.3, where MEM shows better reproducibility in training over a range of learning rates (η), while the other models demonstrate a high sensitivity to the variation in learning rate.

- For the MNIST dataset, the MEM WTA network shows less variation when run multiple times for different learning rates, while obtaining more than 80% accuracy.
- Training the MEM network using the CalTech101 Silhouettes subsets resulted in decreasing learning ability with increasing difficulty of the dataset.
- The other models compared to the MEM model were able to demonstrate learning only for specific learning rates. However, the MEM model was able to successfully learn using the same range of learning rates for all the datasets considered.

Discussion

- Our results show that the MEM-based perceptron utilizes a smooth ReLU like activation function to allow greater reproducibilty of biomolecular computations than existing biomolecular perceptrons.
- MEM-based WTA network exhibits reduced sensitivity to hyperparameters like learning rate, while the other models considered demonstrate learning only for specific learning rates for each dataset and its subsets used.
- MEM logic gates show soft decision boundaries, suggesting a potential tradeoff between accuracy in binary decision-making and reproducibility.

References

1. Anderson, D. F., Joshi, B., and Deshpande, A. On reaction network implementations of neural networks. Journal of the Royal Society Interface, 18(177):20210031, 2021.
2. Moorman, A., Samaniego, C. C., Maley, C., and Weiss, R. A dynamical biomolecular neural network. In 2019 IEEE 58th conference on decision and control (CDC), pp. 1797–1802. IEEE, 2019.
3. Cherry, K. M. and Qian, L. Scaling up molecular pattern recognition with dna-based winner-take-all neural net works. Nature, 559(7714):370–376, 2018.