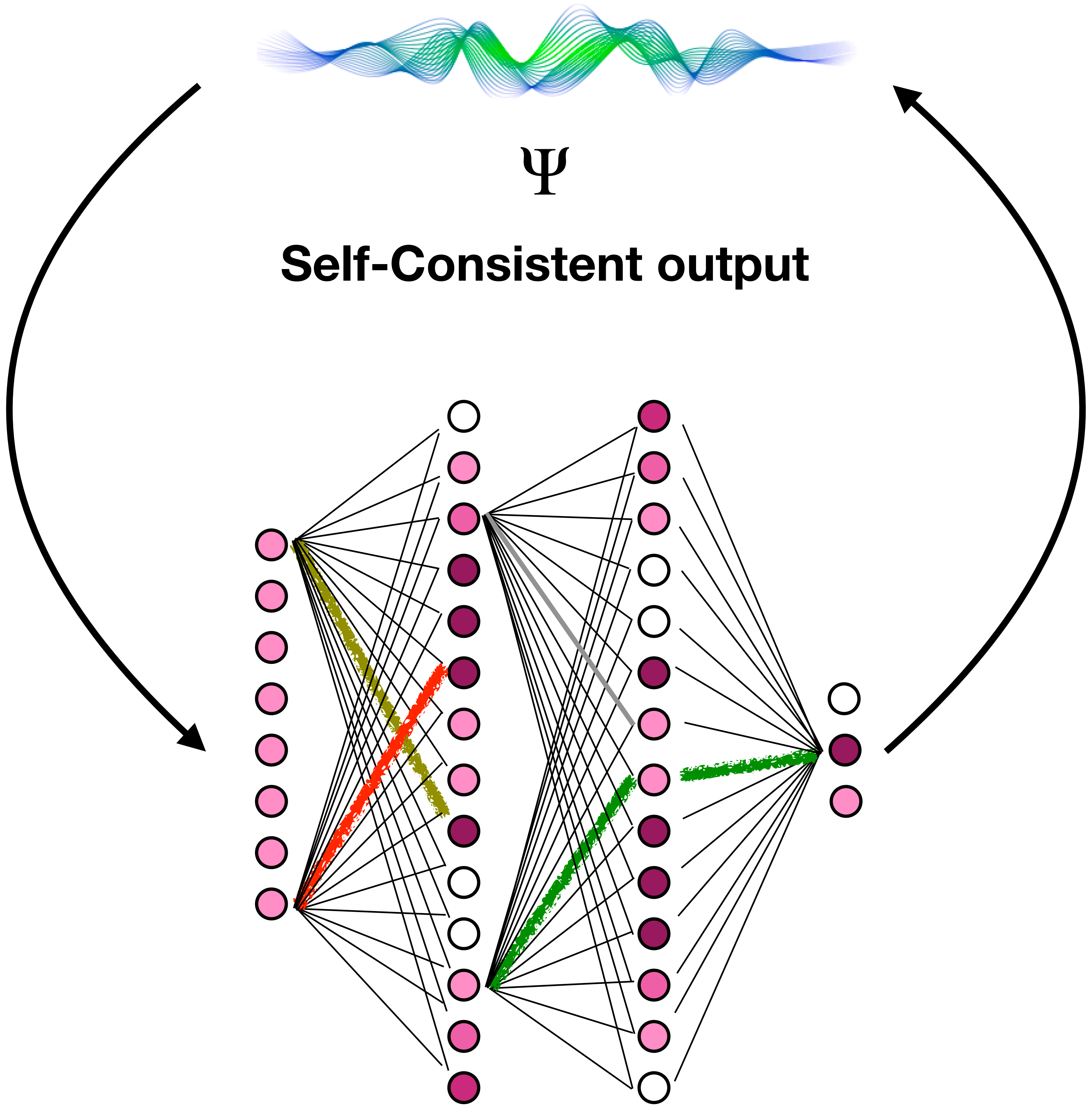
# Physics Guided Machine Learning

## Project Report and Planning - September 3, 2019

BINGHAMTON
UNIVERSITY
STATE UNIVERSITY OF NEW YORK

$$\frac{\partial C_2}{\partial \hat{\Psi}} = \hat{H}^2\hat{\Psi} - 2\hat{H}\hat{\Psi}\hat{E} + \hat{E}^2\hat{\Psi}$$

**Changing cost function**



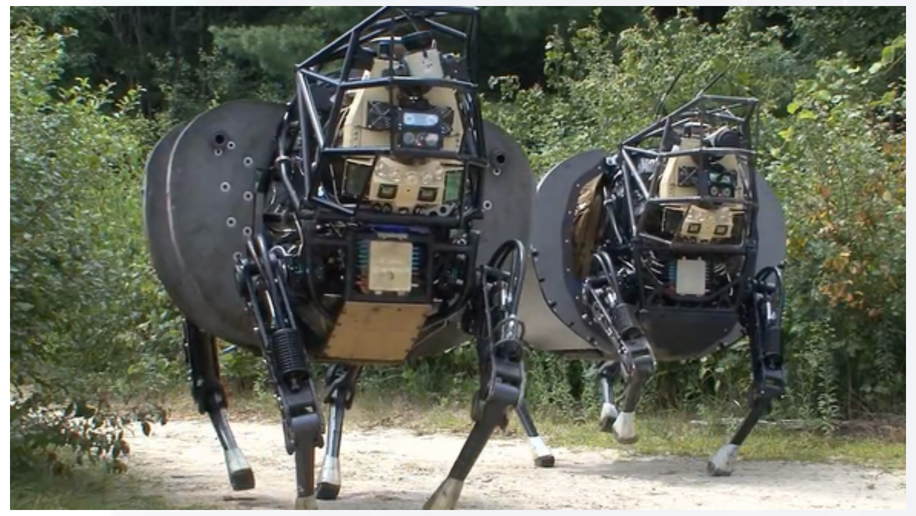

$$\hat{\delta} + = \hat{H}\hat{\Psi} - \hat{\Psi}\hat{E}$$

**Modify error directly**

# *The significance of artificial intelligence*

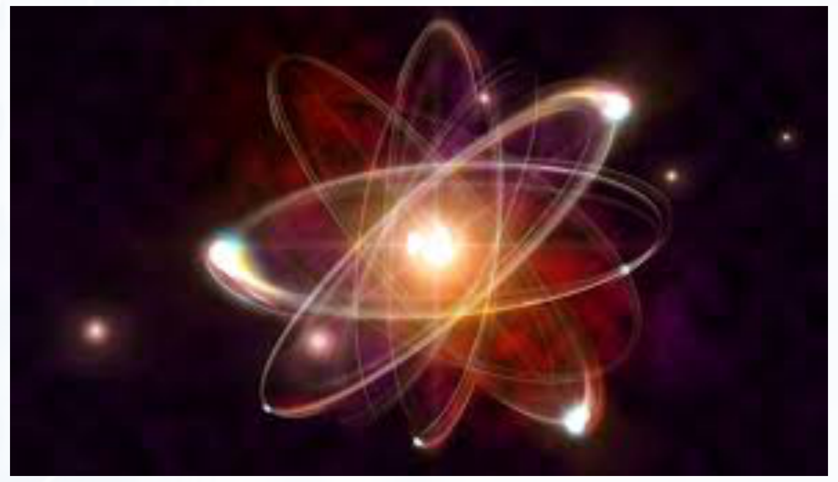
**Facial Recognition**

**National Security**

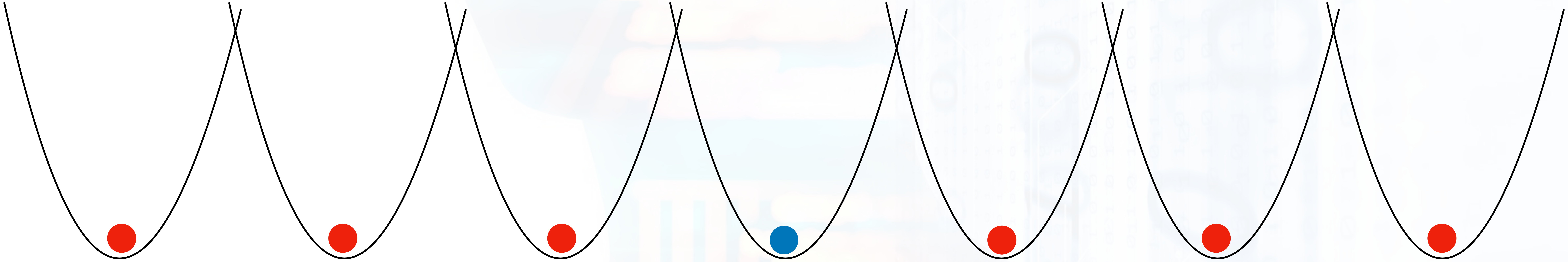


**Financial Markets**

**Quantum Physics**



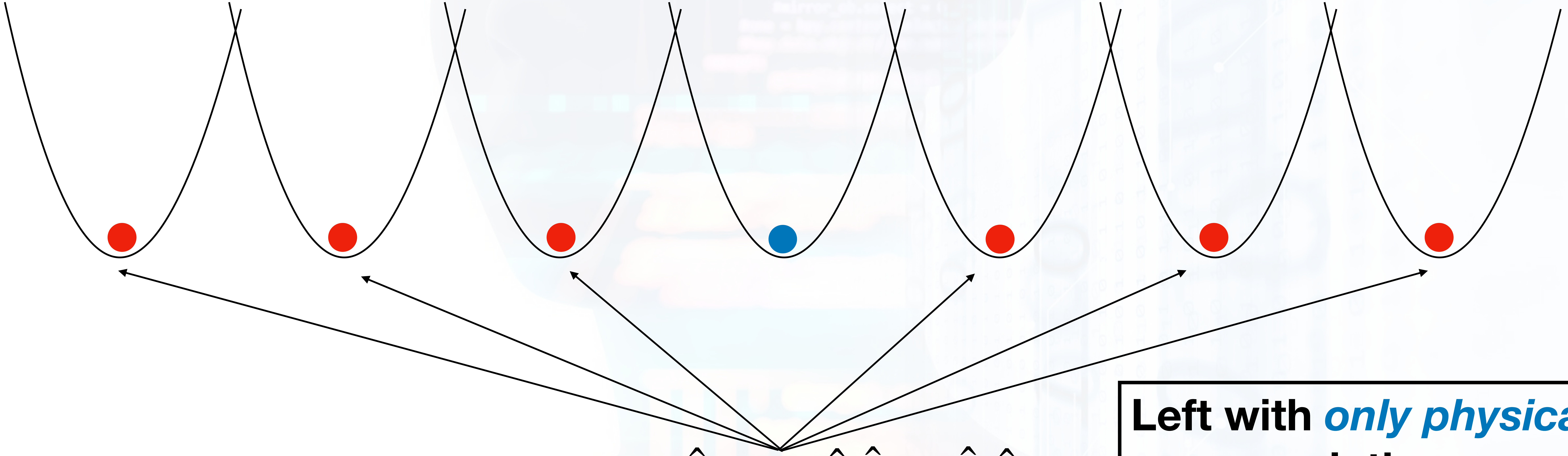
**Can be framed as minimization problem…**



**In actuality, there are *many* solutions**

# *The power of augmented intelligence*

**Given this many solutions… how can we choose just one?**



$$\hat{\delta} + = \hat{H}\hat{\Psi} - \hat{\Psi}\hat{E}$$

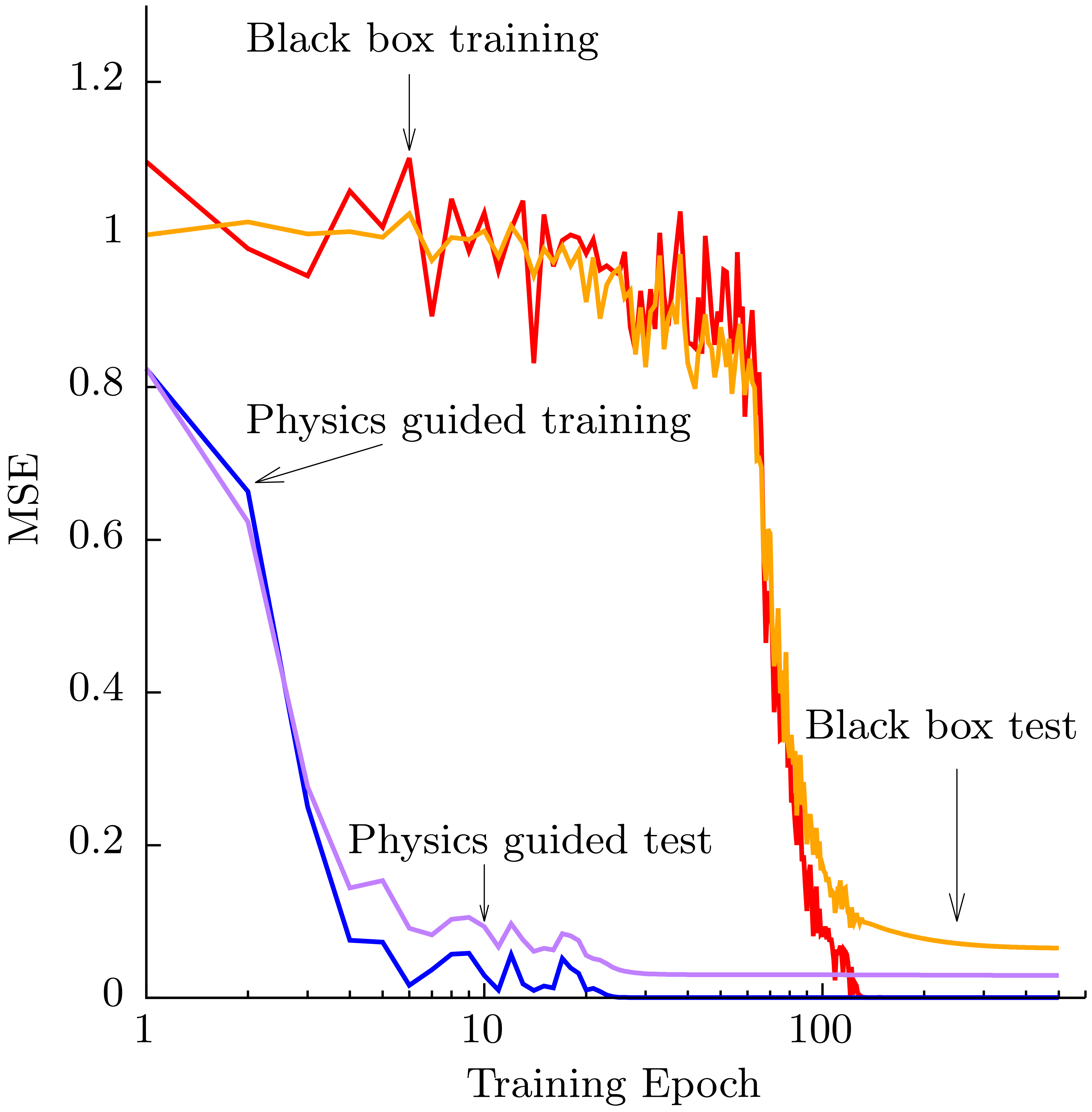
**Left with *only physical* solution**

# Action Items

- State of current results
- Distribution of responsibilities
- Publication targets

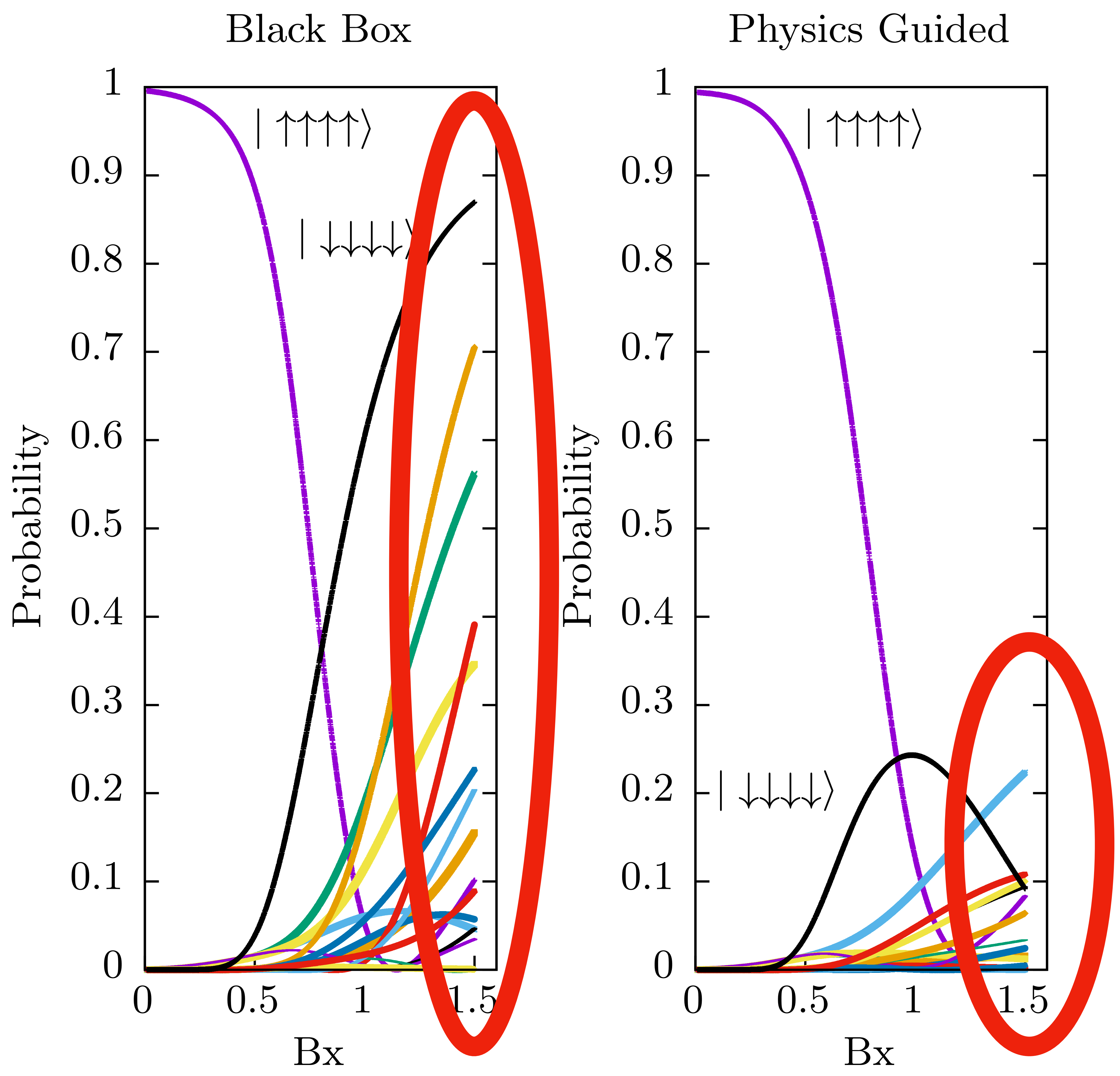
# Central Result 1: *Faster Learning*

- MSE decreases faster in guided machine than for Black Box
- Result achieved by modulating error of output layer



# Central Result 2: *Better Predictions*

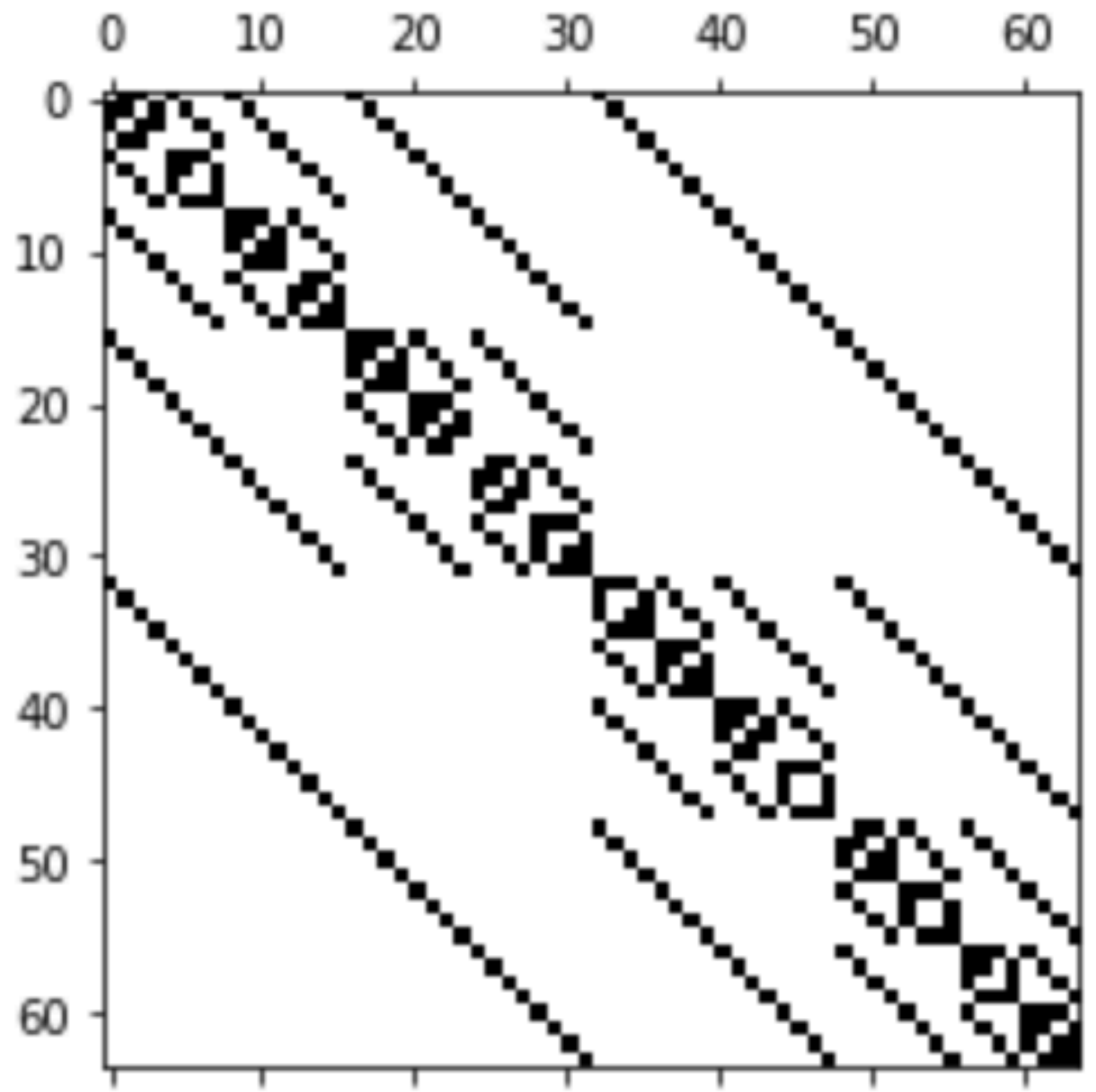
- In ring qubit structures, guided machine efficient at data never seen
- Advancing the field by suggesting machines *can* work outside the domain of training



# Distribution of Work (1) - Data Generation

- Generalized Ising Model
  - Add transverse and longitudinal Field

$$H = J\sum_{i=0}^{N-1}\sigma_i^z\sigma_{i+1}^z - B_x\sum_{i=0}^{N-1}\sigma_i^x - B_z\sum_{i=0}^{N-1}\sigma_i^z$$




**Matrix structure… how to exploit?**

# Distribution of Work (2) - Algorithm Devel

- Sequential Ground State - Lagrange multiplier based
- Matrix Spectrum - Direct modulation of output layer

$$\delta_N^L = \phi\Big(a_N - y_N + 2\lambda a_N^L(1-N)\Big[\sum_m^{N-1}\big[\sum_n^{N-1} a^1_{m\cdot d+n}a_n^L - a_N^L a_m^L\big]\Big]\Big)$$

$$C_2 = \frac{1}{2}||\hat{H}\hat{\Psi} - \hat{\Psi}\hat{E}||_F^2$$

$$\delta_j^L = \Big(a_j^L - y_j + \lambda\sum_i T_j^{(i)}\Big)\Big(1 - \tanh^2(z_j^L)\Big), \forall j < N$$

$$\frac{\partial C_2}{\partial\hat{\Psi}} = \hat{H}^2\hat{\Psi} - 2\hat{H}\hat{\Psi}\hat{E} + \hat{E}^2\hat{\Psi}$$

# Distribution of Work (3) - Implementation

- From scratch C++ for matrix based method (*Chris*)
    - Results for Ising chain using this one
- From scratch Serial GS python (*Matt*)
    - Status?
- Pytorch (*Jie*)
    - Status?

# Notes

- Proof of optimizer
- Speed improvement
- What problem
- Memory issues
- Sparse memory representation
- Plan future meeting - student

**What is the best a standard machine can do?**

# Publication Targets

- Generalizability of results and brevity of story suggest PRL for physics - *algorithm development CS target*?

- Predicting physics (1) - Updating of error (2)

- Abstract submission: Oct 25

APS physics MARCH MEETING 2020
MARCH 2-6 DENVER, CO

- Abstract submission: Oct 11

Society for Industrial and Applied Mathematics is proud to introduce the First Conference on Mathematics of Data Science. This conference will provide a forum to present work that advances mathematical, statistical, and computational methods in the context of data and information sciences and aims to unite researchers who are building mathematical foundations for data science and making principled applications to science, engineering, technology, and society.

siam 2020 Conference on Mathematics of Data Science

# Points of attack to be considered…

- Applicability to density functional theory methods
- Mathematics of eigenvalue problems
- Radar physics not well-defined enough (problem with supervised learning)
- Originality