Lecture 04: Neural network basics

Data C182 (Fall 2024). Week 03. Tuesday Sept 10th, 2024

Speaker: Eric Kim

Announcements

- Welcome to Week 03!
- HW01 released, due Oct 1st!
  - MacOS/Windows: please use Docker to handle setting up the environment (eg installing packages/dependencies). See this Ed post for more details: [link]
  - Linux: feel free to either install the deps yourself, or you can also use Docker
  - Reminder: submit assignments via Gradescope [link]
  - Tip: If you're having trouble getting setup for HW01, please ask in Ed or attend office hours.

Office hours, discussions

- Office hours are active this week! Full OH schedule: [link]
  - Eric Kim OH: Wednesdays, 3PM – 4 PM [Zoom link]
  - Naveen Ashish OH: Wednesdays 1PM – 2PM (Zoom link TBD)
- Discussions active starting this week! Notes + solutions on website: [link]
  - If you still aren't assigned to a discussion section, or you're unable to make your assigned discussion section (eg due to a conflict), please fill out the "2.0" Google Form in this Ed post: [link]
  - Please raise any discussion section assignment issues in this Ed post: [link]
  - Our aim is to get everyone assigned to a section by Week 04 (Sept 16th)
  - That said: feel free to attend any discussion section you prefer. Seats are reserved for those that are officially enrolled in that section.

Midterm

- **Midterm**: Thursday October 24th 2024 (Week 09), 6:30 PM – 8:00 PM
  - In-person exam, pencil + paper.
  - **Physical location**: TBD (likely 10 Evans + another location on campus)
  - **Alternate exam times** will only be given for truly unavoidable, extraordinary circumstances. If you truly can't make this midterm time with a good reason, please write on Ed in a private post ASAP.

Today’s lecture

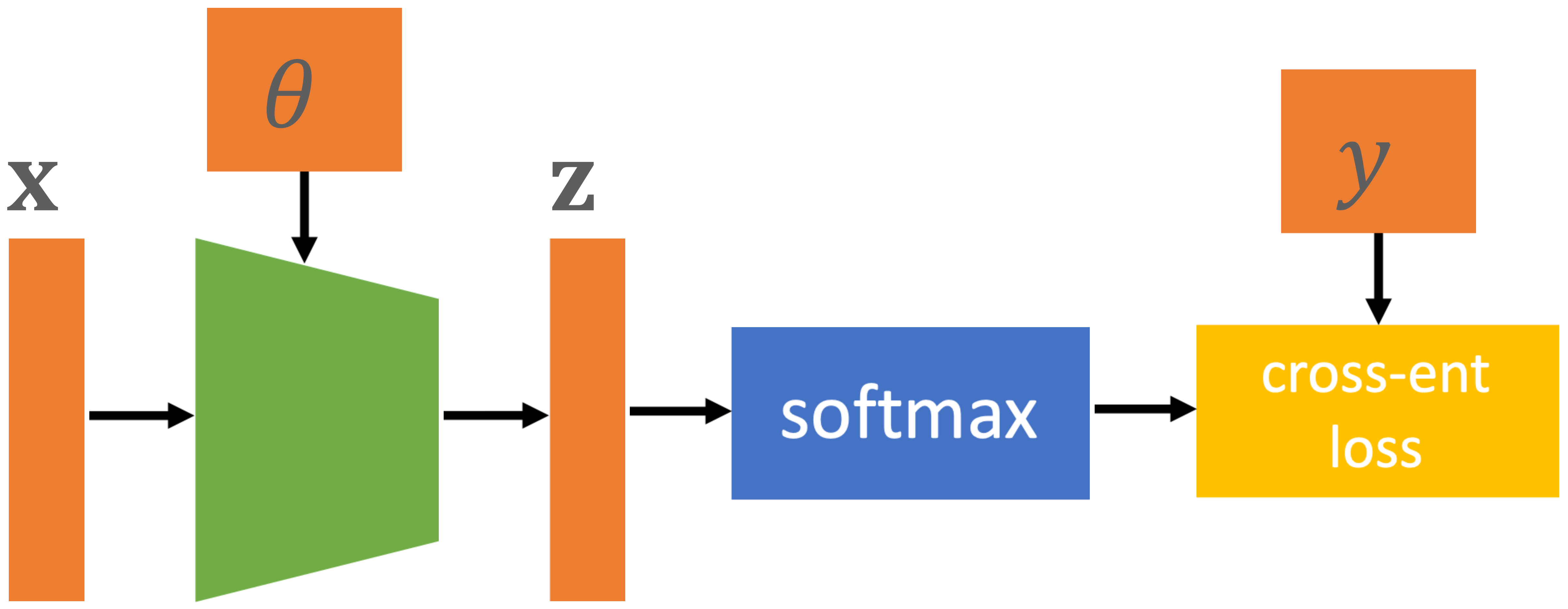
- Some of you may be thinking: “where are the deep neural networks??”
- Today, we’ll start talking about our first basic neural network models
  - We’ll put a full model together in this lecture, mathematically and diagrammatically
- We will then work through the **backpropagation** algorithm for computing gradients of the loss function with respect to the neural network parameters
  - This algorithm relies on reusing gradient values and matrix-vector products
  - Useful to learn and implement once (for the latter, HW1 has you covered), but next lecture you’ll hear from Matt Johnson how deep learning libraries do this for you

Recall: logistic regression

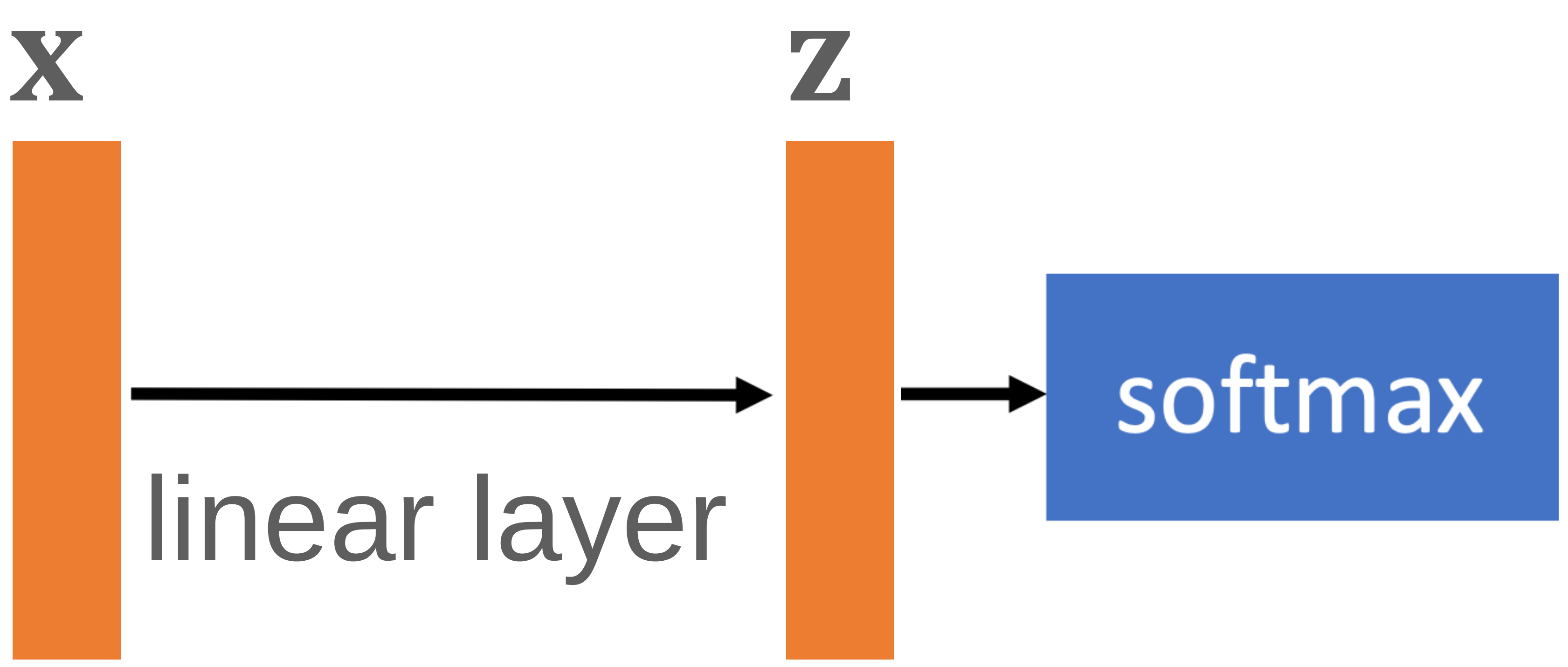
- The “linear neural network”
  - **Setup: Multiclass classification**. Suppose we have K classes ("multiclass", K > 2), and each input sample consist of d input features
  - Given $\mathbf{x} \in \mathbb{R}^d$,define $f_\theta(\mathbf{x}) = \theta^\top \mathbf{x}$,where θ is a $d \times K$ matrix
  - Then, for class $c \in \{0, \ldots, K-1\}$, we have $p_\theta(y = c|\mathbf{x}) = softmax(f_\theta(\mathbf{x}))_c$
    - Remember: $softmax(f_\theta(\mathbf{x}))_c = \frac{\exp f_\theta(\mathbf{x})_c}{\sum_{i=0}^{K-1} \exp f_\theta(\mathbf{x})_i}$
  - Loss function: $\ell(\theta; \mathbf{x}, y) = -\log p_\theta(y|\mathbf{x})$

For a nice review of logistic regression, and how to generalize from binary classification to multiclass (K>2) classification, see: [link]

A diagram for logistic regression



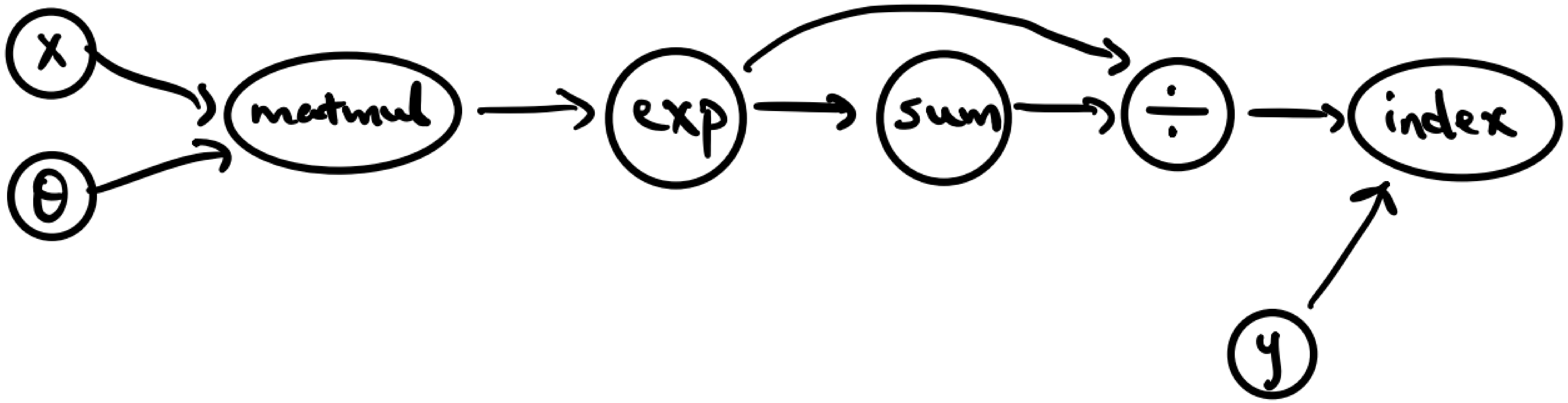
"linear layer"



- Often, we will simplify this diagram:
  - Omit the θ box, the parameters are implicit in the diagram
  - Omit the layer box entirely! Denote it with just the arrow
  - Omit the loss box at the end, if we're drawing "just the model"

Another type of drawing: computation graphs

Computation graphs are more detailed, rigorous graphical representations



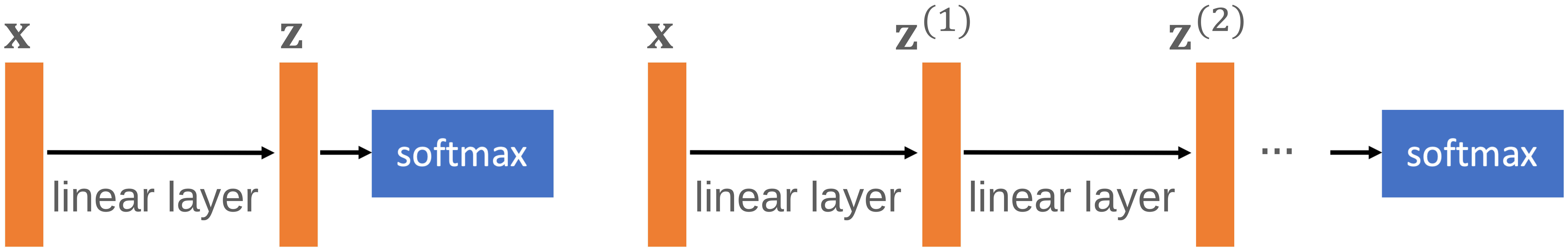
Pictured: the logistic regression model implemented as a series of mathematical "primitive" operations.

you will see variations on the style of drawing, level of detail, etc.

Aside: modern deep learning frameworks "compile" network architectures into a series of "primitive" operators (ex: Tensorflow/pytorch/Caffe/Caffe2). For a glimpse of this, see the "Operators" catalogue for Caffe2: [link]

Neural networks: attempt #1

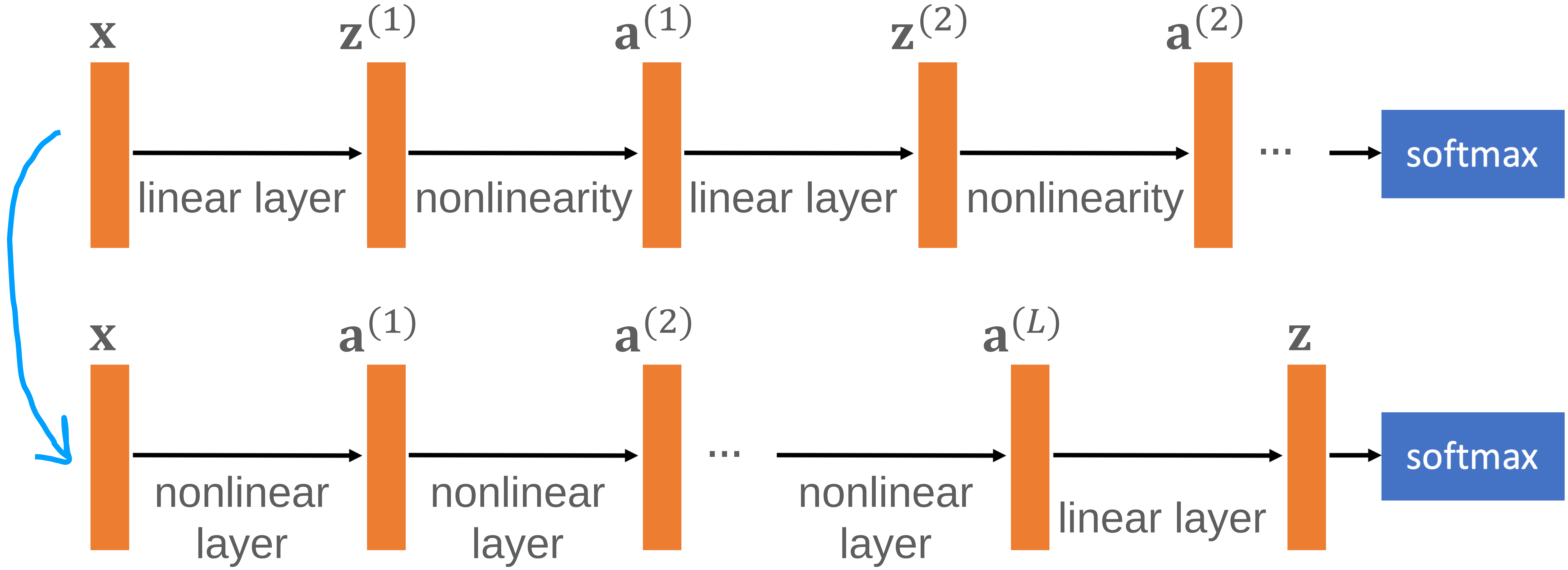
- Our drawing of logistic regression suggests that it is a “single layer model”
  - Are neural networks just more of these layers stacked on top of each other?
  - What’s the issue with this?
  - Composing linear transformations together is still linear!



Making neural networks nonlinear

- One of the main things that makes neural networks great is that they can represent complex non linear functions
- How? The canonical answer: add **nonlinearities** after every linear layer
  - Also called **activation functions**
  - Basically always *element wise* functions on the linear layer output
- Examples: $tanh(\mathbf{z})$, $sigmoid(\mathbf{z}) = \frac{1}{\exp\{-\mathbf{z}\}+1}$, $ReLU(\mathbf{z}) = max\{0, \mathbf{z}\}$

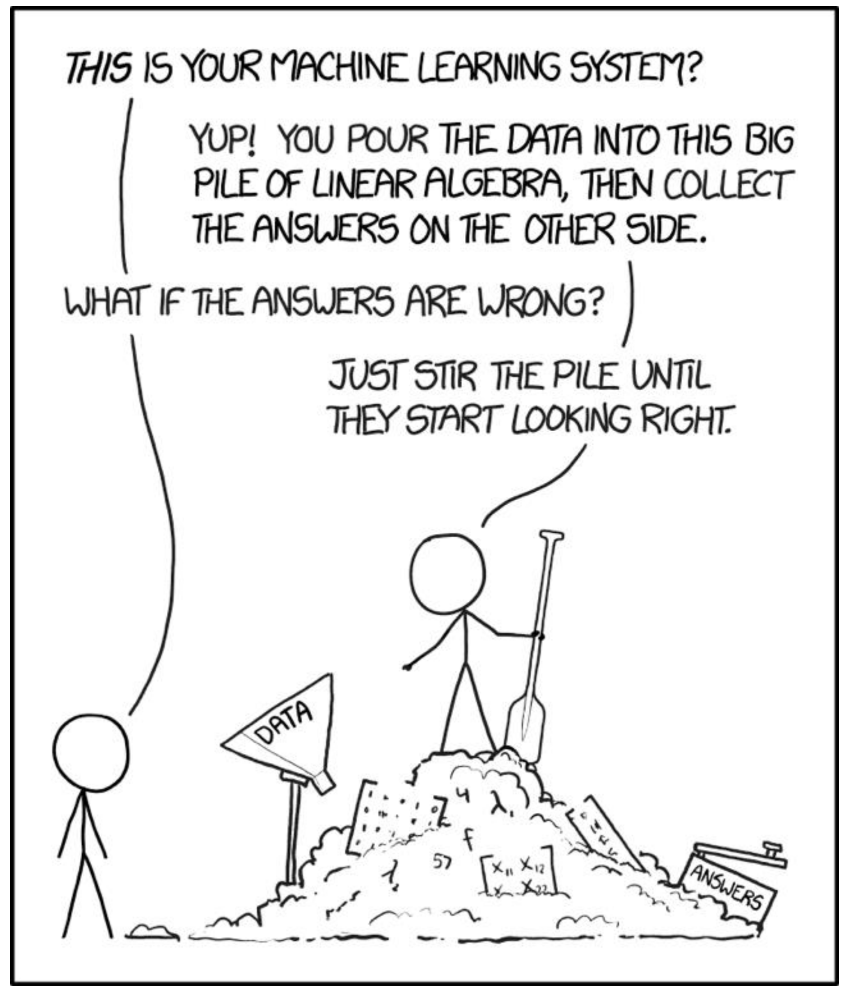
Neural networks: attempt #2



To simplify the diagram, we often "merge" the linear layer with the nonlinear activation function

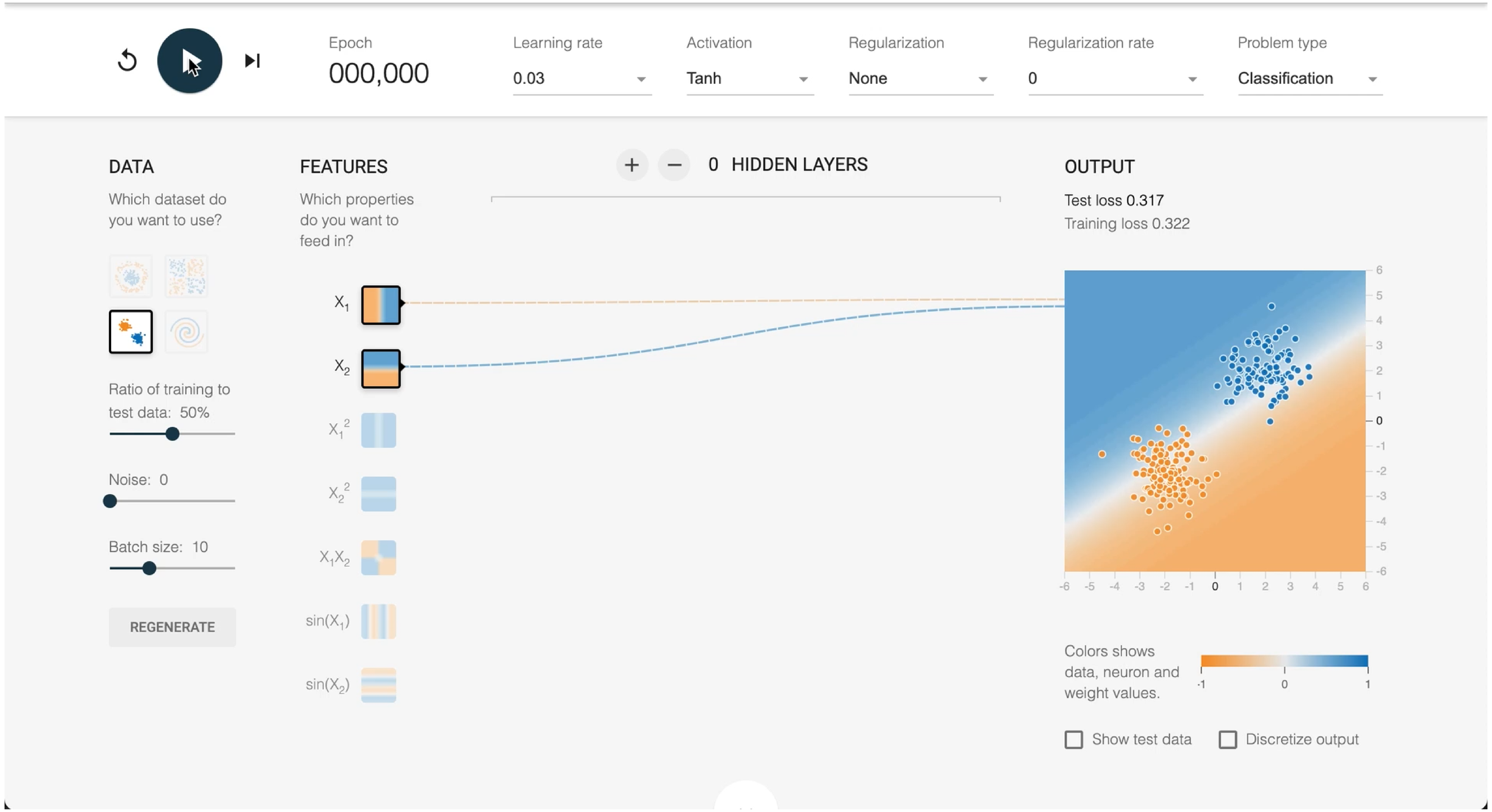
What function is this?

- θ represents all our parameters, e.g., $[\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \dots, \mathbf{W}^{(L)}, \mathbf{b}^{(L)}, \mathbf{W}^{final}, \mathbf{b}^{final}]$
- If our neural network has parameters θ and L **hidden layers**, then it represents the function $f_\theta(\mathbf{x}) = softmax(A^{final}(\sigma(A^{(L)}(\dots\sigma(A^{(1)}(\mathbf{x}))\dots))))$
  - σ is the nonlinearity / activation function
  - $A^i(\mathbf{v}) = \mathbf{W}^i\mathbf{v} + \mathbf{b}^i$ is the i-th linear layer
- What can this function represent? Turns out, a lot



Visualizing neural network functions

- https://playground.tensorflow.org/



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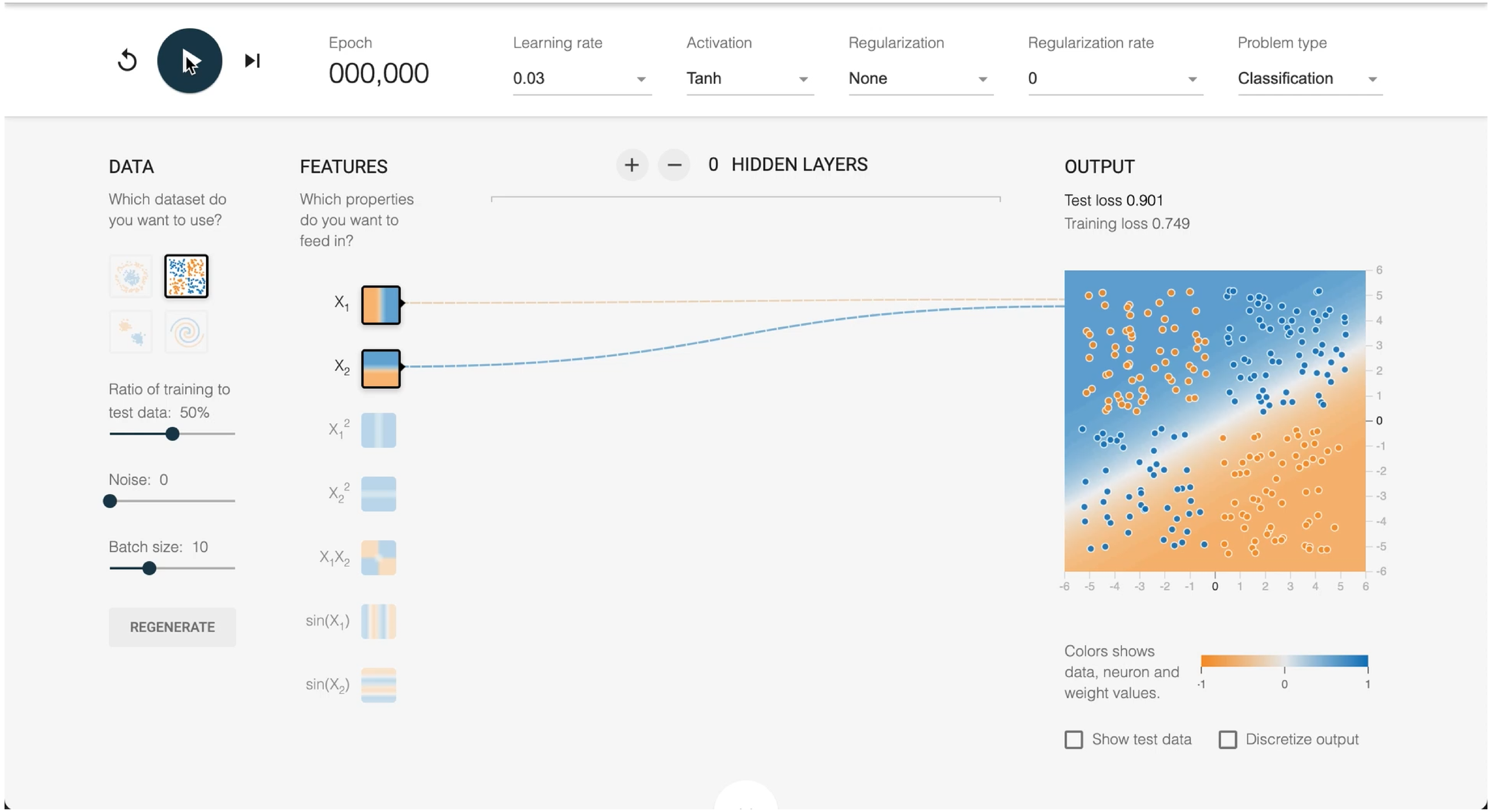

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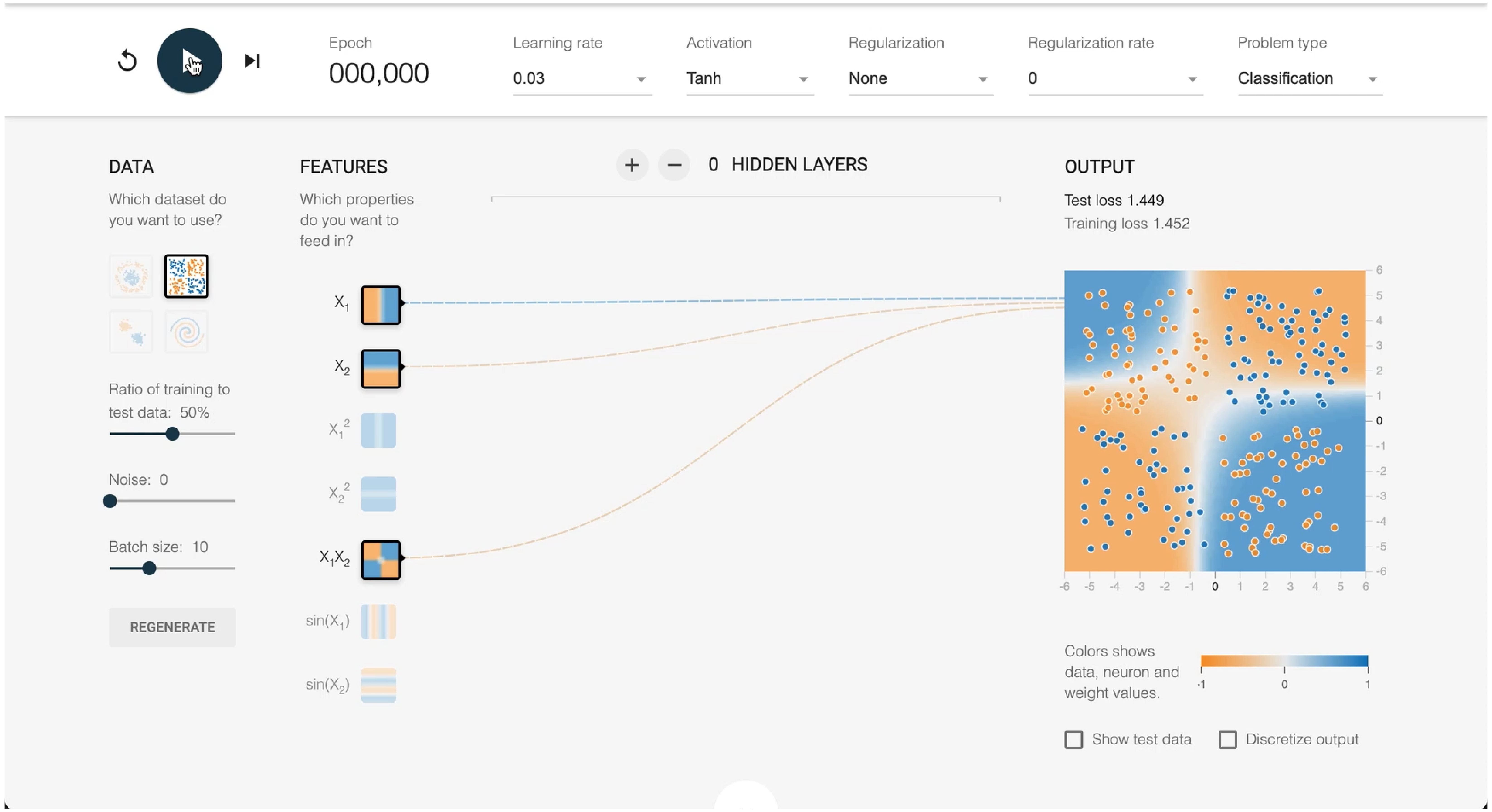

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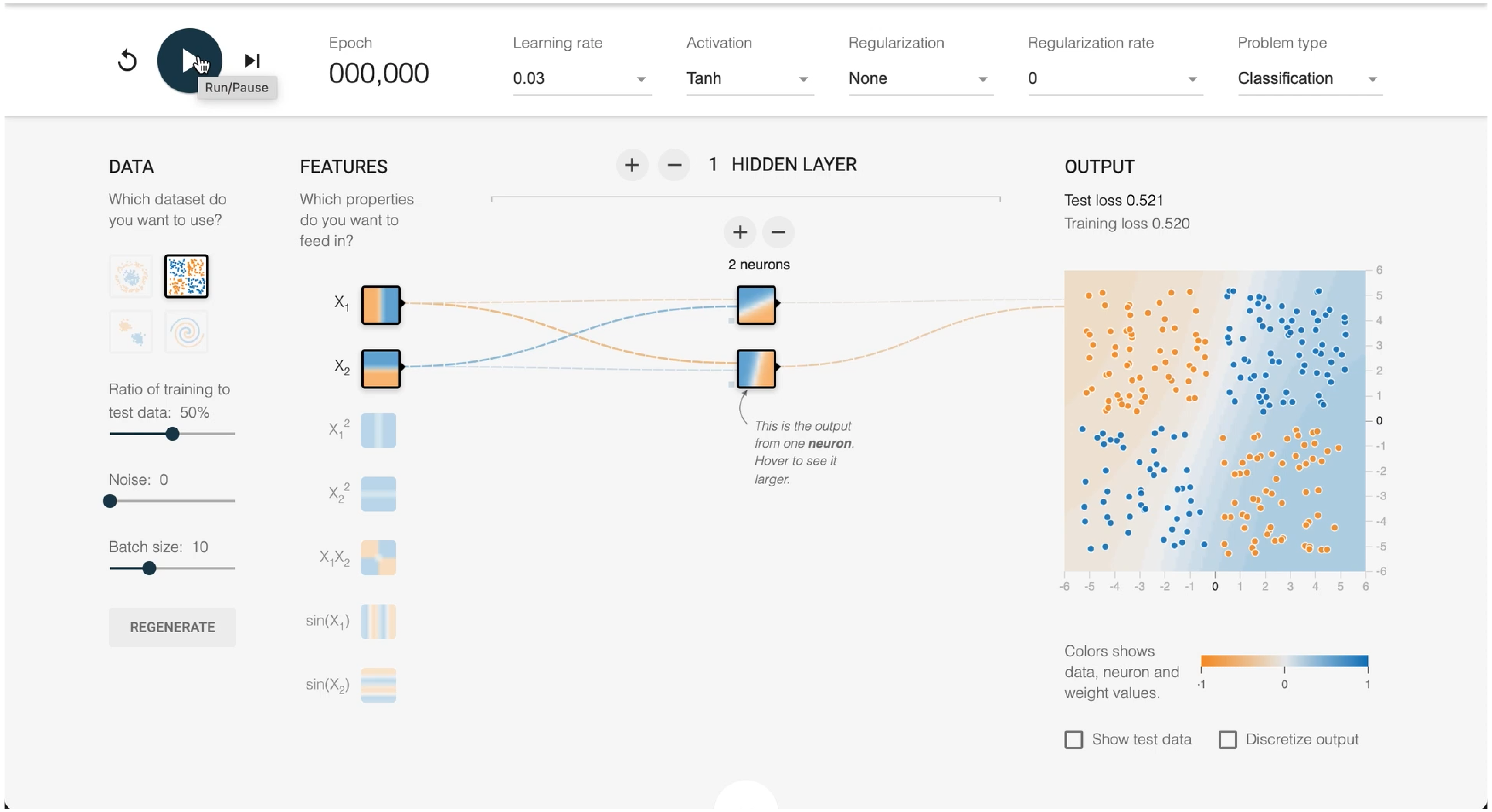

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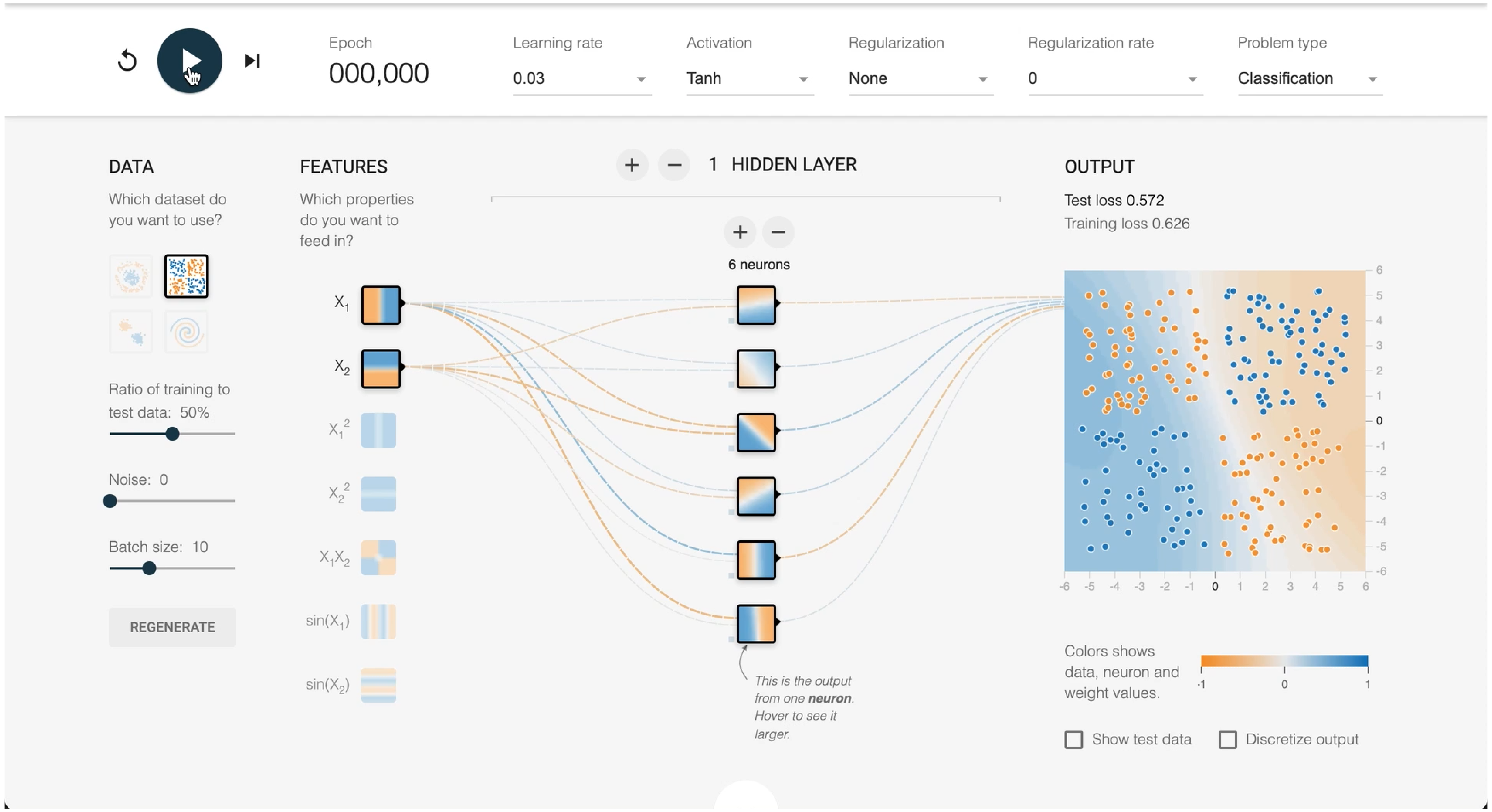
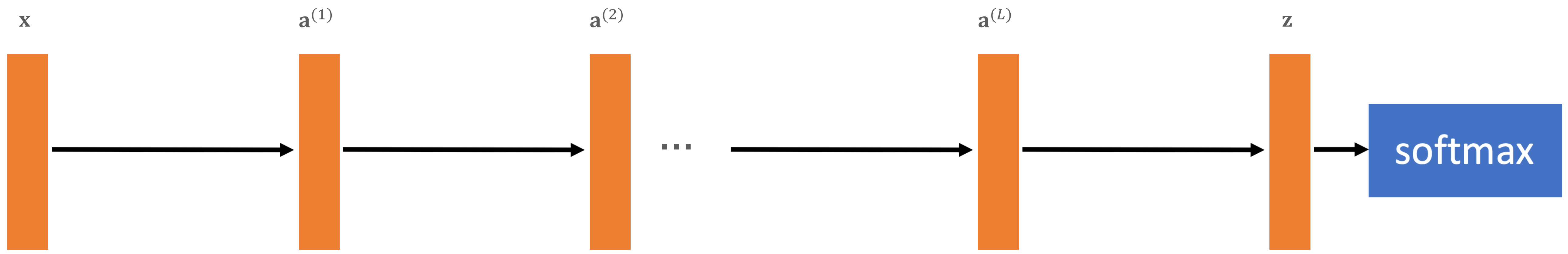


The backpropagation algorithm

Remember: the machine learning method

- (or, at least, the deep learning method)

1. Define your **model**
2. Define your **loss function**
3. Define your **optimizer**
4. Run it on a big GPU



$\ell(\theta; \mathbf{x}, y) = -\log p_\theta(y|\mathbf{x})$ (“cross-entropy”)

$$\theta \leftarrow \theta - \alpha \nabla_\theta \frac{1}{N} \sum_{i=1}^{N} \ell(\theta; \mathbf{x}_i, y_i)$$

wait… we need gradients!

What gradients do we need?

- We want to update our parameters as $\theta \leftarrow \theta - \alpha \nabla_\theta \frac{1}{N} \sum_{i=1}^{N} \ell(\theta; \mathbf{x}_i, y_i)$
- θ represents all our parameters, e.g., $[\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \ldots, \mathbf{W}^{(L)}, \mathbf{b}^{(L)}, \mathbf{W}^{final}, \mathbf{b}^{final}]$
- So we need $[\nabla_{\mathbf{W}^{(1)}} \ell, \nabla_{\mathbf{b}^{(1)}} \ell, \ldots, \nabla_{\mathbf{W}^{(L)}} \ell, \nabla_{\mathbf{b}^{(L)}} \ell, \nabla_{\mathbf{W}^{final}} \ell, \nabla_{\mathbf{b}^{final}} \ell]$
- How do we compute these gradients? Let’s talk about two different approaches:
    - numerical (**finite differences**) vs. analytical (backpropagation)

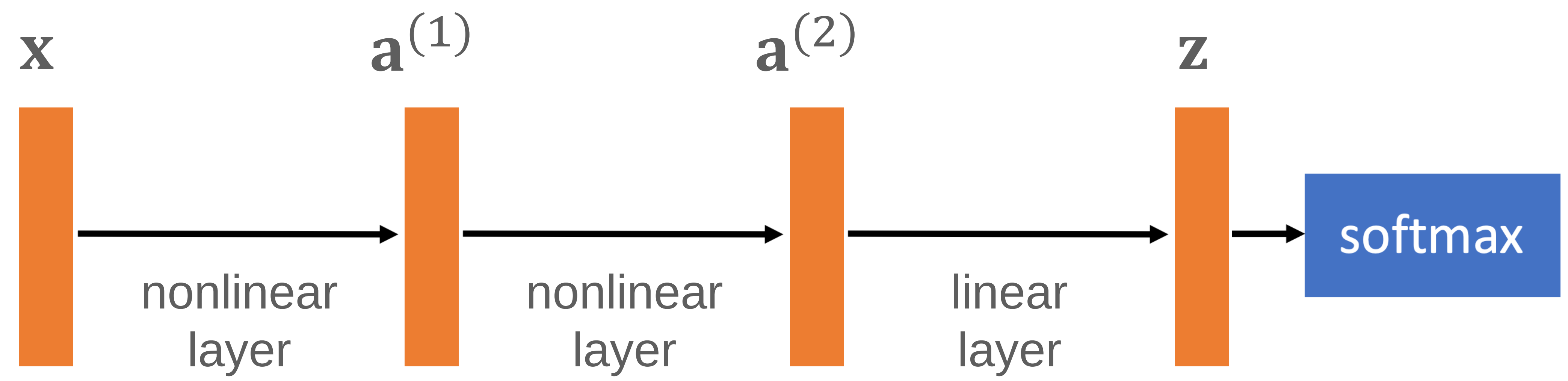
Finite differences

- The method of finite differences says that, for any sufficiently smooth function f which operates on a vector $\mathbf{x}$, the partial derivative $\frac{\partial f}{\partial x_i}$ is approximated by
- $\frac{\partial f}{\partial x_i} \approx \frac{f(\mathbf{x}+\epsilon \mathbf{e}_i)-f(\mathbf{x}-\epsilon \mathbf{e}_i)}{2\epsilon}$, where $\mathbf{e}_i$ denotes a "one hot" vector
- This is the definition of (partial) derivatives as $\epsilon \rightarrow 0$
- Think about how slow this would be to do for all our network parameters… Nevertheless, it can be useful as a method for checking gradients

Computing gradients via backpropagation

- The backpropagation algorithm is a much faster and more efficient method for computing gradients for neural network parameters
  - It made training large neural networks feasible and practical
- Backpropagation works “backward” through the network, which allows for:
  - reusing gradient values that have already been computed
  - computing matrix-vector products rather than matrix-matrix products, since the loss is a scalar!
- It’s pretty confusing the first (or second, or third, …) time you see it

Backpropagation: the math



first, let’s do the “forward pass” through our network, from input to prediction

let’s work with two hidden layers, for concreteness

$$z^{(1)} = W^{(1)} x_i + b^{(1)} \qquad a^{(1)} = \sigma(z^{(1)})$$

$$z^{(2)} = W^{(2)} a^{(1)} + b^{(2)} \qquad a^{(2)} = \sigma(z^{(2)})$$

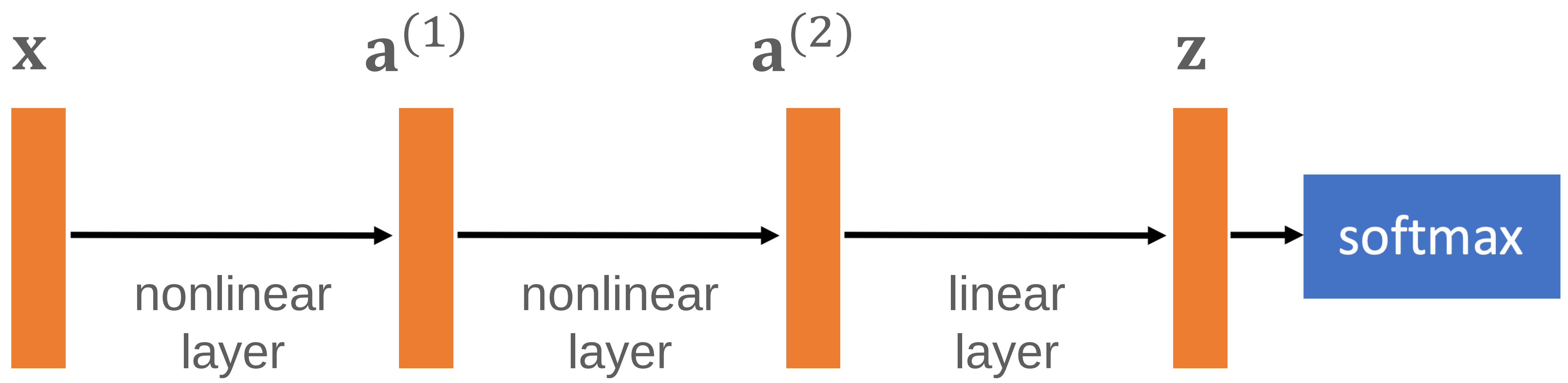
$$z = W^{\text{final}} a^{(2)} + b^{\text{final}}$$

this is a vector

$$p_\theta(y_i \mid x_i) = \frac{\exp z}{\sum_i \exp z} \qquad y_i\text{-th index}$$

this is a number

Backpropagation: the math



$\mathbf{z} = \mathbf{W}^{final}\mathbf{a}^{(2)} + \mathbf{b}^{final}$ represents our "logits" (aka inputs to softmax)

this is a vector

$$p_\theta(y_i | x_i) = \frac{\exp z}{\sum \exp z}$$ y_i - th index

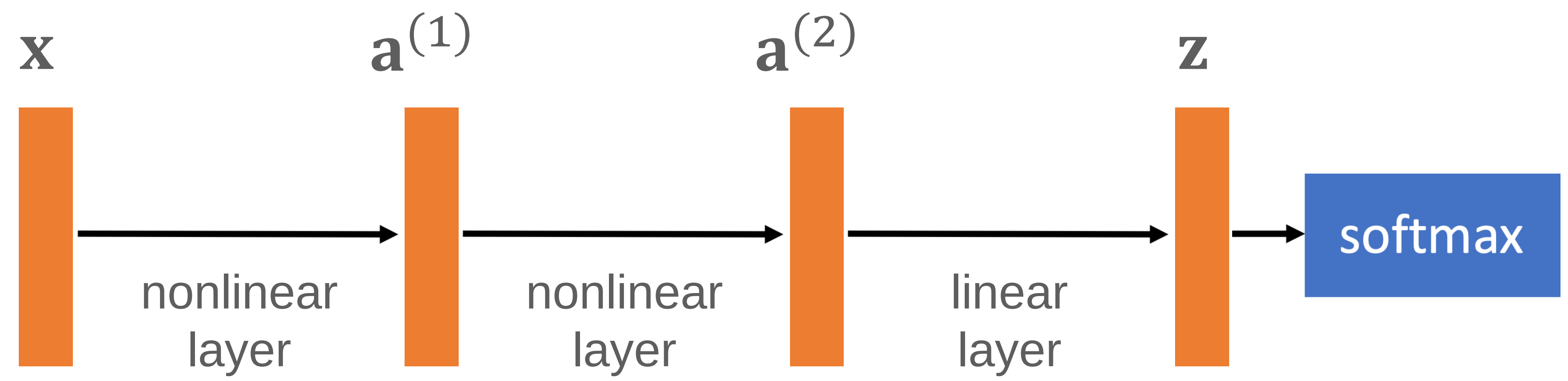
this is a number

$$\log p_\theta(y_i | x_i) = z_{y_i} - \log \sum \exp z$$

$$\ell(\theta; x_i, y_i) = \log \sum \exp z - z_{y_i}$$

want: $\nabla_W \ell$, $\nabla_b \ell$ for all W, b

Backpropagation: the math



first let's look at $\nabla_{\mathbf{W}^{final}} \ell$ and $\nabla_{\mathbf{b}^{final}} \ell$

remember: $\ell = \log \sum \exp \mathbf{z} - \mathbf{z}_{y_i}$,and also $\mathbf{z} = \mathbf{W}^{final} \mathbf{a}^{(2)} + \mathbf{b}^{final}$

By multivariate chain rule: using the matrix shape conventions defined here: [link]

$$\nabla_z \ell = \frac{\exp z}{\sum \exp z} - e_{y_i}$$

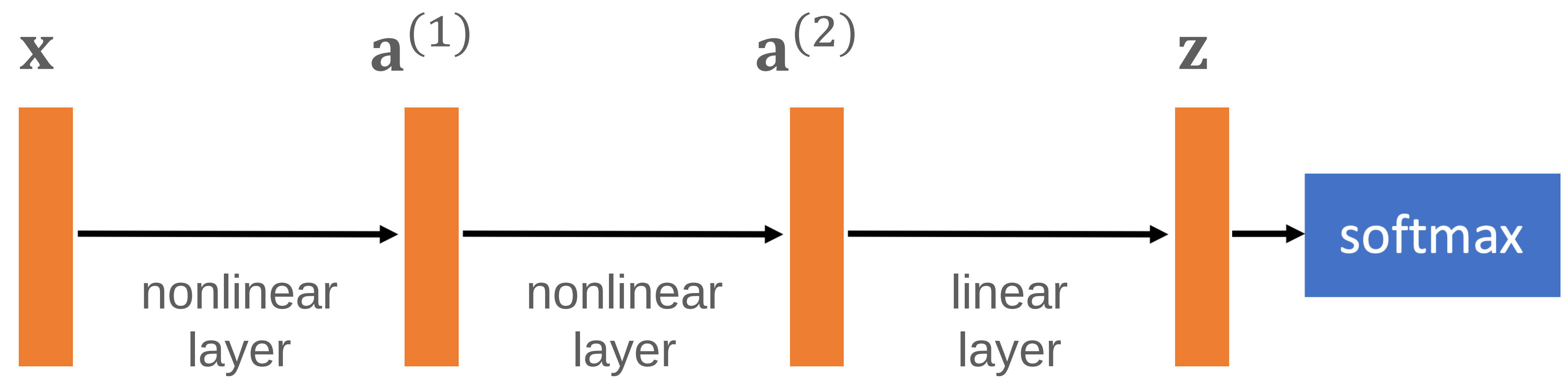
← "one hot" vector

$$\nabla_{a^{(2)}} \ell = \frac{dz}{da^{(2)}} \nabla_z \ell = W^{final\,T} \nabla_z \ell$$

$$\nabla_{W^{final}} \ell = \frac{\overset{K}{dz}}{\underbrace{dW^{final}}_{K \times d_{a^{(2)}}}} \nabla_z \ell = (\nabla_z \ell) a^{(2)T}$$

$$\nabla_{b^{final}} \ell = \frac{dz}{db^{final}} \nabla_z \ell = \nabla_z \ell$$

Backpropagation: the math



now let's look at $\nabla_{\mathbf{W}^{(2)}} \ell$ and $\nabla_{\mathbf{b}^{(2)}} \ell$

remember: $\mathbf{a}^{(2)} = \sigma(\mathbf{z}^{(2)})$, and also $\mathbf{z}^{(2)} = \mathbf{W}^{(2)}\mathbf{a}^{(1)} + \mathbf{b}^{(2)}$

$$\nabla_{z^{(2)}} \ell = \frac{da^{(2)}}{dz^{(2)}} \nabla_{a^{(2)}} \ell = \begin{bmatrix} \sigma'(z_1^{(2)}) & & \\ & \ddots & \\ & & \sigma'(z^{(2)}_{d_{z^{(2)}}}) \end{bmatrix} \nabla_{a^{(2)}} \ell$$

How does the output of my layer change w.r.t. my layer's parameters?

How does the loss change w.r.t. this layer's outputs?

$$\nabla_{W^{(2)}} \ell = \frac{dz^{(2)}}{dW^{(2)}} \nabla_{z^{(2)}} \ell = (\nabla_{z^{(2)}} \ell)\, a^{(1)T}$$

$$\nabla_{b^{(2)}} \ell = \frac{dz^{(2)}}{db^{(2)}} \nabla_{z^{(2)}} \ell = \nabla_{z^{(2)}} \ell$$

$$\nabla_{a^{(1)}} \ell = \frac{dz^{(2)}}{da^{(1)}} \nabla_{z^{(2)}} \ell = W^{(2)T} \nabla_{z^{(2)}} \ell$$

Observation: gradients for a given layer are functions of local things (eg inputs to layer during forward pass, and how the layer's outputs affect the loss gradient)
Suggests a dynamic-programming-like way to implement backpropagation in a way that mirrors the computation graph

a pattern emerges… do you see it?

Backpropagation: the summary

- First, we perform a forward pass and cache all the intermediate $\mathbf{z}^{(l)}$, $\mathbf{a}^{(l)}$
- Then, we work our way backwards to compute all the $\nabla_{\mathbf{W}^{(l)}}\ell$, $\nabla_{\mathbf{b}^{(l)}}\ell$
  - Going backwards allows us to reuse gradients that have already been computed
  - It also results in matrix-vector product computations, which are far more efficient than matrix-matrix product computations
- After all the gradients have been computed, we are ready to take a gradient step
  - Neural network optimization repeats this over and over — more on that next week

Confused?

- Backpropagation can be tricky and unintuitive
- What can help is trying to work out the math on your own to see the patterns
- Implementing it for HW1 should also help solidify the concept
- But, most importantly: we don’t have to do it ourselves these days!
  - Deep learning libraries do it for us (ex: pytorch, tensorflow)