Boosting Simulations of Hot Nuclear Matter with Machine Learning

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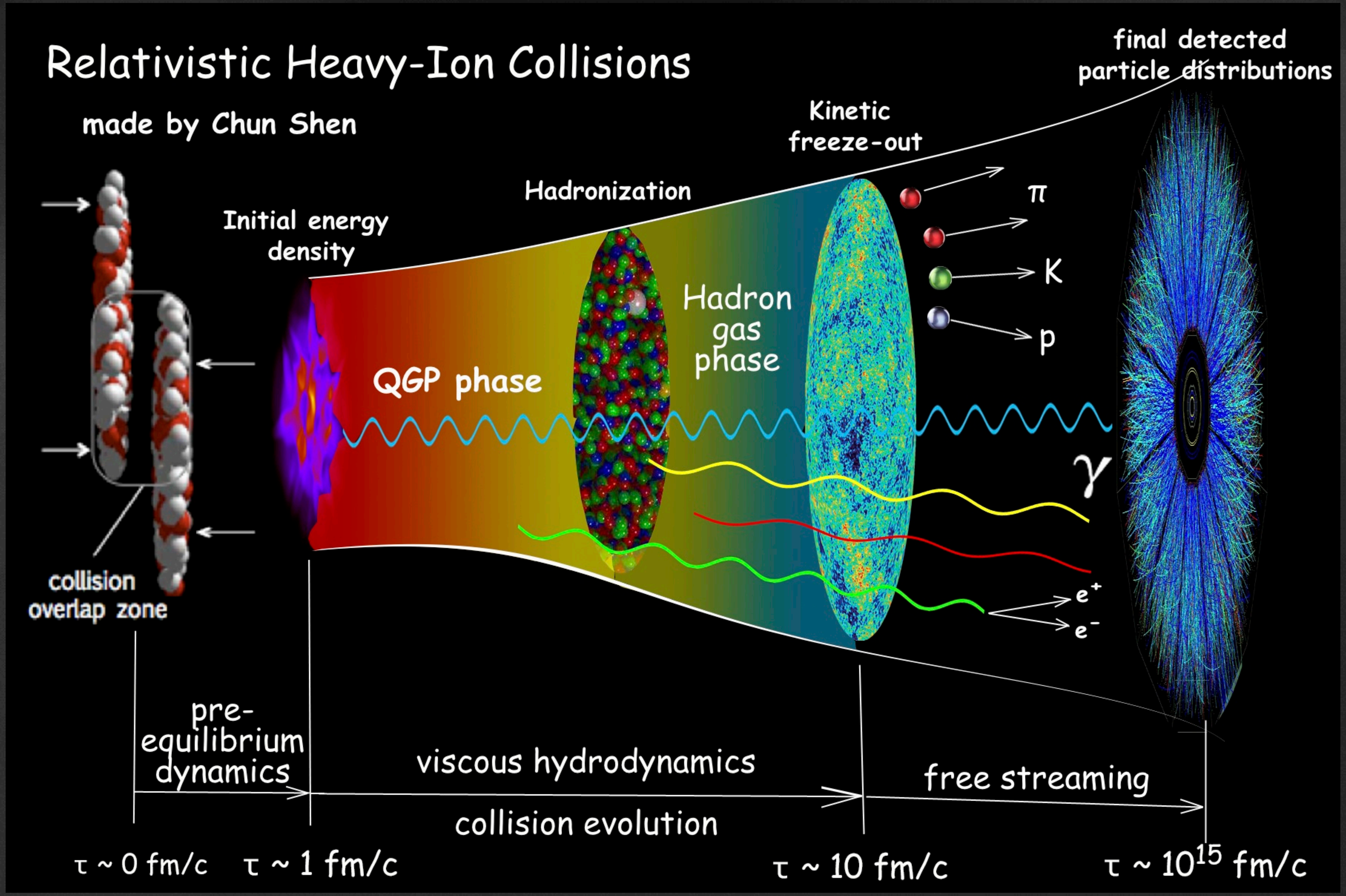
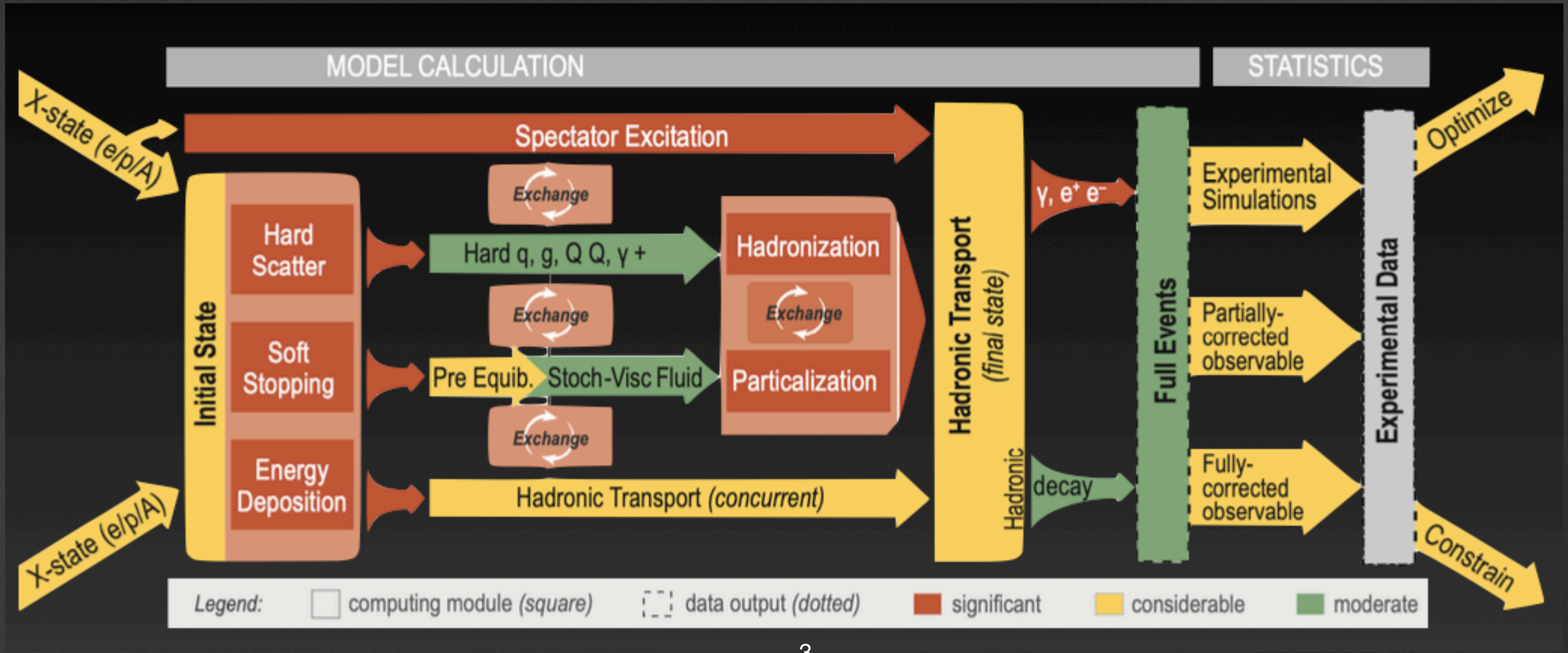
Along with

Numerical Simulations of (3+1)D Hydrodynamics + hadronic transport hybrid model

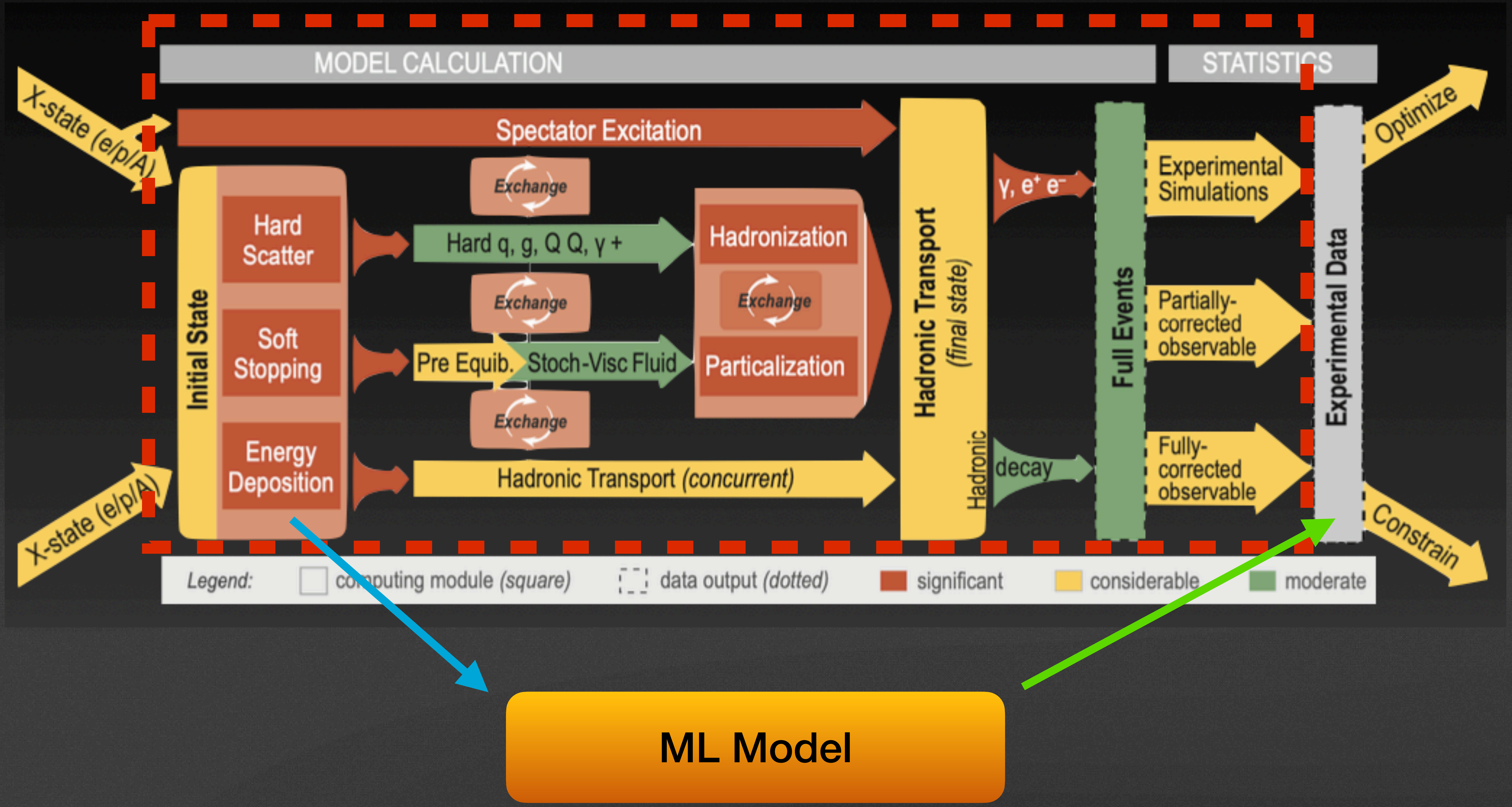


The problem

- Computationally expensive
- Time expensive; a single batch run can take 30+ hours to complete
- 10-100 million events are required to ensure enough statistics for observables
- It is critical to find ways to reduce computational costs

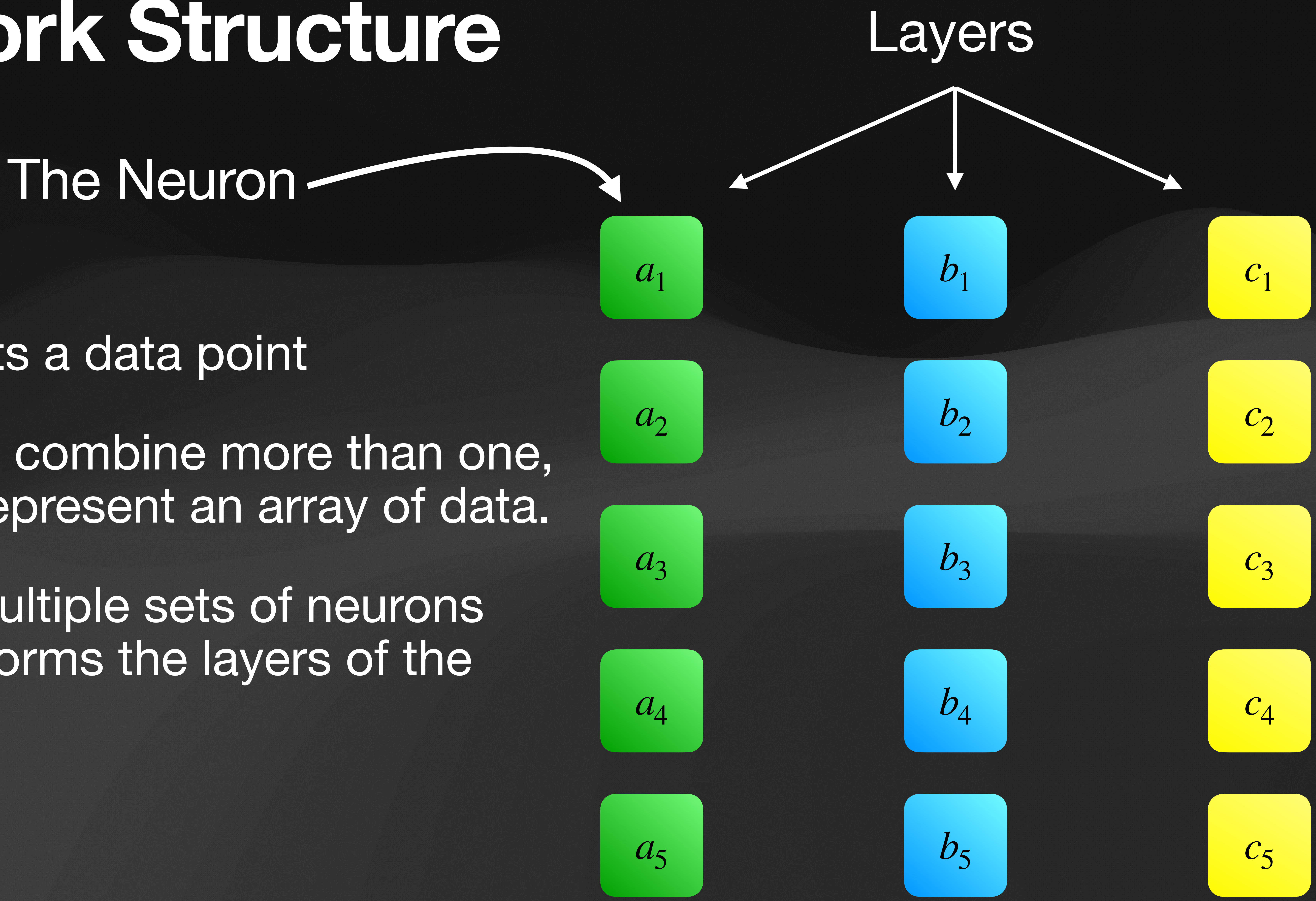


The problem



Can we create a machine learning model that can learn the correlation between the initial state and the final state?

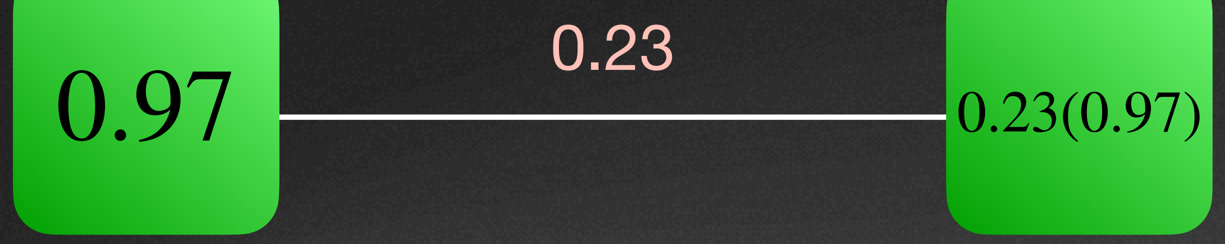
Network Structure



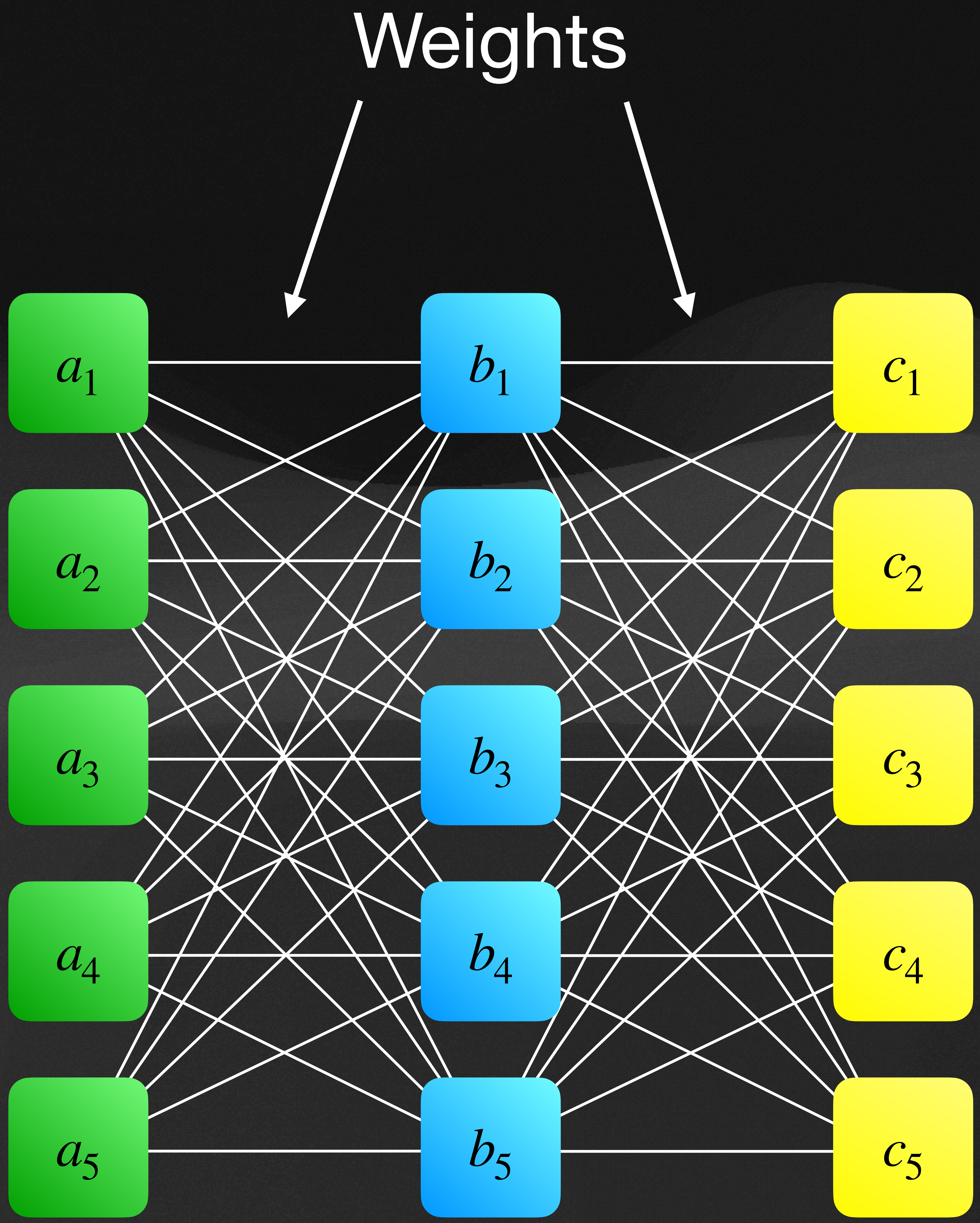
- Represents a data point
- When you combine more than one, you can represent an array of data.
- Placing multiple sets of neurons together forms the layers of the network

Network Structure

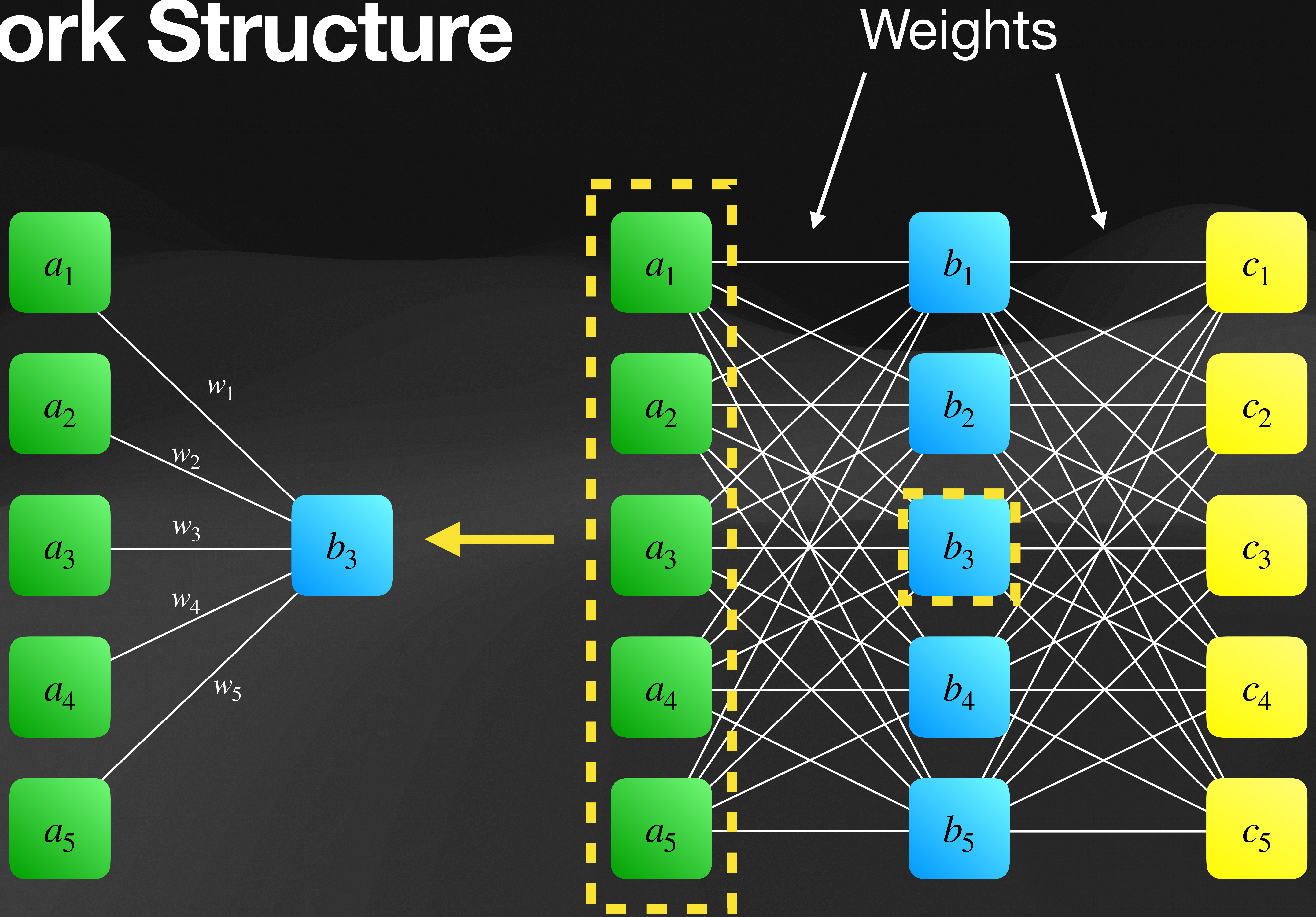
Each neuron in connected by a weight



The weights are the parameters that we are training!

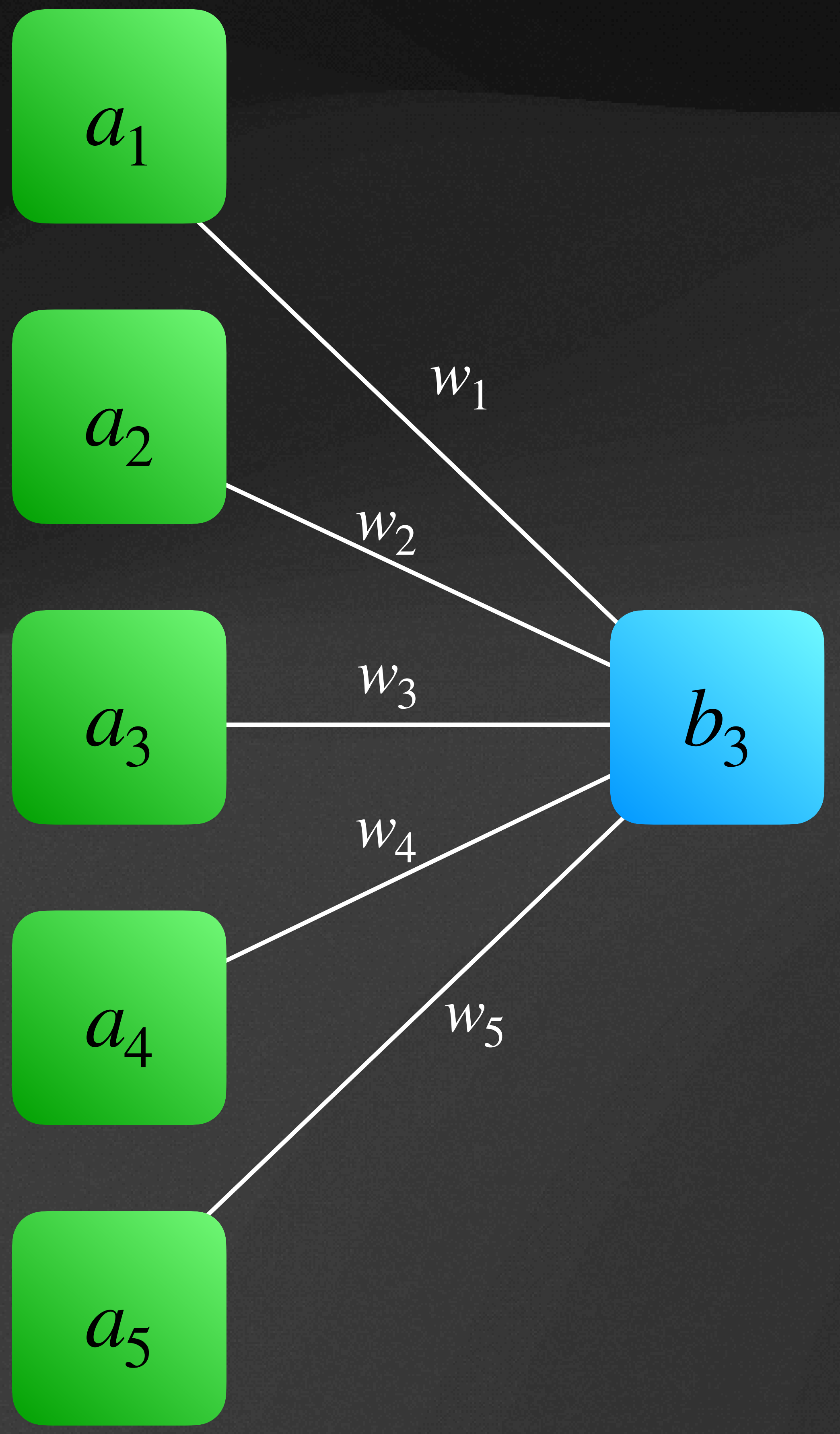


Network Structure



Network Structure

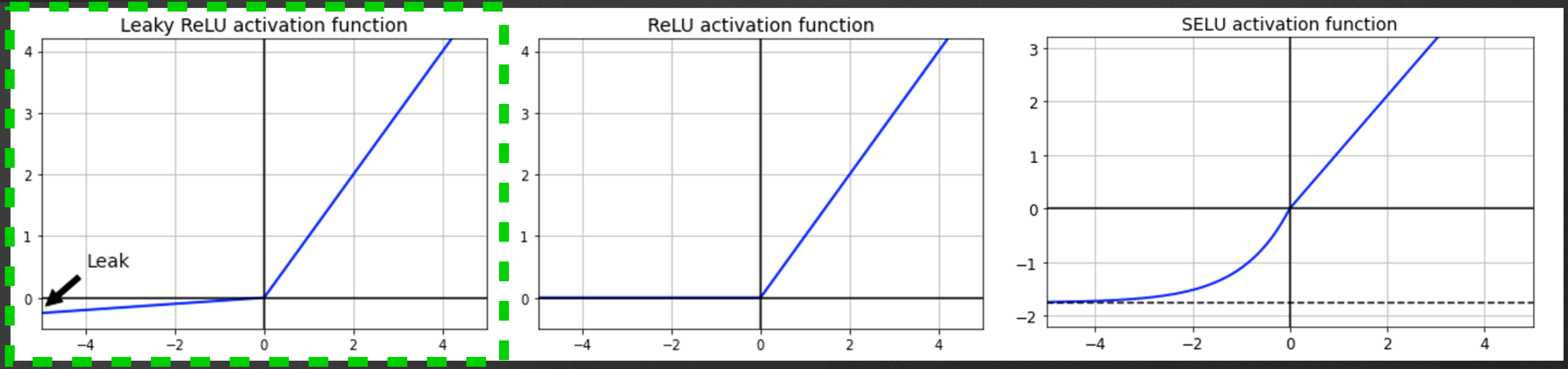
b_j is the linear
combinations of all of its
weights and connections



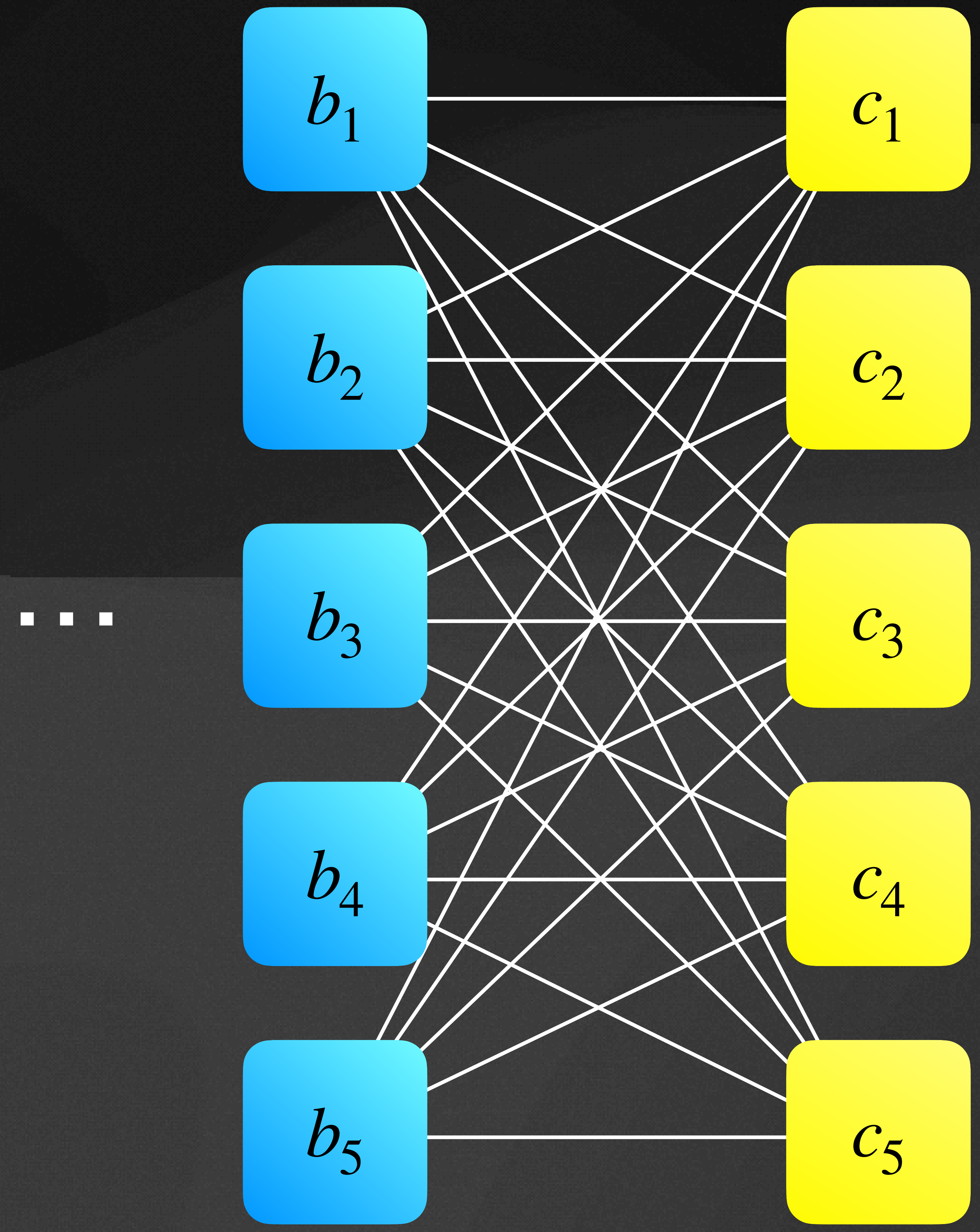
$$b_j = \sum_{i=1}^{n} a_i w_i$$

Non-linearity

$$b_j = ReLU\left(\sum_{i=1}^{n} a_i w_i\right)$$



Error Calculation



$$l_n = (x_n - y_n)^2$$

Model Output

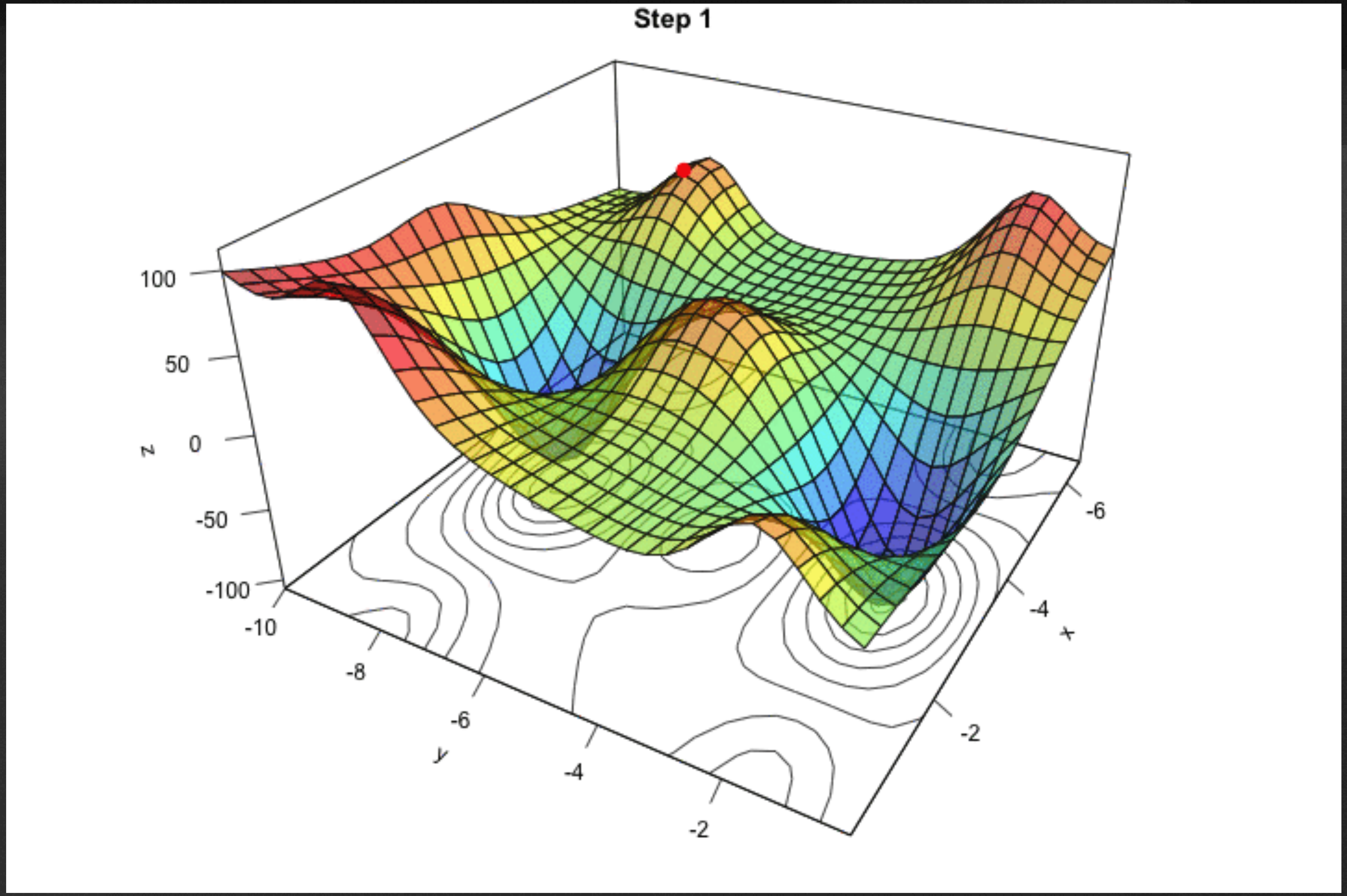
Real Data

$$l(x, y) = L = \{l_1, l_2, \ldots, l_N\}^{\mathsf{T}}$$

Traversing the 'loss surface'

Optimization Algorithms traverse the 'loss surface' to look for the global minimum over L

Loss Surface

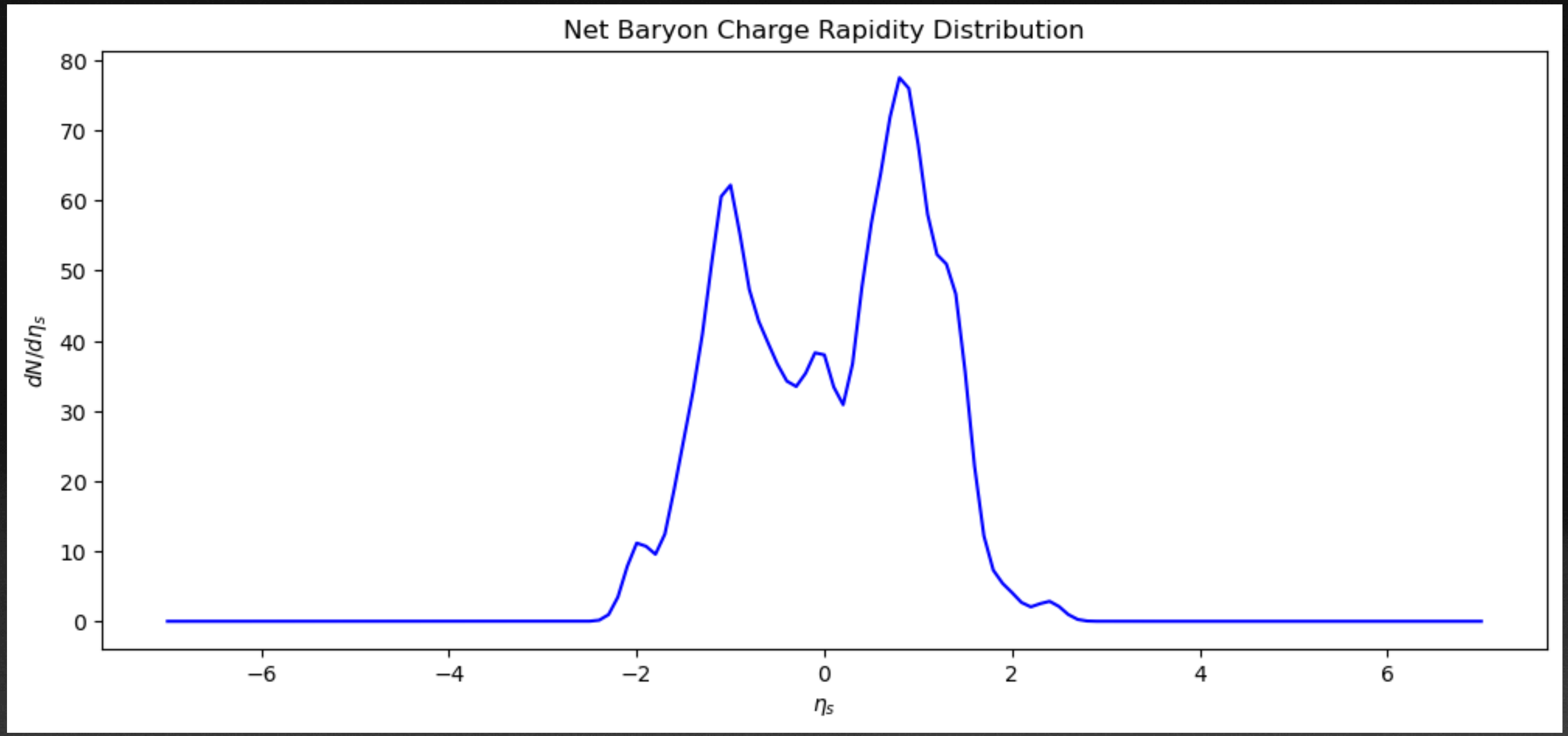


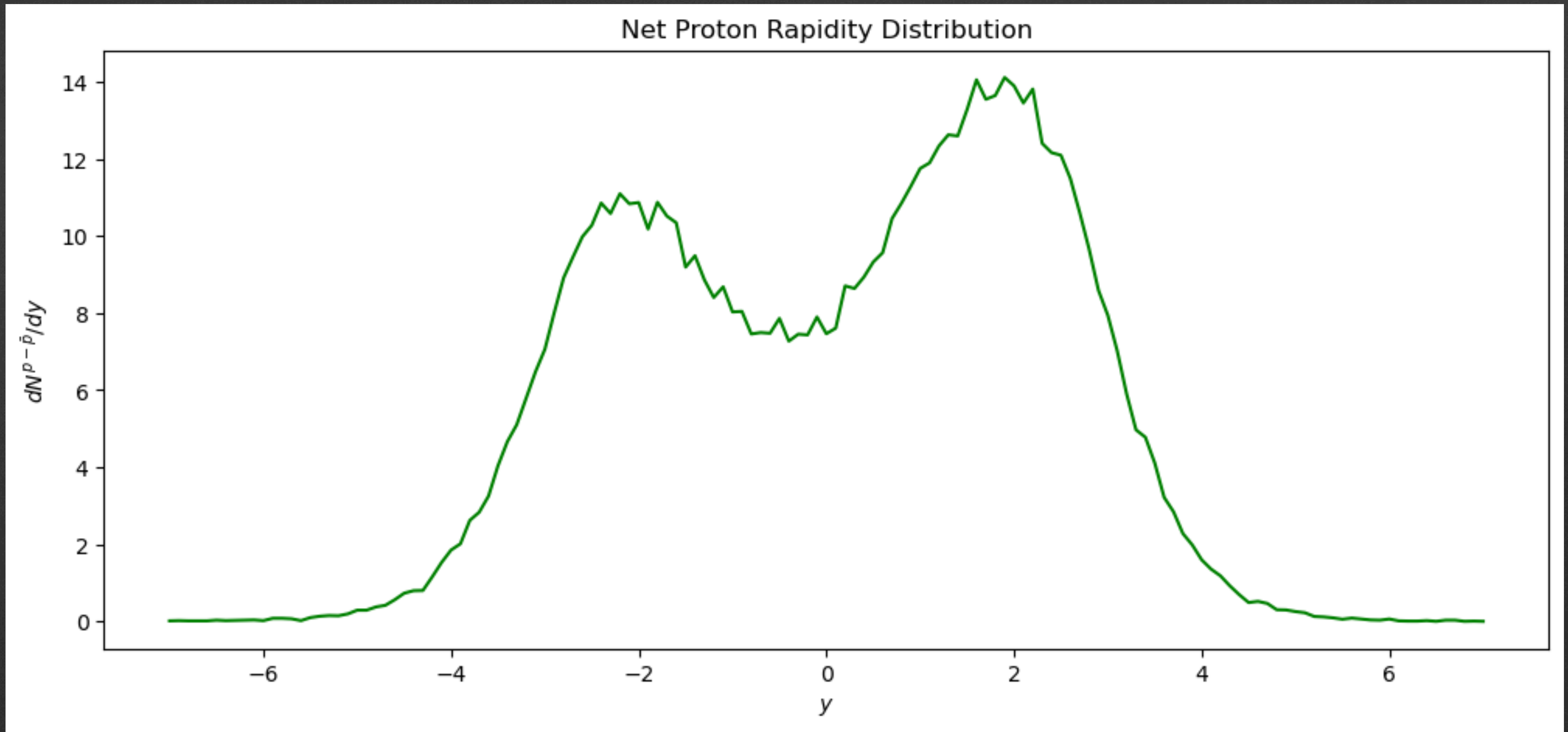
Common Optimizers:

- Gradient Decent (Depicted)
- Stochastic Gradient Decent
- Adam
- Adamax

It starts here

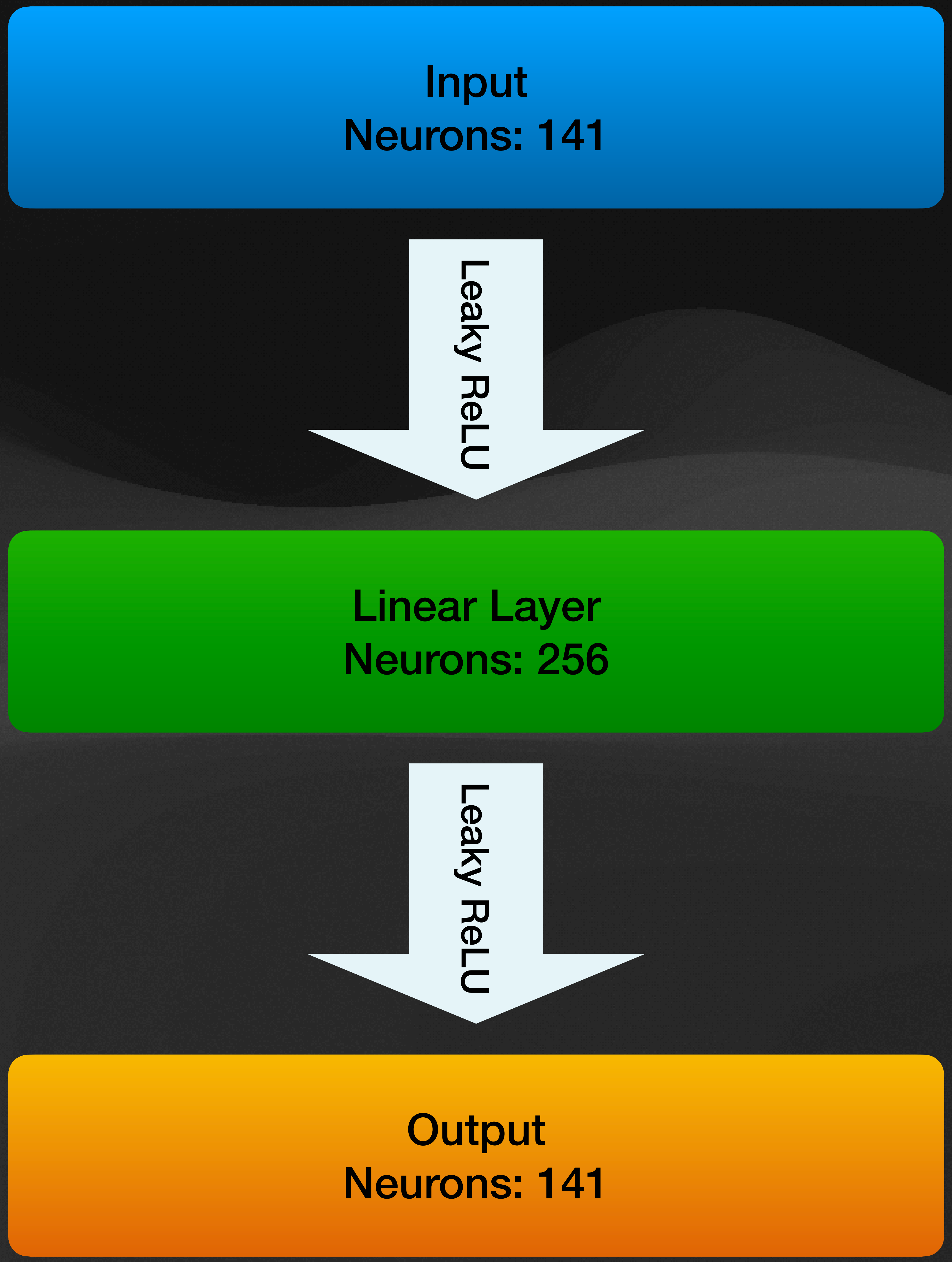
- Au + Au collisions
- 19.6 GeV





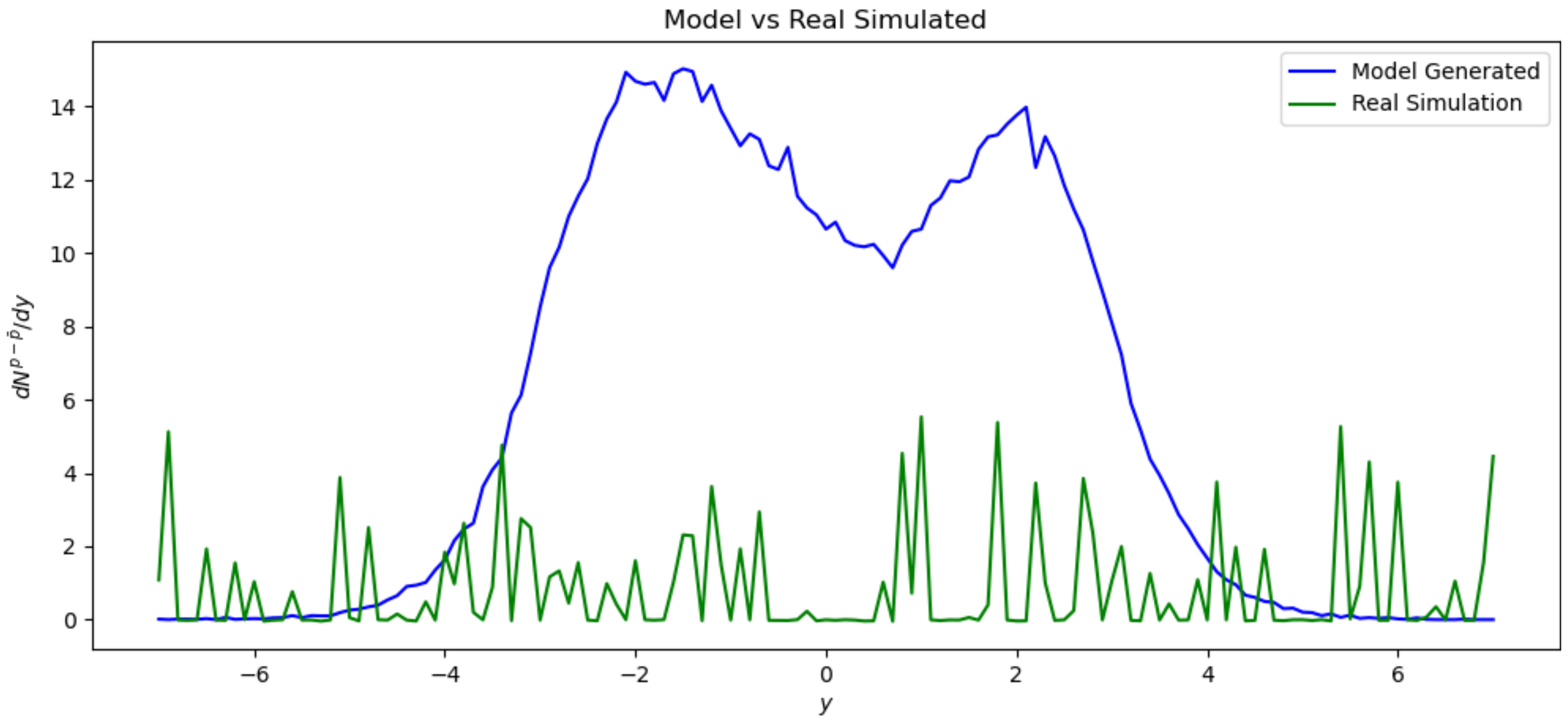
Structure

- Trained on 5,000 pre-simulated initial and final states
- 3 fully connected layers
- Leaky ReLU reduces 'dead neurons'
- Roughly analogous to a polynomial regression

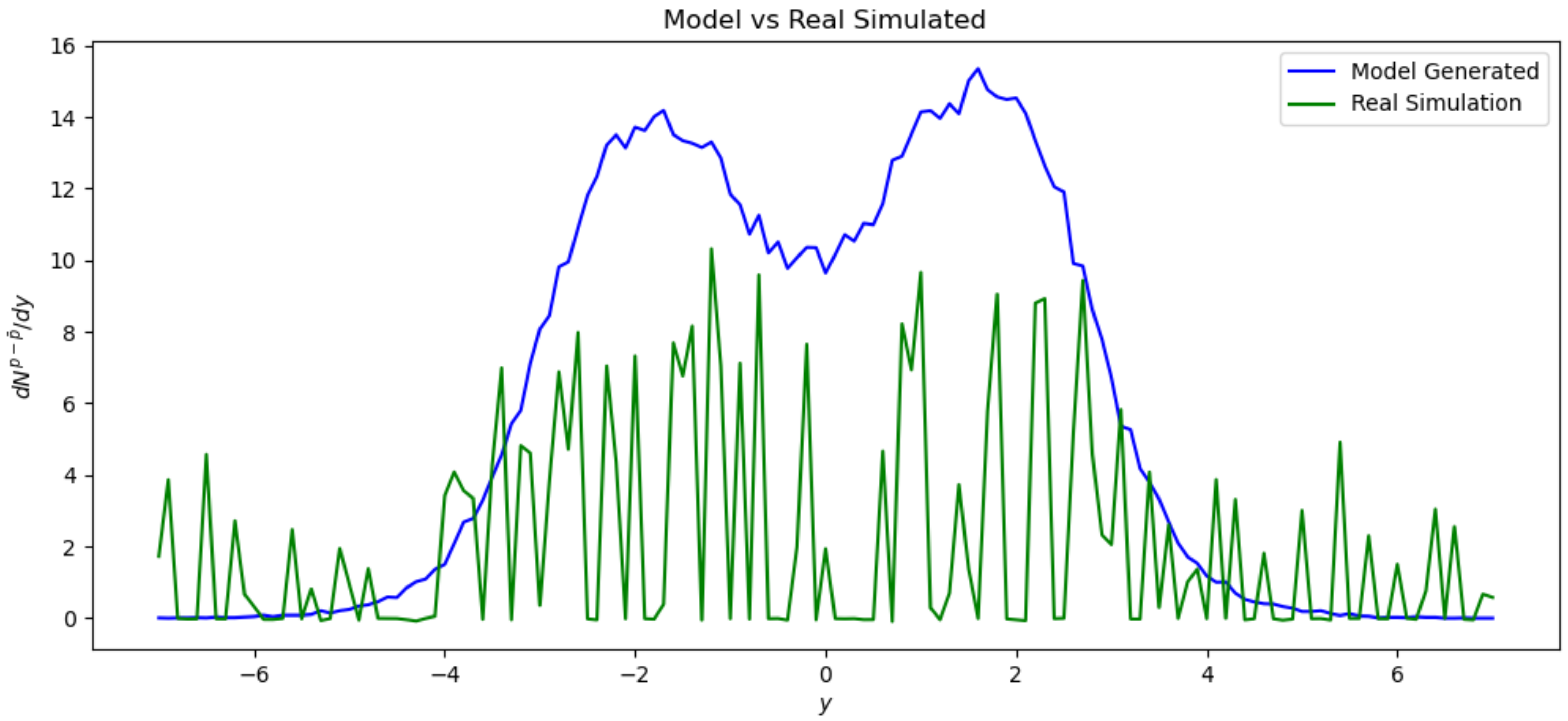


Training iterations

Step 1

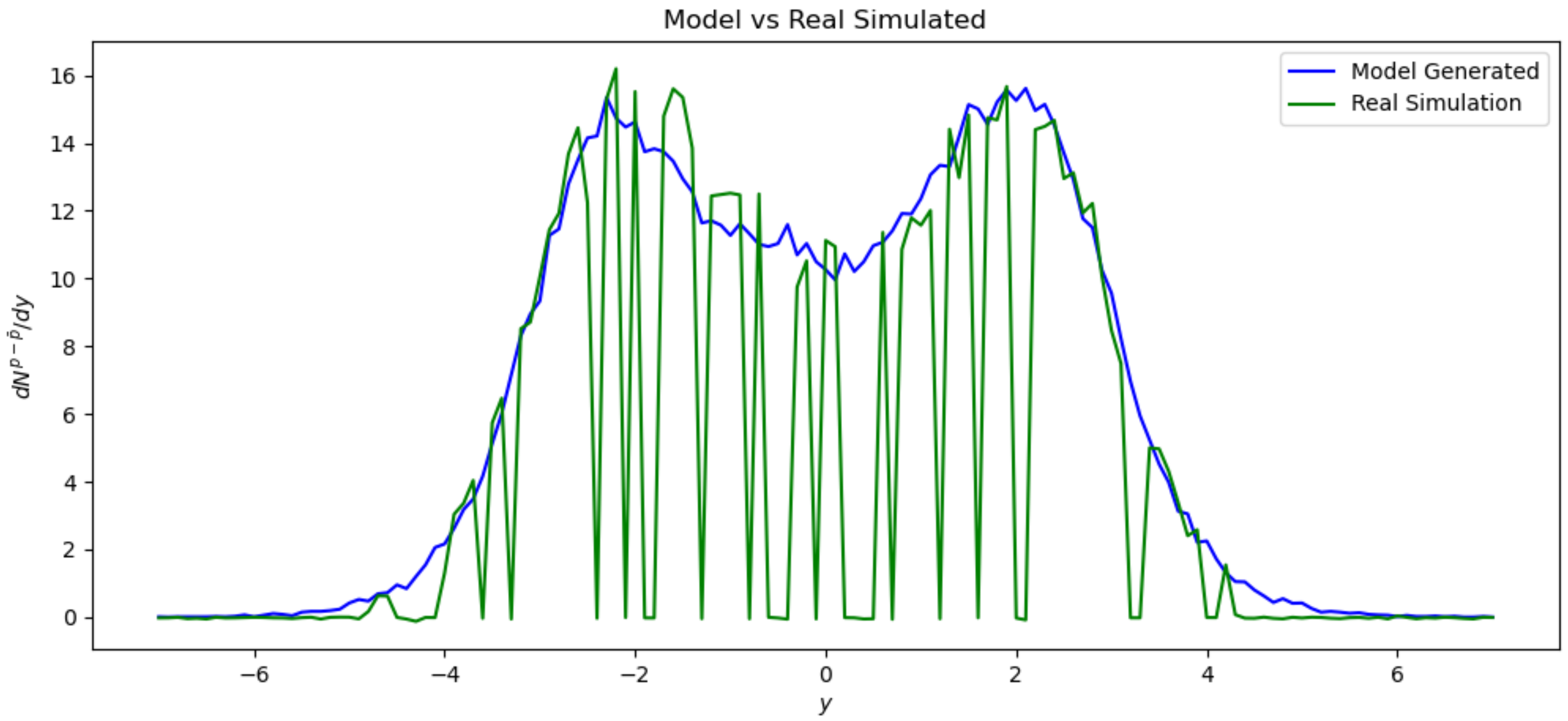


Step 17

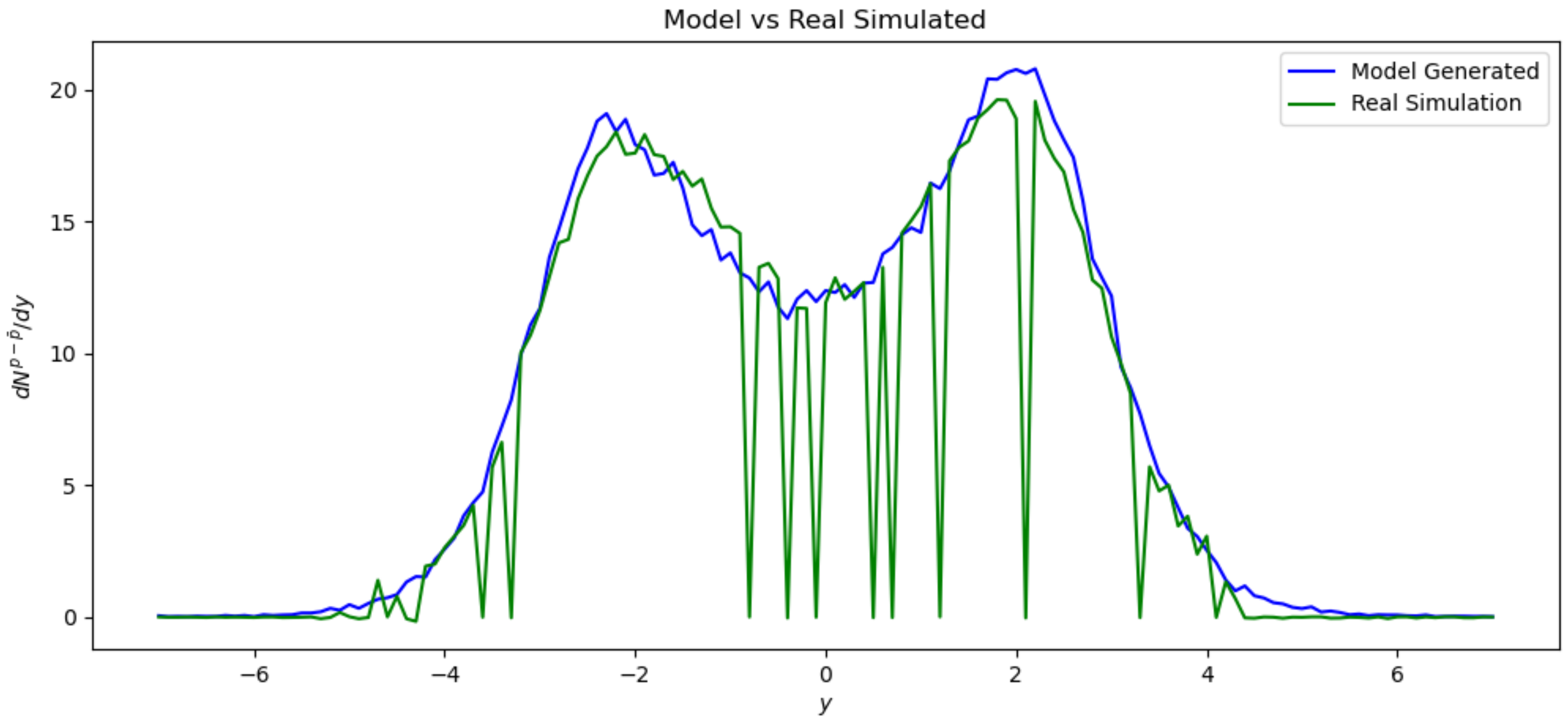


Training iterations

Step 58

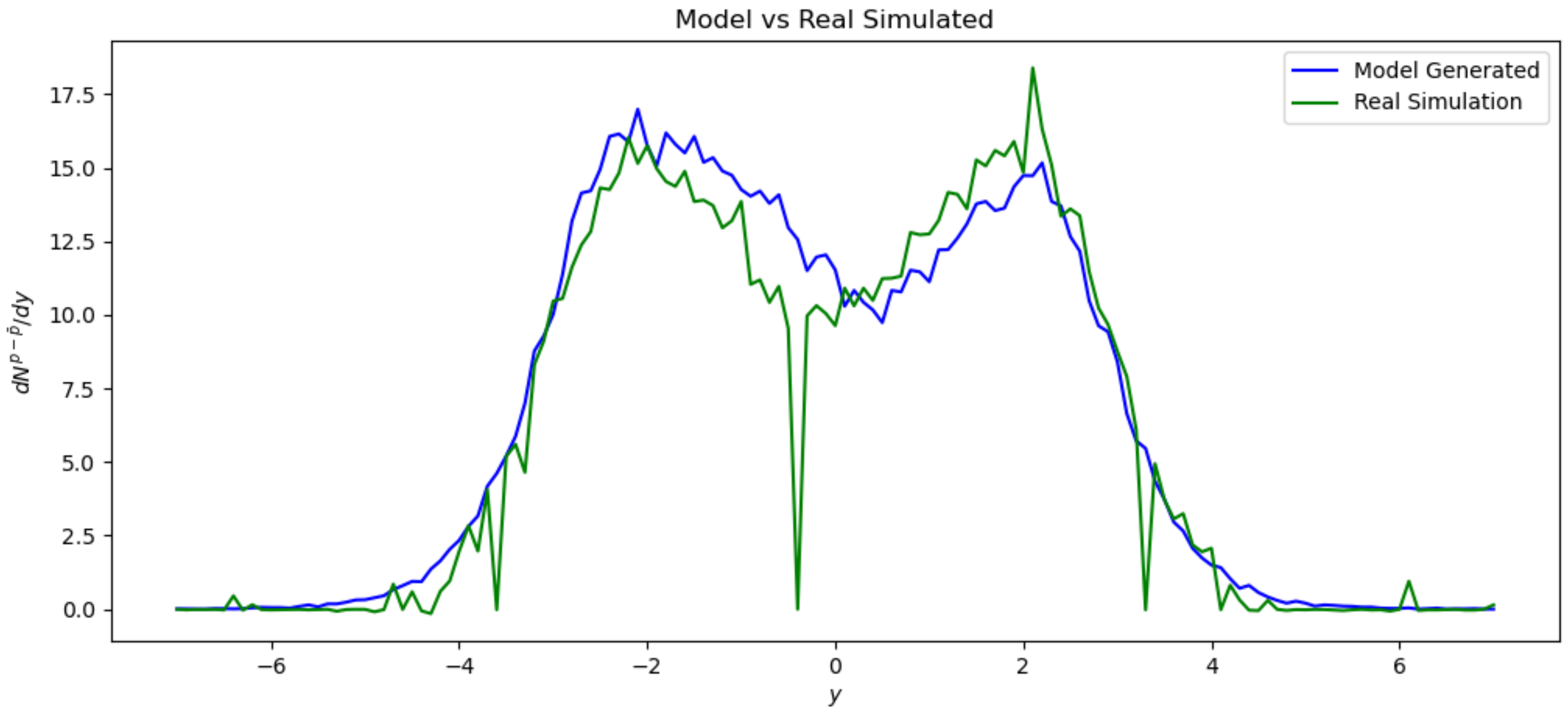


Step 433

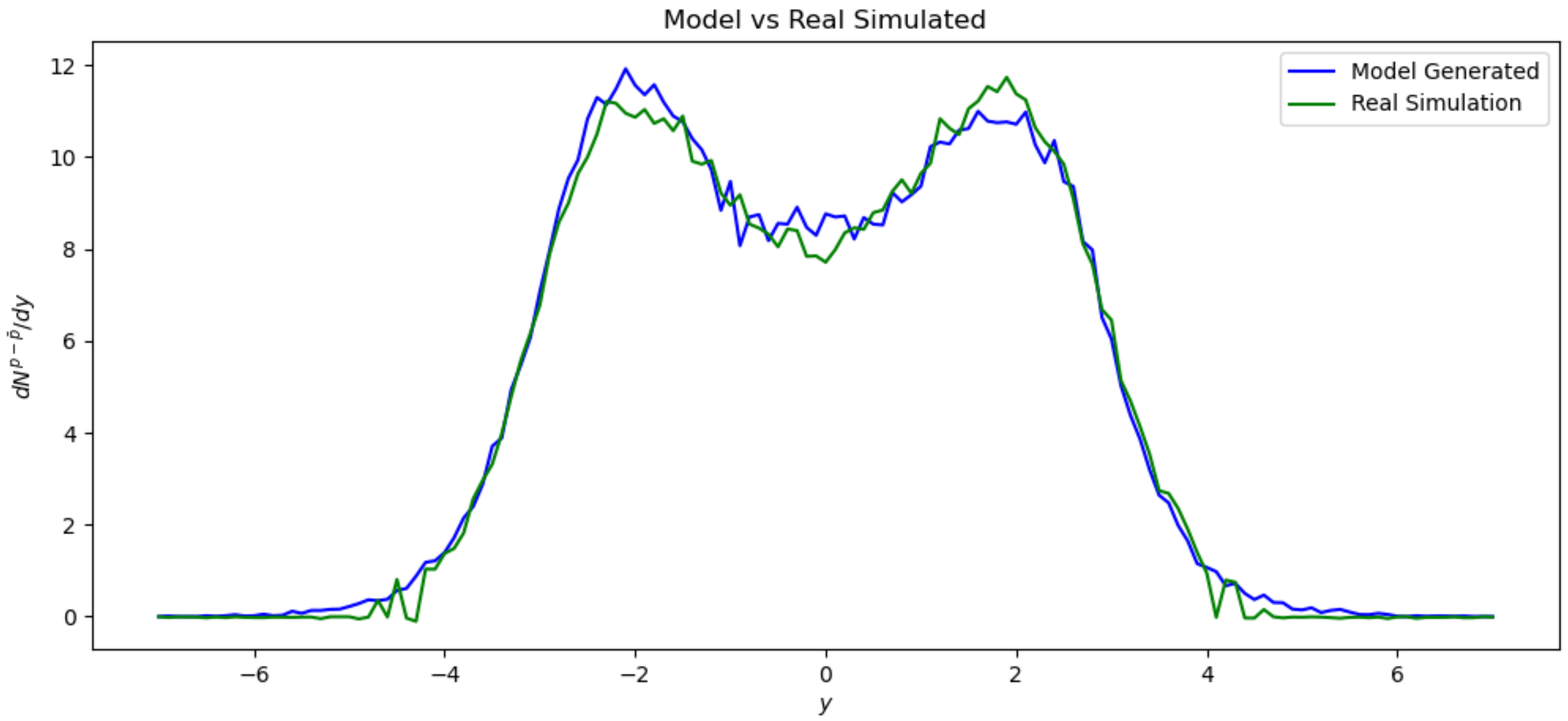


Training iterations

Step 603

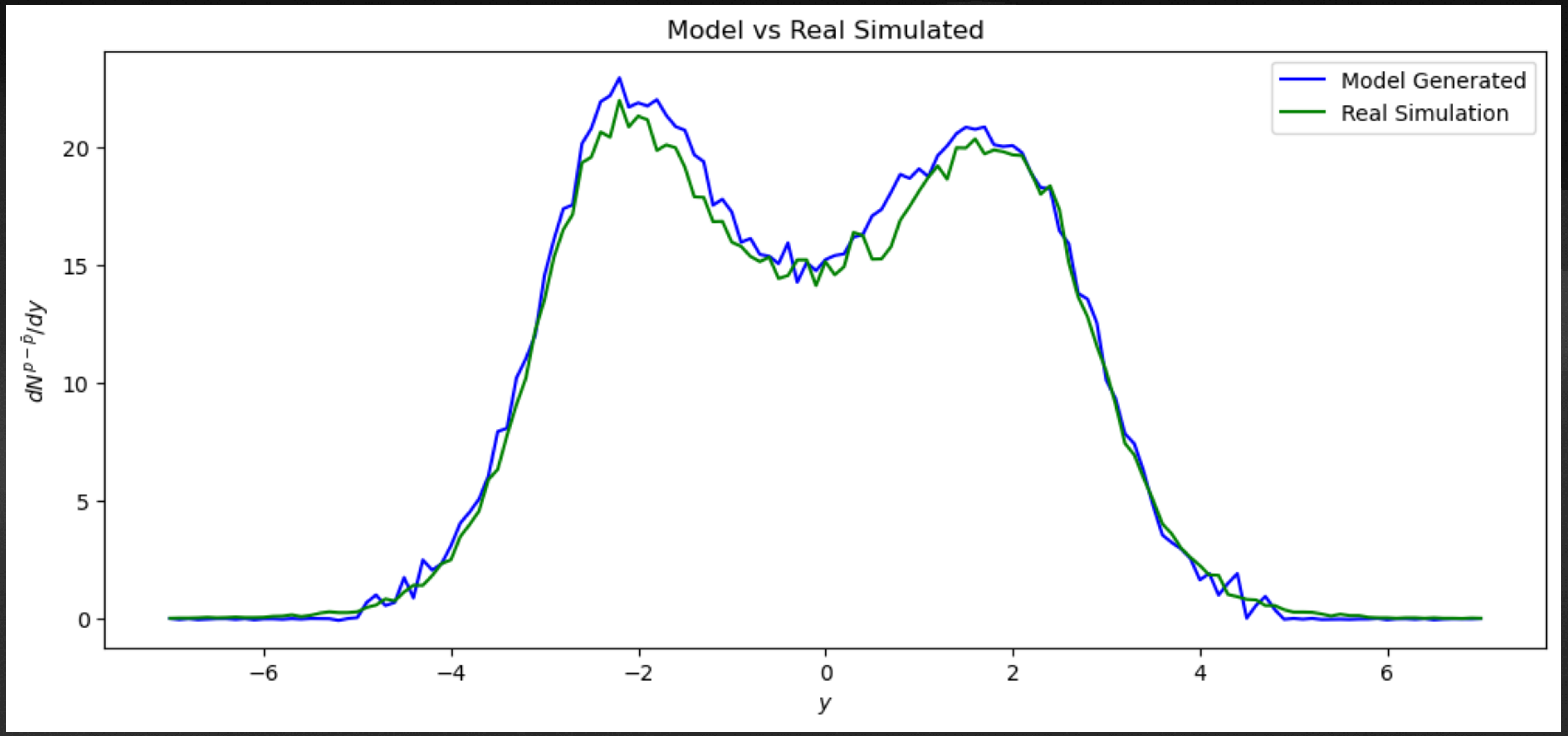


Step 942



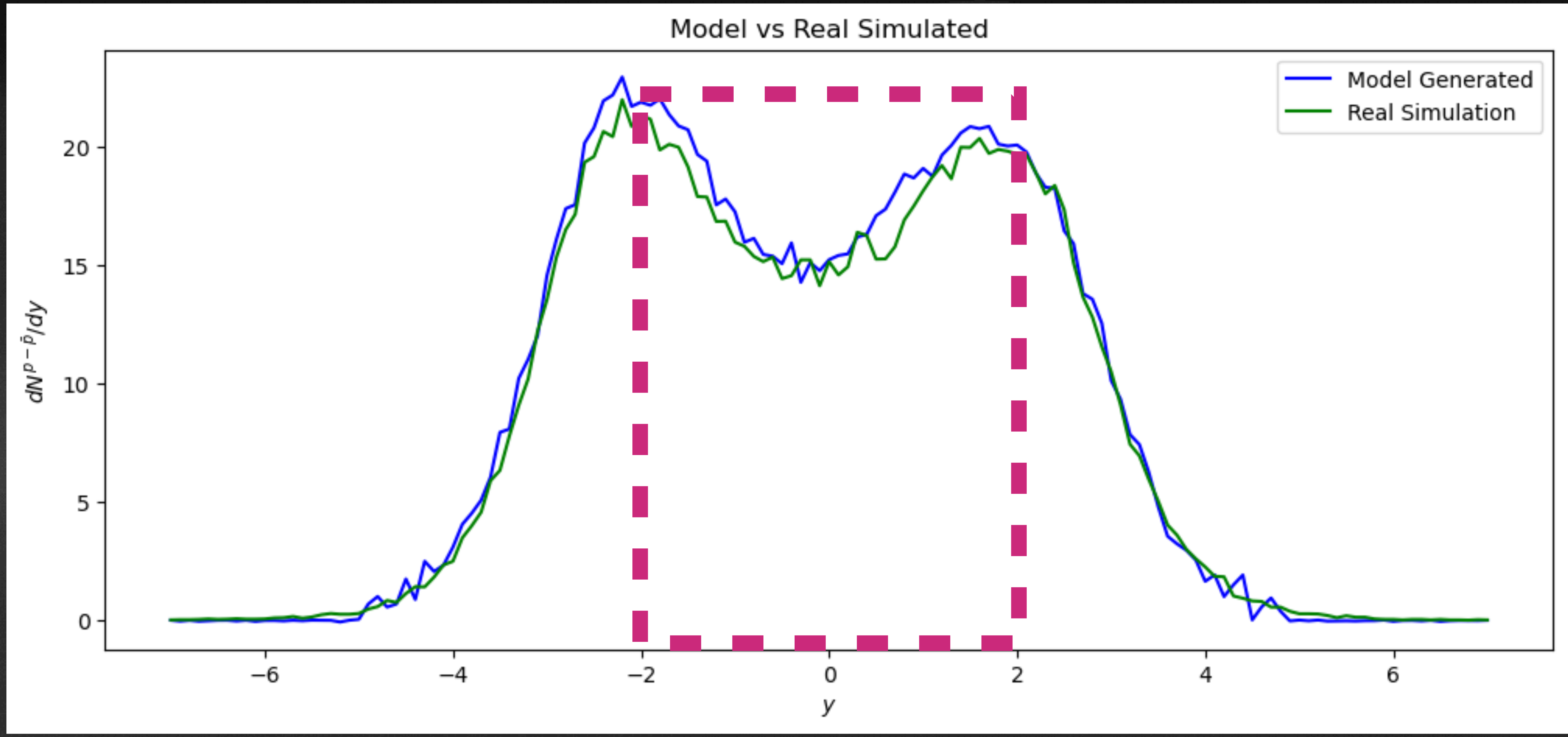
Model Validation

- Model is shown new initial states that it was not trained on
- We can compare the expected output versus the generated output
- Spikes/noise is already accounted for as statistical fluctuations

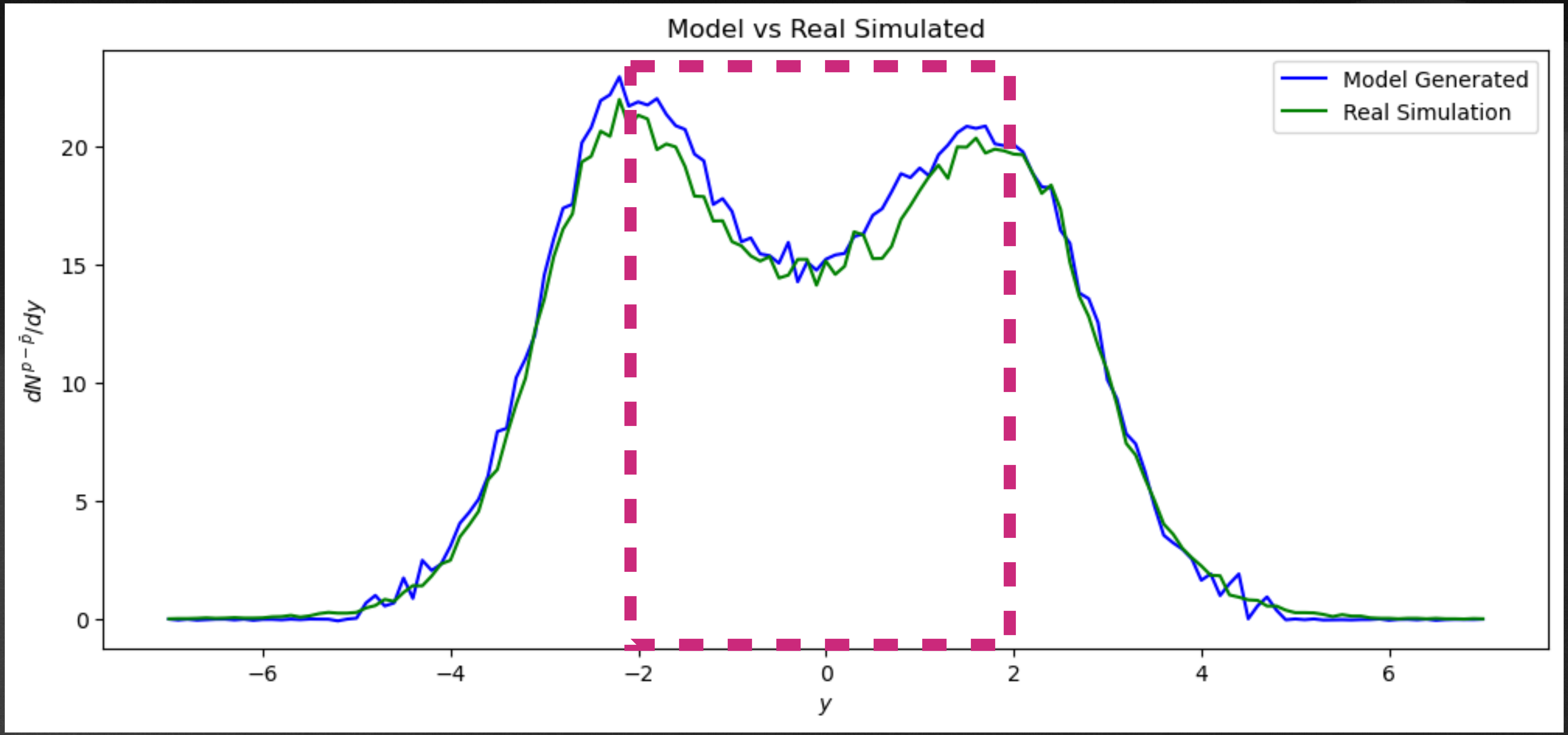


Model Validation

- Model is shown new initial states that it was not trained on
- 5,000 validation events
- We can compare the expected output versus the generated output
- Spikes/noise is already accounted for as statistical fluctuations

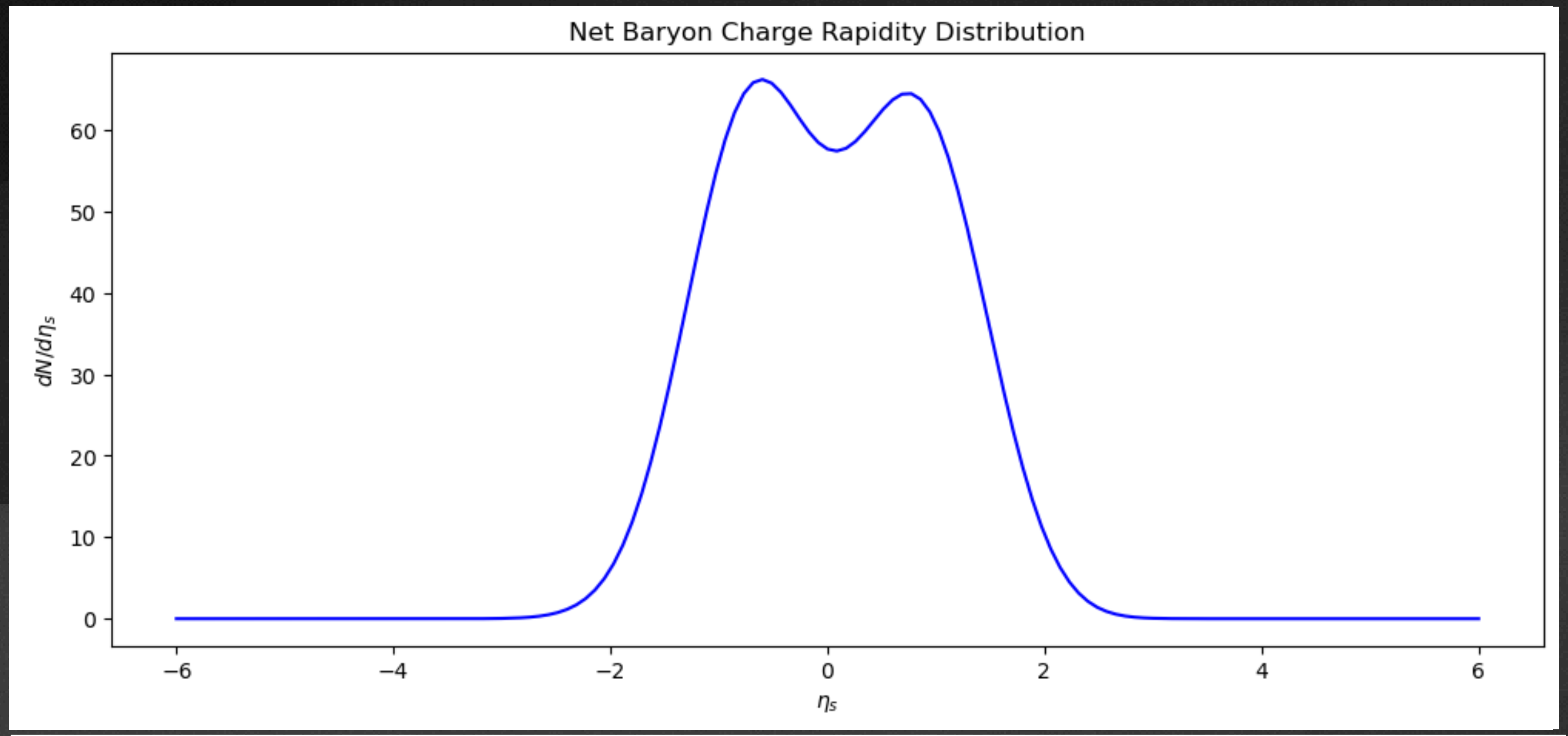


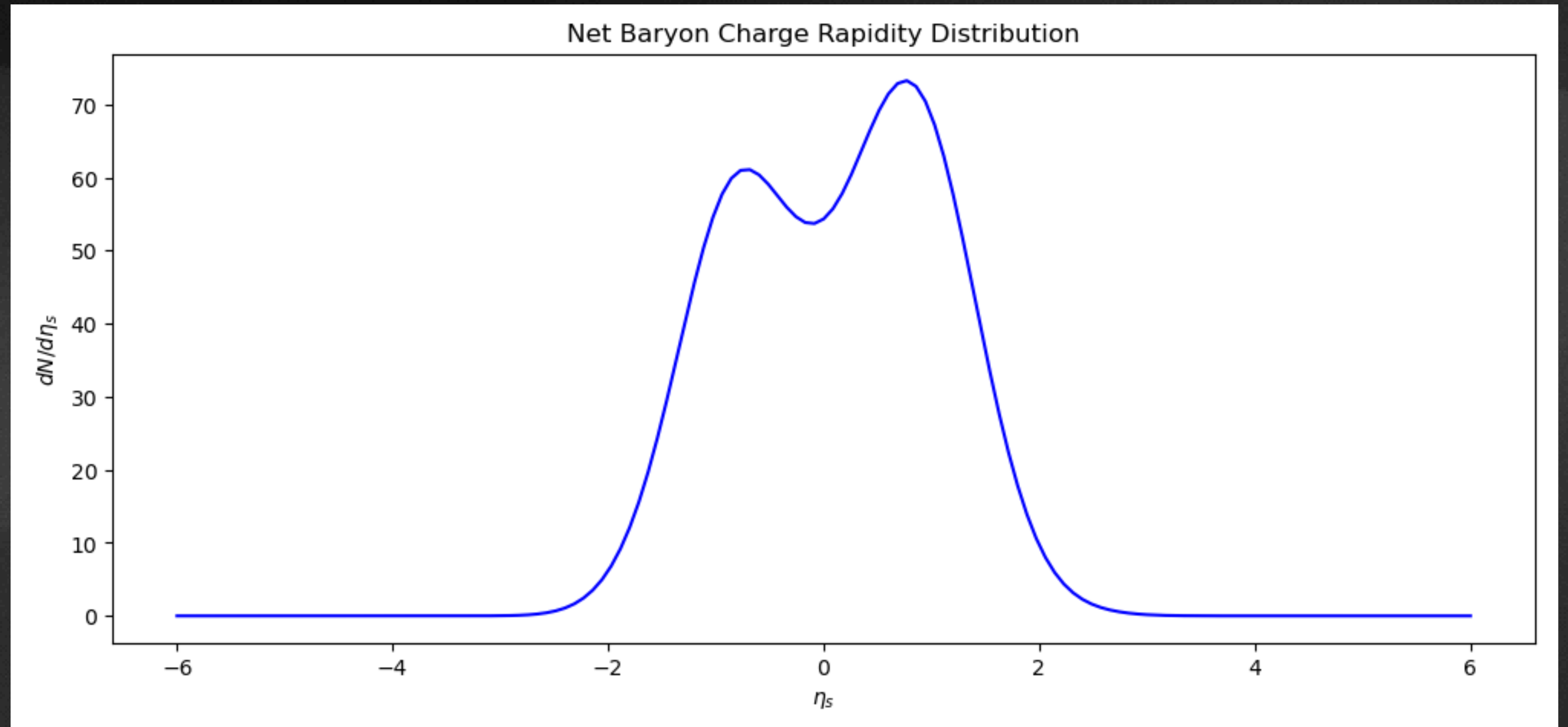
Model Validation

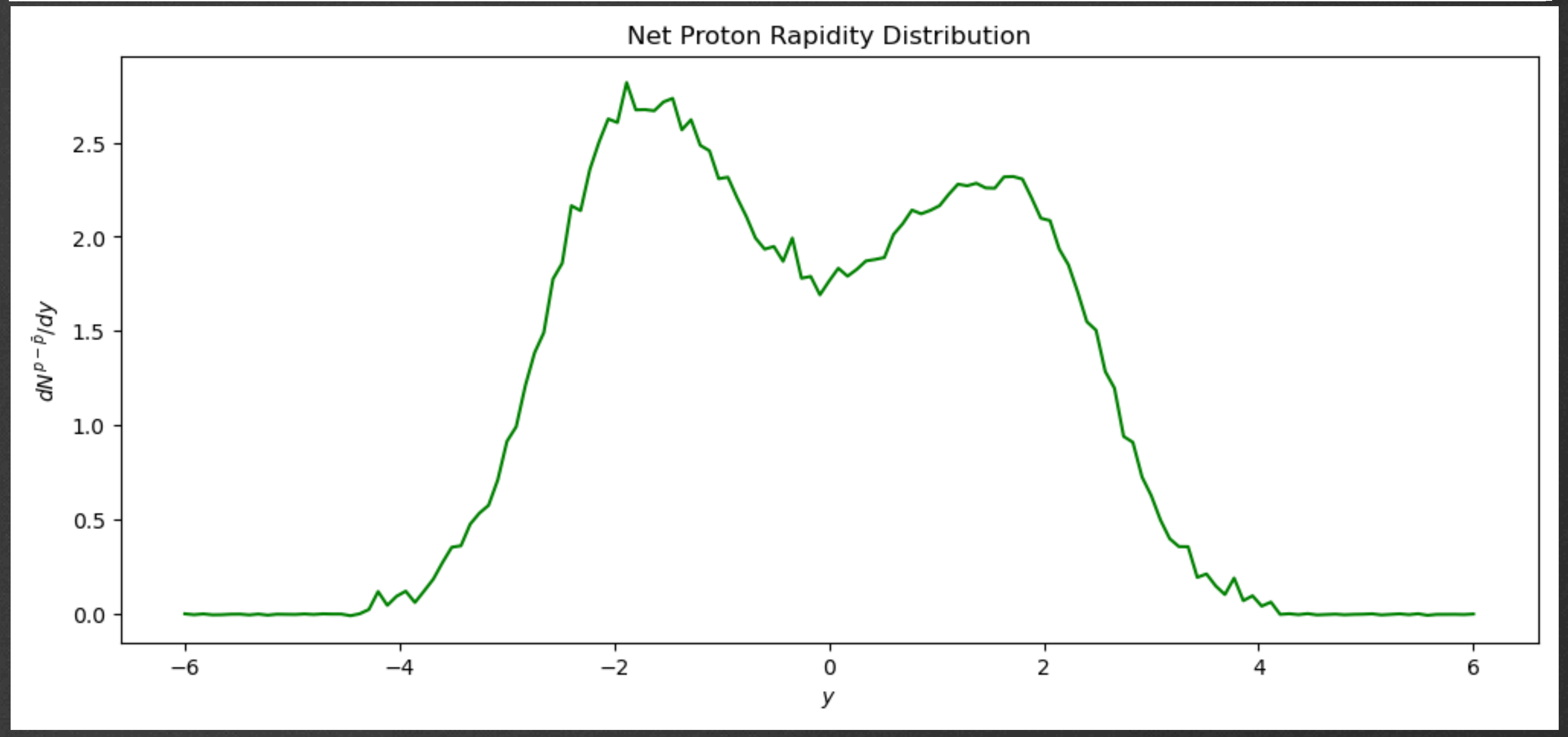


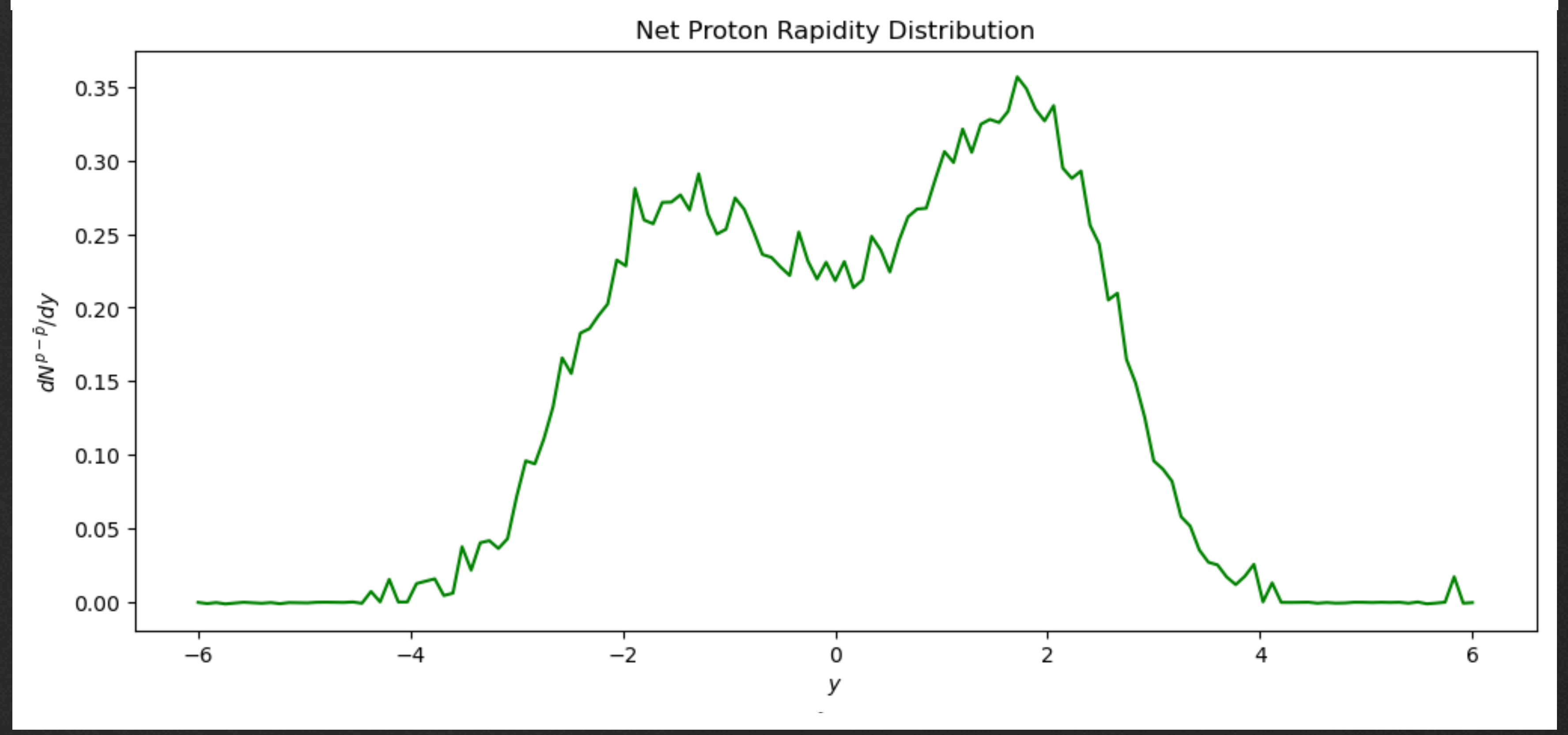
Results

```
└─$ python main.py -d datasets/nB_etas_distribution_N_141.dat
{'gridNx': 141, 'model': 'baryon_model_19.6gev.pt'}
(100000, 1, 141)
Run time: 7.484050035476685 seconds
```





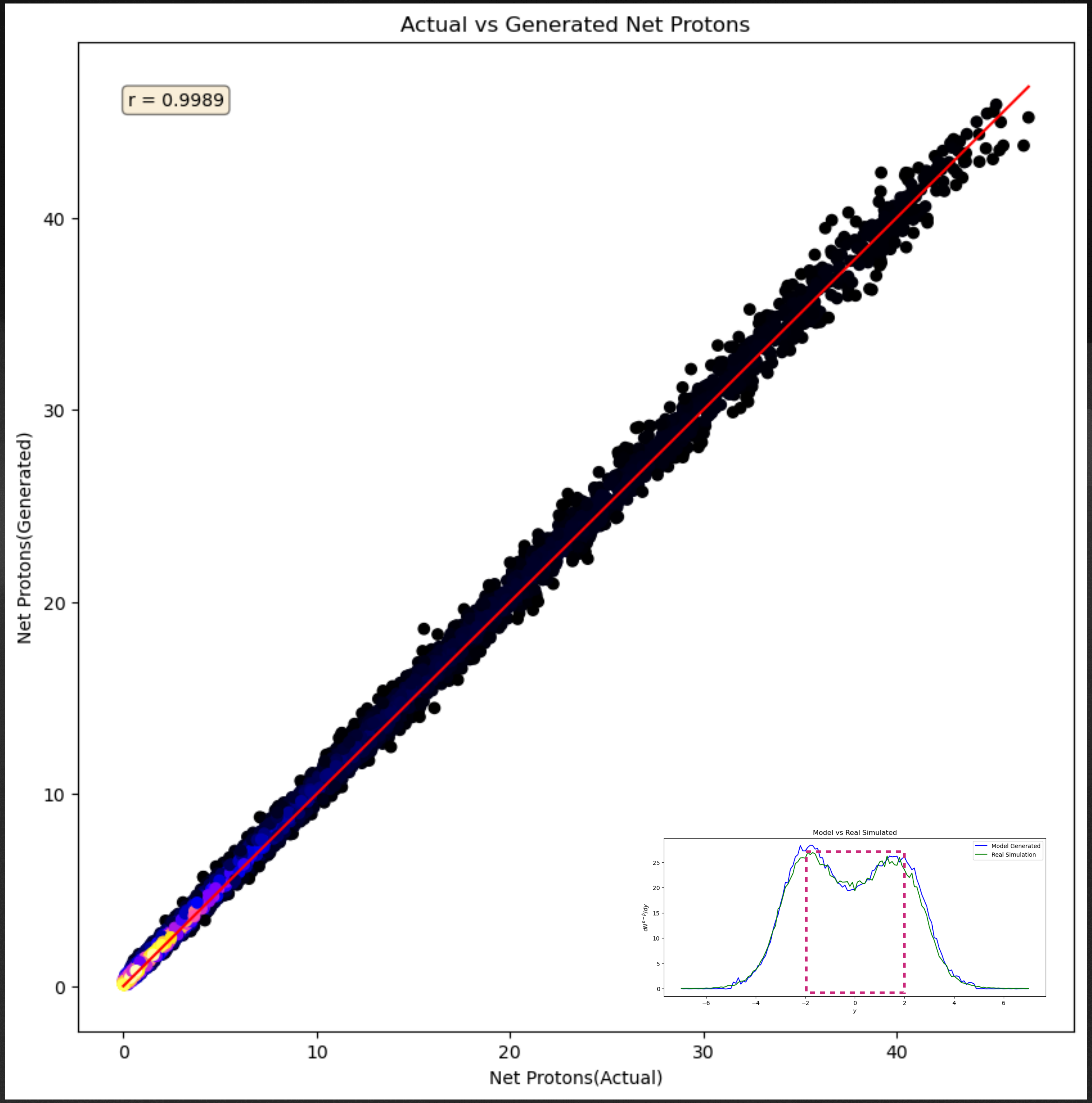




Model Validation

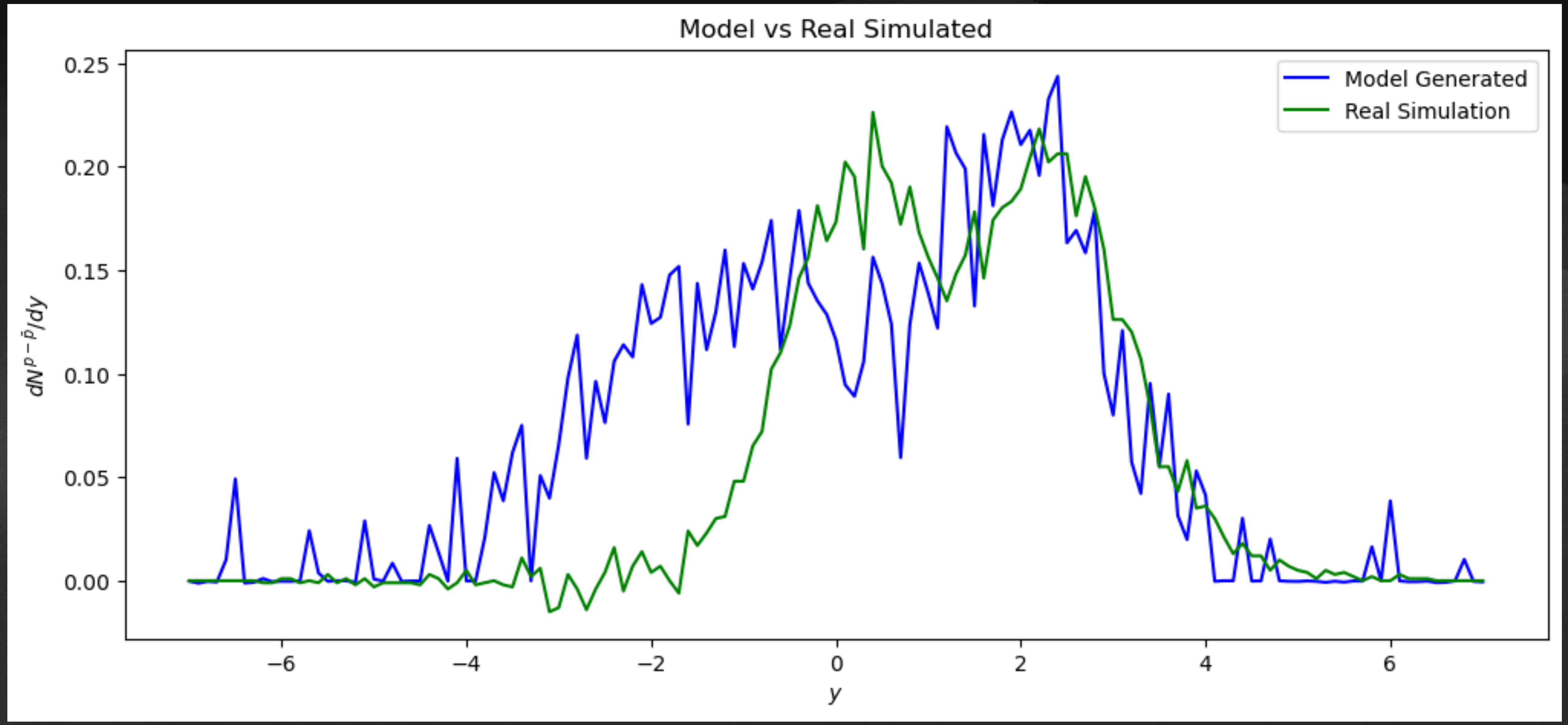
Real simulations vs model generated area for $[-2,2]$

	Real Final State	Generated Final State
Mean	3.17 +- 0.35	3.23 +- 0.36
Varience	14.22 +- 0.50	13.51 +- 0.44
Skew	1.25 +- 0.74	1.14 +- 0.61
Kurtosis	3.60 +- 4.05	3.20 +- 2.90



A note on model generalization

- Minimum Bias — Peripheral collisions get worse
- May not be a significant problem outside of model generalization



Conclusion

- 1,000,000 final states can be generated in less than 30 seconds
- $O(10^5)$ speed up from 30 hours to a few seconds on an event-by-event basis

Future Plans:

- Calculate high-order cumulants for net protons at the RHIC BES program
- Expand neural network emulation for anisotropic flow vector $v_n(\eta)$
  - A more complex design may be needed
- Deploy neural network emulation as low fidelity simulations for Baysian Interface analysis

Questions?