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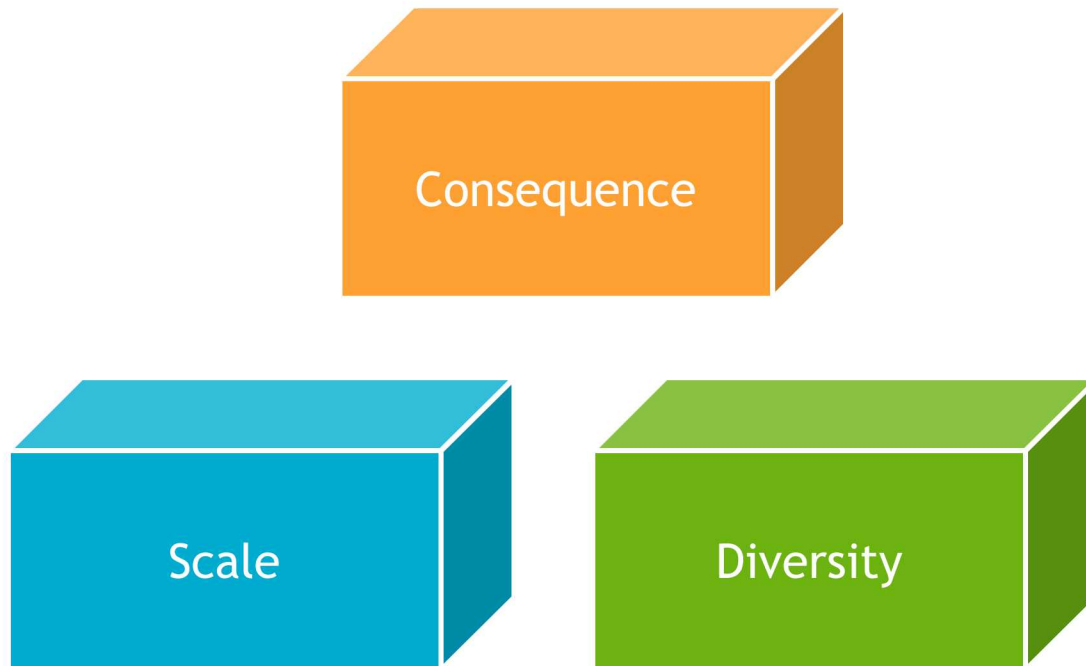
Machine Learning in the Presence of Noise : Early Experiments

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Many Sandia efforts are premised on idea that AI solutions will be instrumental in delivering these requirements



Sandia has a goal of creating a bridge between the broader world of AI and our missions

Extending and developing AI algorithms

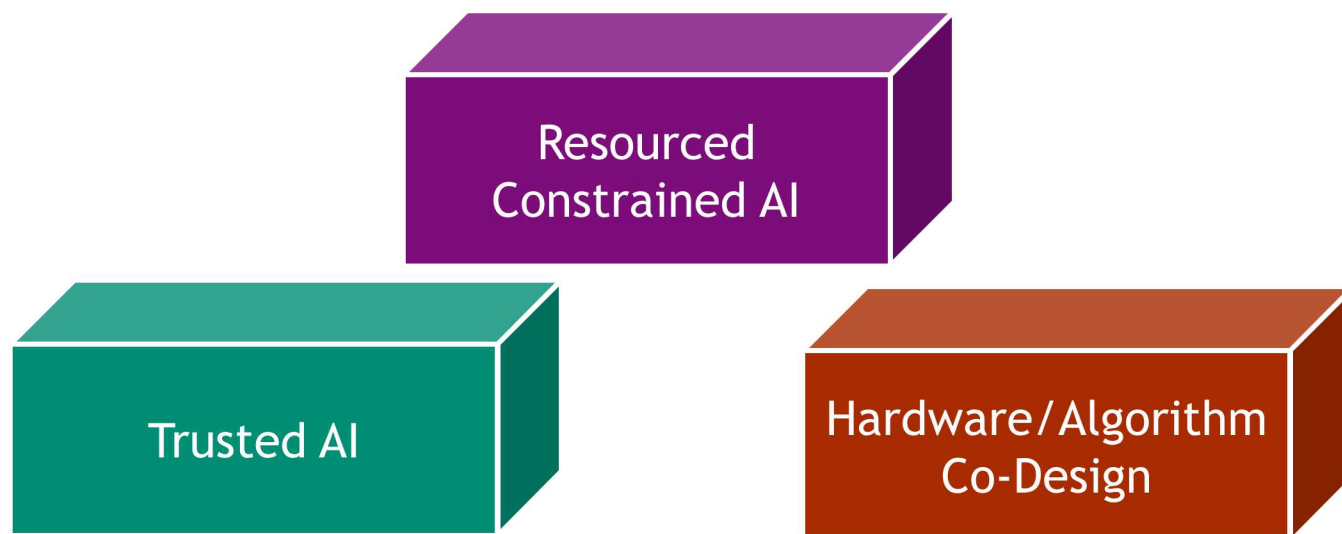
Evaluating novel hardware and accelerators

Explore brain-inspired sensor technology

Identifying opportunities for novel AI impact

Developing tools and analyses suitable for widespread adoption of emerging AI technologies

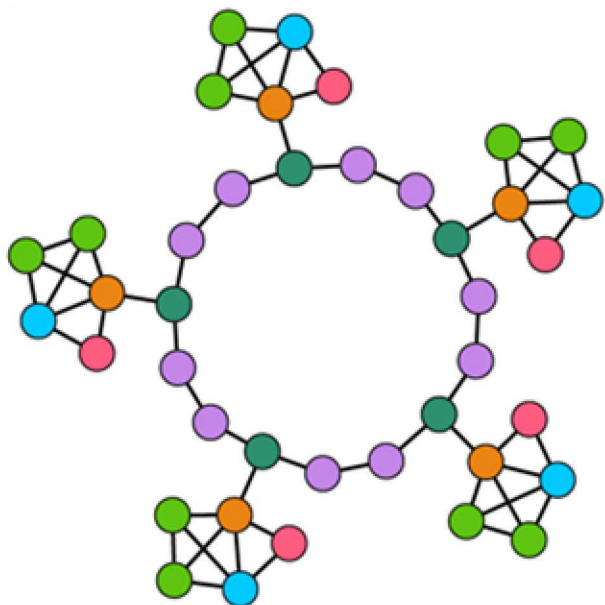
Capabilities



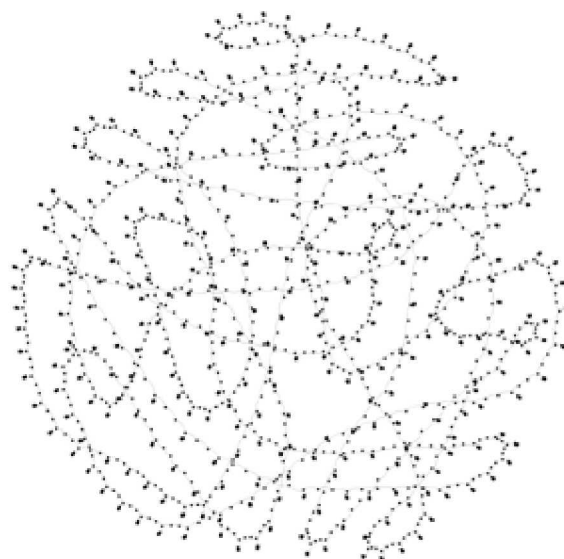
Challenges



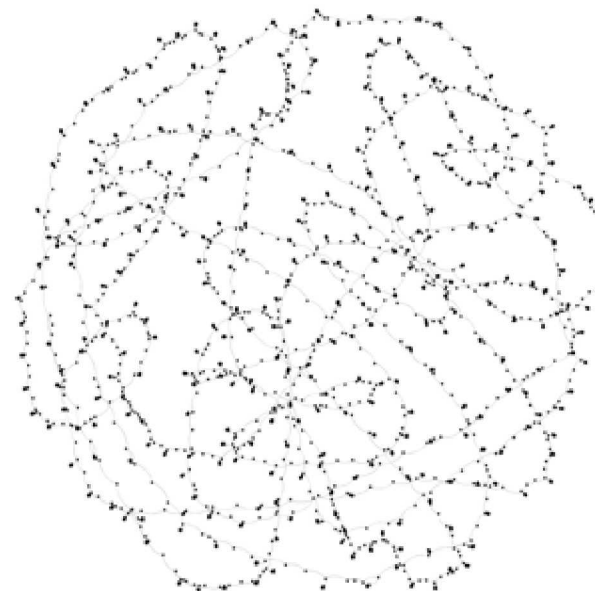
Graph Neural Networks



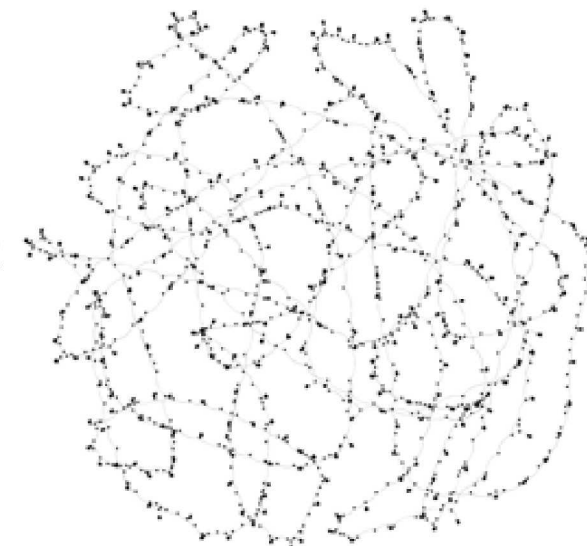
Ring of Houses



Larger graph



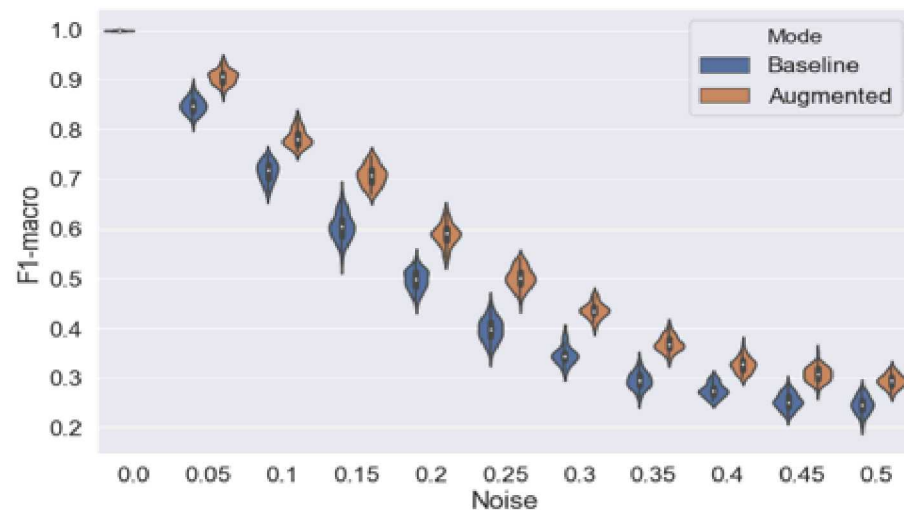
Distance-2 noise



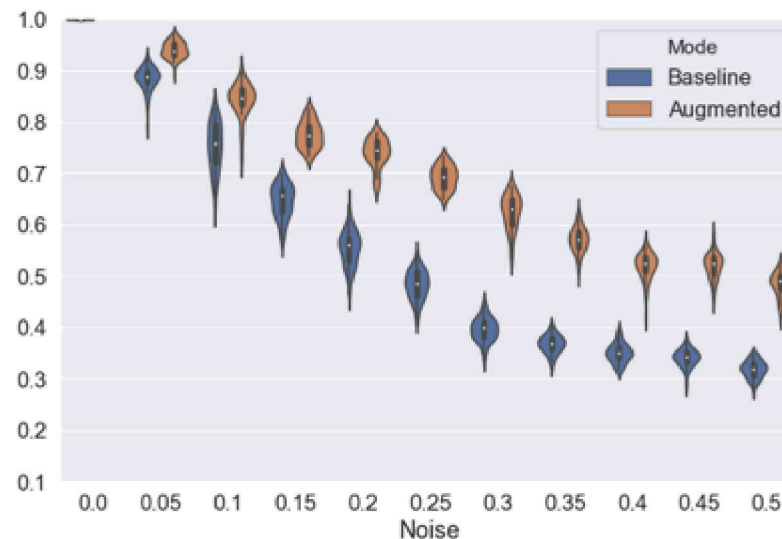
Distance-3 noise

- Graph Neural Networks (GNNs) are a powerful abstraction for learning embeddings on graph structured data
- GNNs have been used in several domains including drug discovery, material science, molecular toxicity prediction
- Evaluate a powerful GNN (Xu et al. 2018) in the presence of noise

Graph Neural Networks – Noisy Data



Test F1 score of GIN model with varying levels of structural noise added to input graph, across 3 different modes of noise constraint.



Augmented vs. non-augmented training (baseline) for node classification on Gp. Y-axis is F1 score, x-axis is random edge addition ratio.

- GNNs can predict the six classes with perfect accuracy with no noise
- The class prediction accuracy drops quite fast even at the presence of small amount of noisy edges 0.1-0.15
- The prediction accuracy can be improved by training on augmented noisy graphs

“How Robust are Graph Neural Networks to Structural Noise”, J. Fox, S. Rajamanickam, DLGMA workshop, AAAI 2019.