



Exceptional service in the national interest

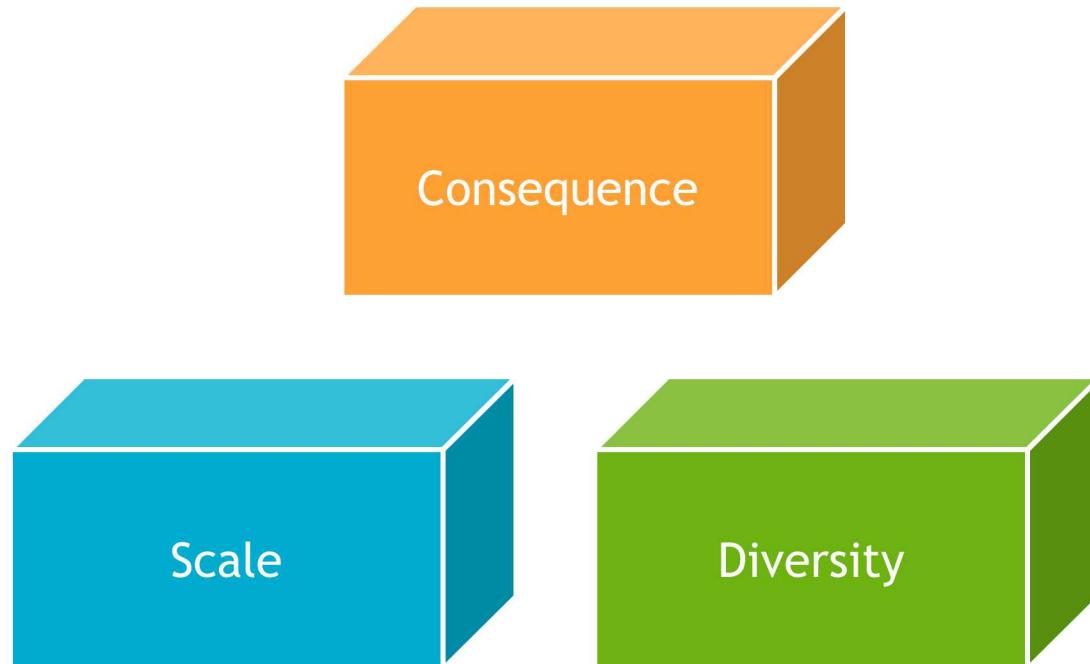


## Machine Learning in the Presence of Noise : Early Experiments

Presented by: Siva Rajamanickam  
srajama@sandia.gov

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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**

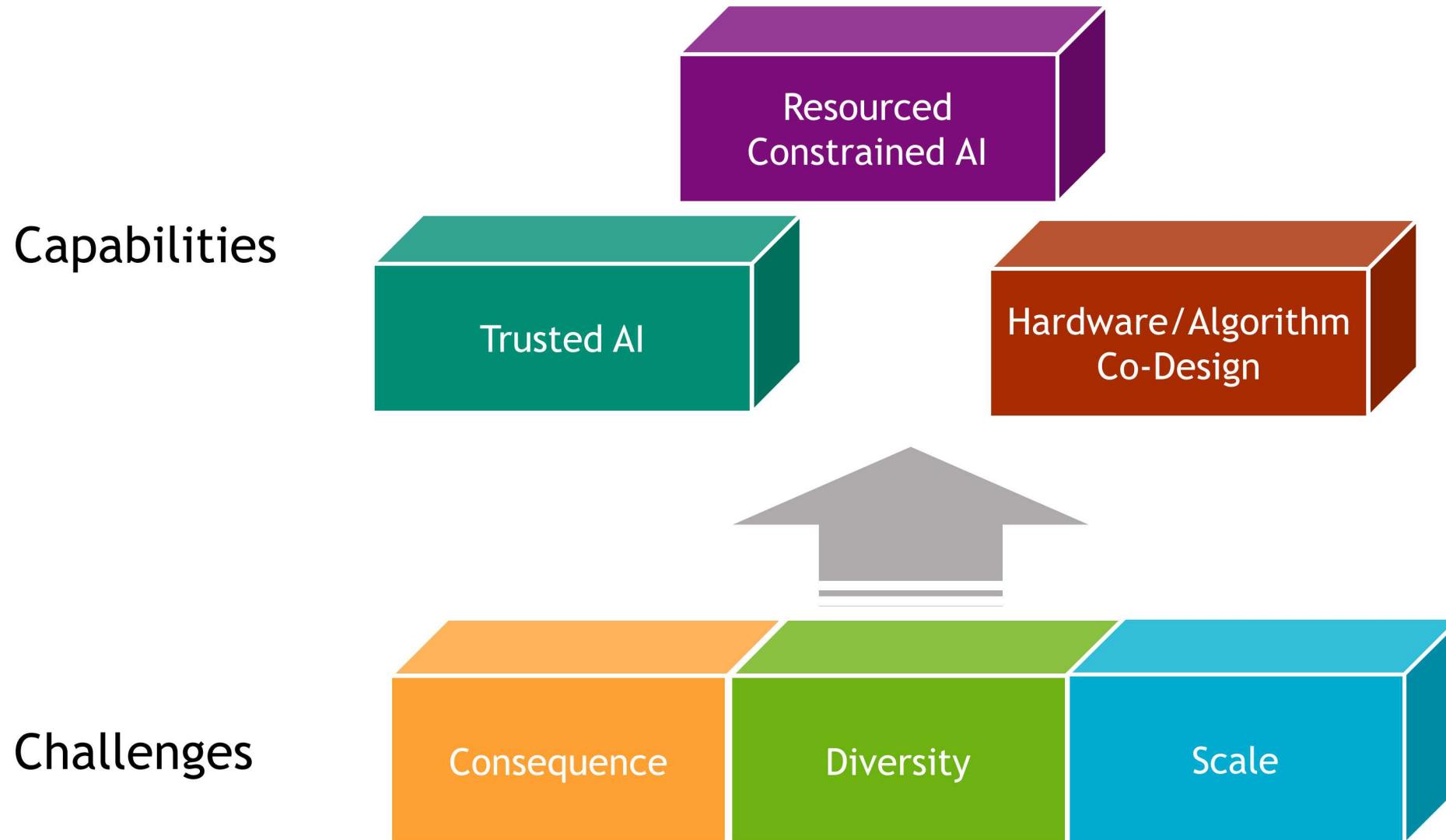
Extending and developing AI algorithms

Evaluating novel hardware and accelerators

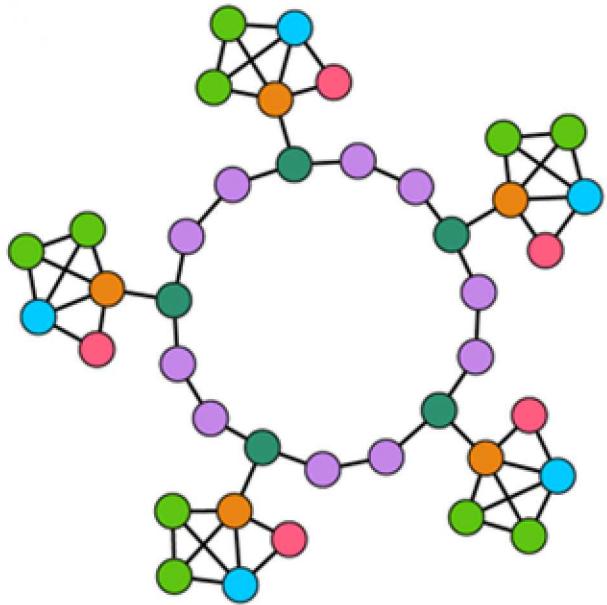
Explore brain-inspired sensor technology

Identifying opportunities for novel AI impact

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



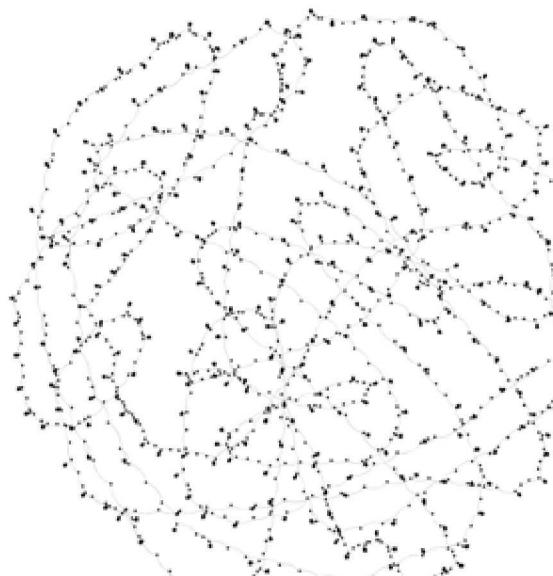
# Graph Neural Networks



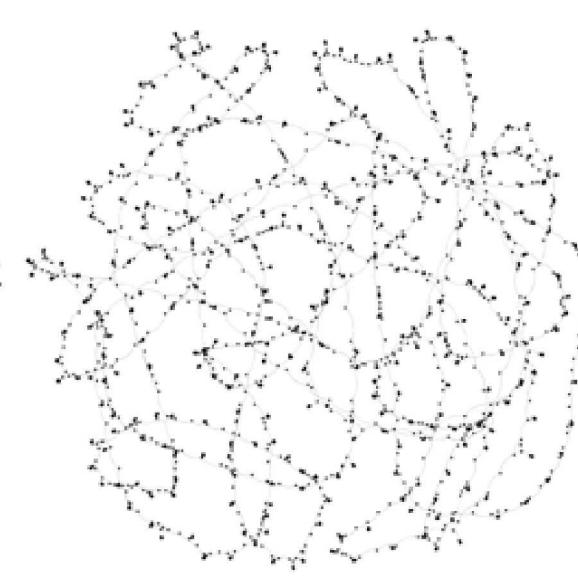
Ring of Houses



Larger graph



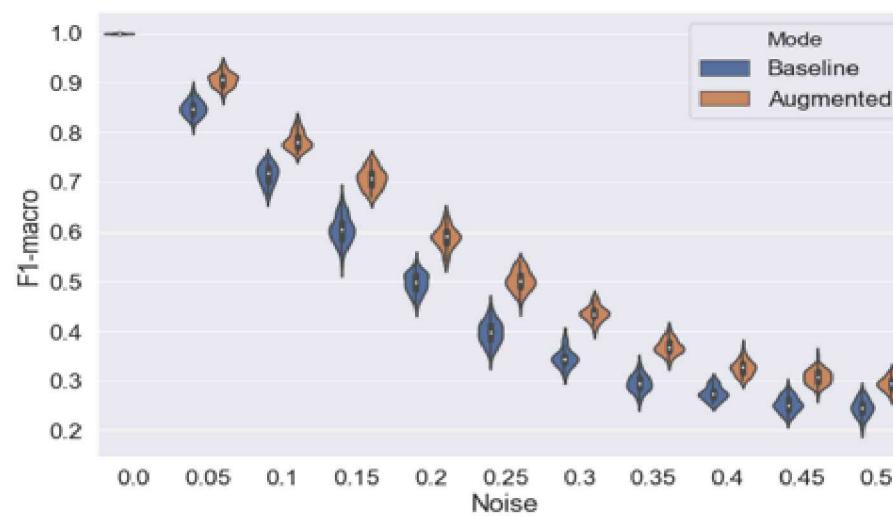
Distance-2 noise



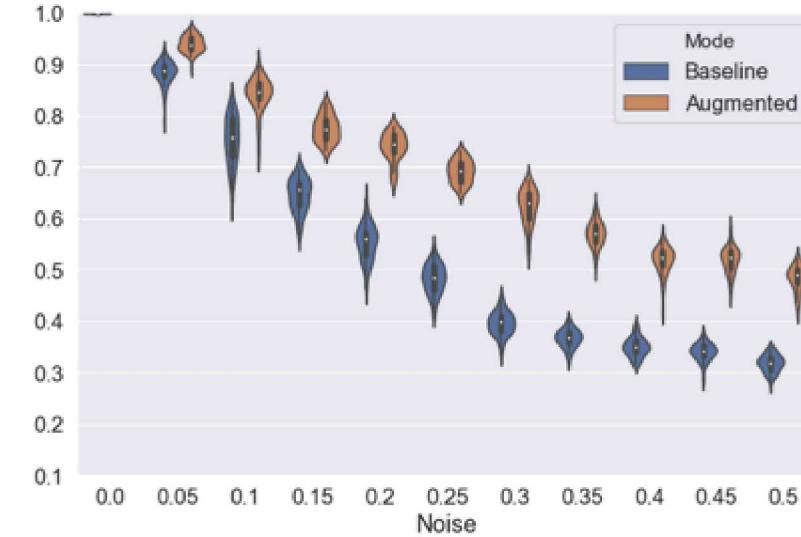
Distance-3 noise

- 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