Machine Learning for Neutrino Identification

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NuSTEAM Workshop

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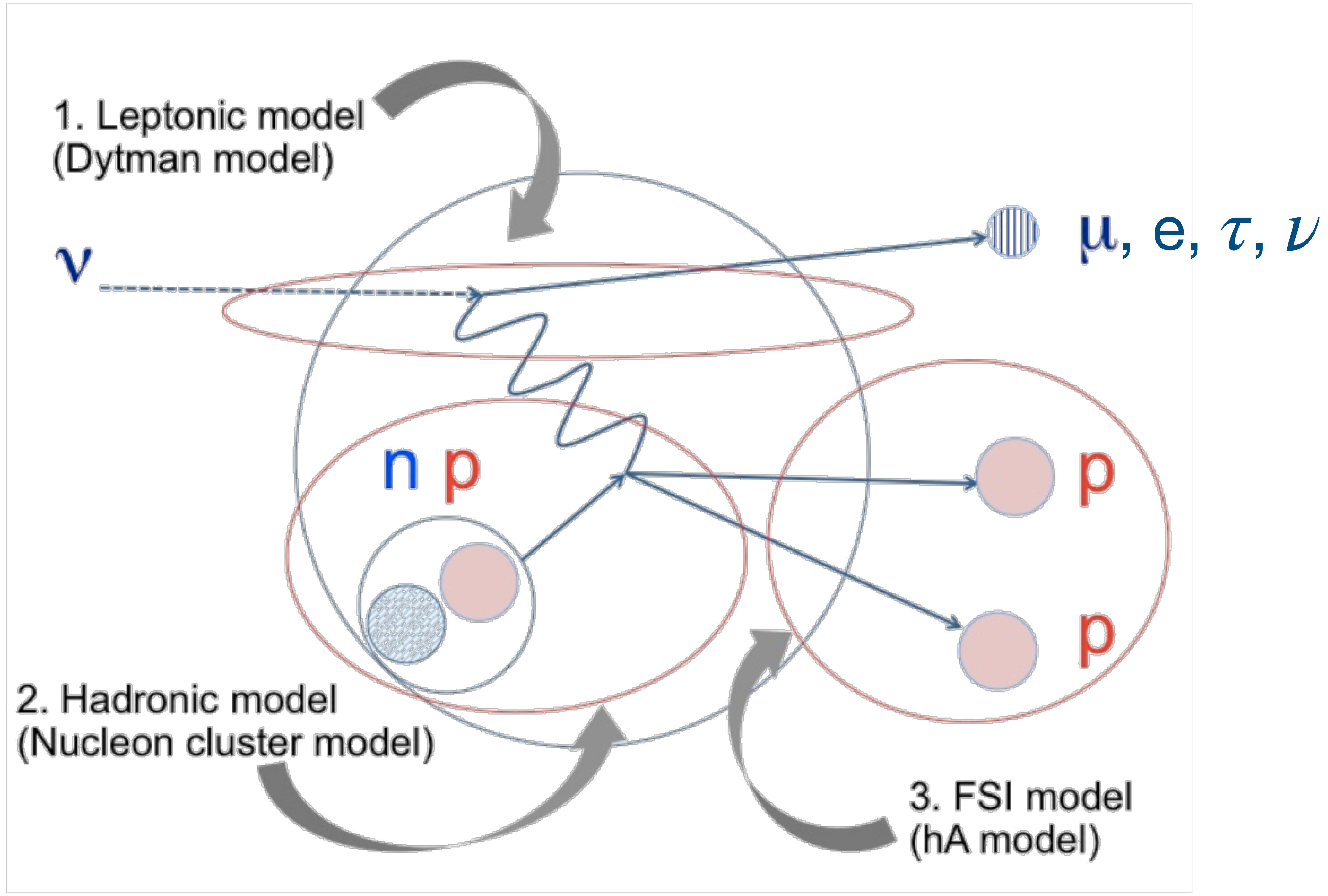
Prerequisites

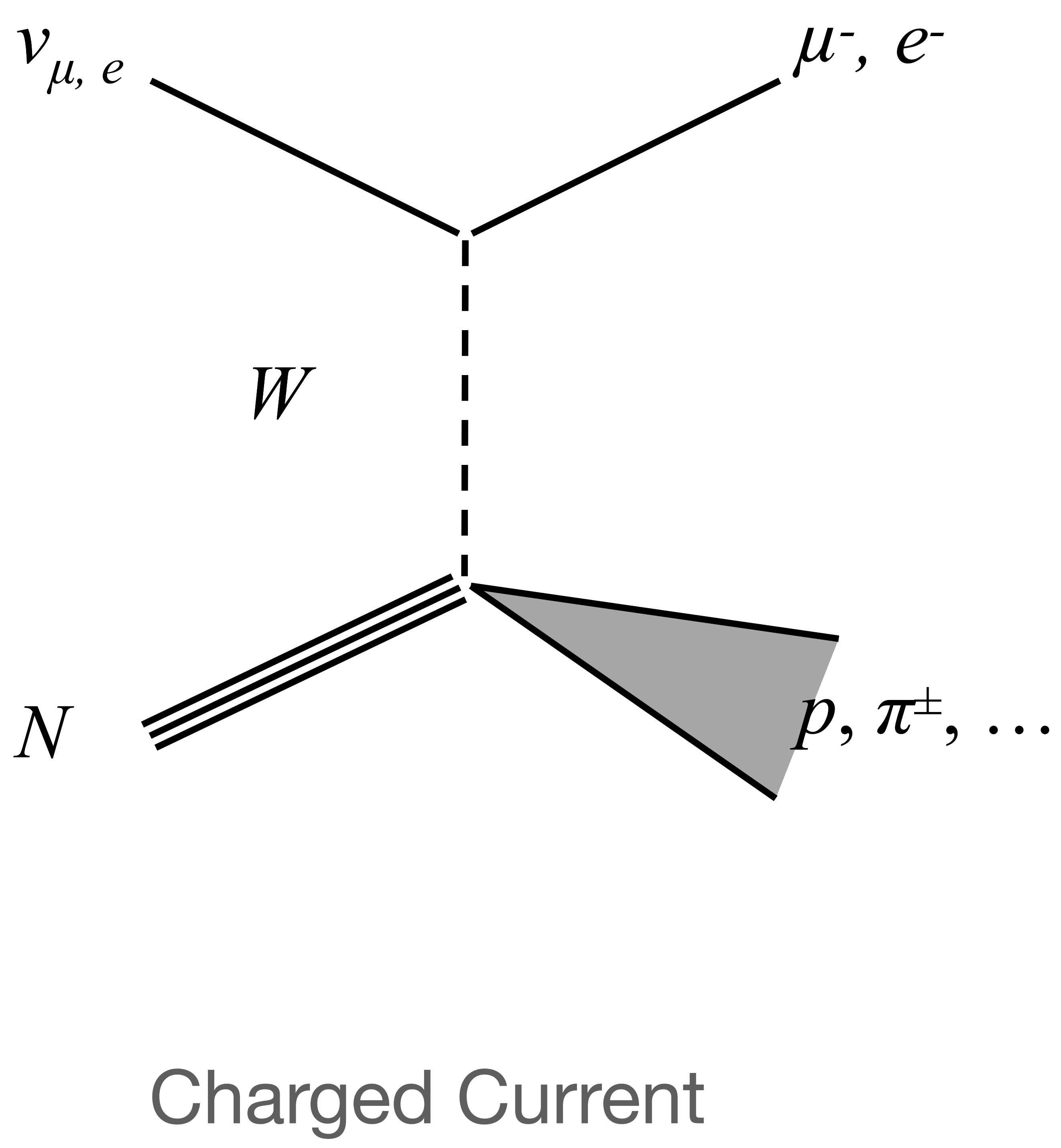
- Types of Neutrino Interactions - ν_e CC , ν_μ CC, ν_τ CC, ν_x NC
- LArTPC detectors
- What neutrino interactions look like
- Why would we want to identify different types?

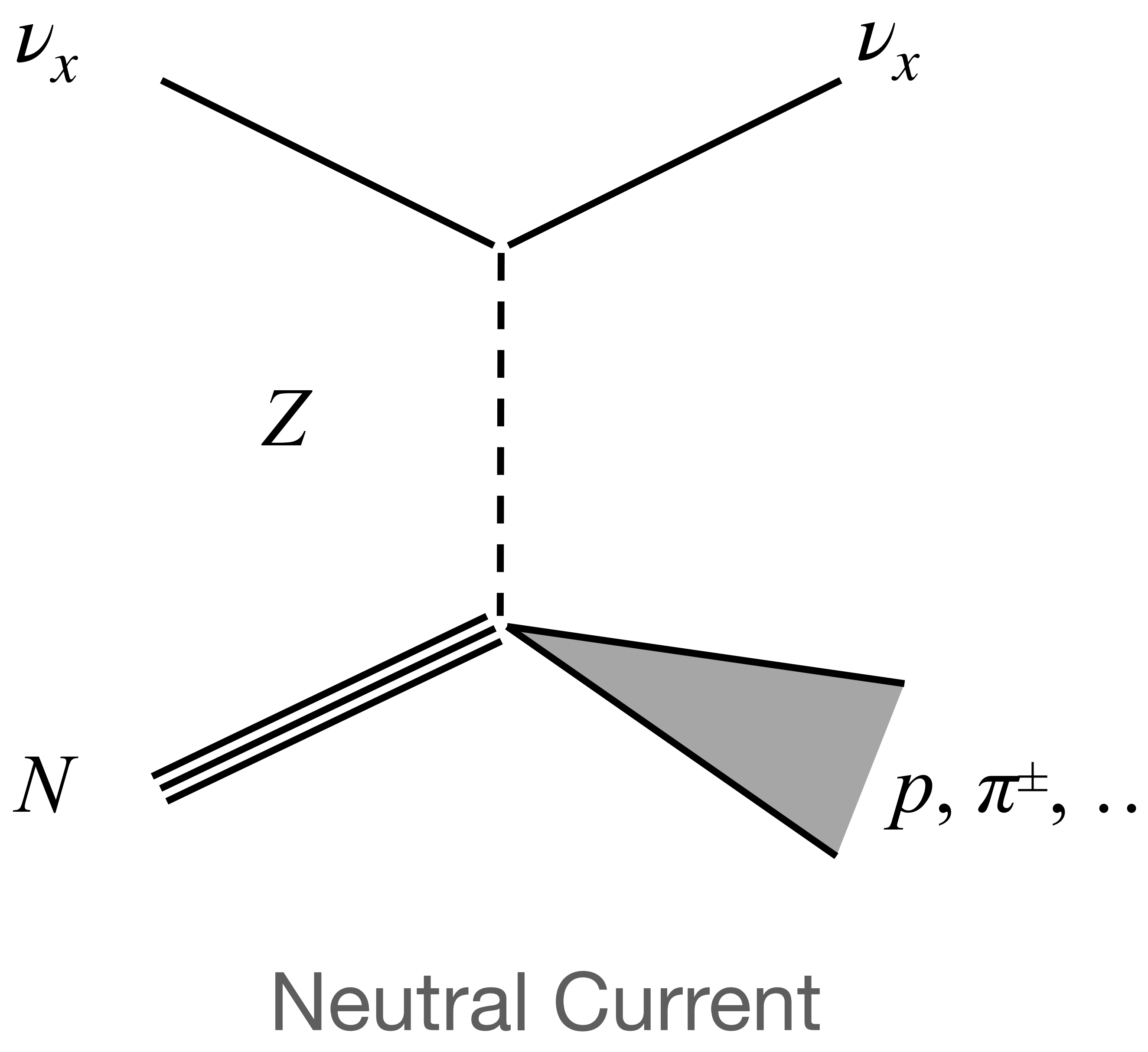
Outline

- Curve fitting/Classification/Regression
- Gentle introduction to Neural Networks
- Predicting type of neutrino interactions in LArTPCs
- Hands-on demo

Types of ν-Interactions



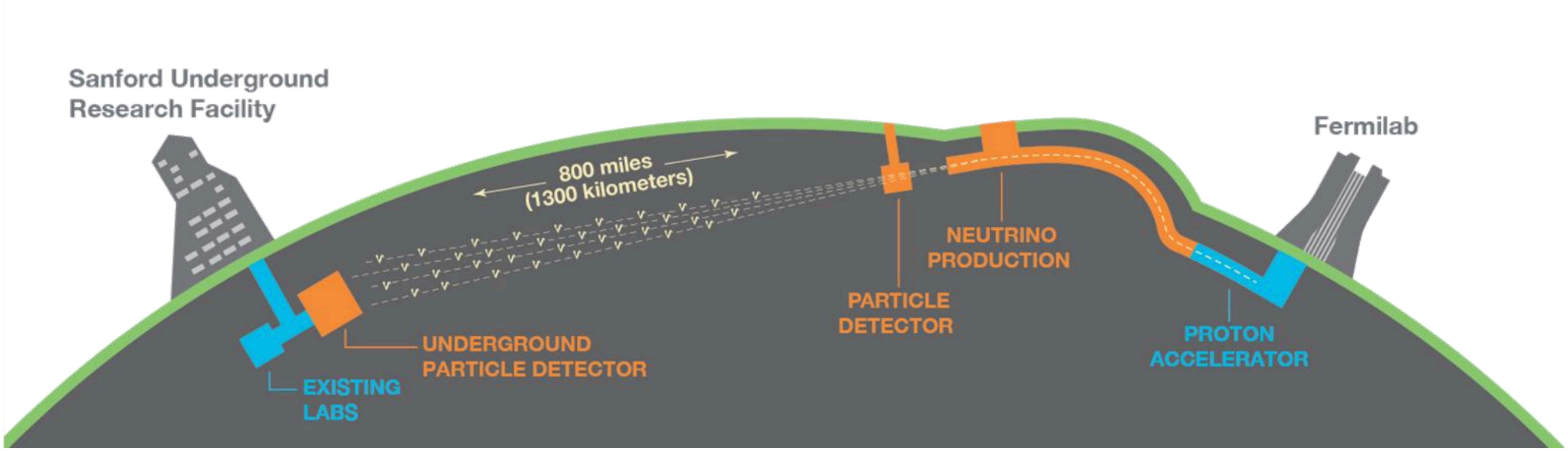




- Different interactions look characteristically different
- Hadronic output (coming from the nucleus) broadly similar
- Interactions mainly differ in the nature of the final-state lepton
- Presence or absence of detected lepton tells us about type of interaction

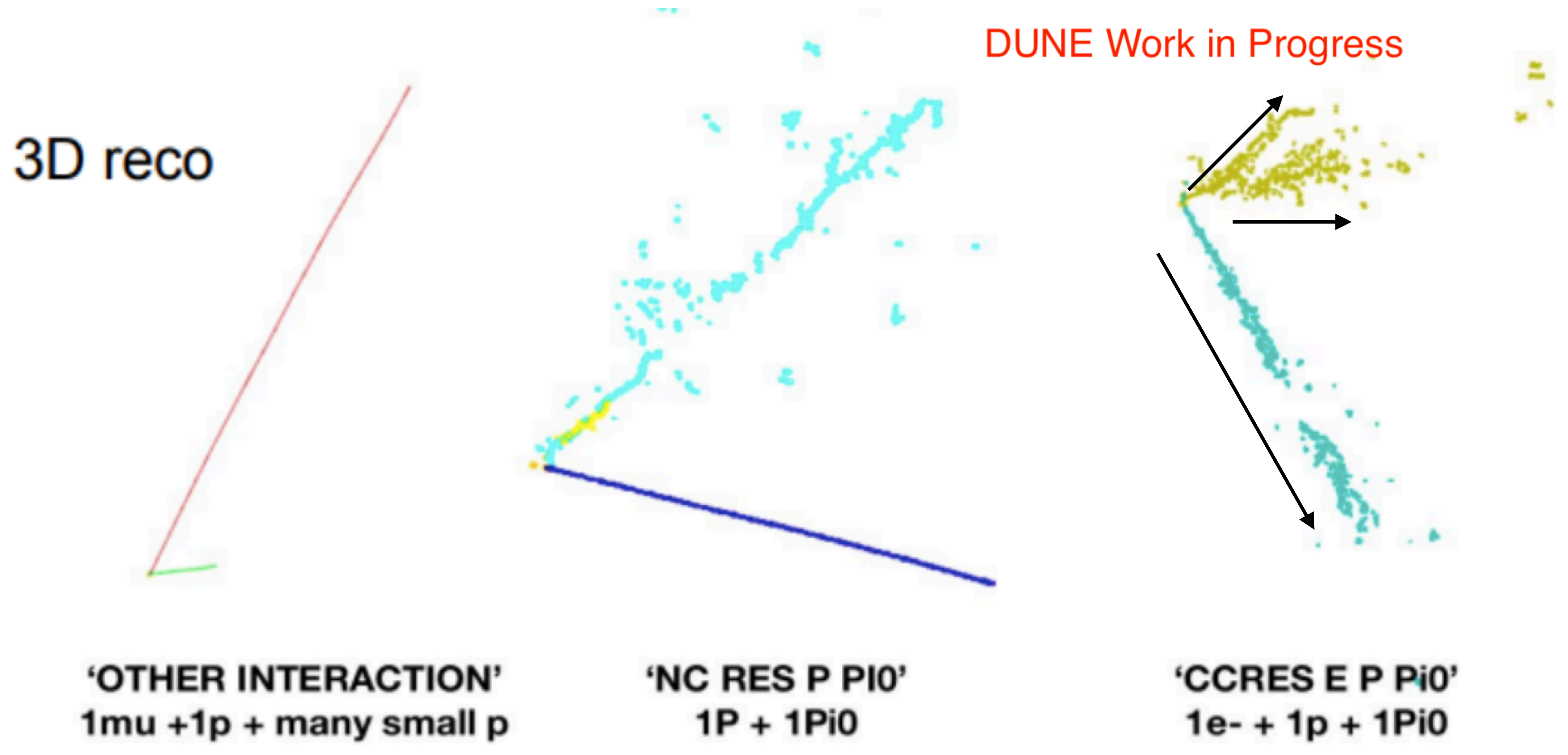
Identifying Neutrinos

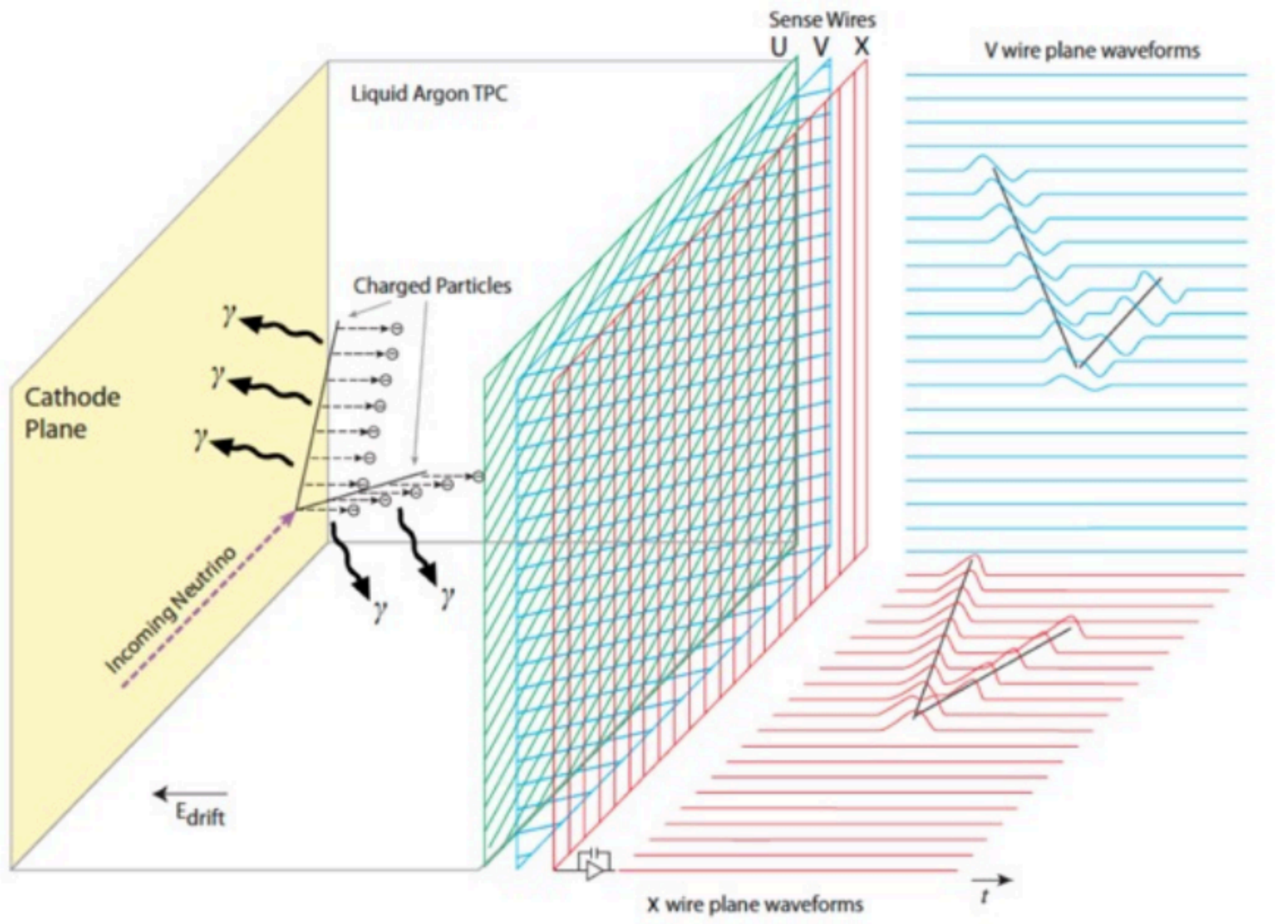
- Fundamental objective of any neutrino oscillation experiment
- Neutrinos change flavor, tagging flavor is crucial to understand what's happening
- We have an idea of how many ν_μ , ν_e we start off with from beam, identify and count how many there at FD => measure probability



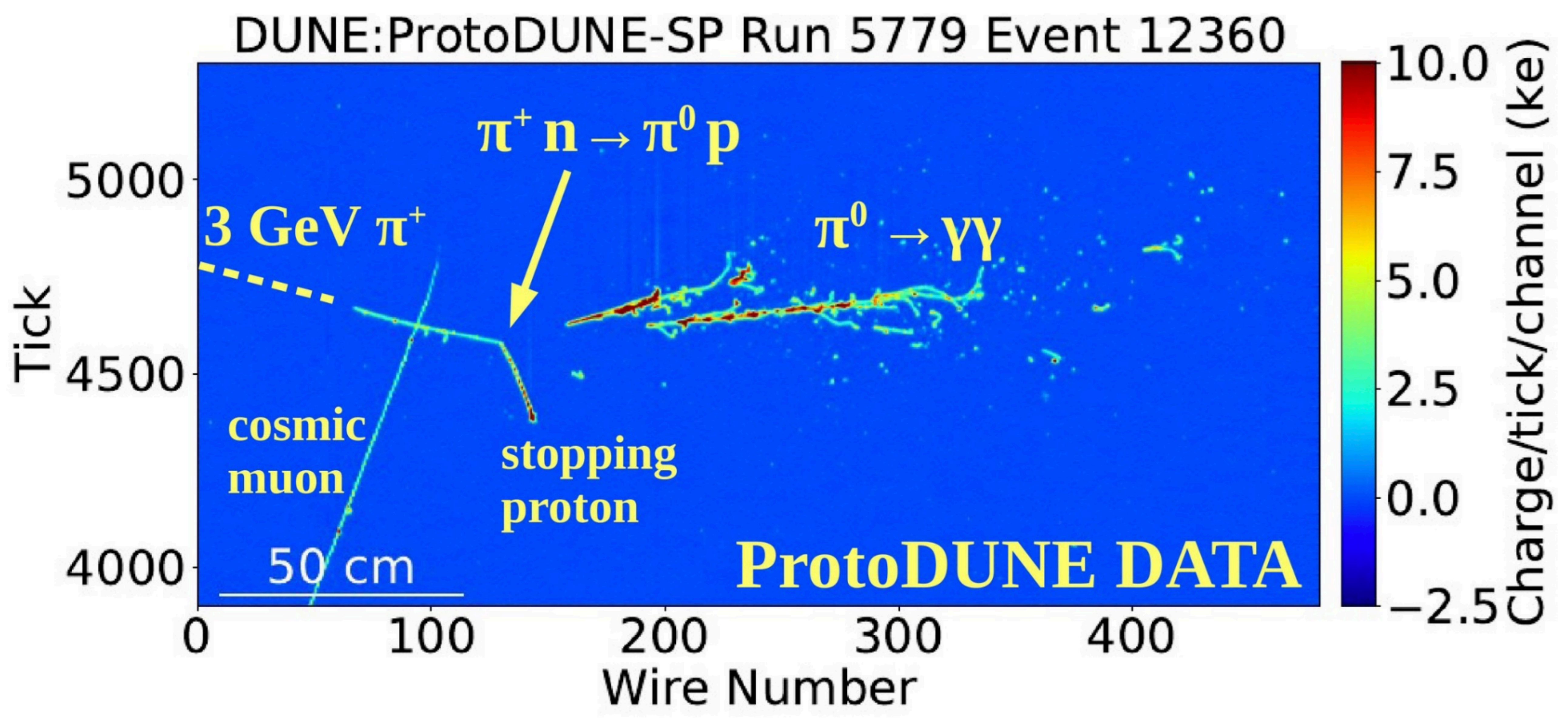
$$P(\nu_\alpha \to \nu_\beta) = \delta_{\alpha\beta} - 4\sum_{i>j}^{3} \Re(U^*_{\alpha i} U_{\beta i} U_{\alpha j} U^*_{\beta i}) \sin^2(\frac{\Delta m^2_{ij} L}{4E_\nu}) + 2\sum_{i>j}^{3} \Im(U^*_{\alpha i} U_{\beta i} U_{\alpha j} U^*_{\beta i}) \sin(\frac{\Delta m^2_{ij} L}{4E_\nu}$$

ν-Interactions in LArTPCs

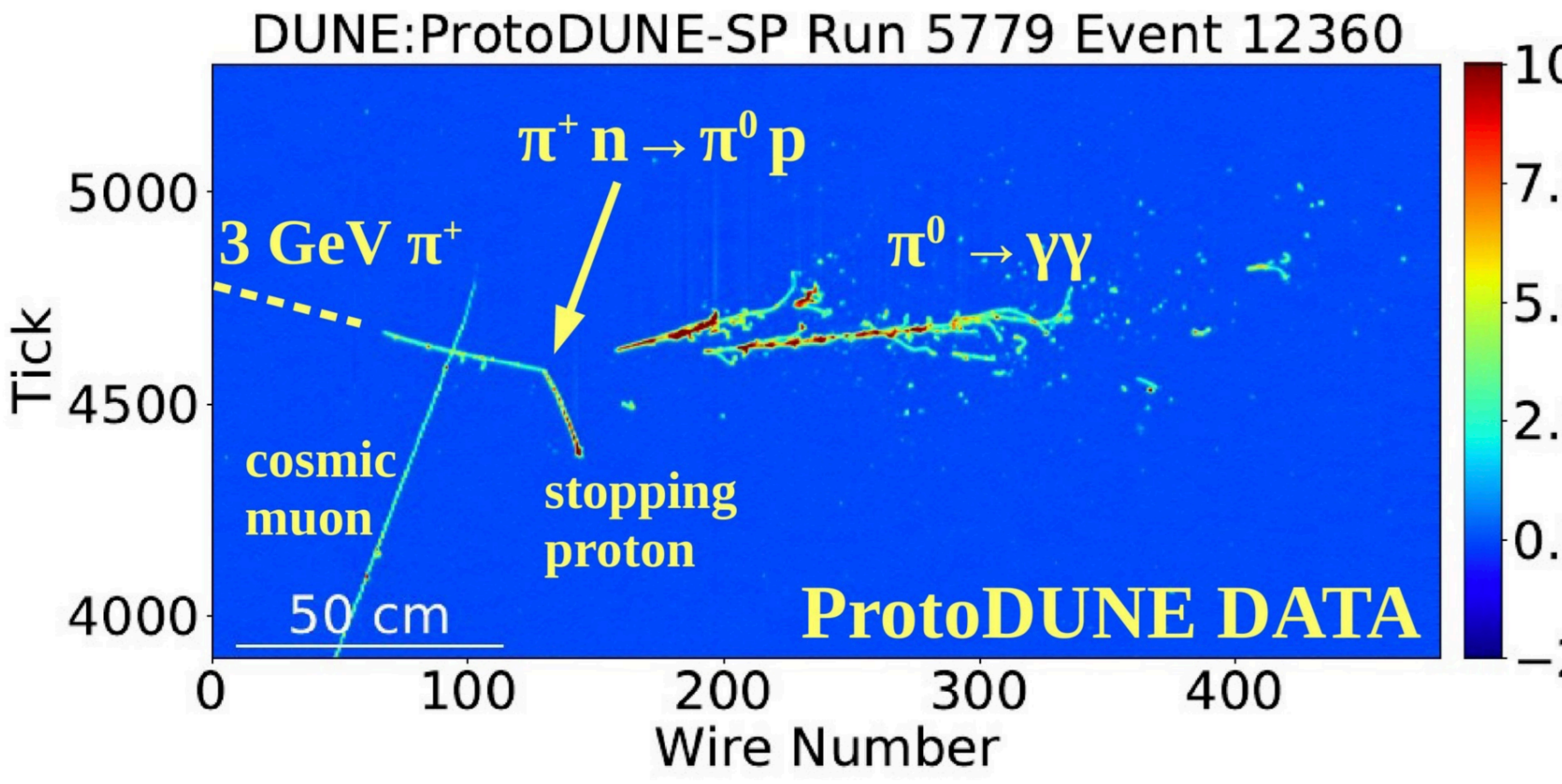


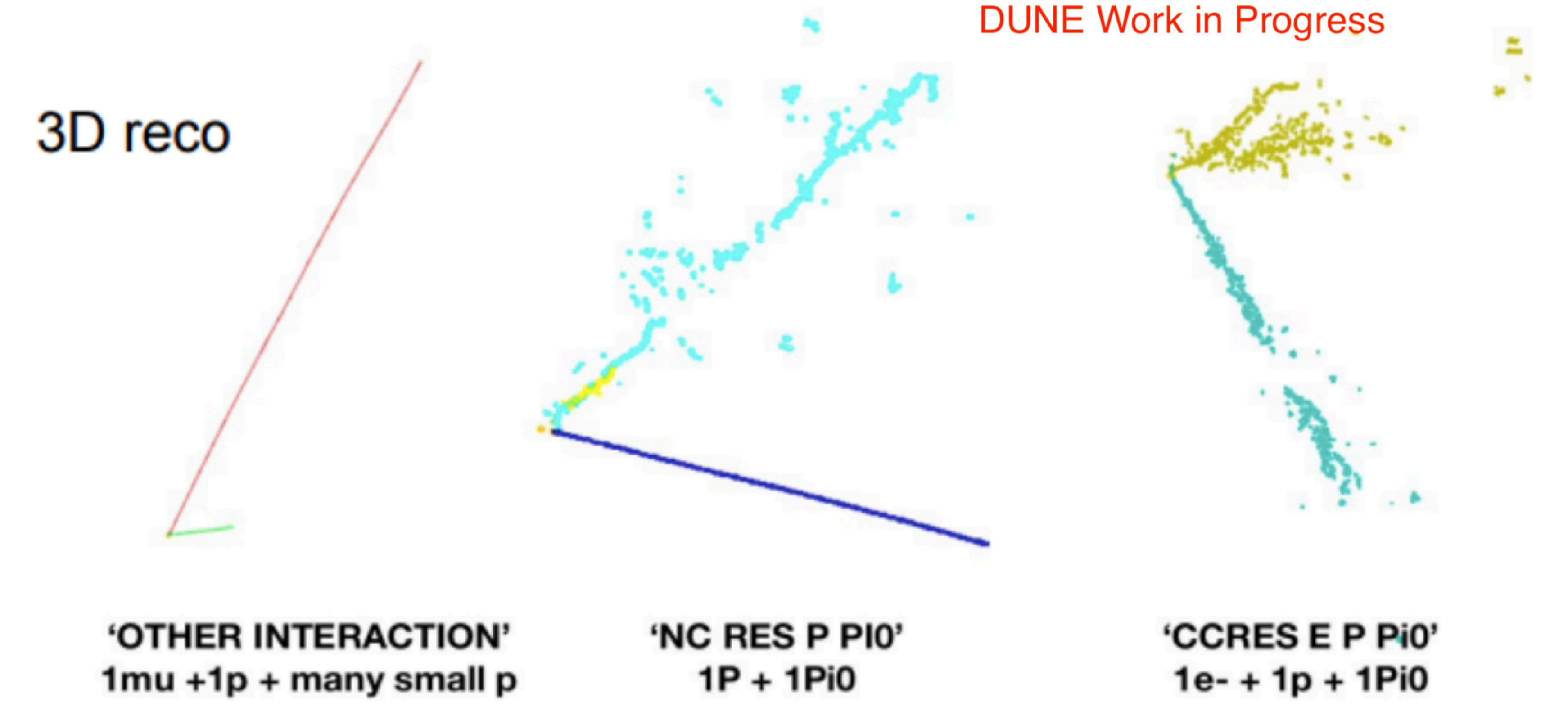


- Broadly track-like or shower-like
- LArTPCs give us exquisite detail
- But mistakes can easily be made!



Issues to deal with





- Neutrino interactions are messy at our energies!
- A decision flow can be something like this :
  - If you identify a μ (usually a long, straight track) => $\nu_\mu CC$
  - If you identify an e (shower like) => $\nu_e CC$
  - If you don't see either => NC
- But :
  - Sometimes don't see two γ's from π^0 (one is short and buried in the other), can be confused as e
  - $\pi^\pm$ are often long and straight too, can be confused as μ
  - Other messy stuff
- We need automated tools to tell them apart! Can't sift through each one manually..

Curve Fitting

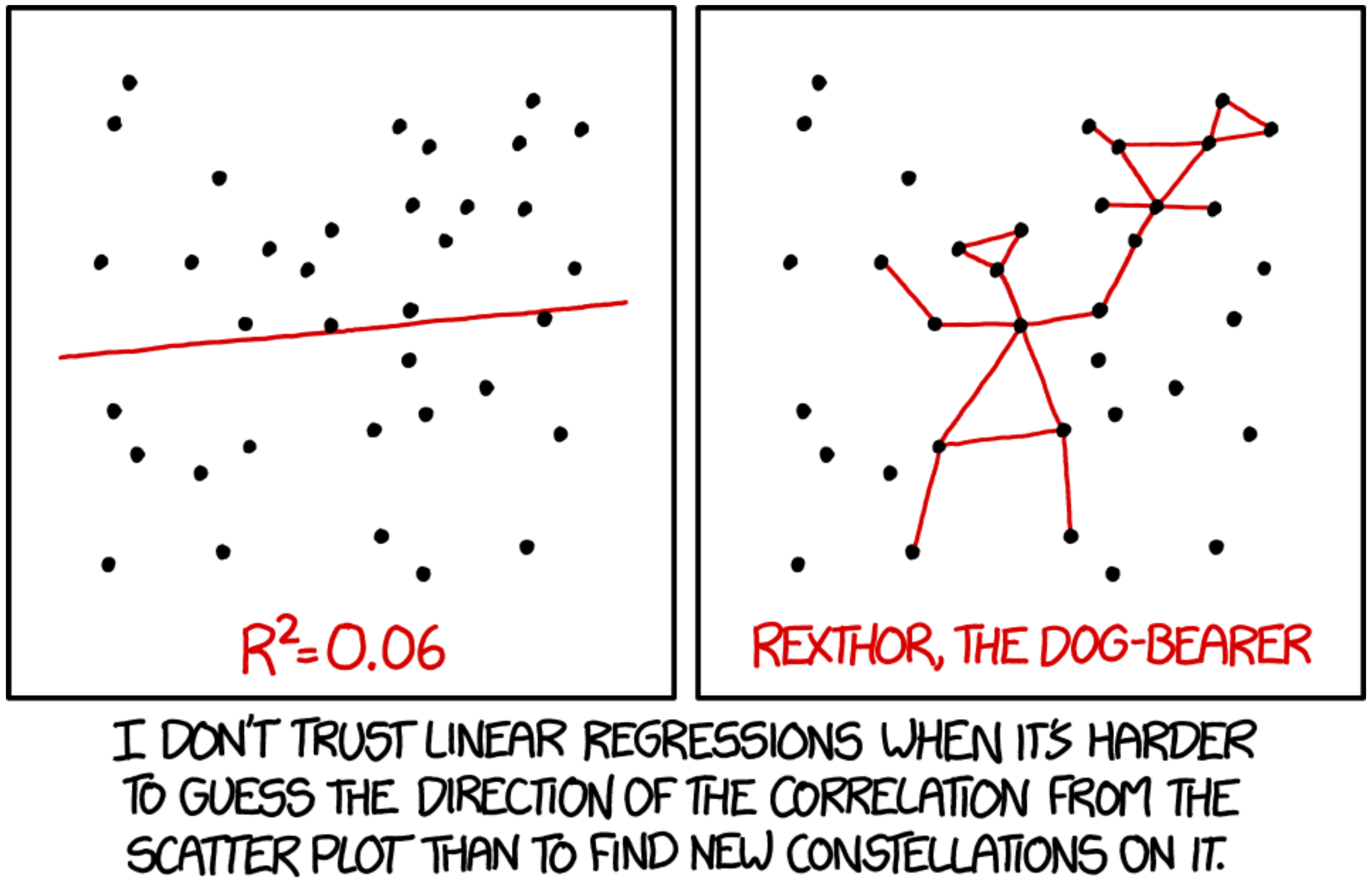
https://xkcd.com/2048/

- Teasing out relationships between observables
- Data is usually always noisy
- Often have to make assumptions about what its supposed to look like : linear, quadratic, something fancy etc.
- Not always easy to justify!

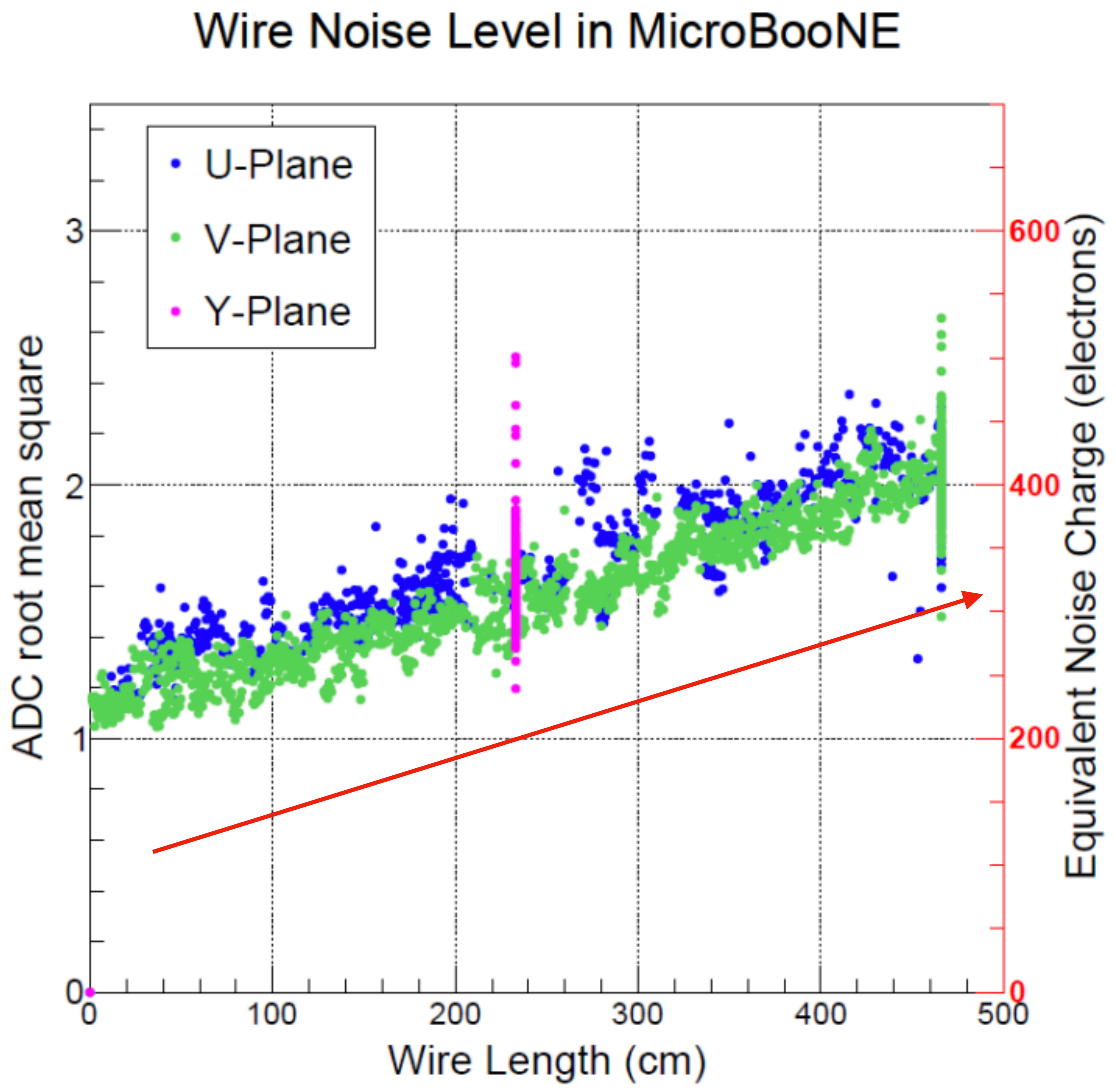
Parametric Fitting

- $y = f(\vec{x}, \vec{\theta})$
  - Eg : $y = ax^2 + bx + c$, where $\vec{\theta} \equiv (a, b, c)$
- Choose $\vec{\theta}$ based on some measure denoting how good/bad the fit is ("loss function")
  - Eg : $\vec{\theta}$: $\min |\hat{y} - f(\vec{x}, \vec{\theta})|^2$ ("least square distance")
- Overfitting :
  - Can be caused by having too many parameters (d.o.f) describing low-dimensional data
  - Fits well to given noisy data but doesn't generalize!

https://xkcd.com/1725/



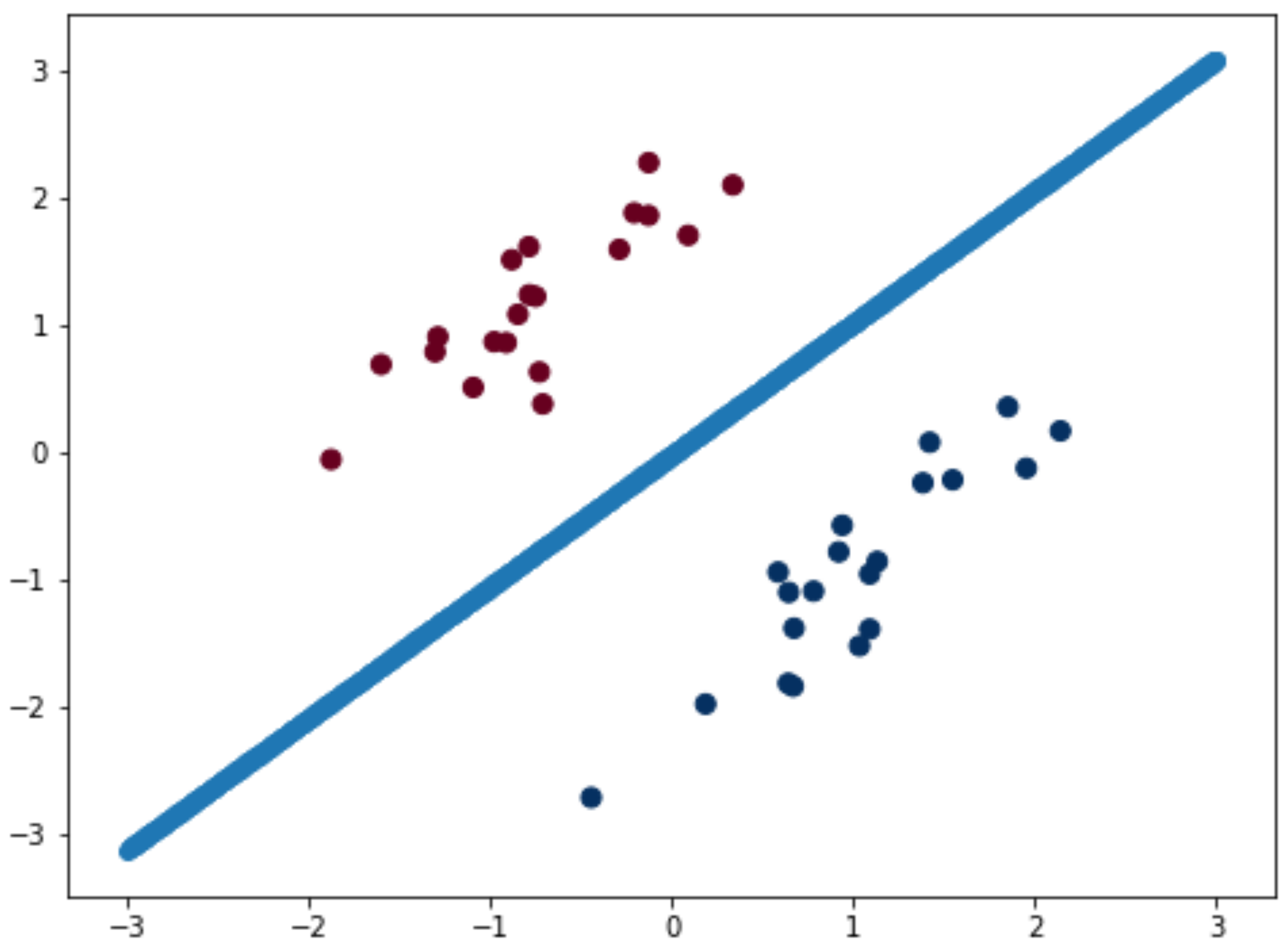
- Teasing out relationships between observables
- Data is usually always noisy
- Potential for spurious, nonsense results if not careful!

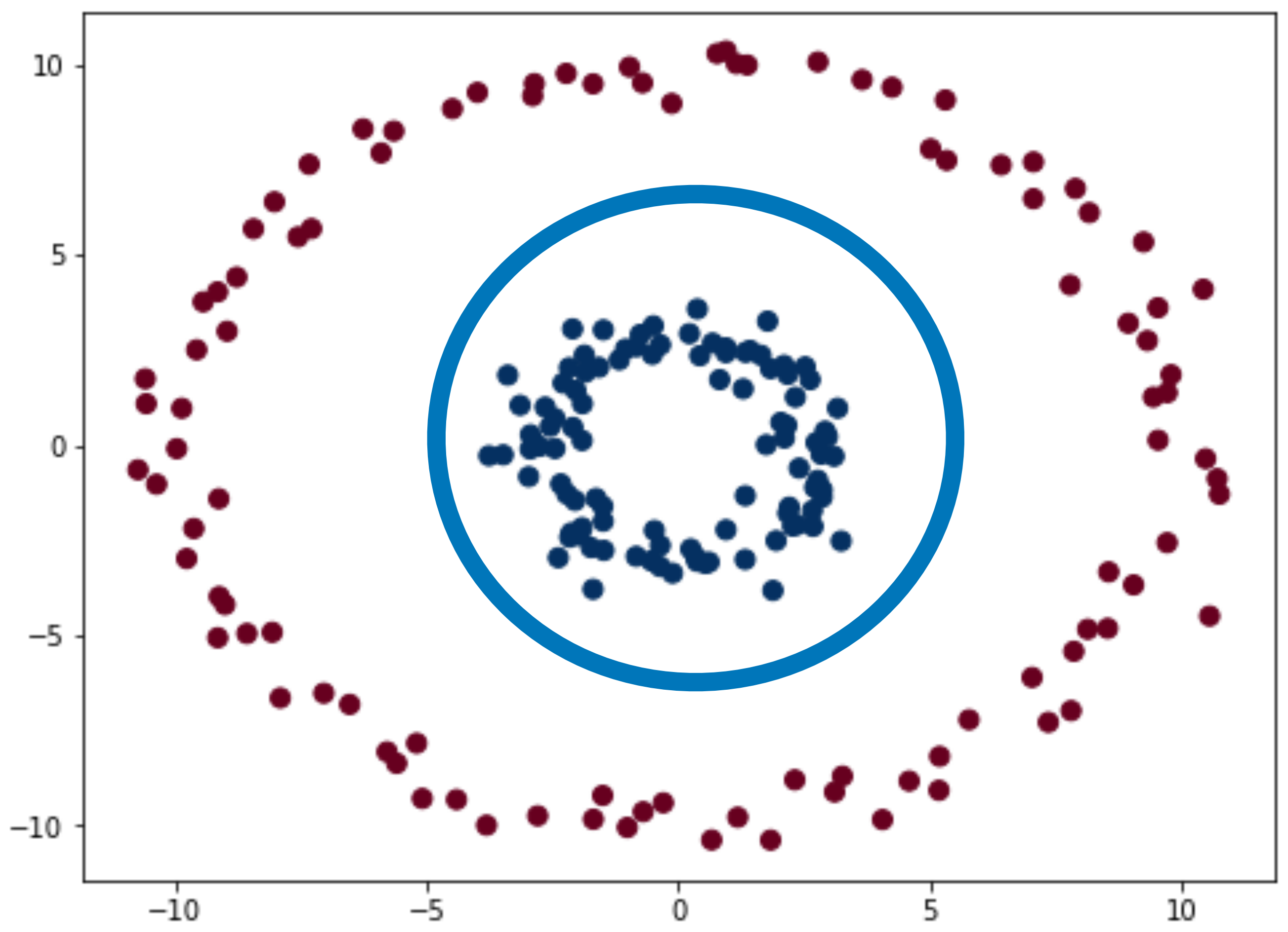


- But how to choose parametric form? Need to carefully assess which one works for given problem and what assumptions are being made
- Problem becomes worse when working with high-dimensional data and no reason to believe a parametric form even exists
  - Eg : Predict how movies are going to perform based on various inputs (choice of actors, marketing budget, script etc)
- Sophisticated techniques that are automatically able to “learn” what’s best. Can predict with astounding accuracy in many cases
- More complexity $\not\Longrightarrow$ automatically better! Still prone to overfitting, biases, bad assumptions etc

Regression vs Classification

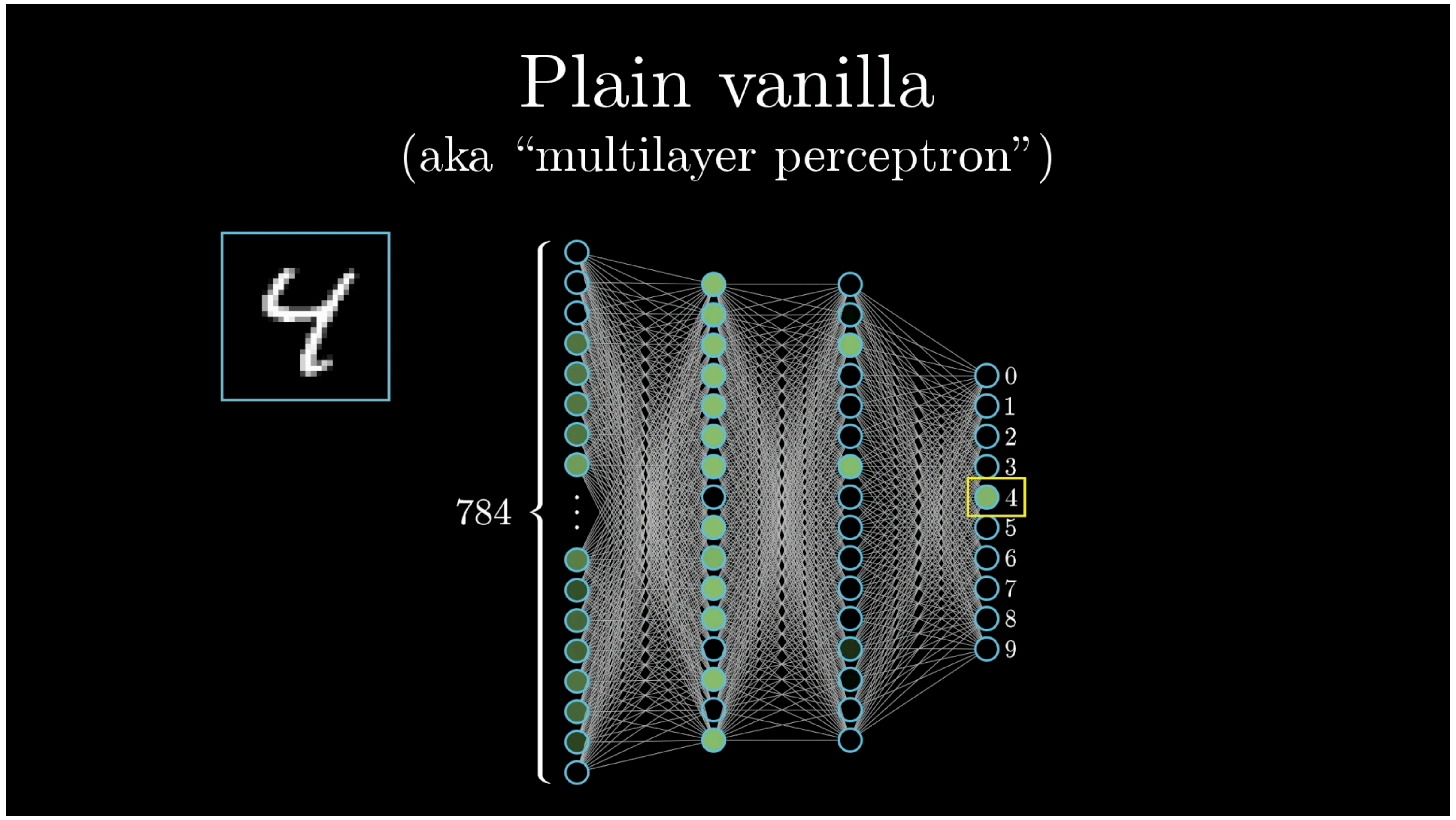
- Regression - Predict a continuous variable, for eg. the energy of the neutrino that interacted in the detector
  - Parametric methods : Find $\overrightarrow{\theta}$: $\min |\hat{y} - f(\overrightarrow{x}, \overrightarrow{\theta})|^2$: Choice of f can be pre-determined or automatically "learnt"
  - Complex problems require complex f, often very non-linear
- Classification - Predict one of many possible <u>discrete</u> labels, for eg. ν_e CC , ν_μ CC, ν_τ CC, ν_x NC
- Classification is also curve-fitting in a way!





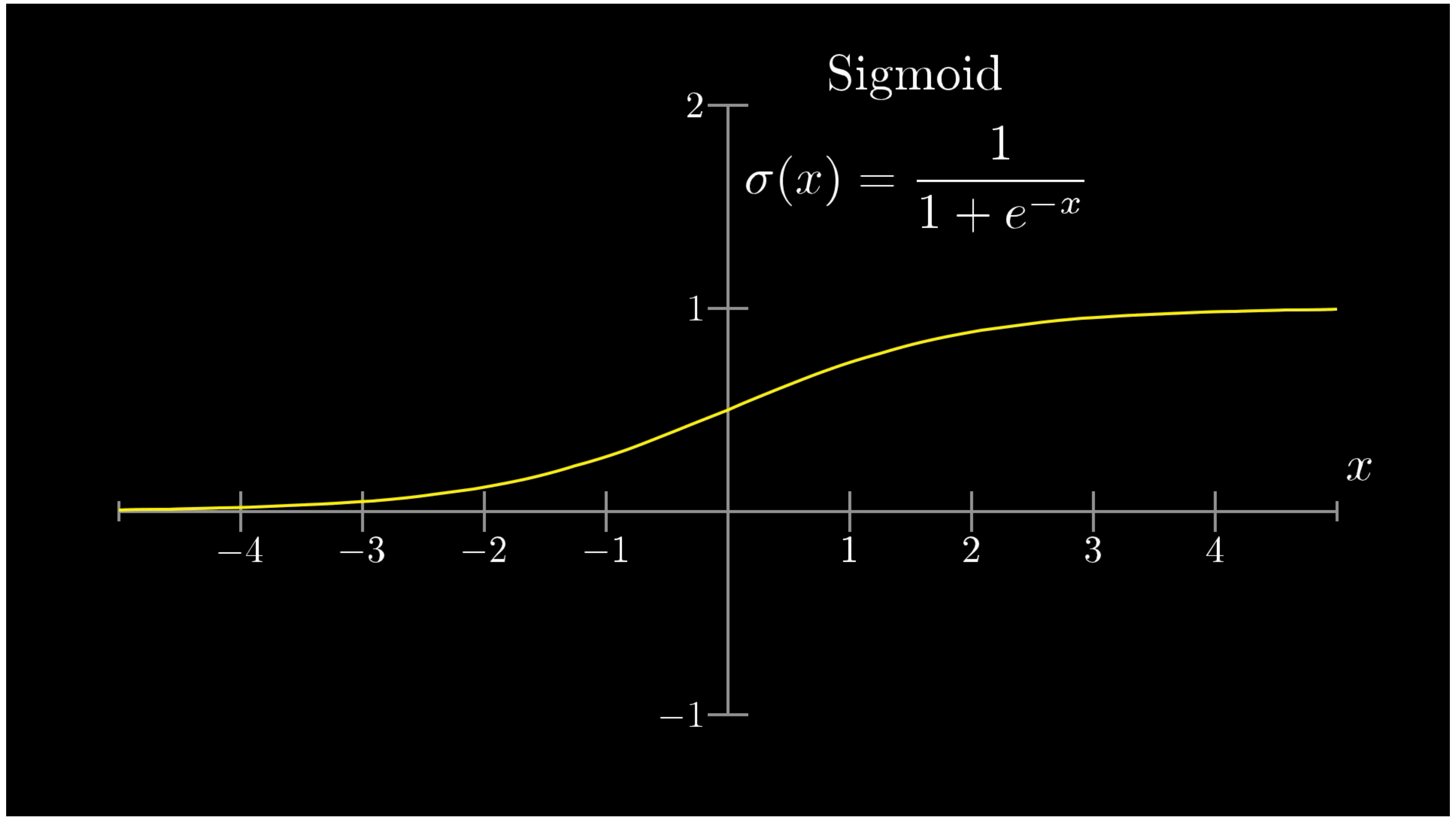
- Now, we want f and $\overrightarrow{\theta}$ that best <u>discriminates</u> between data coming from different labels
  - "Decision boundary"
- Essentially a regression problem for the probability of given data to belong to one label or the other
- Again, f can be relatively simple or highly complicated depending on context
- Involves another loss-function that minimizes "probability error", can be least-squares as before

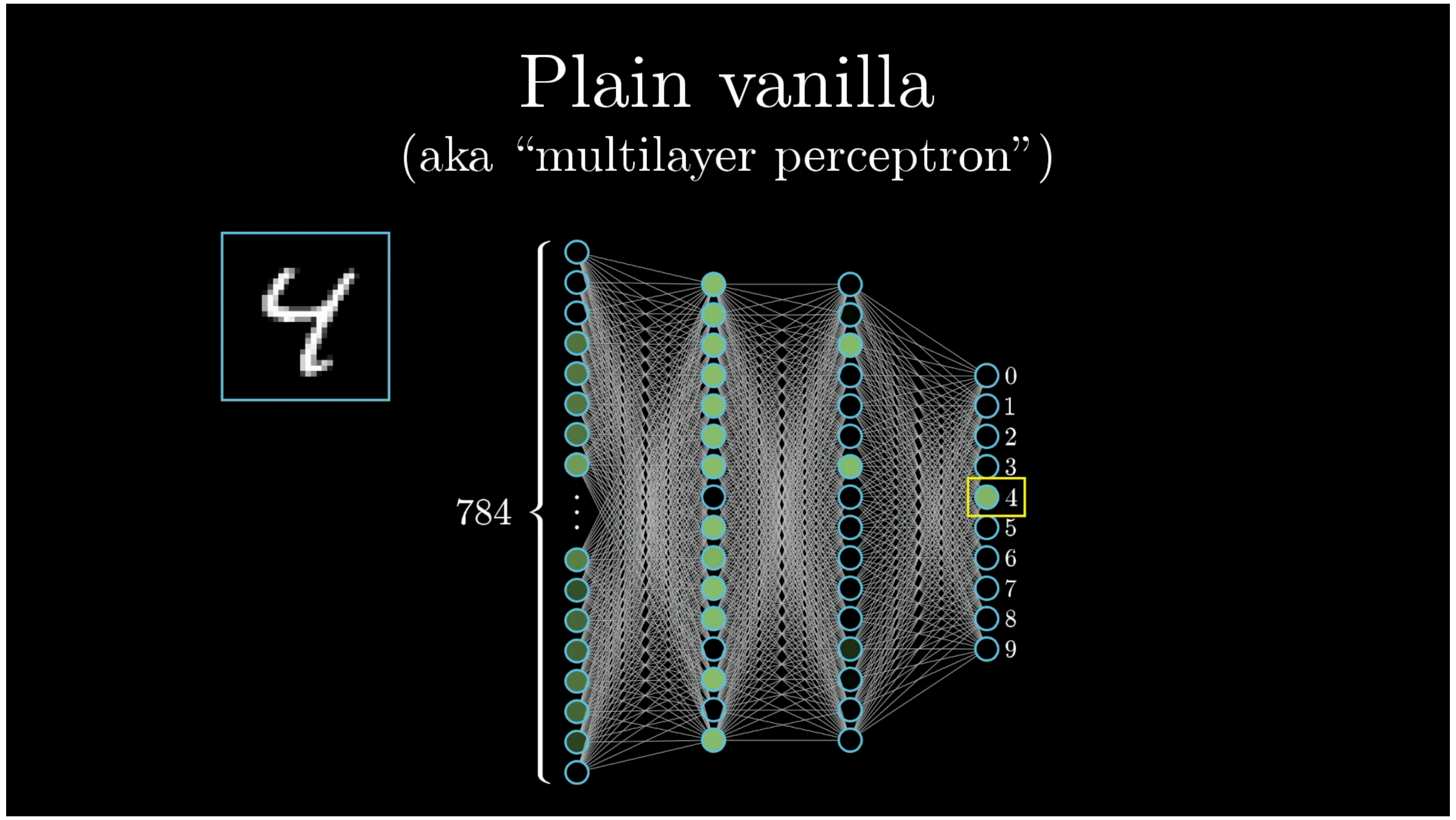
Neural Networks



- Essentially devices that can spit out arbitrarily complex functions in many dimensions
- Network of “neurons” to mimic structure of human brain
- Consider for eg, input 28x28 (=784 pixels) image where each pixel has a number b/w (0, 1) denoting how bright that pixel is
- The neurons (1 for each pixel) in the first (“input”) layer can just be “brightness” values in that pixel

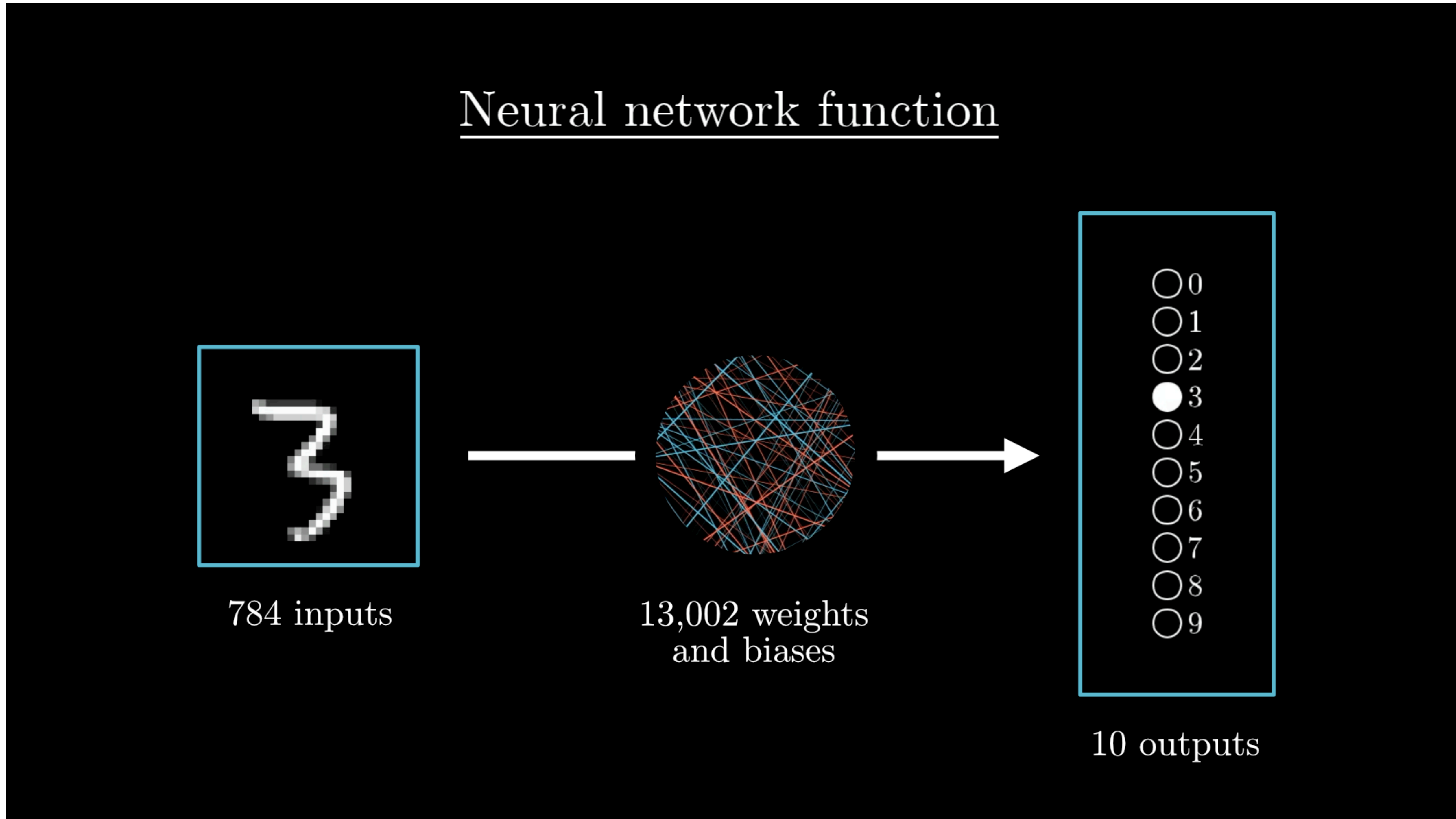
- For a neuron in the 2nd layer, calculate its response as :
  - $a_0^{(1)} = \sigma(w_{0,0}a_0^{(0)} + w_{0,1}a_1^{(0)} + w_{0,2}a_2^{(0)} + \ldots w_{0,n}a_n^0 + b_0)$
  - Where $a_i^{(0)}$ represents the value of the i^{th} neuron in the 0^{th} layer
  - $w_{0,i}$ represents the strength of the connection between $a_0^{(1)}$ and $a_i^{(0)}$ (“weights”)
  - b_0 is a bias parameter
  - σ is a so-called activation function, designed to ensure values in each neuron are within a certain range, for eg between (0, 1) typically for classification





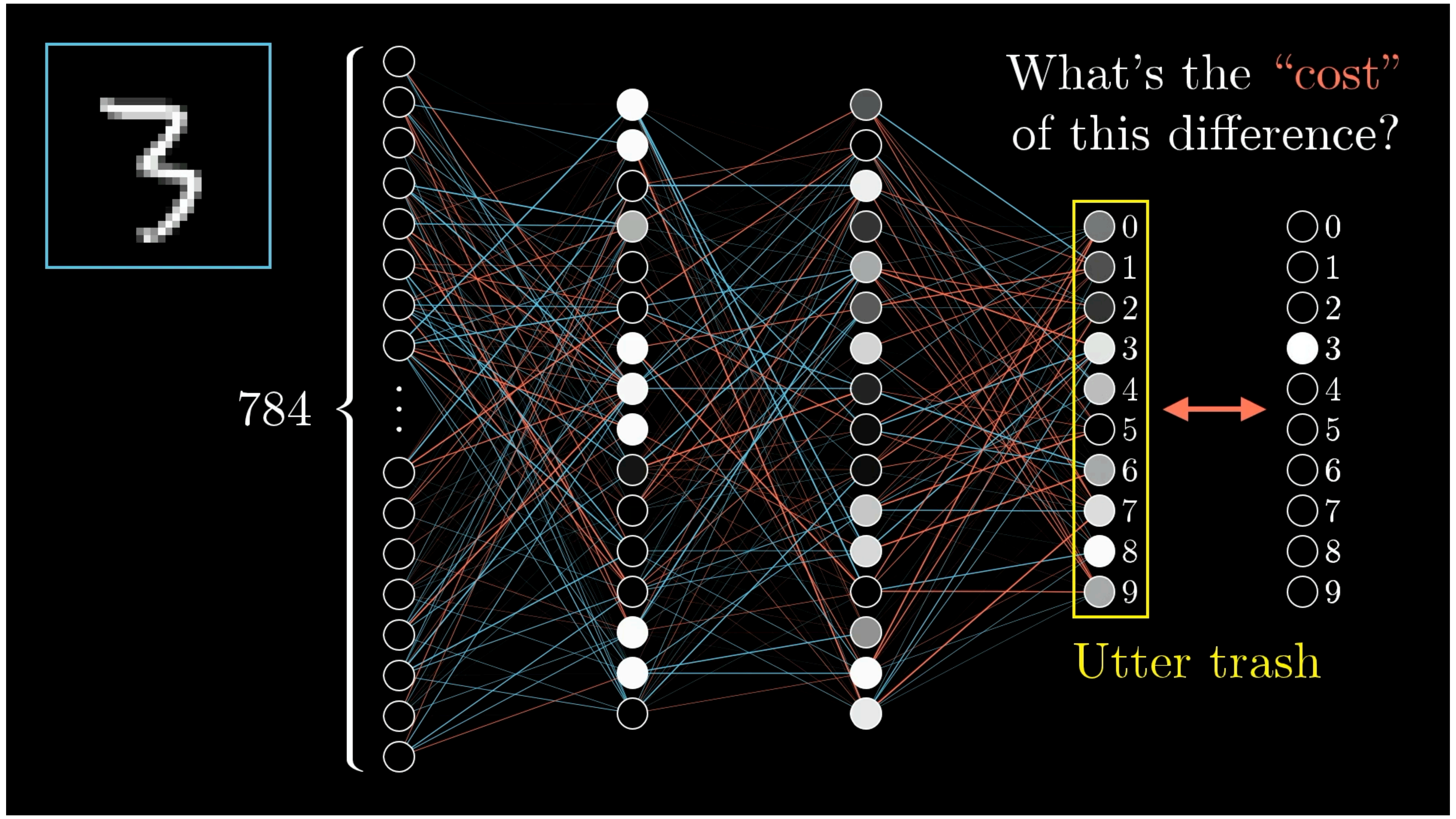
- In our eg, the final ("output") layer has 10 neurons
  - 1 for each digit we want to predict (0-9) based on input image of 784 pixels
- Lets assume 2 hidden layers, each with 16 neurons

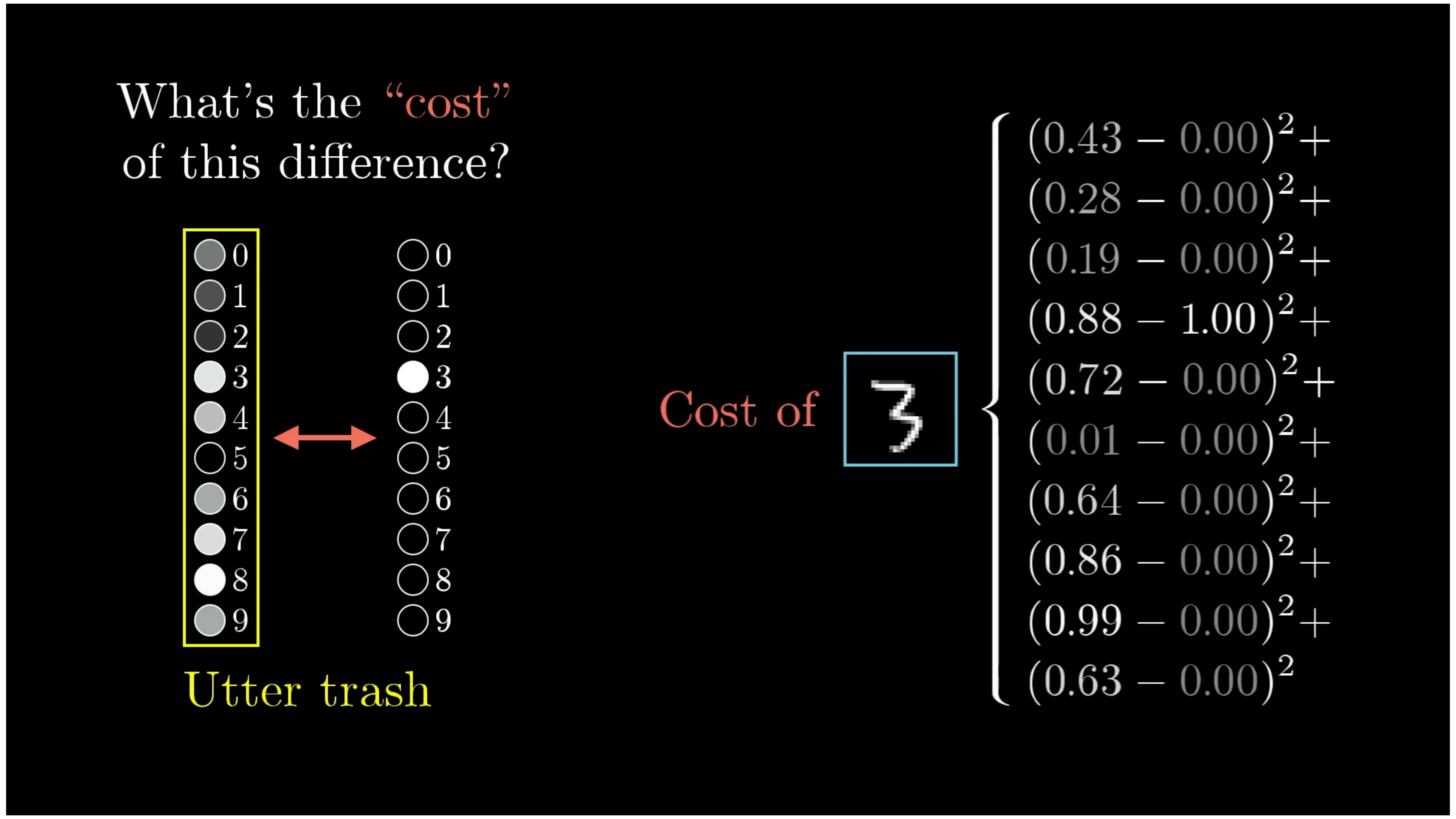
- => (784*16 + 16*16 + 16*10) = 12960 w parameters ("weights")
- => (16 + 16 + 10) = 42 b parameters ("biases")
- Total = 13002 parameters
- Find w and b values such that we get the best predictions
- Curve fitting in 13002 dimensions!



Training

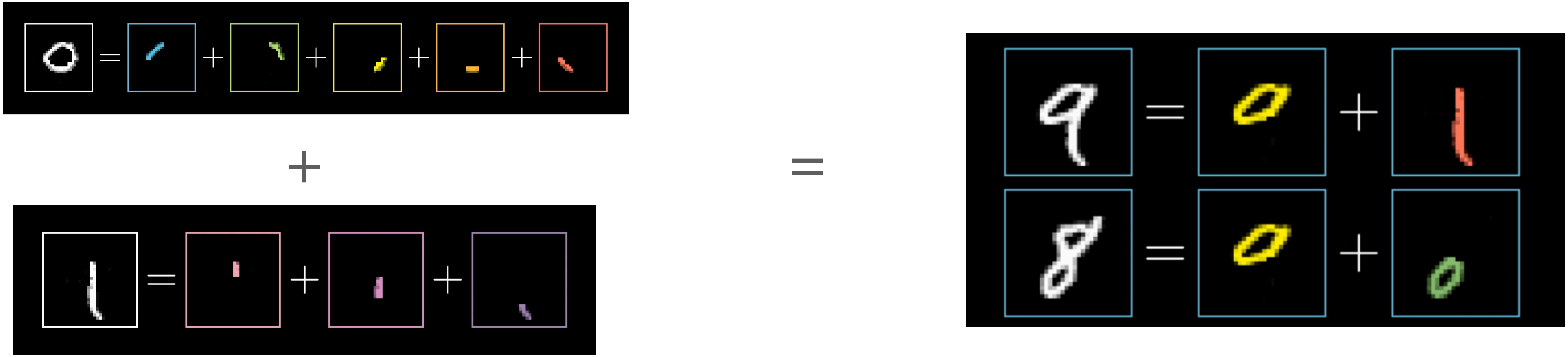
- Process of finding best w and b values referred to as "training the network"
- What do we mean by "best"?
    - For some w and b, each neuron in output layer contains value between (0, 1)
    - A probability measure denoting how confident the network is about the input image corresponding to that label
    - Can define loss function exactly as before ("least-squares") as
    - $L(w, b) = \sum_{i=0}^{9} (\hat{y}_i - o_i(w, b))^2$ and minimize this





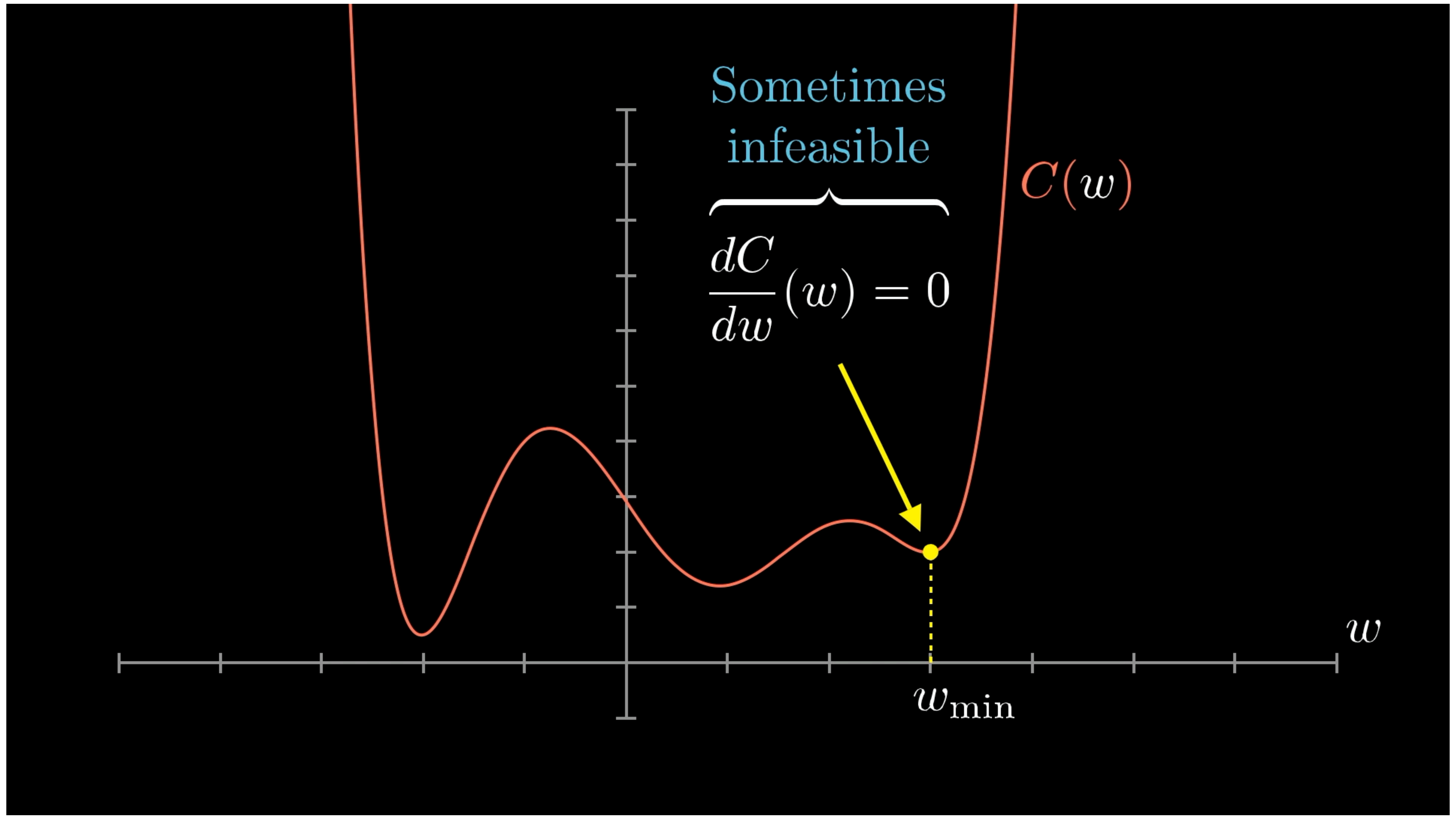
Why so complex?

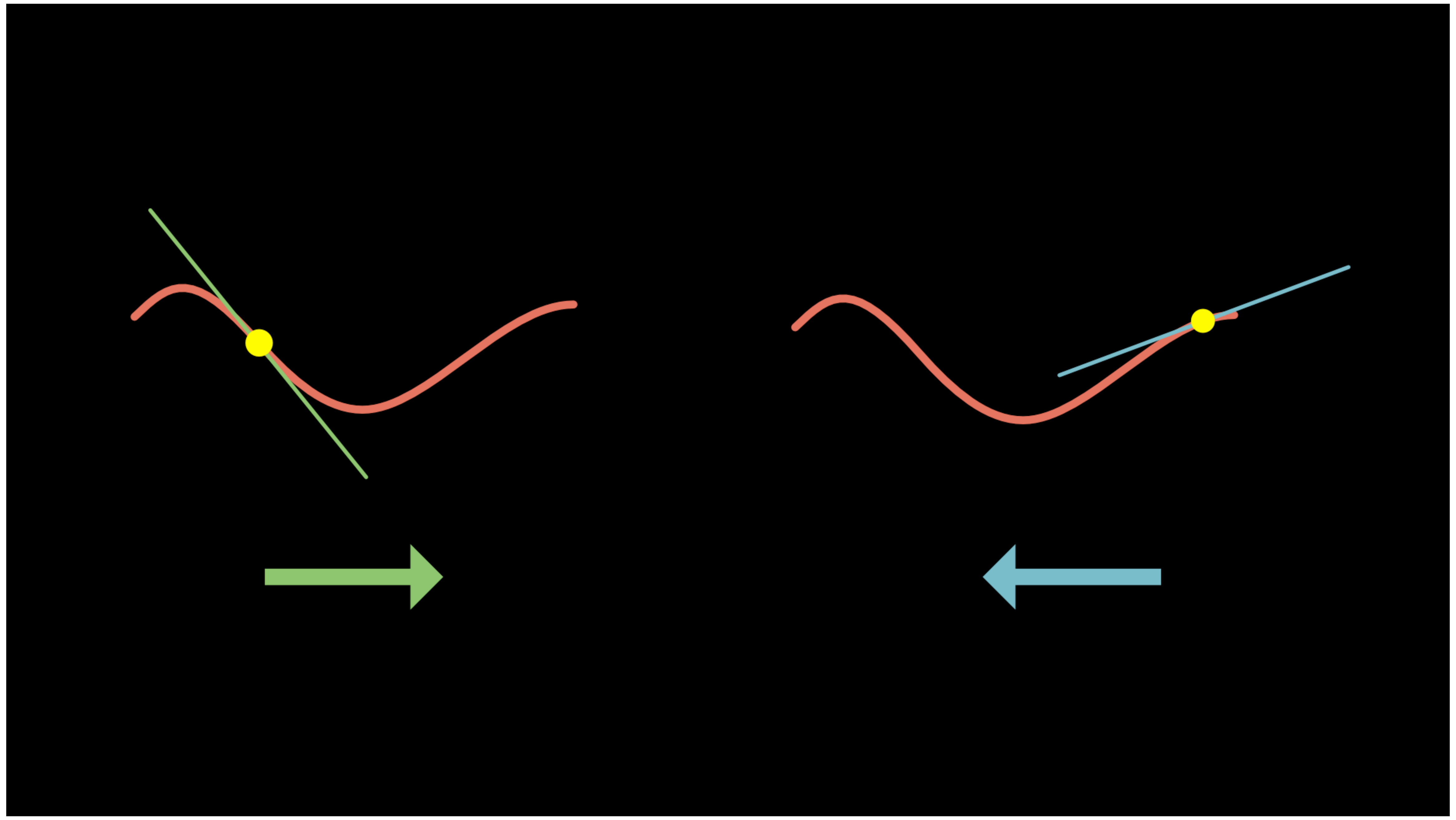
- Our brains can easily recognize patterns/digits even if the images were a bit fuzzy
- But its a hard problem! We need ~13000 parameters to be able to describe arbitrary decision boundary shapes
- Could imagine the neural network decision flow as :
  - 2nd layer of neurons detect edges of image where pixels are bright
  - 3rd layer of neurons combines these edge pixels in various shapes, for eg loops or lines
  - Final layer might try to correlate number of loops or lines to the actual digits, for eg, 2 loops 0 lines => label “8” etc
- As we feed in more data during the training phase to optimize the loss function, network can get better and better at figuring out these patterns



Gradient Descent

- Algorithm to minimize loss-function, $L(w, b)$ and find best w, b
- $L(w, b)$ has 13,002 input parameters but outputs a single number
- Finding a minimum for such a function is also complicated!
- Gradient descent — "ball rolling down a hill"
- Non-convex optimization : not guaranteed to find global minimum
- Try starting the ball at different starting points. Also "stochastic GD" — try to make ball jump across valleys

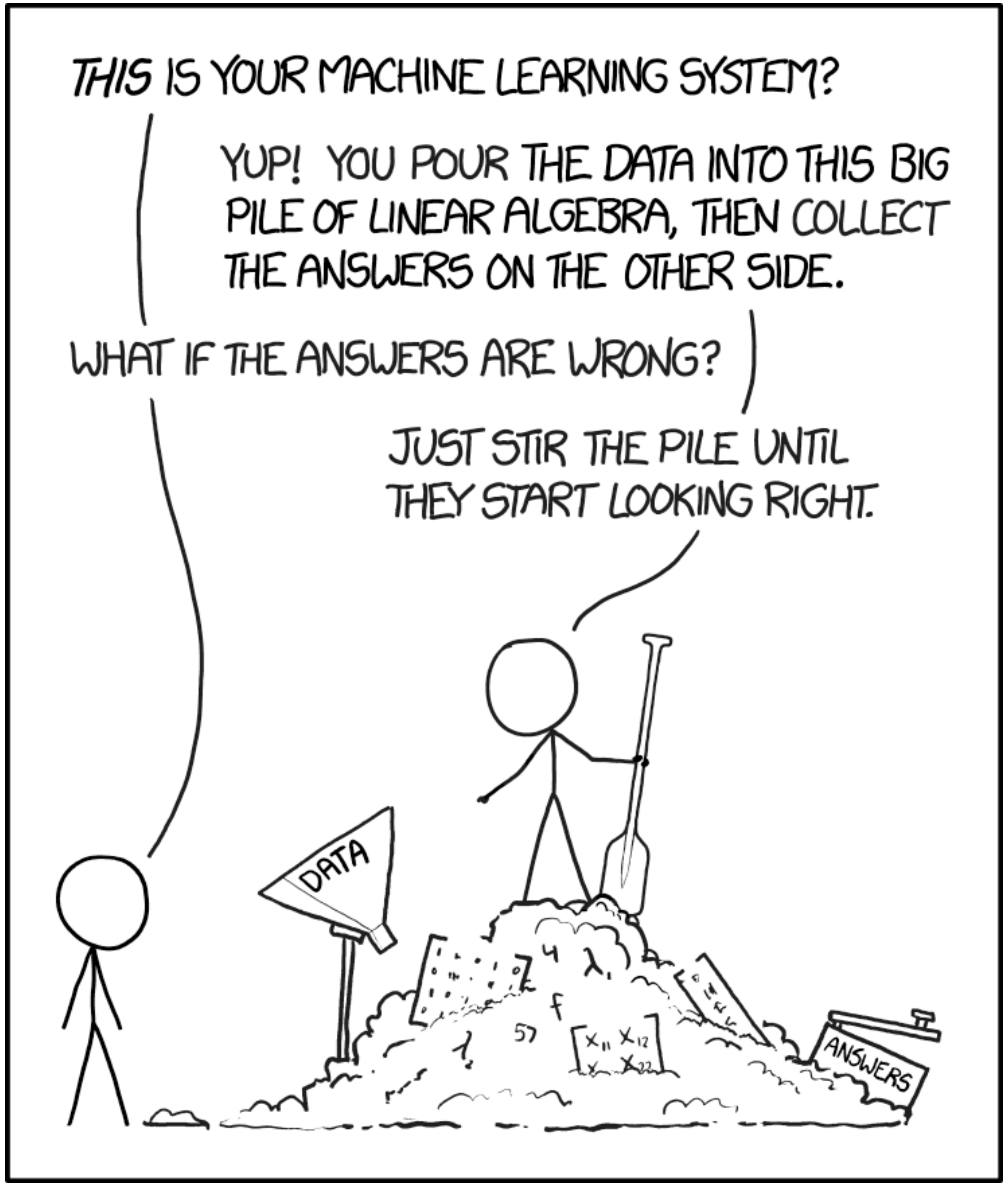




What’s the takeaway

https://xkcd.com/1838/

- Forced to deal with complexity
  - Large dimensionality, unknown parametric relationships
- Overfitting : network starts to predict based on spurious features it learns from training data
  - For eg, it might decide the digit in image on particular handwriting styles and not generalize to other styles — “bias”
  - But its hard to know what it learns! ~Black box
- We never assess network performance on training dataset
- Always keep a fraction of data separate and then see how trained network performs (“Test dataset”)
  - If training errors are very different from test errors, we may have issues
- Also good practices, shuffling dataset before training, cross-validation, i.e change up training and test data for different iterations
- Playing around with GD parameters etc

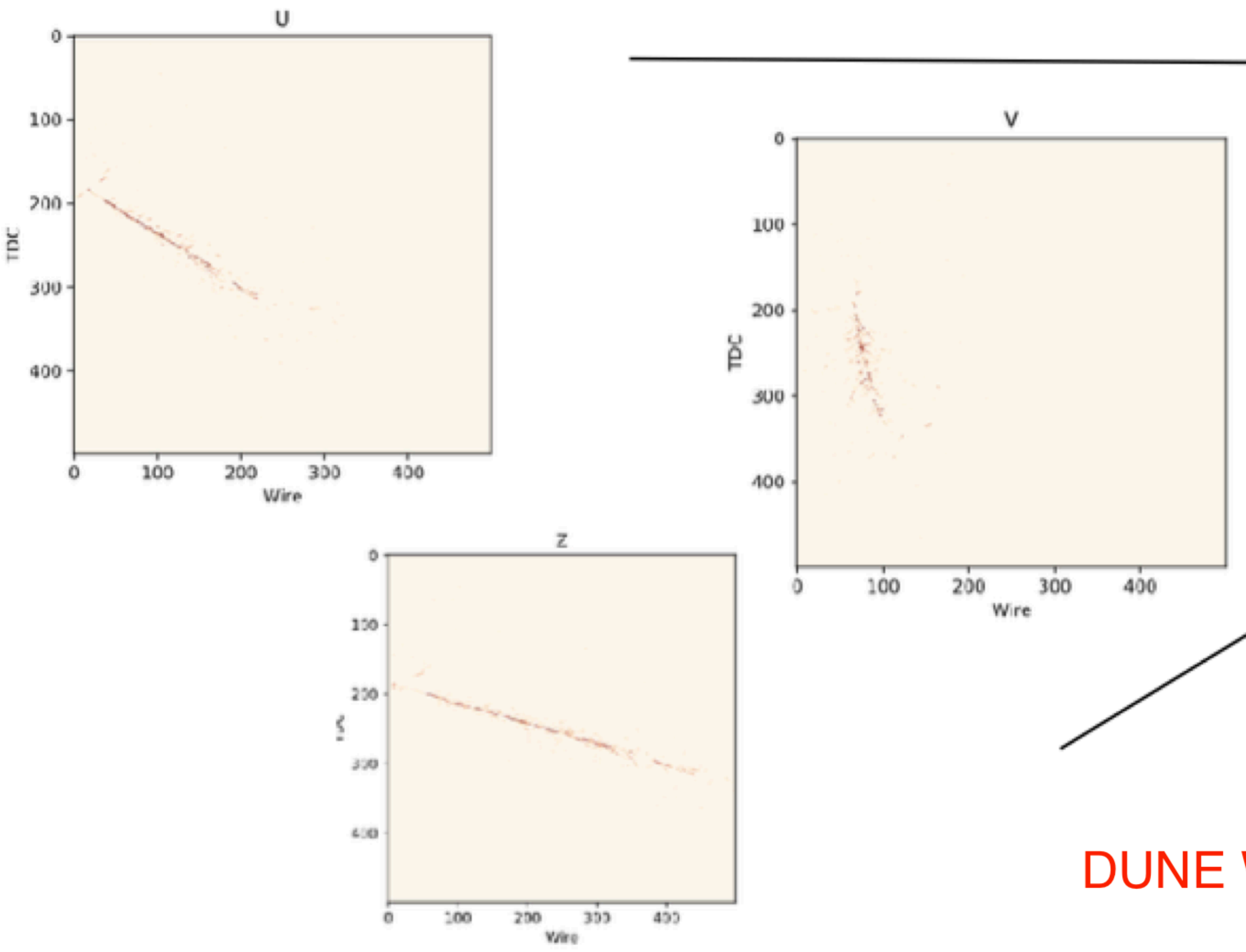


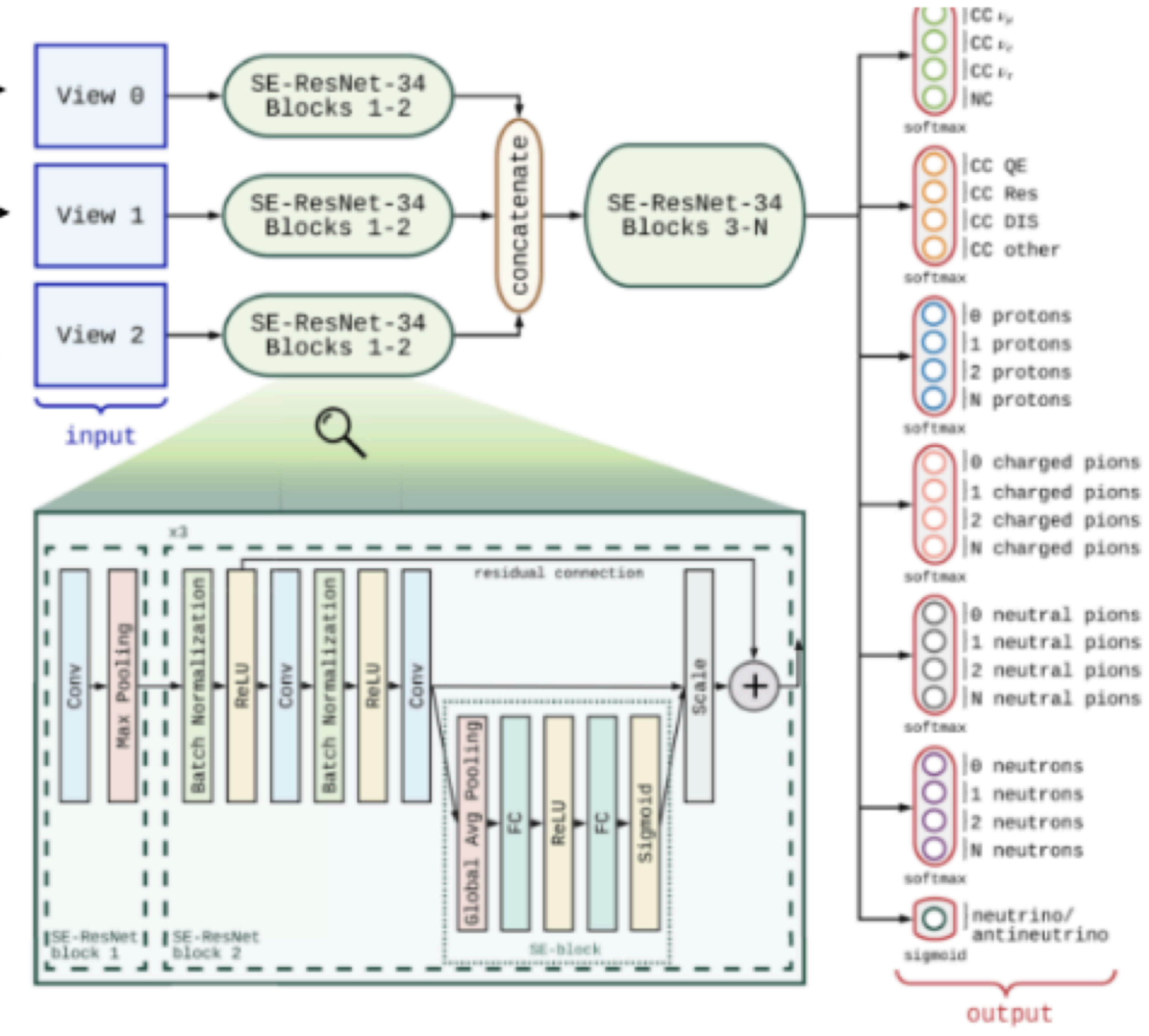
Neutrino Flavor Tagging

- Classification problem
- We use “deep neural networks”, particularly a brand called convolutional neural networks
  - Trained on ~6 million total events across ν_e CC , ν_μ CC, ν_τ CC, ν_x NC
  - ~22 million parameters (>> 13000!), “softmax” activation function to squish neurons to b/w (0, 1)
  - Trained for a week using Nvidia GPU clusters. Actually, most modern GPUs can handle these kinds of payloads but sometimes need more than 1
  - Three input images, each 500 x 500 = 250,000 pixels

$$\sigma(\vec{z})_i = \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}$$

- Output is a score b/w (0, 1) for each of 4 flavor labels : ν_e CC , ν_μ CC, ν_τ CC, ν_x NC. Also has scores for other features of interaction

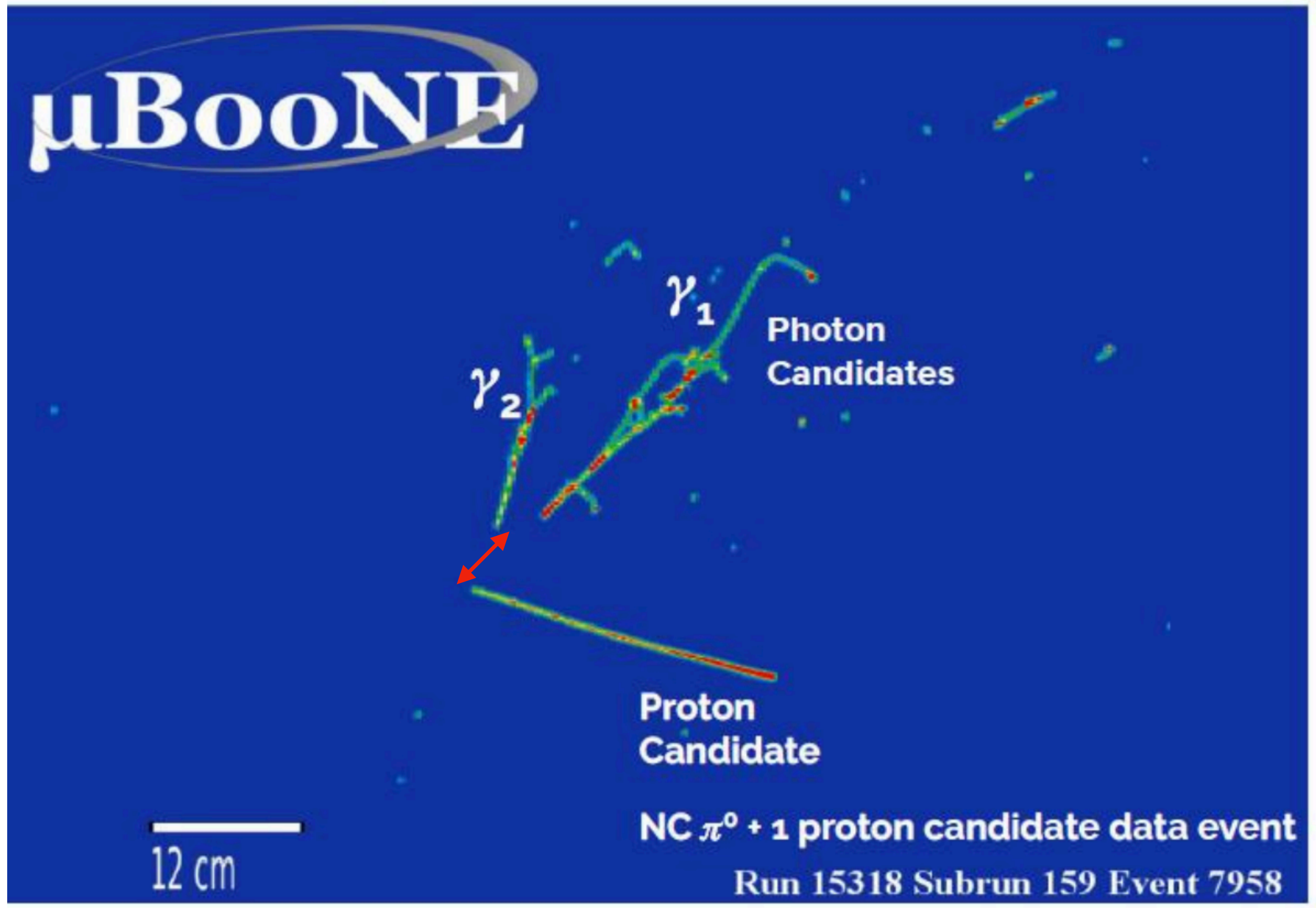


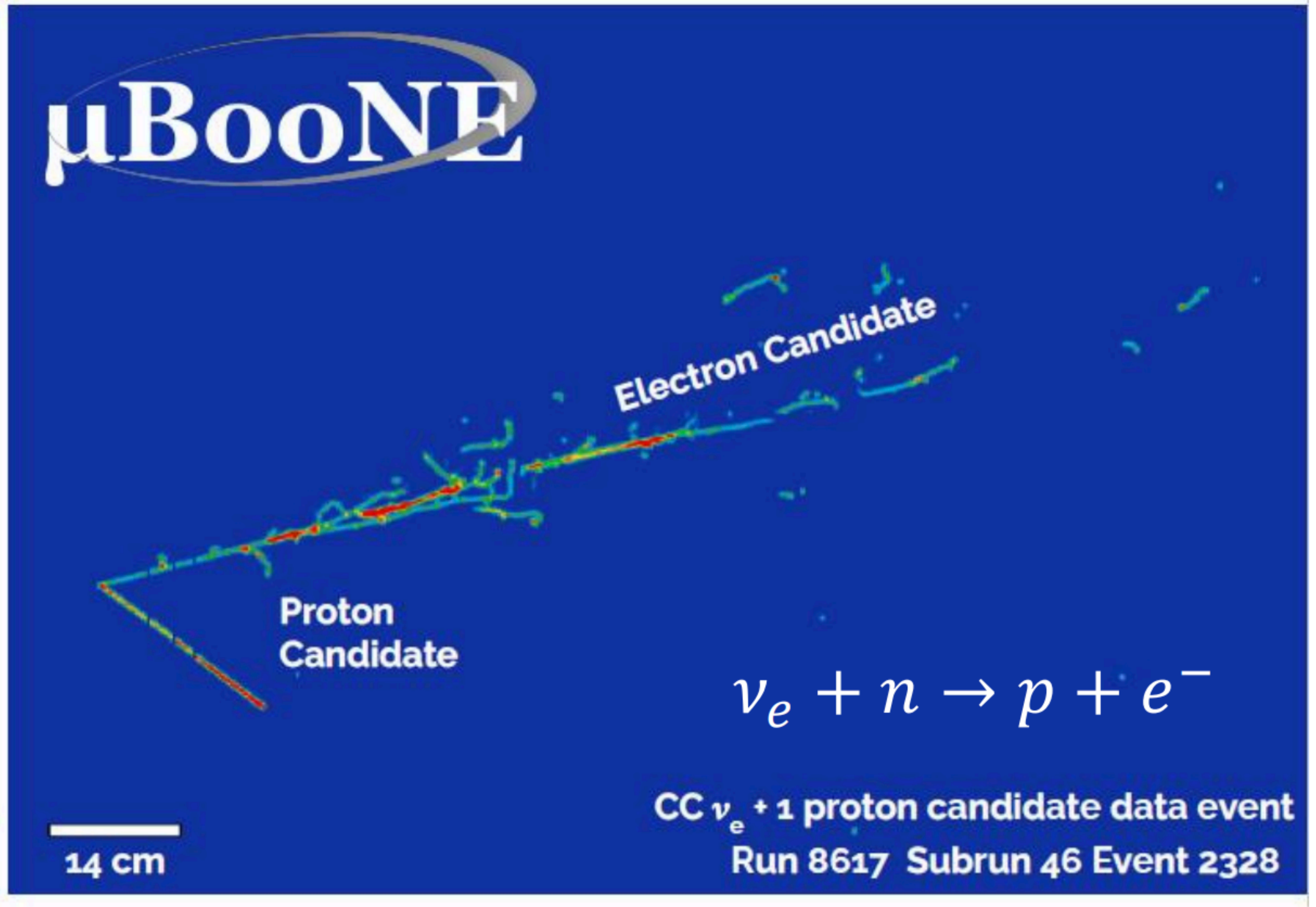


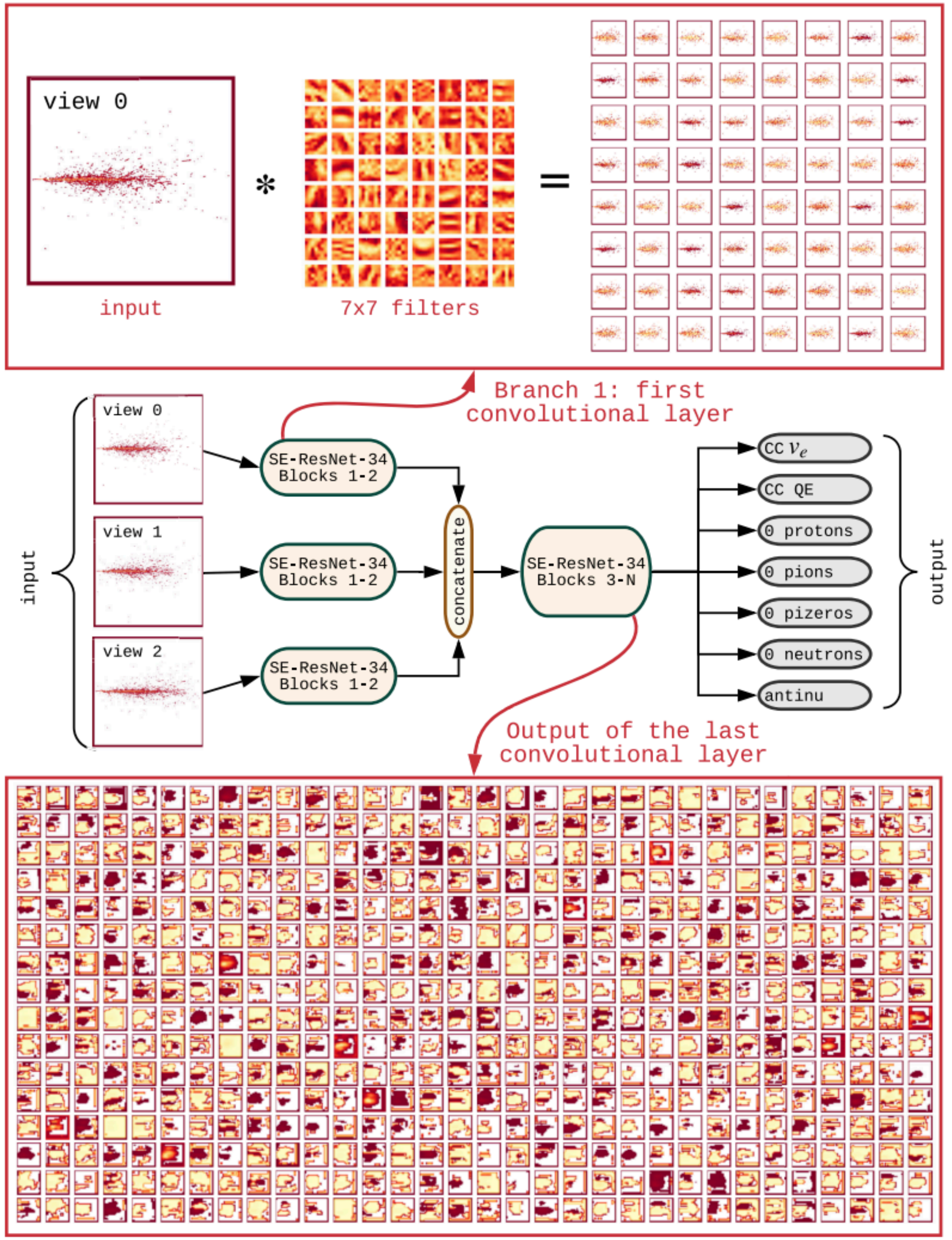
DUNE Work in Progress

Why Deep?

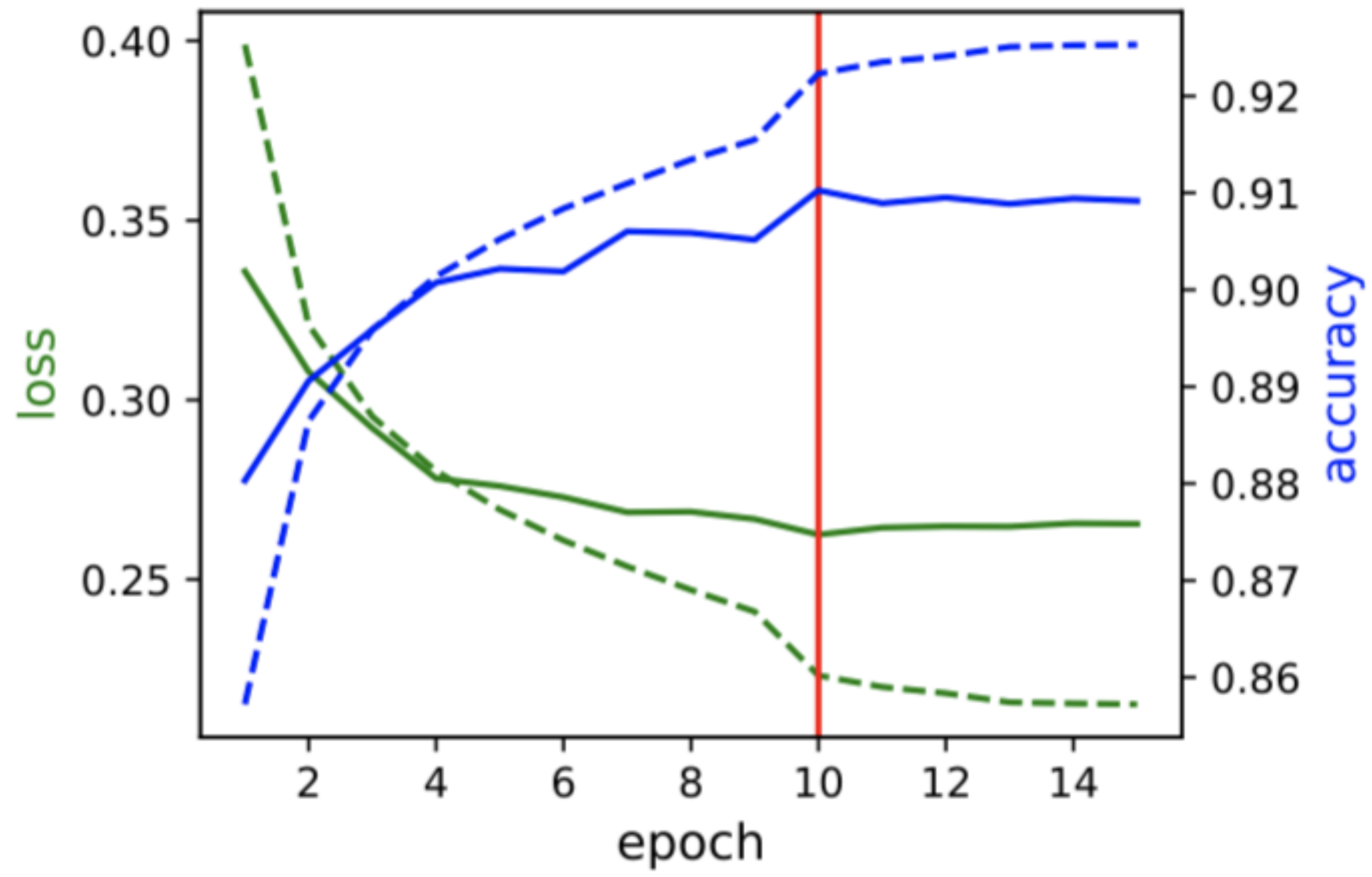
- Previously, traditional approaches involve using set of human-engineered features as input, even to a shallower neural network
    - Examples of useful features for our problem : number of showers, gap from vertex, number of tracks
- Deep neural networks are able to figure these out themselves and their increasing depth also allows them to catch features we may have missed
    - We get more accurate networks, but possibly at the cost of not knowing as much about what its doing.
    - Validation is key to building trust! If established, we can reap the benefits
- Again, context is key. Sometimes it pays to build a less complicated network — active area of research



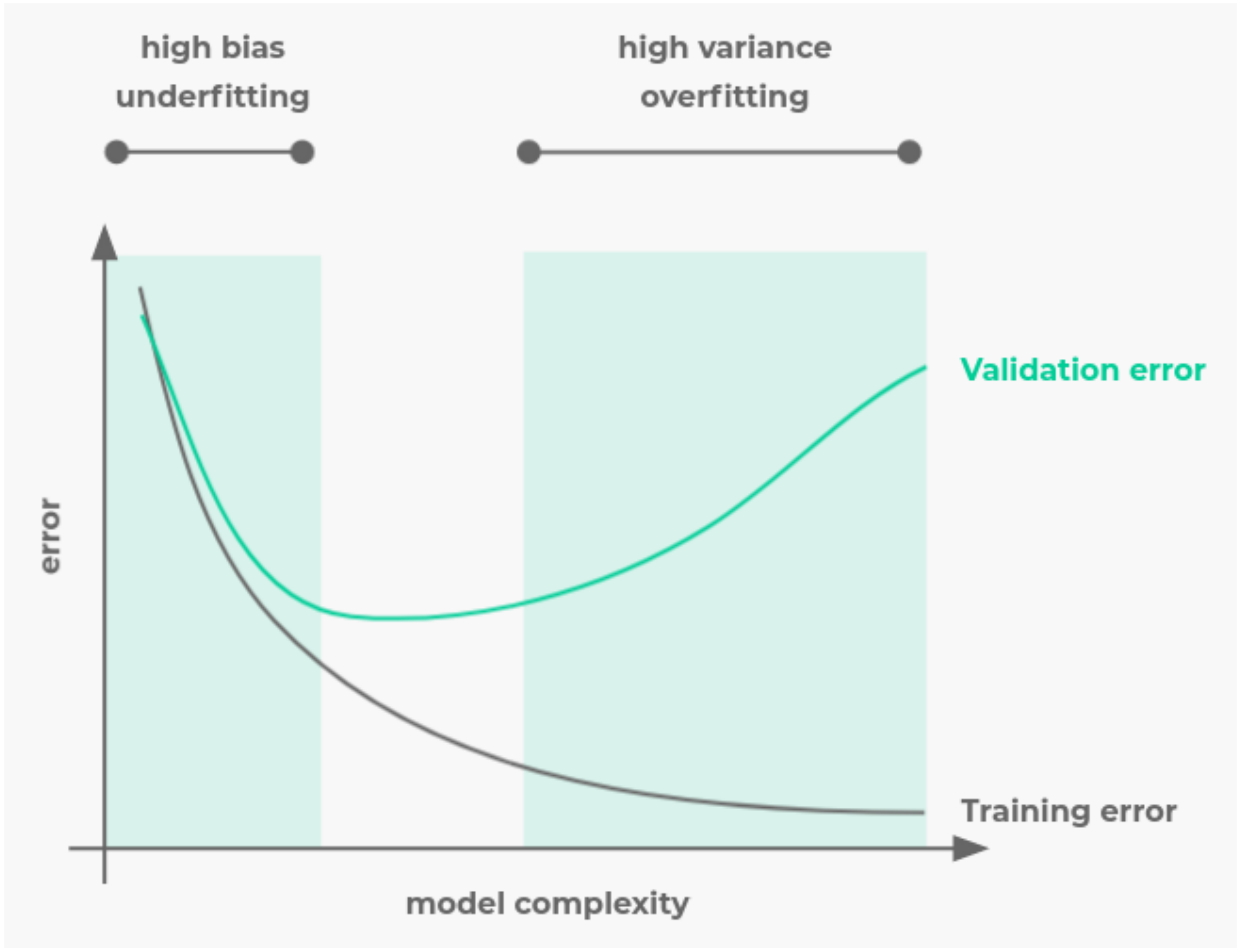




- Extracted features end up looking a bit like this
- Pretty abstract, hard to interpret
- Training process is actually done over multiple iterations
- Works something like this :
    - Split dataset into 90% "training", 10% "test". Don't touch test dataset until after all the training is done
    - For each iteration ("epoch"), further split "training" into 80% actual training, 10% validation dataset after shuffling randomly
    - Feed the 80% into neural network in batches of 64, evaluate loss-function for each batch
    - Tune w, b after each batch using Gradient Descent
    - Once all the 80% dataset is exhausted, evaluate result on validation dataset ("accuracy", "loss")
    - Now re-shuffle the 90% again into a different training and validation set and start all over again



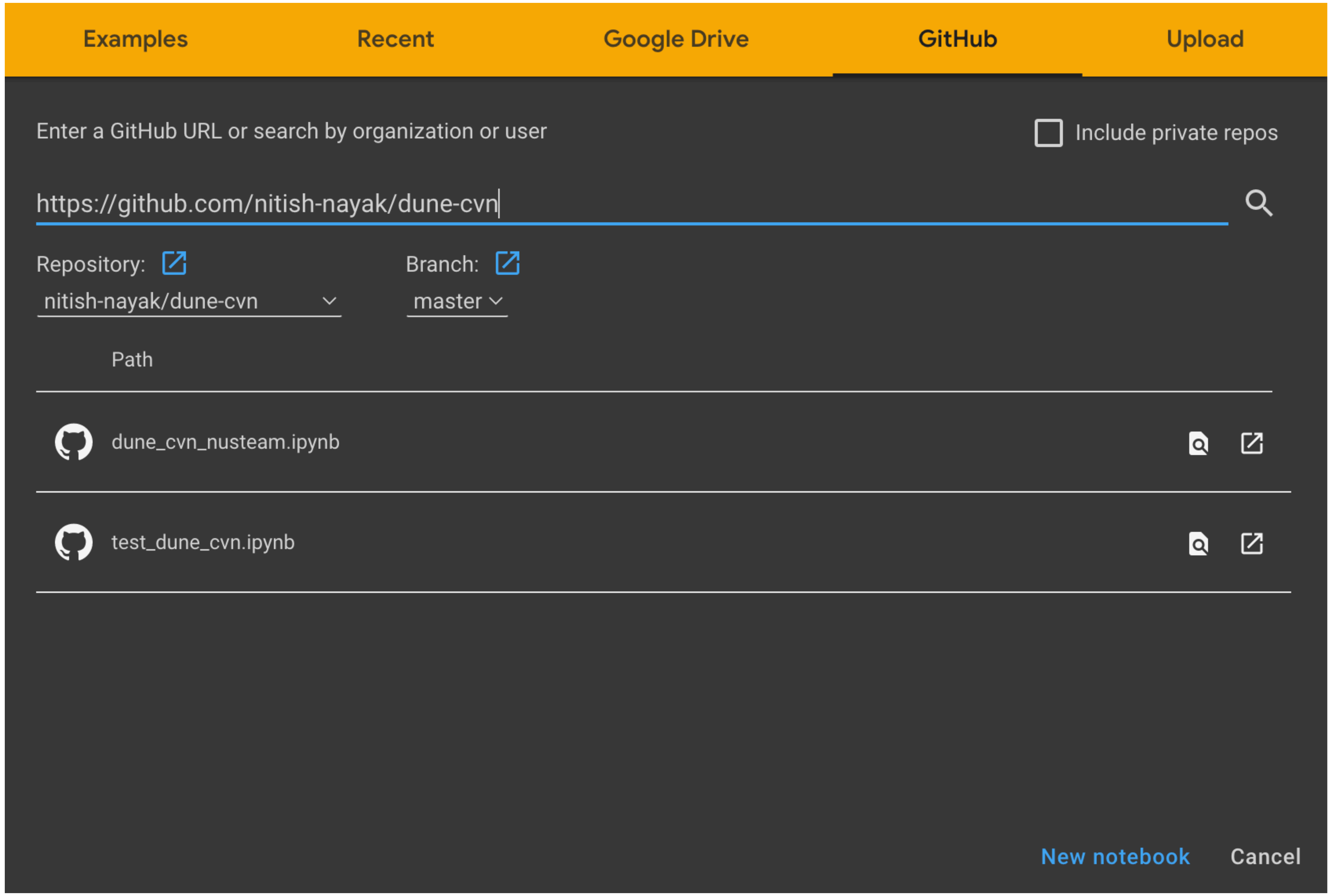
Doesn't look like this!



- Dashed is on training dataset, solid is on validation dataset
- Notice we haven't even touched the remaining 10% test dataset
  - This is because we've been using information from the validation set to inform the training
  - To stay truly unbiased, we need to finally evaluate on events the network has never seen
- For now, we stop training when things stop improving after a few epochs/iterations
- Notice also that it flatlines — this is a good sign that there's no overfitting!
- If we're confident the training went well, we can then look at the test dataset and assess the performance and see if we get similarly accurate results

Lets test things out!

- As a demo, we will test out the CNN network used in [https://journals.aps.org/prd/abstract/10.1103/PhysRevD.102.092003]
- We can do all this on the browser itself, hopefully without having to install anything
  - Go to https://colab.research.google.com/
  - In the pop-up, go to the GitHub tab and type in url : https://github.com/nitish-nayak/dune-cvn
  - You should see two .ipynb files (Python notebooks)
  - Select “dune_cvn_nusteam.ipynb”



Further Reading/Homework

- Borrowed heavily from 3Blue1Brown's excellent neural network explainer :
  - https://www.3blue1brown.com/topics/neural-networks
  - Youtube playlist : https://www.youtube.com/watch?v=aircAruvnKk&list=PLZHQObOWTQDNU6R1_67000Dx_ZCJB-3pi
- Other references :
  - https://towardsdatascience.com/a-visual-introduction-to-neural-networks-68586b0b733b
  - https://towardsdatascience.com/artificial-neural-networks-for-total-beginners-d8cd07abaae4
  - https://towardsdatascience.com/conv-nets-for-dummies-a-bottom-up-approach-c1b754fb14d6
  - https://www.youtube.com/watch?v=YRhxdVk_sIs
- Build and train your own CNN :
  - https://github.com/josephlee94/intuitive-deep-learning/blob/master/Part%202:%20Image%20Recognition%20CIFAR-10/Coding%20Companion%20to%20Intuitive%20Deep%20Learning%20Part%202%20(Annotated).ipynb
  - https://medium.com/intuitive-deep-learning/build-your-first-convolutional-neural-network-to-recognize-images-84b9c78fe0ce