Study of Neural Network Size Requirements for Approximating Functions Relevant to HEP

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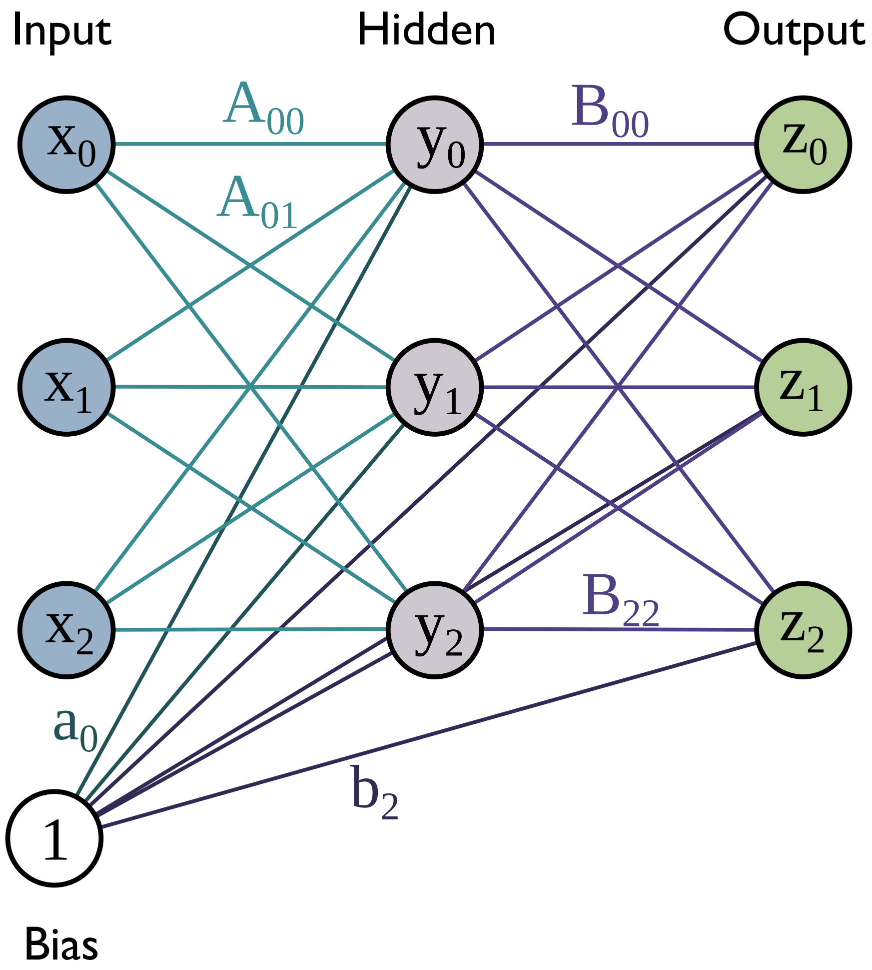
Deep Learning

- Neural networks as function approximator
- Learns from map of inputs and outputs
- Outputs given by

$$y_j = h\left(\sum_{i=0}^{2} A_{ji} x_i + a_j\right)$$

$$z_k = \sum_{j=0}^{2} B_{kj} y_j + b_k$$

$$h(x) = \begin{cases} 0 & x \leq 0 \\ x & x > 0 \end{cases}$$



Deep Learning in HEP

Inspiration

- Machine learning approaches are already used to solve classification problems in HEP
- "Searching for Exotic Particles in High-Energy Physics with Deep Learning" (P. Baldi et al., 2014)

Questions

- How big does the network have to be?
  - This effects how effectively we survey hyperparameter space
  - Too big – overfitting
  - Too small – can't fit

Deep Learning Study

- Examine basic functions
  - Vector to Vector
  - Vector to $Vector^2$
  - Vector to $|Vector|^2$
- Used toy model to generate reasonable parameters for momentum vectors
  - Inputs standardized for training

- Network training
  - GPUs
  - Keras with Theano
  - 5 trials (trained on 1 million samples, validated on 10,000)
  - MSE loss function
  - Adam optimizer with default parameters
  - Batch size: 1000 Epochs: 5000
  - Saved model from best epoch

Vector to Vector

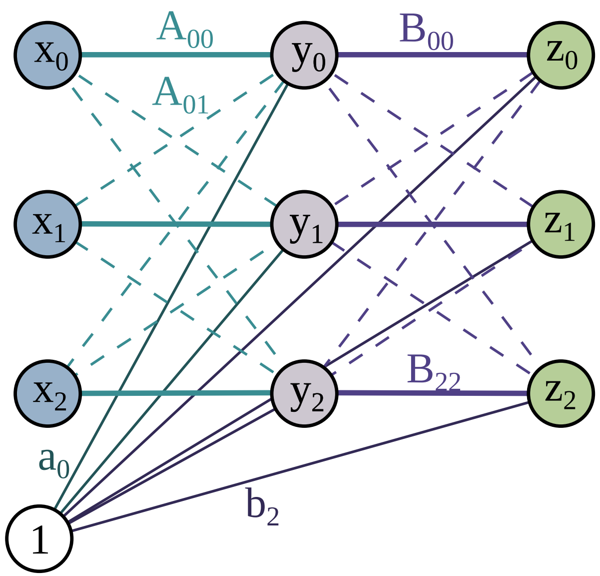
Mapping a vector onto itself

The solution needs to satisfy…

$$AB = I \qquad Ba + b = 0$$

Obvious solution:

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad a = \begin{bmatrix} -x_{0,min} \\ -x_{1,min} \\ -x_{2,min} \end{bmatrix} \qquad B = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad b = \begin{bmatrix} +x_{0,min} \\ +x_{1,min} \\ +x_{2,min} \end{bmatrix}$$



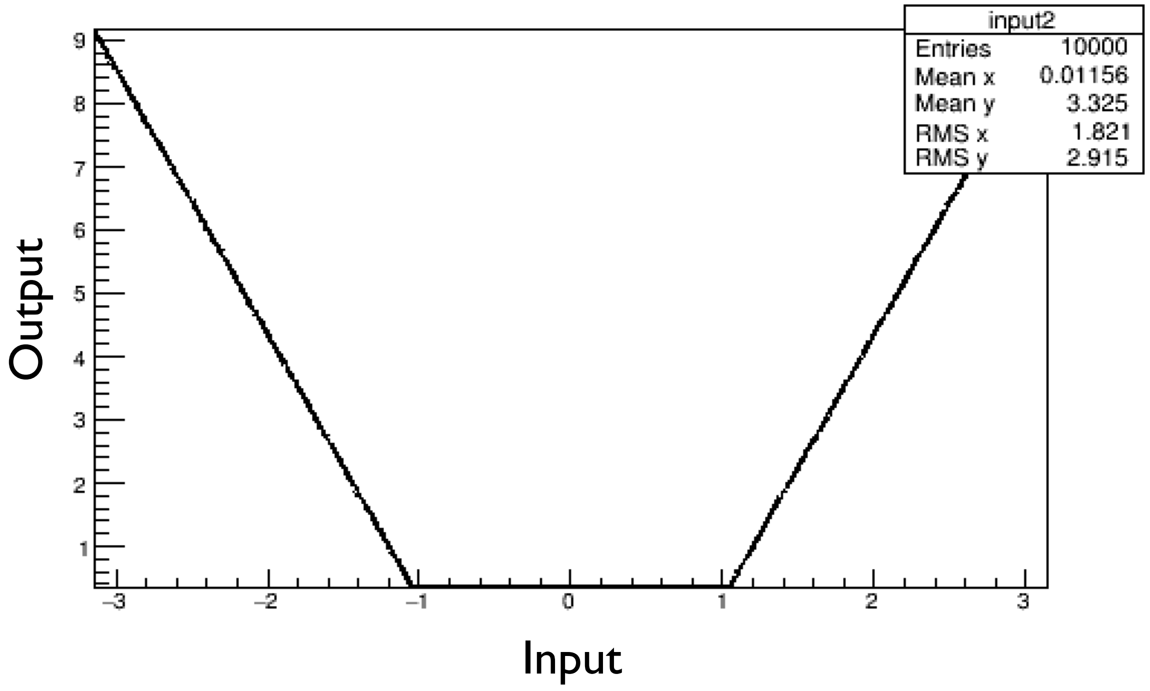
What the NN training actually found (one trial):

$$A = \begin{bmatrix} 0.711 & 0.279 & 0.266 \\ 0.023 & 0.494 & -0.102 \\ -0.091 & 0.354 & 0.471 \end{bmatrix} \qquad a = \begin{bmatrix} 1.474 \\ 1.929 \\ 1.448 \end{bmatrix} \qquad B = \begin{bmatrix} 1.313 & -0.182 & -0.782 \\ -0.009 & 1.754 & 0.386 \\ 0.260 & -1.354 & 1.682 \end{bmatrix} \qquad b = \begin{bmatrix} -2.294 \\ -1.154 \\ -2.203 \end{bmatrix}$$

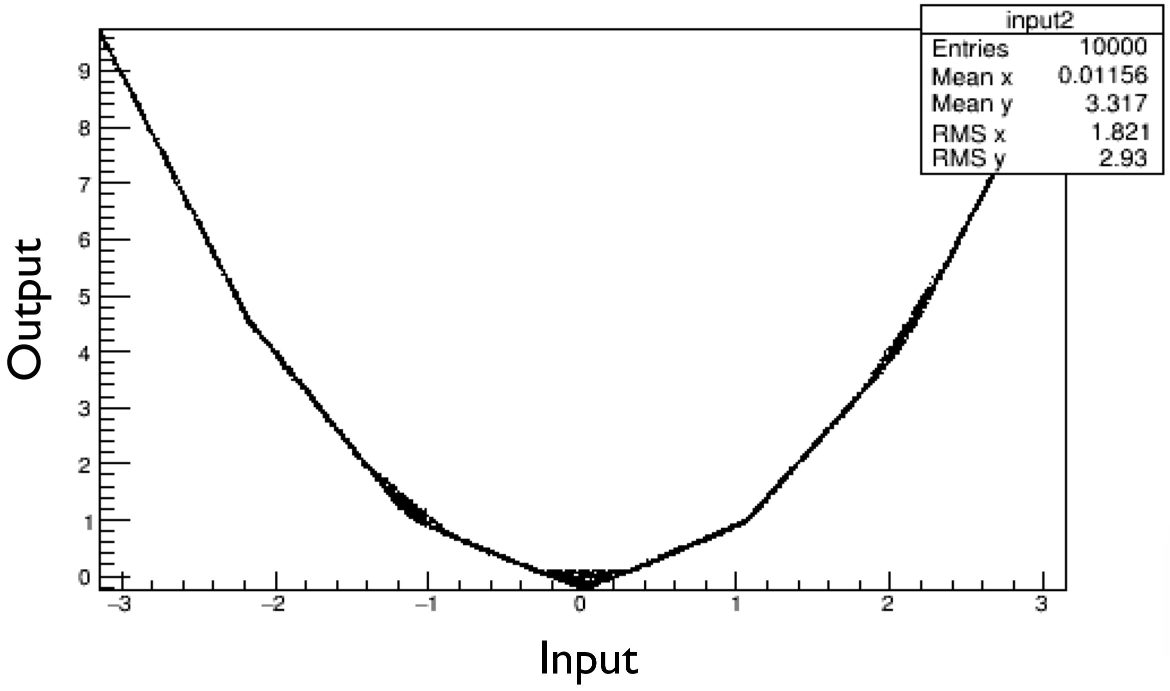
NN finds a correct solution even if it is not the simplest solution (fewest non-zero weights).

Vector to Vector^2

3 Nodes

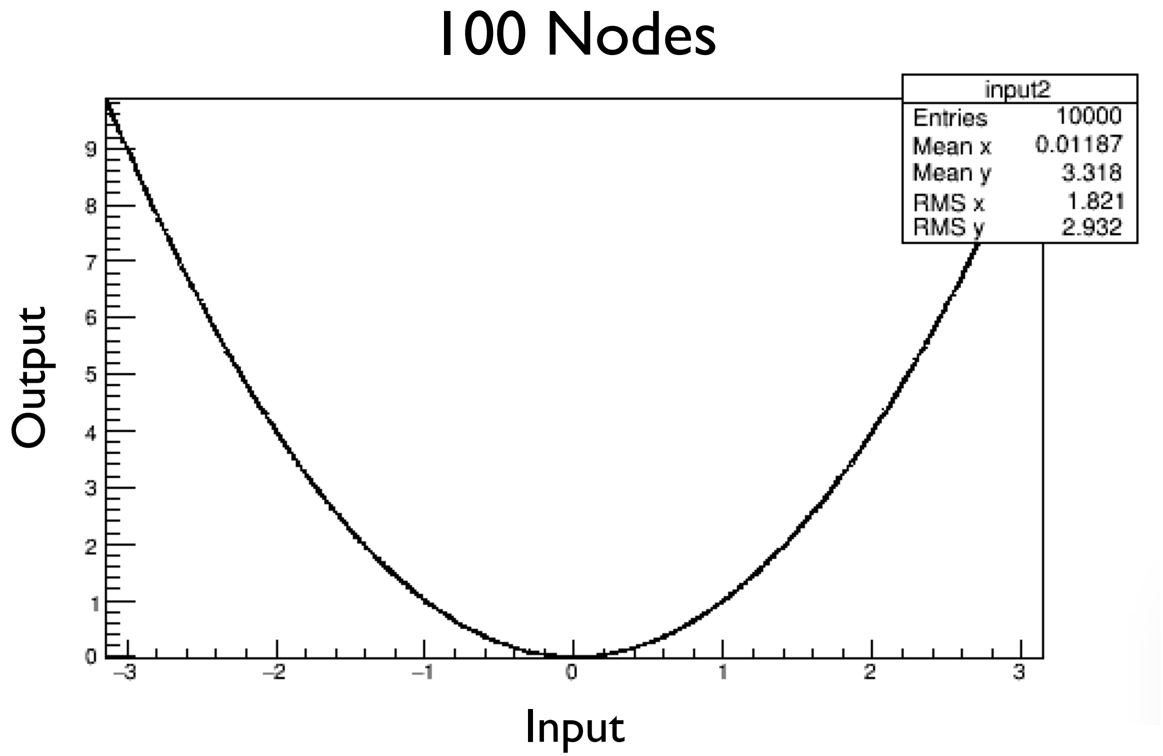


25 Nodes



In networks with few nodes, we can see the segments used to approximate the function.

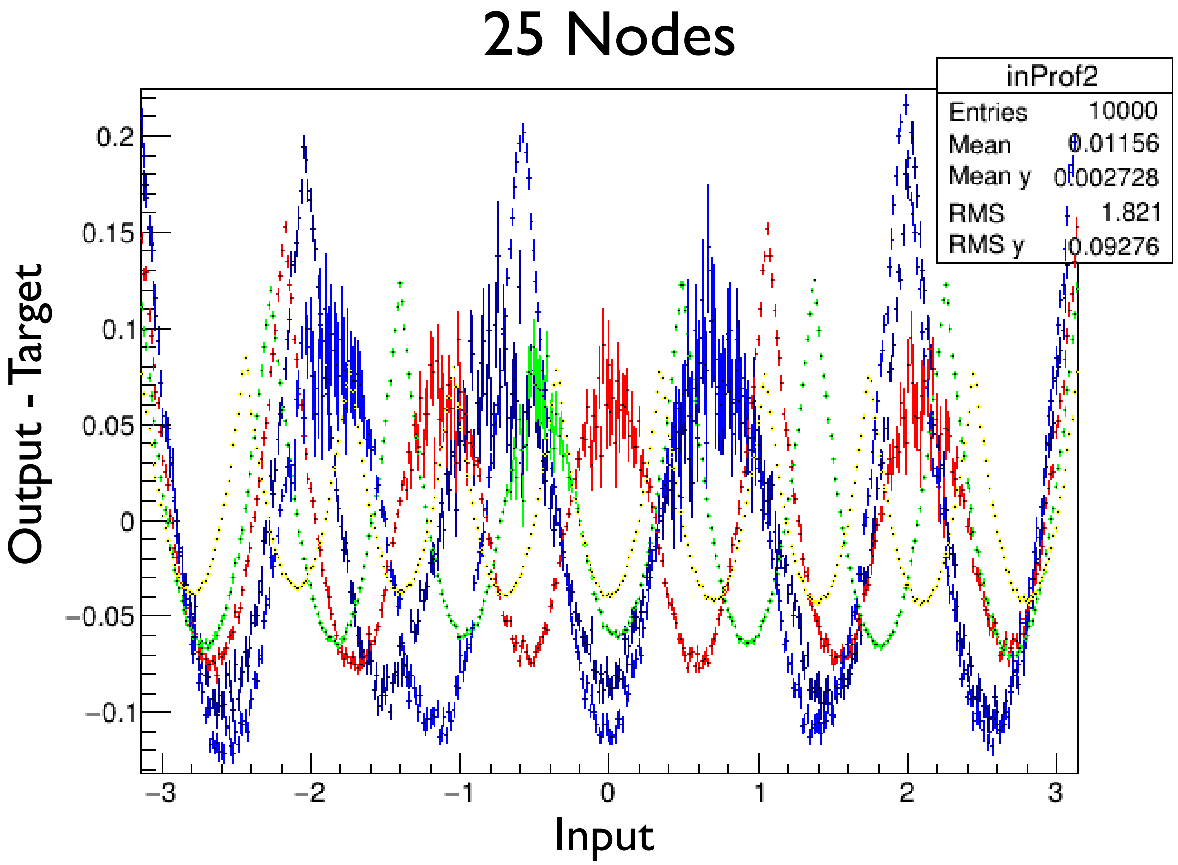
Vector to Vector^2



As the number of nodes increases, the curve becomes smoother.
This indicates a better approximation of the function V^2.

Vector to Vector^2

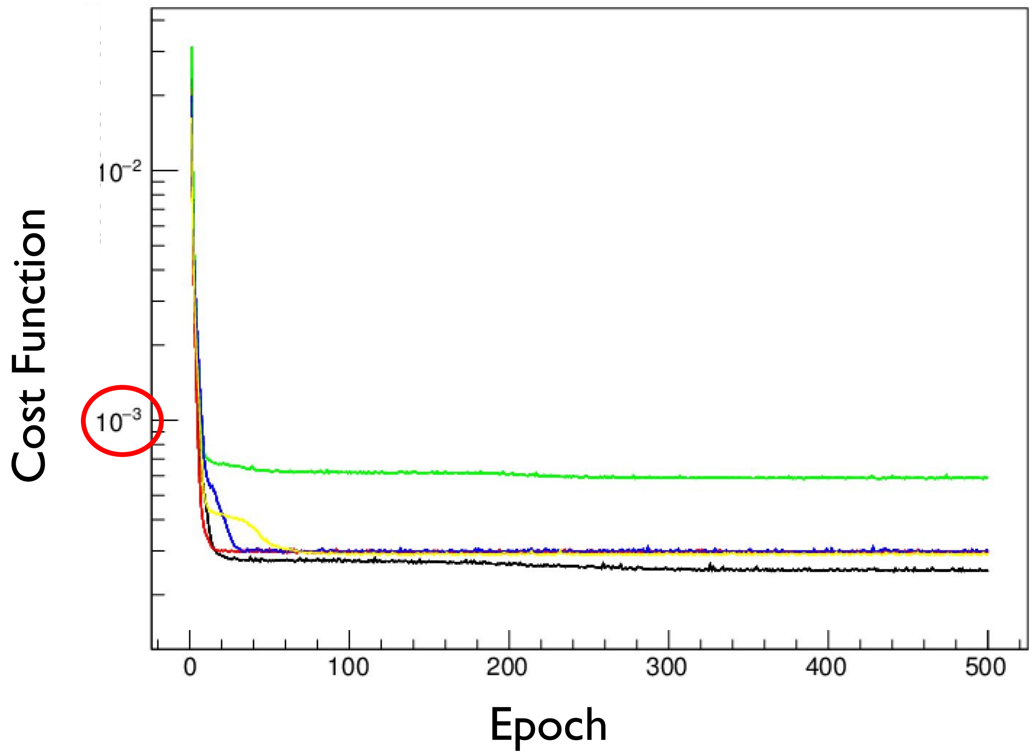
- Zero crossings correspond to the segments used to approximate V^2
  - Divided among the 3 variables (not always evenly)
  - Suspect this is from ReLU case where all inputs < 0 and gradient becomes 0.
  - Initial weights also play a role



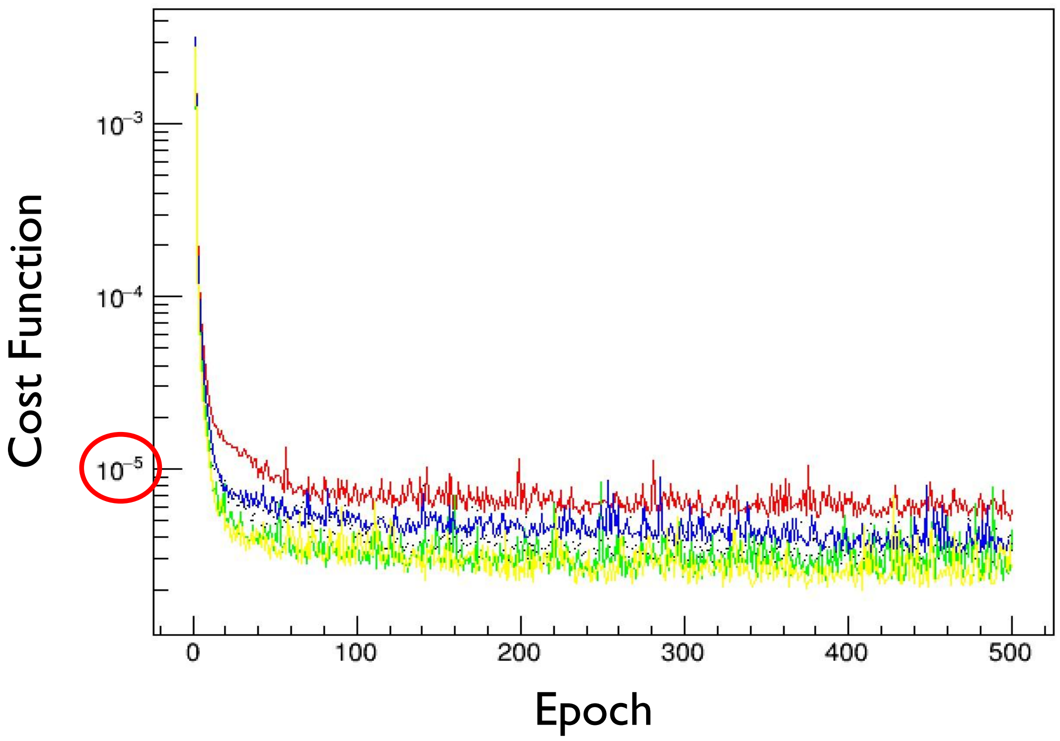
Vector to Vector^2

Network performances

25 Nodes

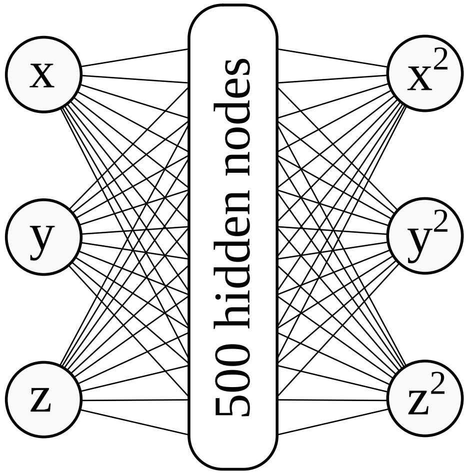


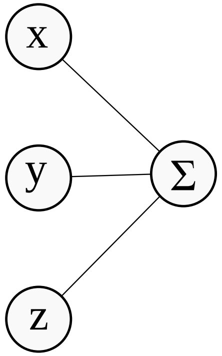
100 Nodes

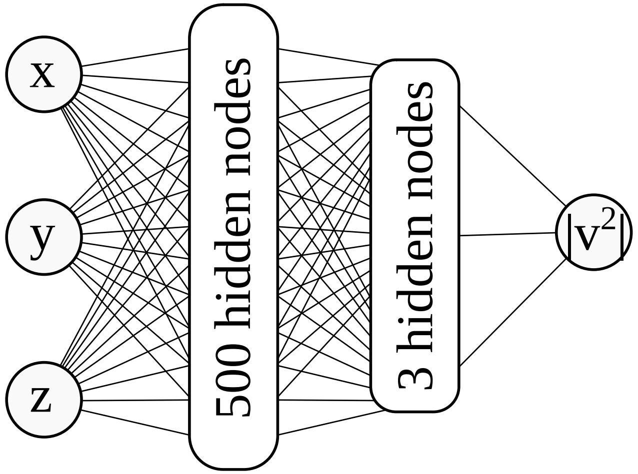


Vector to $|Vector|^2$

- Intuitive Strategy
  - Use the best networks from V to V^2
    - One layer with 500 nodes
  - Add a summation layer that adds the V^2 outputs
    - One layer with 3 nodes







Vector to |Vector|^2

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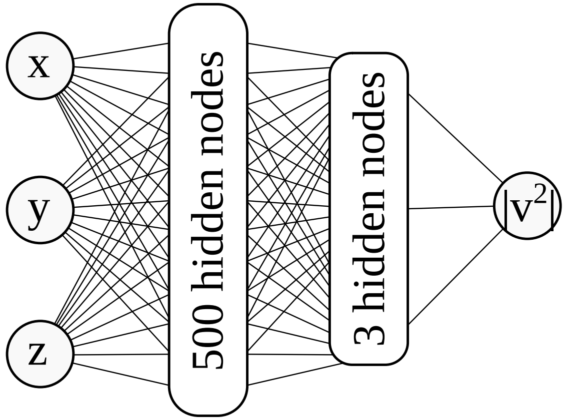
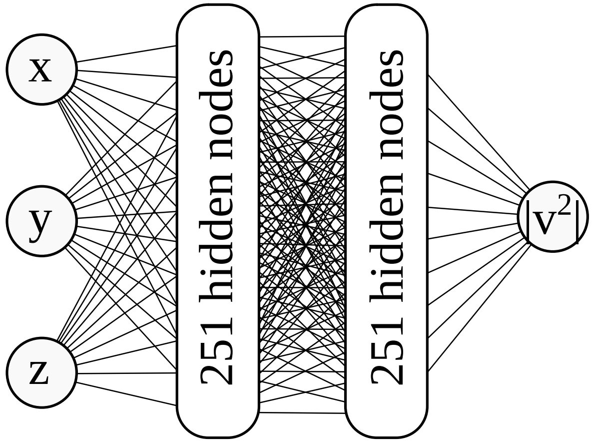
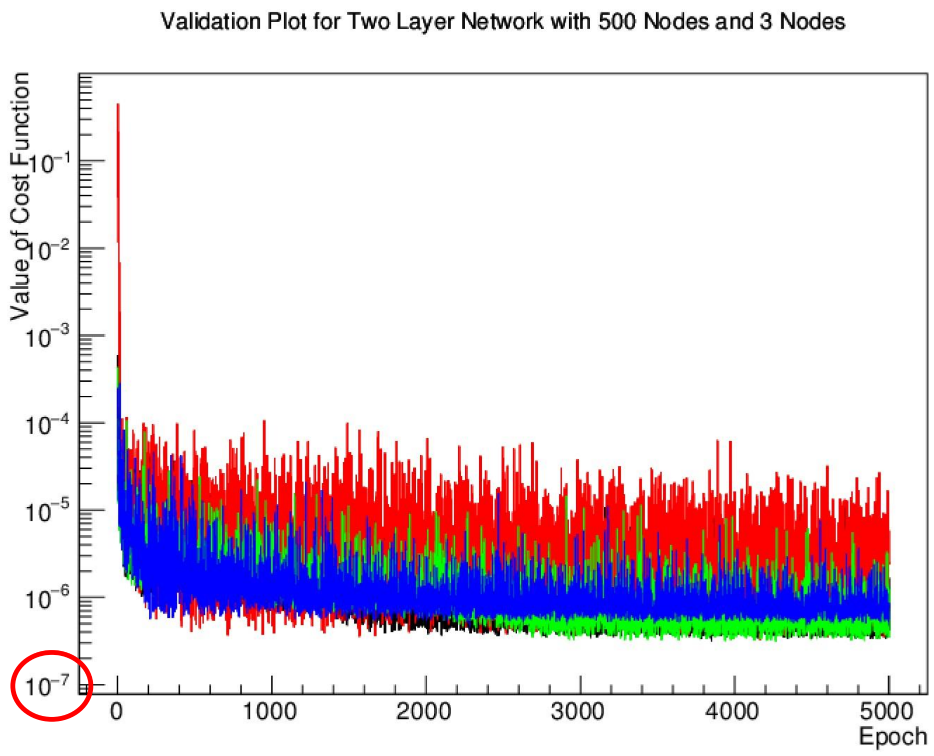


- Alternative Strategies
  - Tried many, for example, add a layer, but keep the total nodes constant

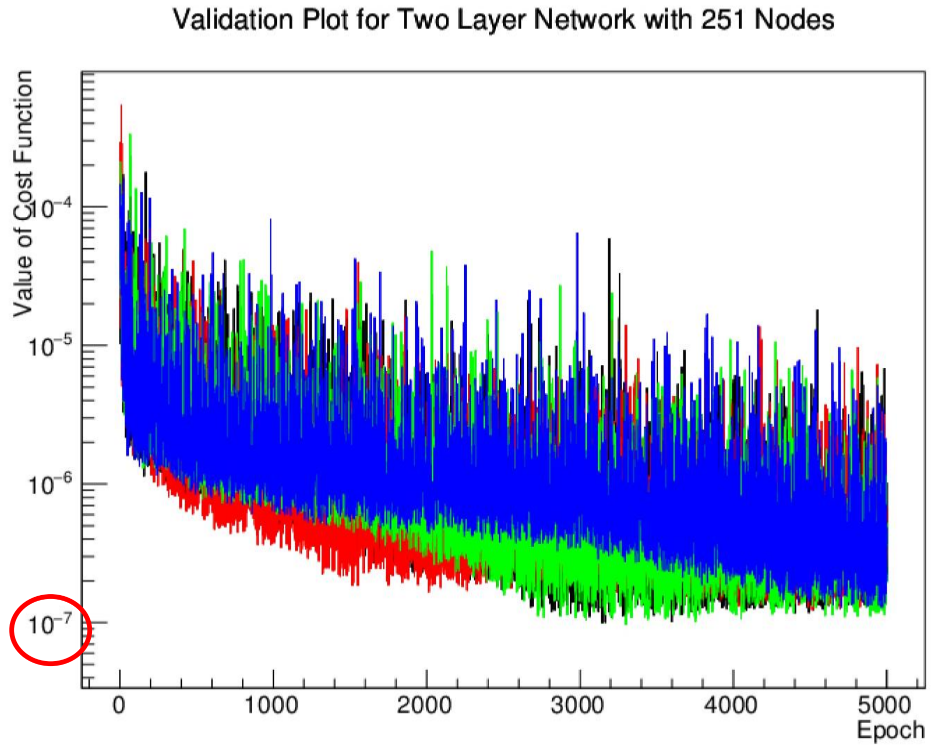


Vector to $|\text{Vector}|^2$

Intuitive



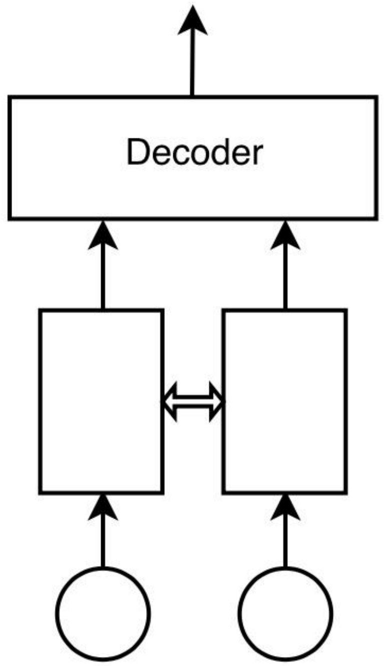
Alternative



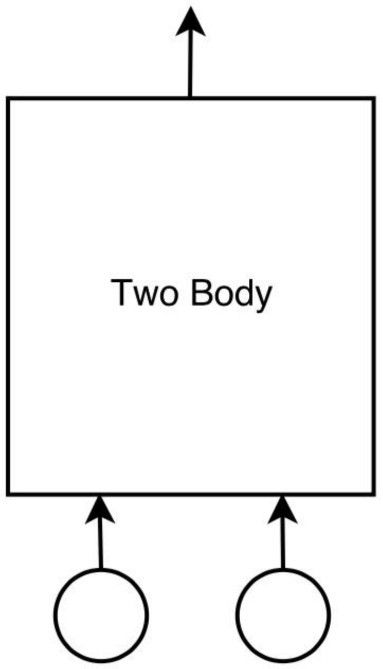
Future Work

Ask questions similar to Vector to $|\text{Vector}|^2$ experiment, but this time taking multiple four vectors as inputs.

Intuitive



Unstructured



Conclusions

- NN's find solutions to problems that aren't always the most intuitive
- It is important to understand the fundamentals of NN behavior before applying them to more complicated problems
  - We can develop better intuition for creating networks that work for HEP analysis
- Do we guide the network towards the solutions we'd like or give it free reign?

Questions?