Introduction to Neural Networks

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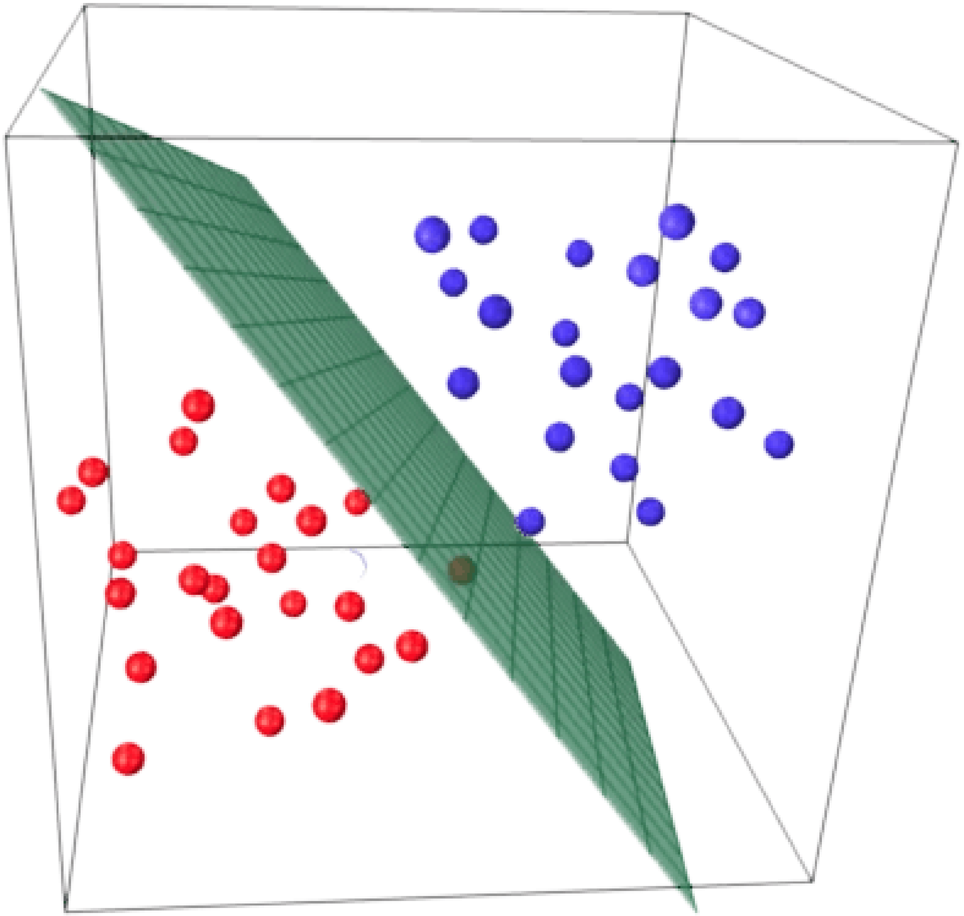
Review: Linear Models

- Examples: Linear regression, logistic regression, softmax regression
- Test time: Make a prediction based on learned parameters
  - E.g., linear regression: $y_{\text{pred}} = w^\top x + b$, after learning *w* and *b*
- Training time: Learn model parameters
  - Use gradient descent to minimize average loss over training dataset
  - E.g., linear regression:

$$\nabla_w L(w, b) = \frac{1}{n} \sum_{i=1}^{n} 2(w^\top x^{(i)} + b - y^{(i)}) \cdot x^{(i)}$$

Review: Linear Models

- Pro: Easier to understand what model is doing
- Pro: Optimizes convex loss function, gradient descent guaranteed to work
- Con: Can **only learn linear function of input features**
  - Workaround #1: Add more features—but this **requires manual tweaking**
  - Workaround #2: Use kernels, but **only adds more features in pre-defined ways**



Method for learning features from data

Powerful family of non-linear functions

Set of building blocks to create complex models

Method for learning features from data

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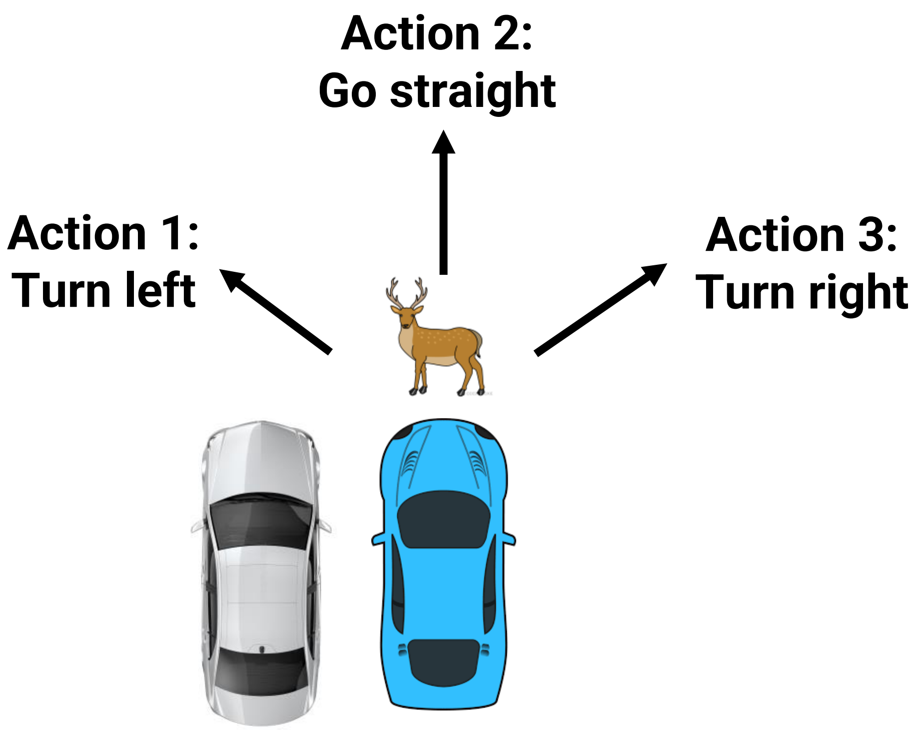
Set of building blocks to create complex models

Deep Learning

Machine Learning using Neural Network models

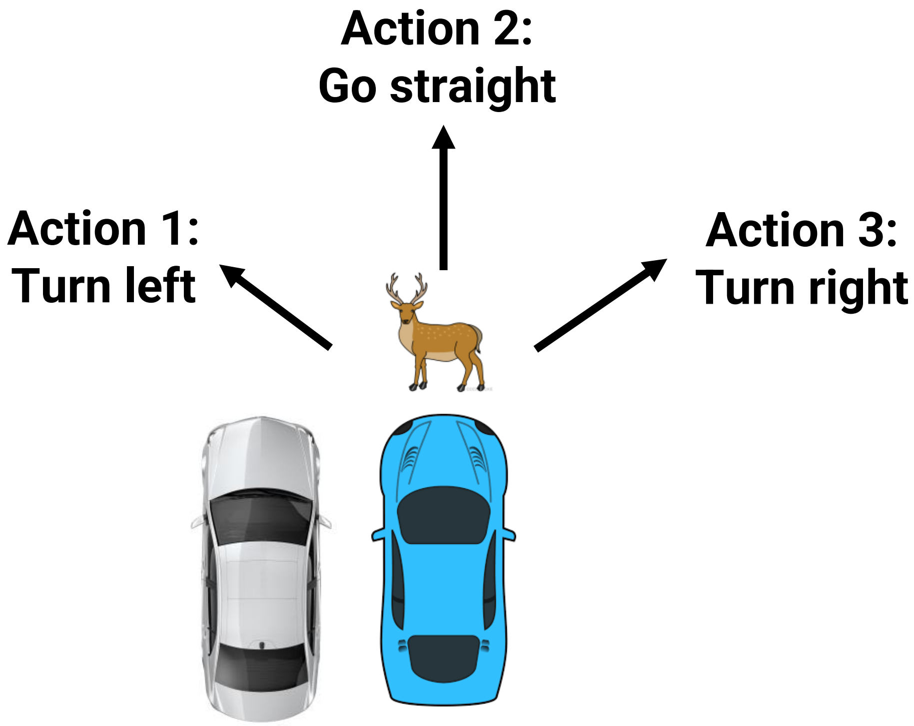
Method for learning features from data

A (toy) self-driving car example



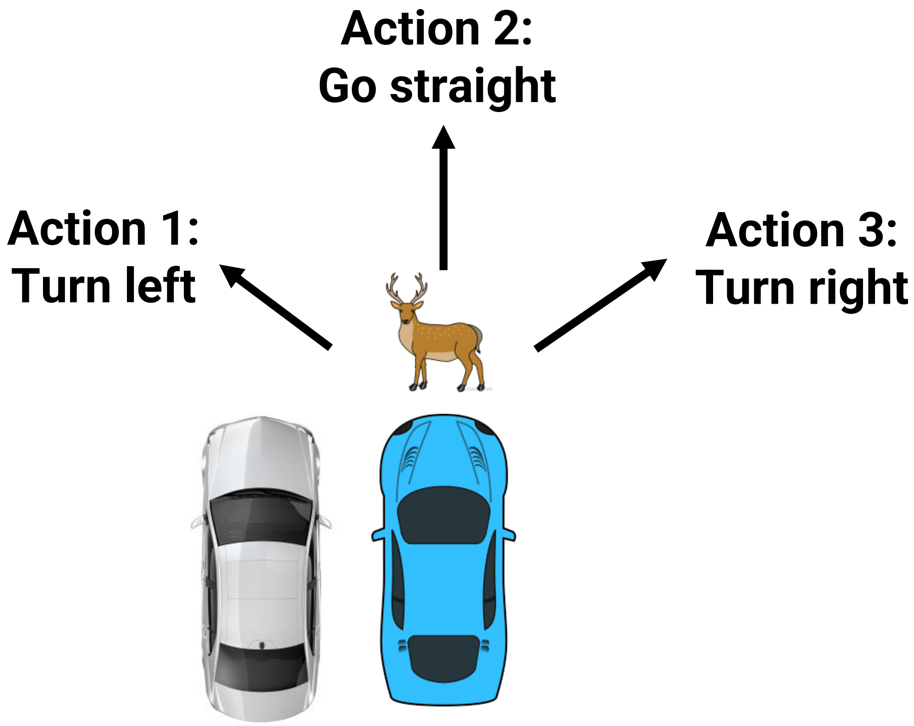
- Three-way classification problem: Go left, straight, or right?
- What features are important here?
  - Is front clear?
  - Is left clear?
  - Is right clear?

A (toy) self-driving car example



- Suppose we had these features:
  - $z = [z_1, z_2, z_3]$
  - z_1 = 1 if front is clear, 0 else
  - z_2 = 1 if left is clear, 0 else
  - z_3 = 1 if right is clear, 0 else
- With this, we can do softmax regression:
  - Score for "straight": $20\ z_1 - 10$
  - Score for "left": $10\ z_2 - 10$
  - Score for "right": $10z_3 - 10$
- Behavior
  - If everything is clear, go straight
  - If front is blocked, go left or right if those are clear
  - If everything is blocked, all equally bad

A (toy) self-driving car example



- How can we write the feature "is front clear"?
- Checking if the front is clear **is itself a machine learning problem**
  - Input = camera image/lidar data, Output = whether there is an obstacle
  - Obstacle near or far away?
  - Hard obstacle or a plastic bag?
- Can we make our features the outputs of another "classifier"?

Feature learning

Input x

Classifier 1:
Is front clear?

Classifier 2:
Is left clear?

Classifier 3:
Is right clear?

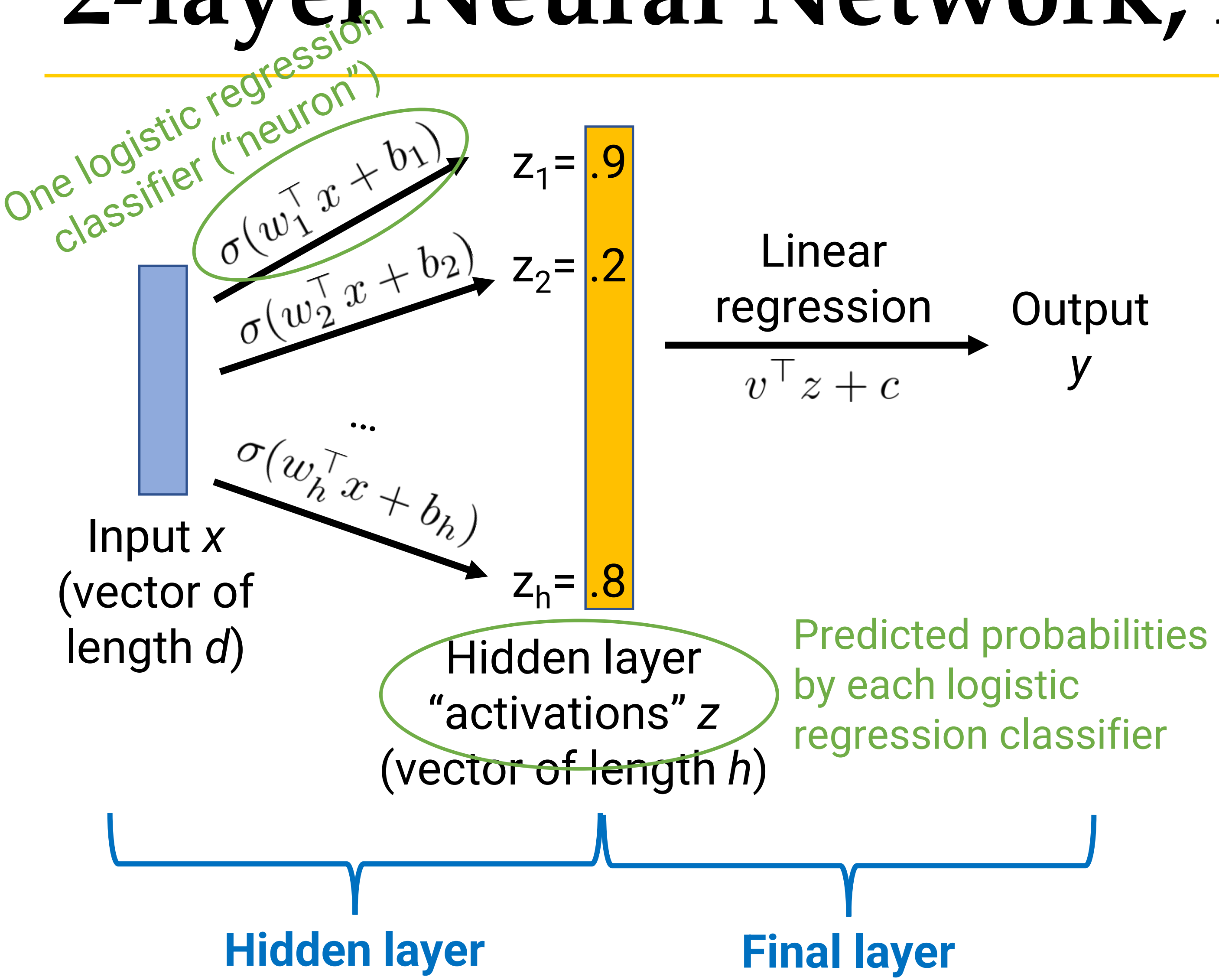
$$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

Classifier 4:
Where to go?

Output y
Turn left

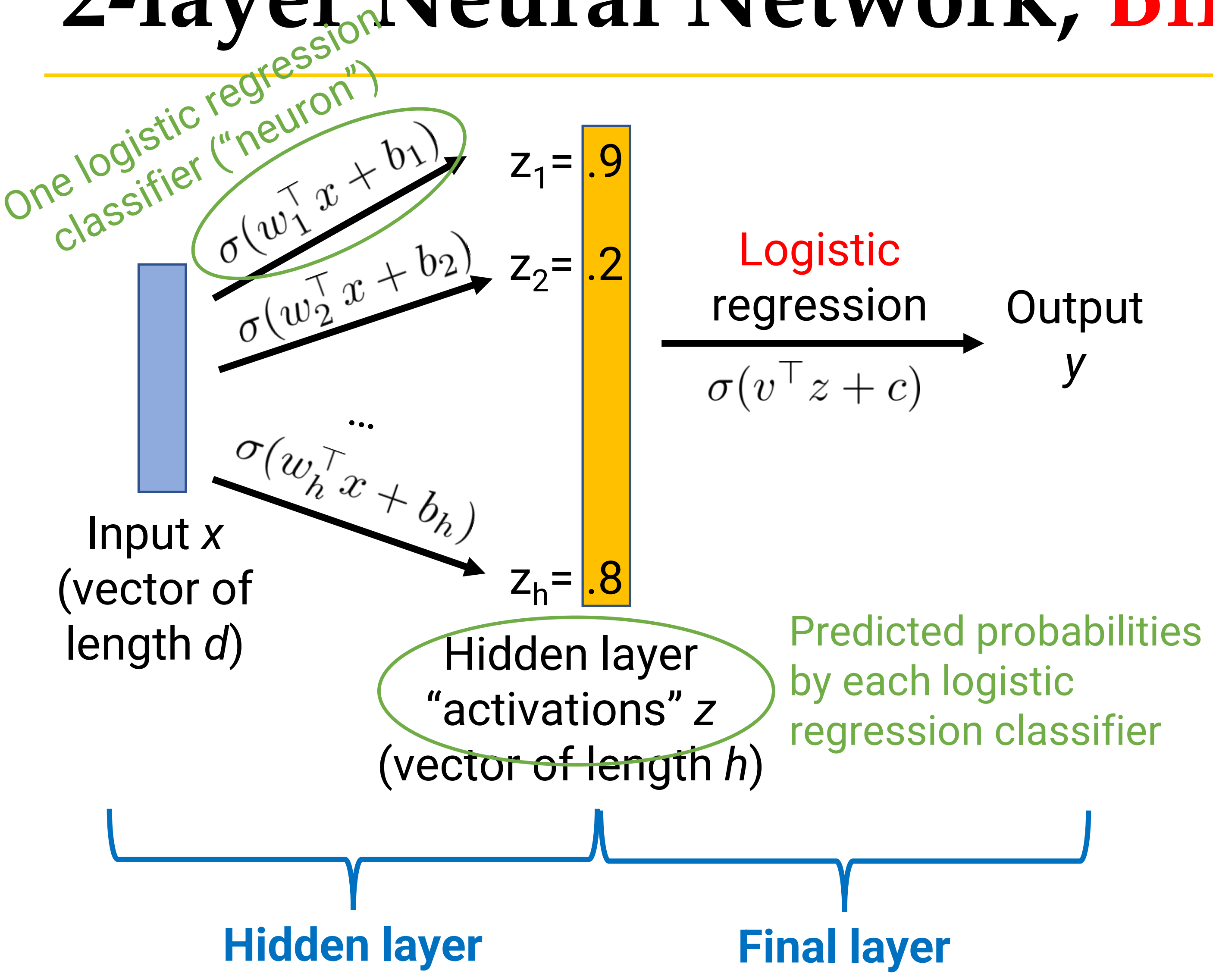
This is a neural network!

2-layer Neural Network, Regression



- Hidden layer = A bunch of logistic regression classifiers
  - Parameters: $\boldsymbol{w_j}$ and $\boldsymbol{b_j}$ for each classifier, for each *j=1, …, h*
  - *h* = number of neurons in hidden layer ("hidden nodes")
  - Produces "activations"= learned feature vector
- Final layer = linear model
  - For regression: linear model with weight vector ***v*** and bias ***c***

2-layer Neural Network, Binary Classification



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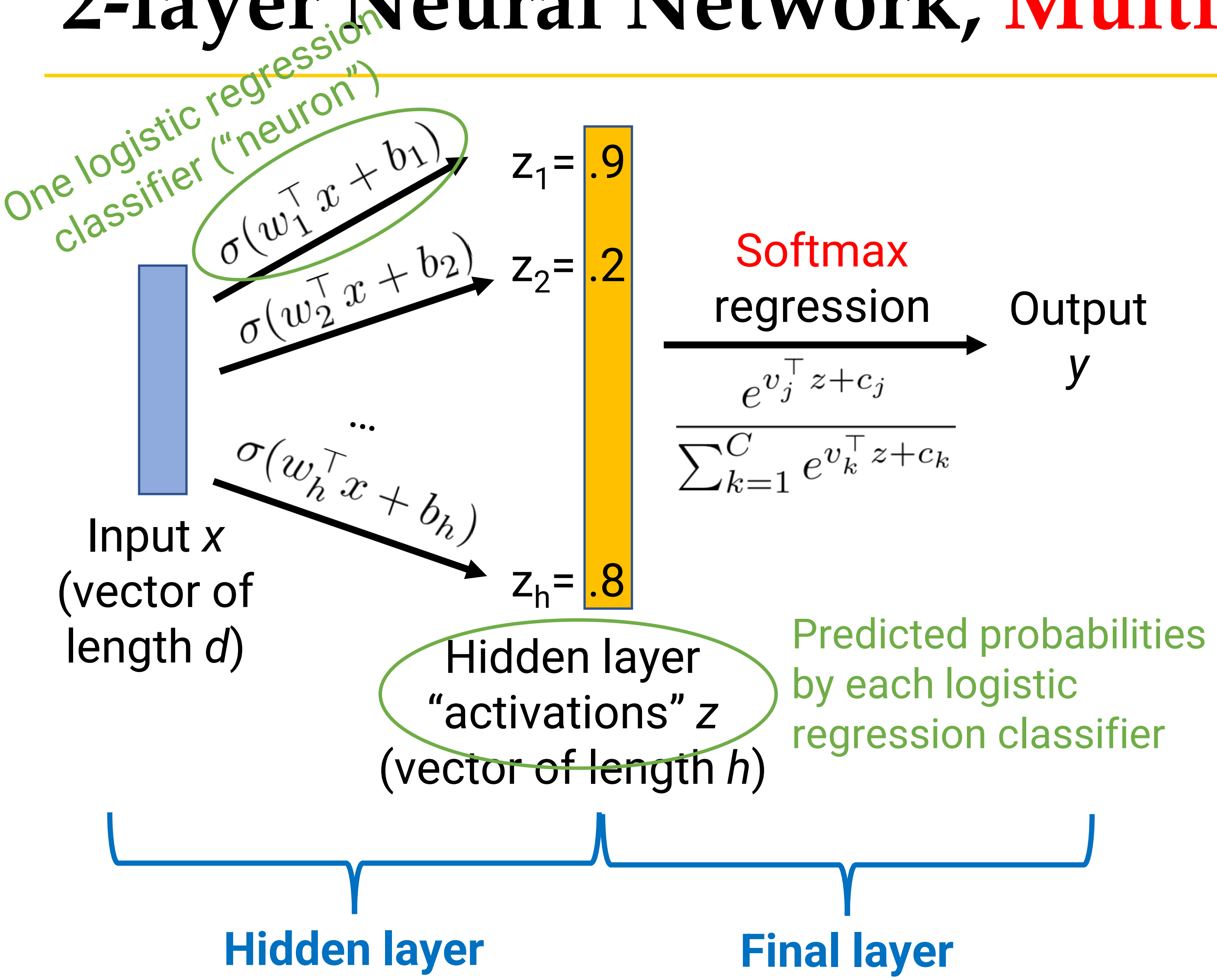
  - Produces "activations"= learned feature vector
- Final layer = linear model
  - For binary classification: linear model with weight vector ***v*** and bias ***c***
  - **Only final layer changes when changing to a different task**

2-layer Neural Network, Multi-Class Classification



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  - Produces "activations"= learned feature vector
- Final layer = linear model
  - For multi-class classification: linear model with weight vector $\boldsymbol{v_k}$ and bias $\boldsymbol{c_k}$ for each class *k*
  - **Only final layer changes when changing to a different task**

Feature Learning with Neural Networks

Input x

Classifier 1:
Is front clear?

Classifier 2:
Is left clear?

Classifier 3:
Is right clear?

$$\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

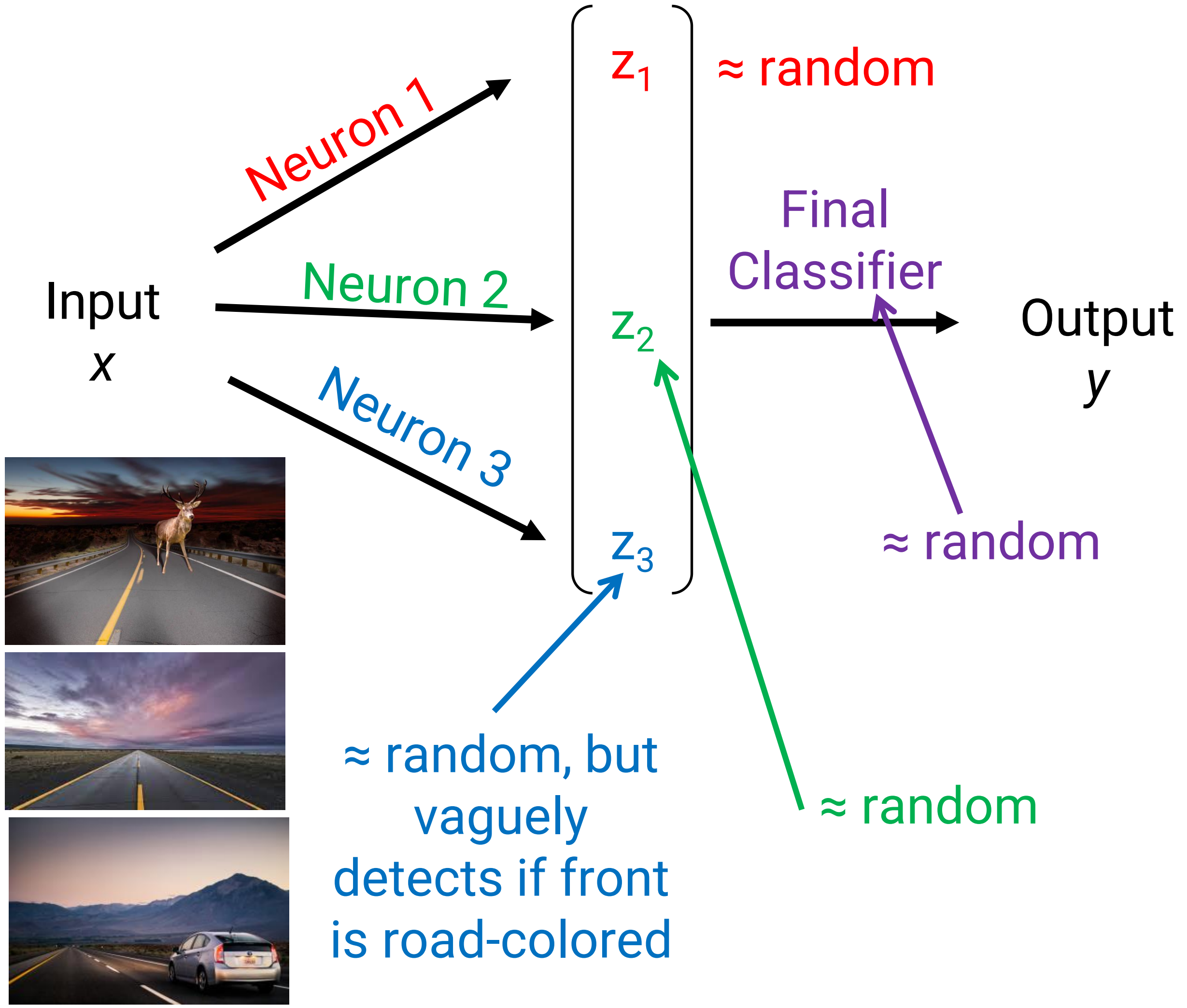
Classifier 4:
Where to go?

Output y
Turn left

Learn a classifier whose output is a good feature
We don't tell the model what classifier to learn
Learn from data that "is front clear" is a useful concept

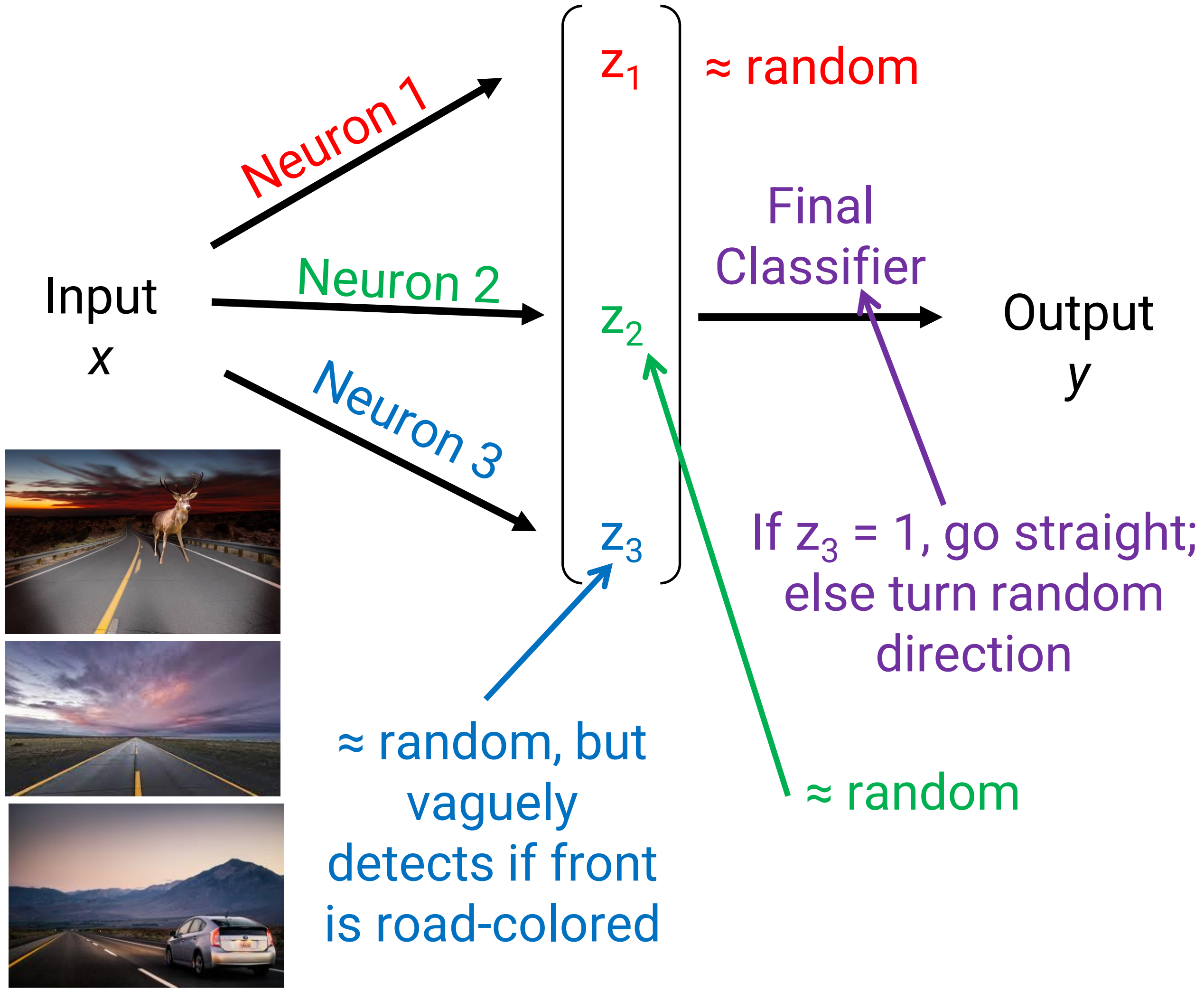
Learn to classify based on features
(same as linear model)

Feature Learning with Neural Networks



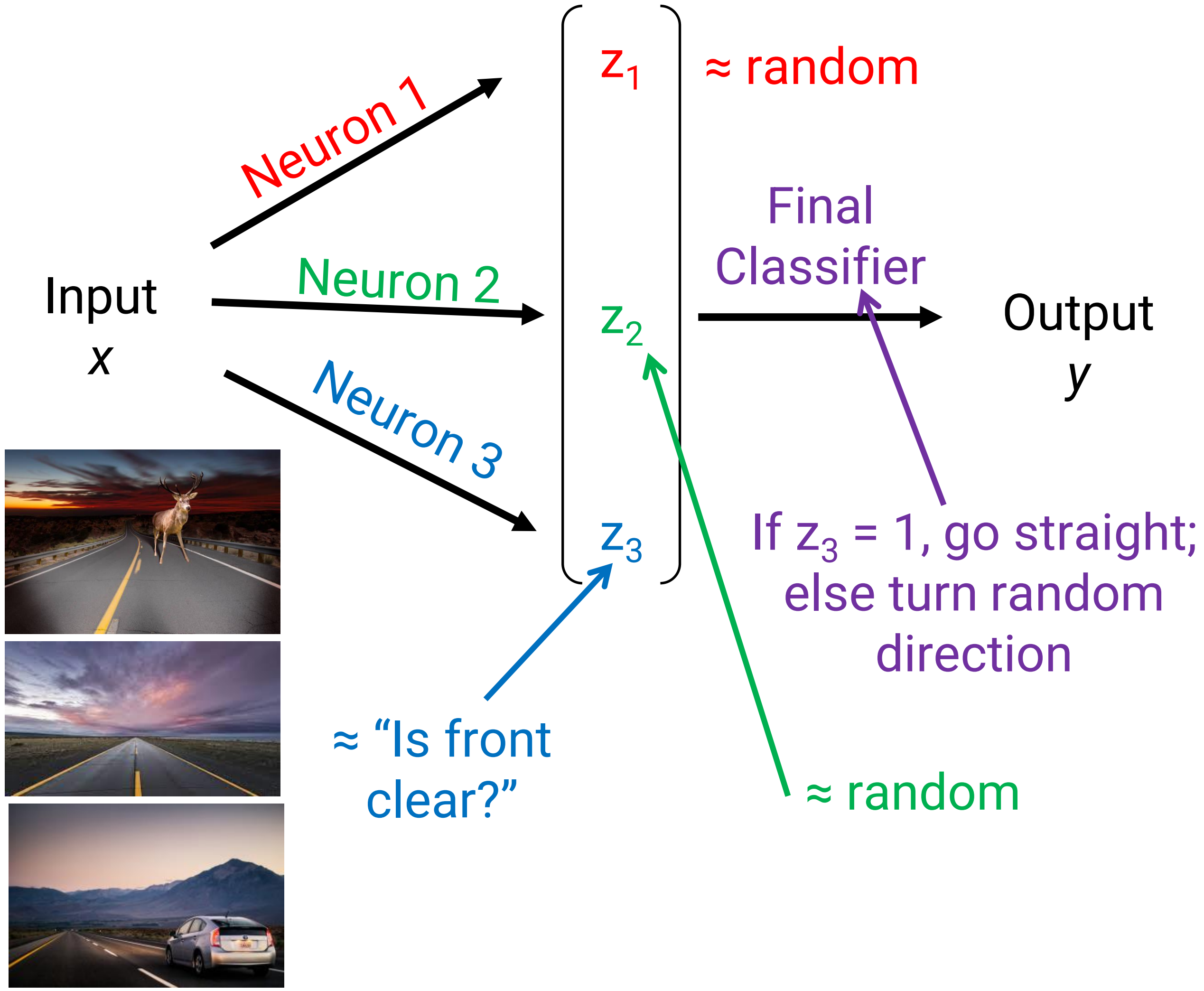
- Plan: Train neural networks to mimic training data via gradient descent
- Initially, each neuron makes random classification “predictions.” Some by chance are mildly useful

Feature Learning with Neural Networks



- Plan: Train neural networks to mimic training data via gradient descent
- Initially, each neuron makes random classification “predictions.” Some by chance are mildly useful
- Final layer learns to use the most useful neurons to make final prediction

Feature Learning with Neural Networks



- Plan: Train neural networks to mimic training data via gradient descent
- Initially, each neuron makes random classification "predictions." Some by chance are mildly useful
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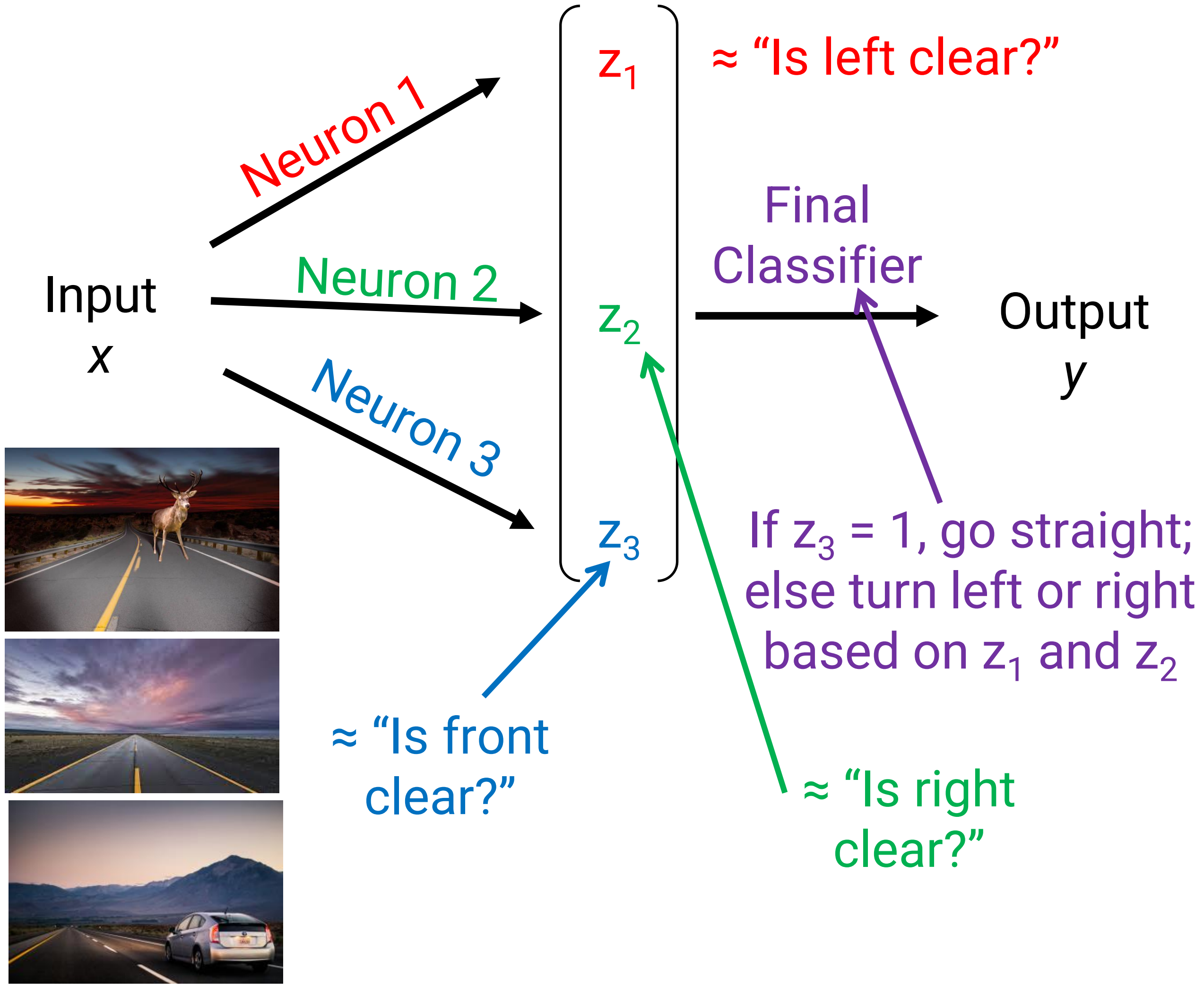
- The neurons that get used are incentivized to become better, to improve final accuracy

Feature Learning with Neural Networks



- Plan: Train neural networks to mimic training data via gradient descent
- Initially, each neuron makes random classification "predictions." Some by chance are mildly useful
- Final layer learns to use the most useful neurons to make final prediction
- The neurons that get used are incentivized to become better, to improve final accuracy
- Other neurons slowly change to surface useful information not already captured by other neurons
- Eventually, learned features are very useful and final layer can predict well!

Summary: Neural Networks as Feature Learners

- Neural networks **learn new features from data**
- Each learned feature is the output of a classifier using the original input features
- These classifiers can be “trained” to produce features that help the final layer make good predictions

Announcements

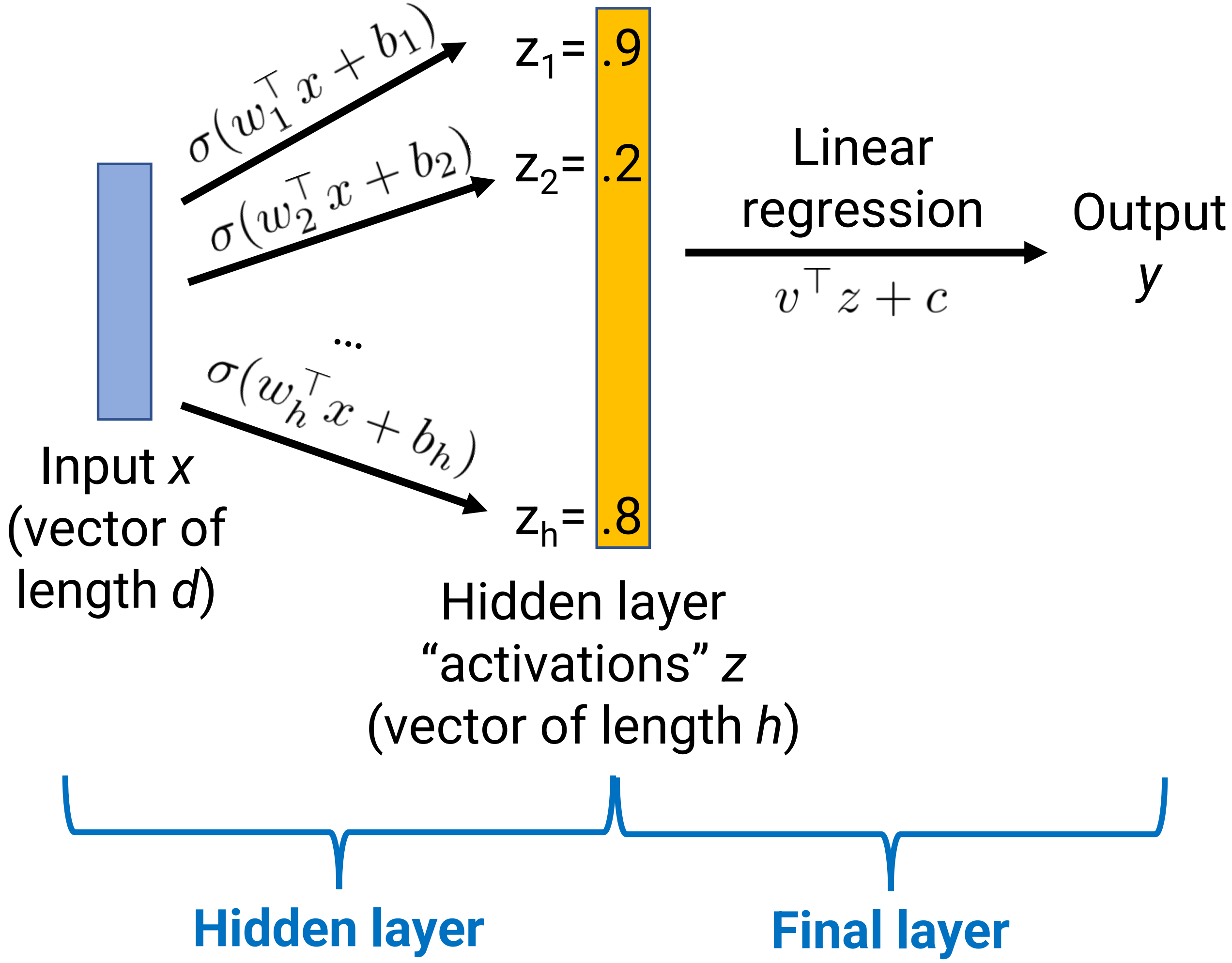
- Project proposals due next Tuesday @ 11:59pm
  - Submit as one group on gradescope (one submission per group)
- Section tomorrow: Cross-validation and evaluation metrics
  - Useful for project proposal when discussing how to evaluate your model
- Homework 2 released soon, Due Thursday March 6

Powerful family of non-linear functions

Neural Networks are Non-linear Functions

- Second view: Neural networks compute a **non-linear** function of input to make predictions
  - As a result, neural networks can learn many functions that linear models cannot
- In most other ways, neural networks are **very similar** to their linear counterparts!
  - E.g., Training is mostly the same

2-layer Neural Network, Regression



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  - Parameters: $\boldsymbol{w_j}$ and $\boldsymbol{b_j}$ for each classifier, for each *j=1, …, h*
  - *h* = number of neurons in hidden layer ("hidden nodes")
  - Produces "activations"= learned feature vector
- Final layer = linear model
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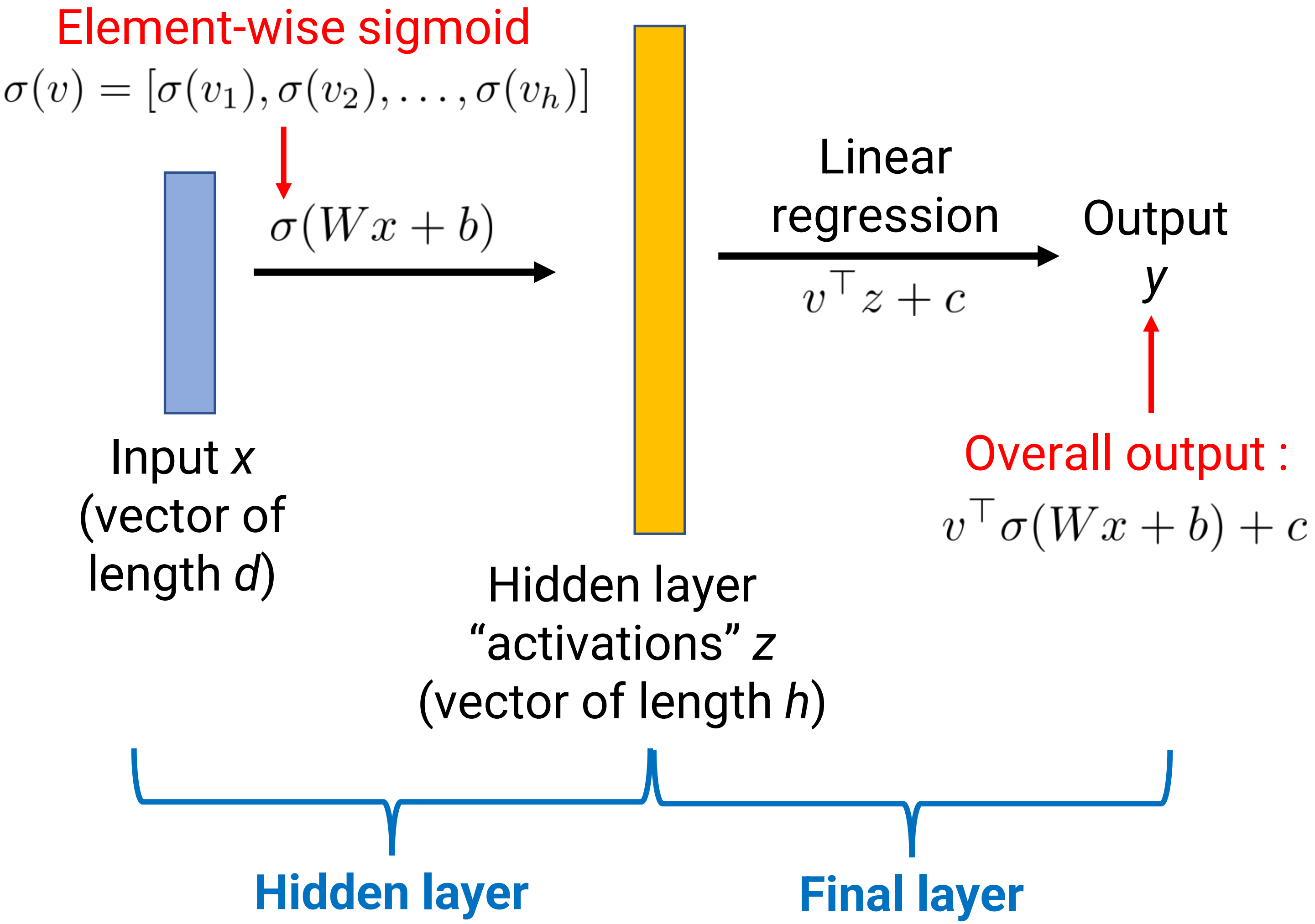
2-layer Neural Network in Matrix Form



- Hidden layer = A bunch of logistic regression classifiers
  - Parameters: $\boldsymbol{w}_j$ and $\boldsymbol{b}_j$ for each classifier, for each j=1, …, h
  - Equivalently: matrix ***W*** (h x d) and vector ***b*** (length h)
  - h = number of neurons in hidden layer ("hidden nodes")
  - Produces "activations"= learned feature vector
- Final layer = linear model
  - For regression: linear model with weight vector ***v*** and bias ***c***
- **Parameters of model are** ***θ = (W, b, v, c)***

Training Neural Networks

Linear Regression

- Model's output is

$$g(x) = w^\top x + b$$

- (Unregularized) loss function is

$$\frac{1}{n}\sum_{i=1}^{n}(g(x^{(i)}) - y^{(i)})^2$$

Regression w/ Neural Networks

- Model's output is

$$g(x) = v^\top \sigma(Wx + b) + c$$

- **Use same loss function**, in terms of g!

$$\frac{1}{n}\sum_{i=1}^{n}(g(x^{(i)}) - y^{(i)})^2$$

Training objective for both types of models:

$$\frac{1}{n}\sum_{i=1}^{n}\ell\left(y^{(i)}, g(x^{(i)})\right), \ \text{where } \ell(y, u) = (y - u)^2$$

Also applies for logistic regression, softmax regression, etc.

Training Neural Networks

General loss function: $\frac{1}{n}\sum_{i=1}^{n}\ell\left(y^{(i)}, g(x^{(i)})\right)$

Model's output, depends on all model parameters θ (includes all layers)

- How to minimize? Gradient Descent!

$$\theta \leftarrow \theta - \eta \cdot \underbrace{\frac{1}{n}\sum_{i=1}^{n}\nabla_\theta \ell\left(y^{(i)}, g(x^{(i)})\right)}_{\text{Average of per-example gradients}}$$

- In practice, use a variant of traditional gradient descent
  - (Will discuss in 2 classes)

Importance of "Non-linearities"

With sigmoid,
overall output is:

$$v^\top \sigma(Wx + b) + c$$

Without sigmoid,
overall output is:

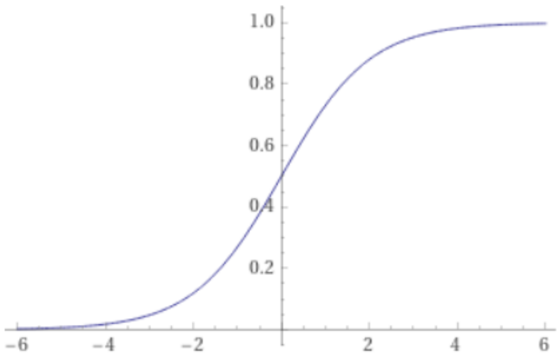
$$v^\top (Wx + b) + c$$

$$= (v^\top W)x + (v^\top b + c)$$

- Having the sigmoid is very important!
- What if we skipped the sigmoid?
- Result: Just another way to write a linear function!
  - New "weight" is $v^T W$
  - New "bias" is $v^T b + c$
- Having a **simple non-linear function** (like sigmoid) between the two linear operations enables us to learn a **complex non-linear function**!

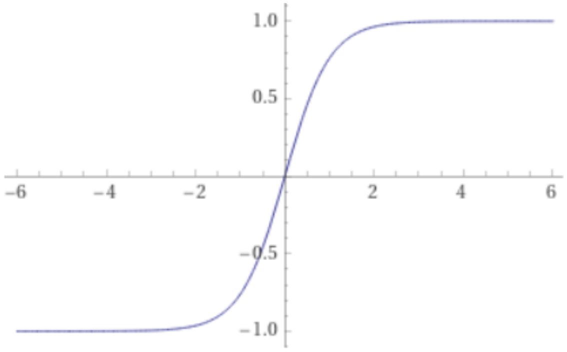
Options for Non-linearities

Sigmoid



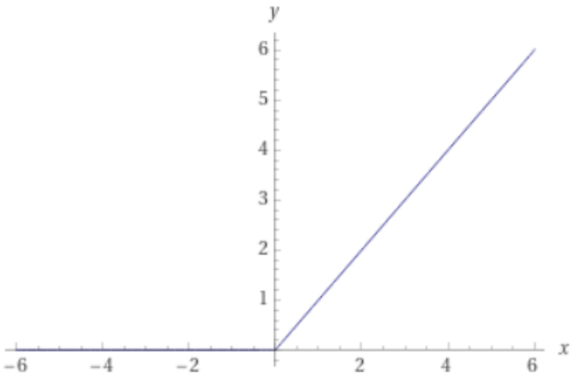
$$\sigma(z) = \frac{1}{1+e^{-z}}$$

Tanh



$$\tanh(z) = \frac{e^{2z}-1}{e^{2z}+1}$$

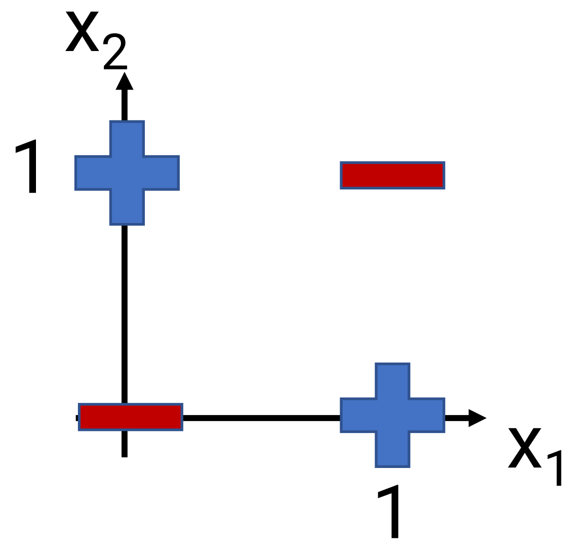
ReLU



$$\mathrm{ReLU}(z) = \max(z, 0)$$

- Many options work, just must be differentiable (for gradient descent)
  - Sometimes called "activation functions" or just "non-linearities"
- In practice: tanh and ReLU often preferred
  - Tanh: Better than sigmoid because outputs centered around zero
  - ReLU: Very fast to compute

Non-linearities make NN's more expressive



- XOR: Classic binary classification problem that can't be solved by linear classifier
- A 2-layer neural network can solve it!
  - I can choose values for the parameters that lead to perfect classification on this dataset
  - Conclusion: Neural networks are **more expressive** than linear models

$x_1 \xrightarrow{\sigma(100 \cdot (-x_1 - x_2 + 0.5))} z_1$ ≈1 if both are 0, ≈0 else

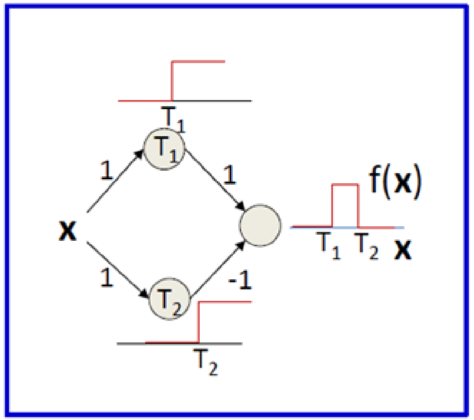
$x_2 \xrightarrow{\sigma(100 \cdot (x_1 + x_2 - 1.5))} z_2$ ≈1 if both are 1, ≈0 else

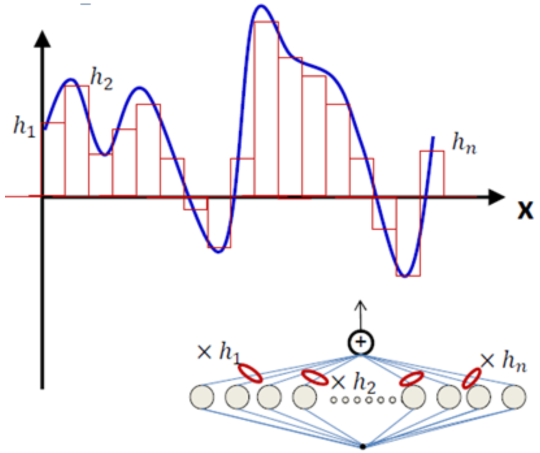
$\xrightarrow{0.5 - z_1 - z_2}$ < 0 if XOR(x_1, x_2) = 0

> 0 if XOR(x_1, x_2) = 1

Universal Approximation

- Fact: **Any function** can be approximated by a 2-layer neural network with enough hidden units
- 2-layer neural networks are thus "**universal approximators**"
  - Note: Also true for k-NN, SVM with RBF kernel…
- Proof sketch
  - First layer learns a bunch of indicator-like features like "is x > 1?", "is x > 2?", etc.
  - This divides space into a bunch of buckets of width 1
  - Second layer assigns correct value to each bucket
  - If you have enough hidden units, you can make buckets really small and approximate a function very well

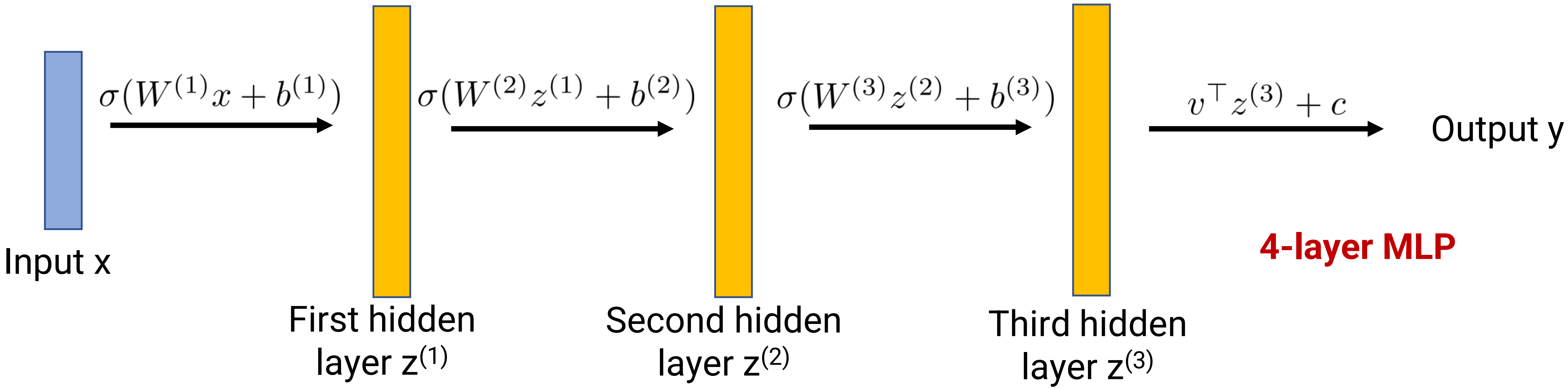




Summary: Neural Networks as Non-linear Functions

- Neural Networks are a type of **learnable non-linear function**
  - Contrast with previous models, which are learnable linear functions
- Constructed from multiple layers, each of which have their own learnable parameters
- Non-linearities between layers make the model much more expressive—can represent **any function** with a big enough network and right choice of parameters
  - Whereas linear models just cannot learn certain functions, like XOR
- Learning process works the same way as for linear models

Multi-Layer Perceptron (MLP)



- What we saw so far is called a “2-layer perceptron”
- But we can add more layers!
  - Corresponds to more complex feature extractor
  - In practice, making networks “deeper” (more layers) often helps more than making them “wider” (more hidden units in each layer)
  - Layers are “fully connected” as each neuron depends on every neuron in previous layer

Set of building blocks to create complex models

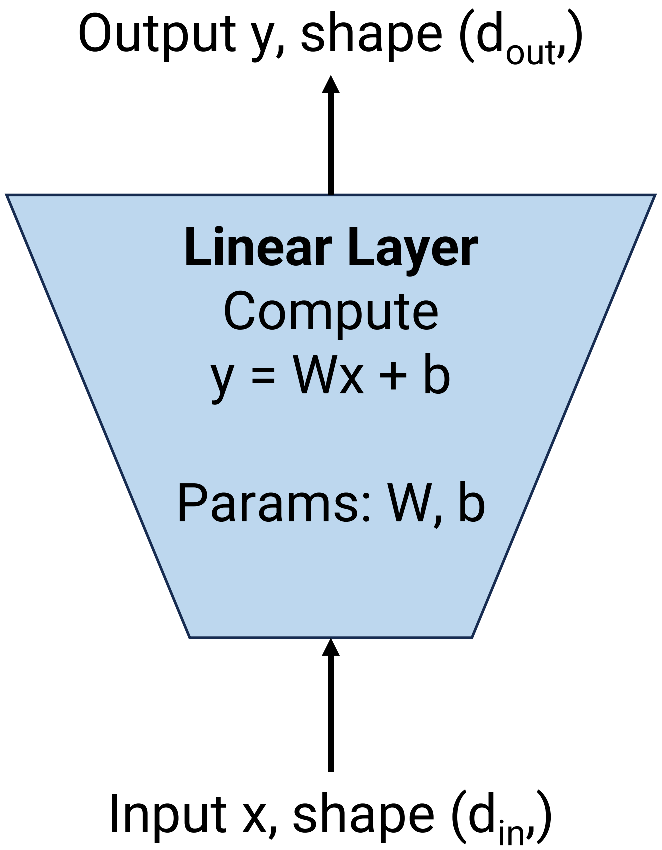
Deep Learning as a Set of Building Blocks

- Neural Network = Many “layers” stacked on top of each other
  - Each “layer” takes in some input and computes some output
  - Simplest layers are basic building blocks, can build more complex layers from those
  - Arrangement of layers is called an “architecture”
- Deep Learning: **Design suitable neural architectures with various reusable building blocks**
  - This is the view of most deep learning programming libraries like pytorch

The Basic "Building Blocks"

(1) Linear Layer

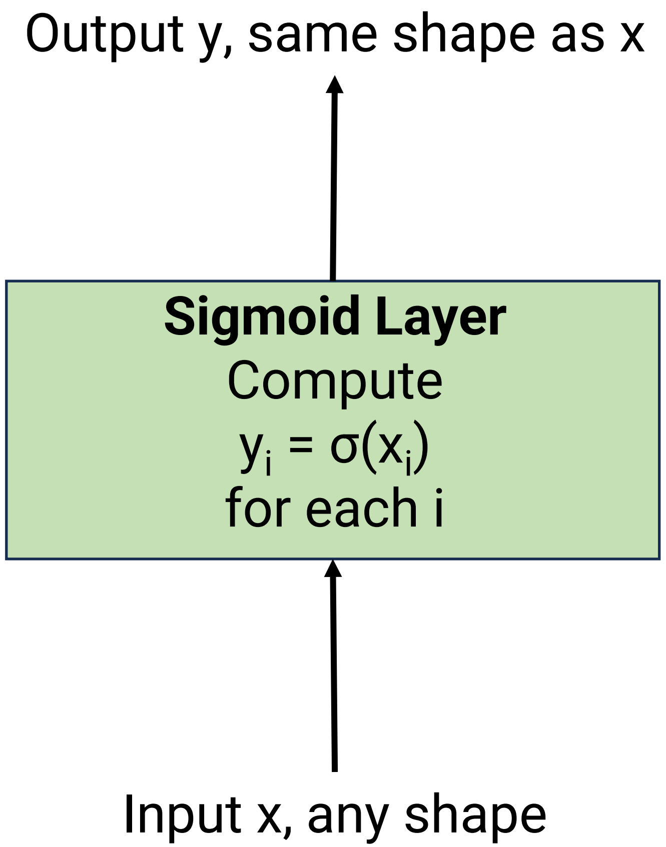
- Input x: Vector of dimension d_{in}
- Output y: Vector of dimension d_{out}
- Formula: y = Wx + b
- Parameters
  - W: d_{out} x d_{in} matrix
  - b: d_{out} vector
- In pytorch: nn.Linear()



The Basic "Building Blocks"

(2) Non-linearity Layer

- Input x: Any number/vector/matrix
- Output y: Number/vector/matrix of same shape
- Possible formulas:
  - Sigmoid: $y = \sigma(x)$, elementwise
  - Tanh: $y = \tanh(x)$, elementwise
  - Relu: $y = \max(x, 0)$, elementwise
- Parameters: None
- In pytorch: torch.sigmoid(), nn.functional.relu(), etc.



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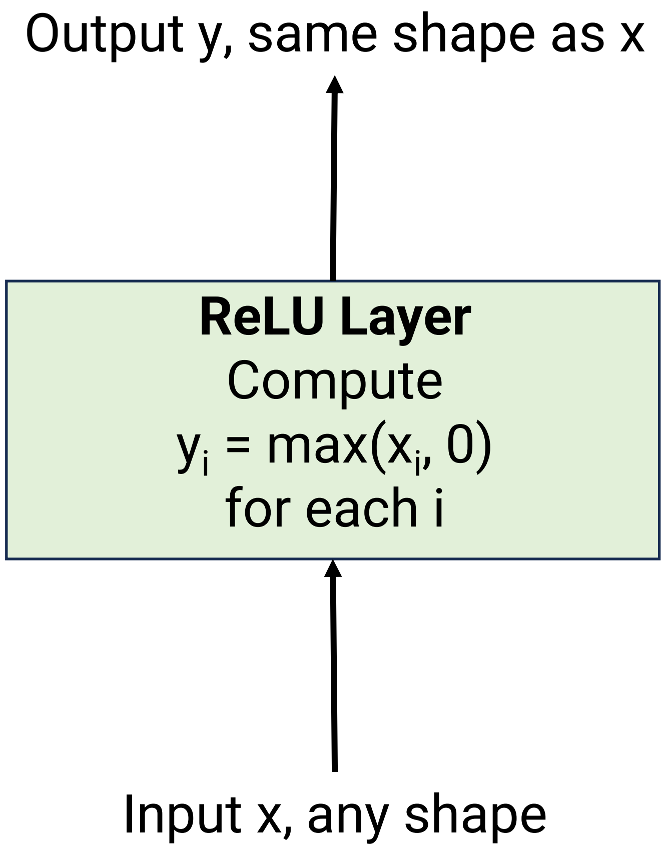


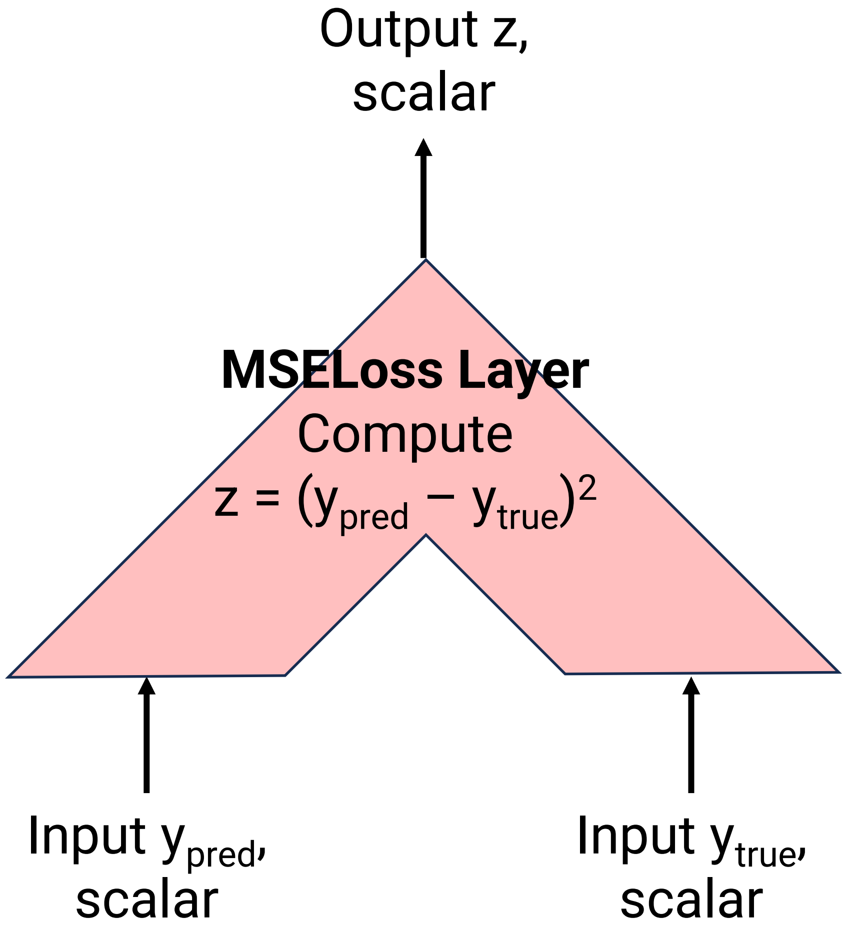
The Basic "Building Blocks"

(3) Loss Layer

- Inputs:
  - y_{pred}: shape depends on task
  - y_{true}: scalar (e.g., correct regression value or class index)
- Output z: scalar
- Possible formulas:
  - Squared loss: y_{pred} is scalar, $z = (y_{pred} - y_{true})^2$
  - Softmax regression loss: y_{pred} is vector of length C,

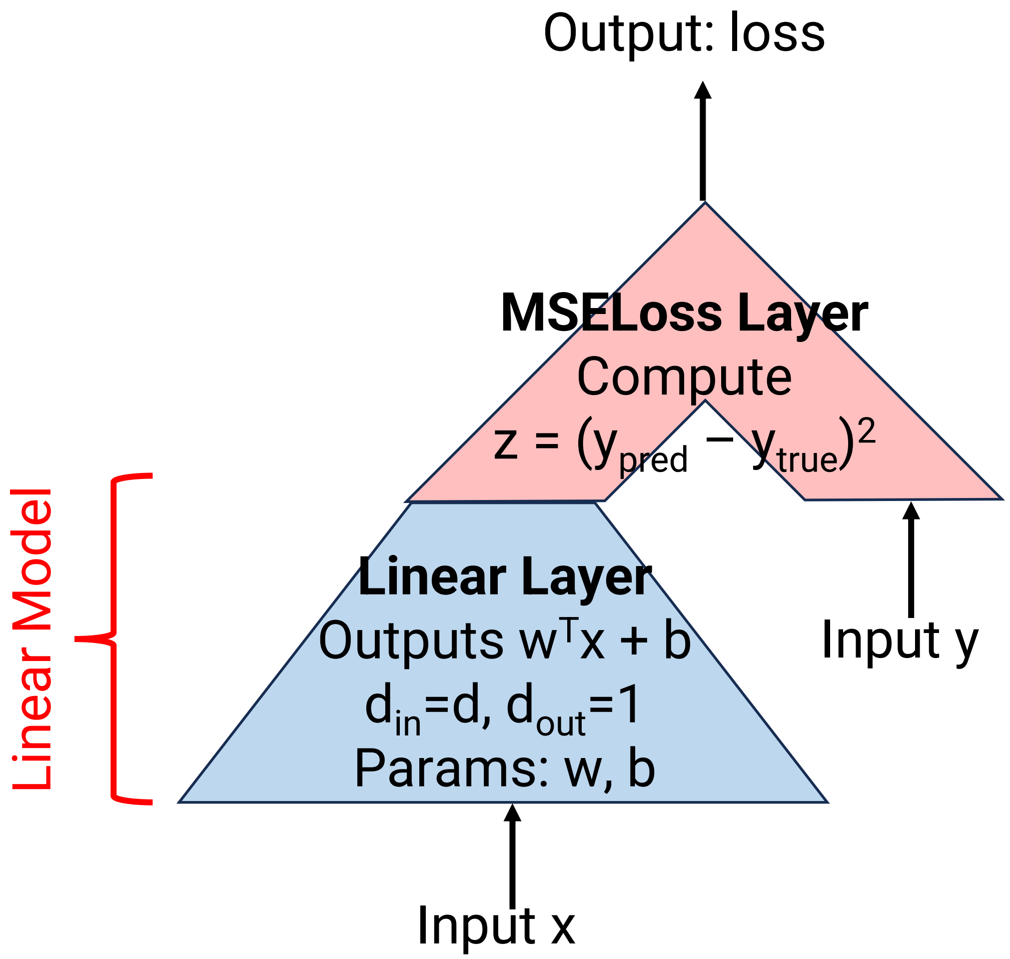
$$z = -\left(y_{\text{pred}}[y_{\text{true}}] - \log \sum_{i=1}^{C} \exp(y_{\text{pred}}[i]) \right)$$

- Parameters: None
- In pytorch: nn.MSELoss(), nn.CrossEntropyLoss(), etc.



Building Linear Regression Training Loop

- Step 1: Compute the loss on one example at a time
  - Training example is (x, y)
  - x is vector of length d, y is scalar



Building Linear Regression Training Loop

- Step 1: Compute the loss on one example at a time
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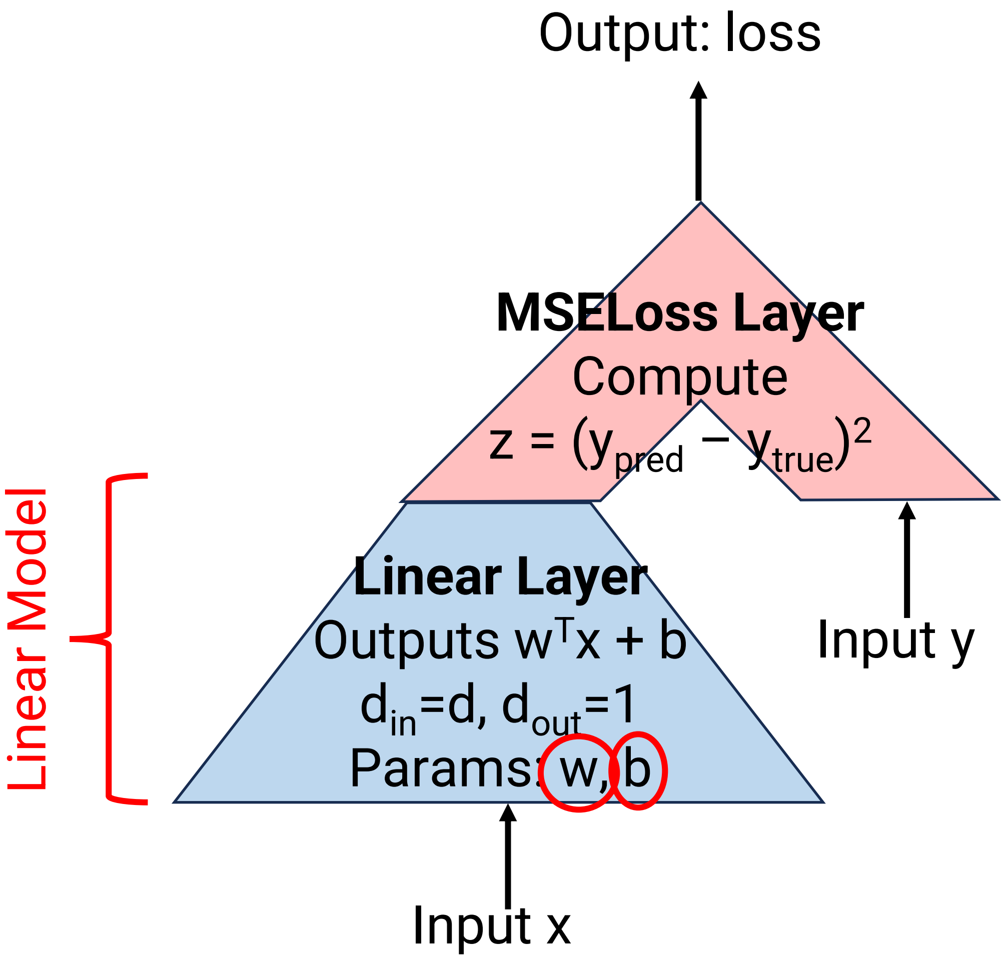
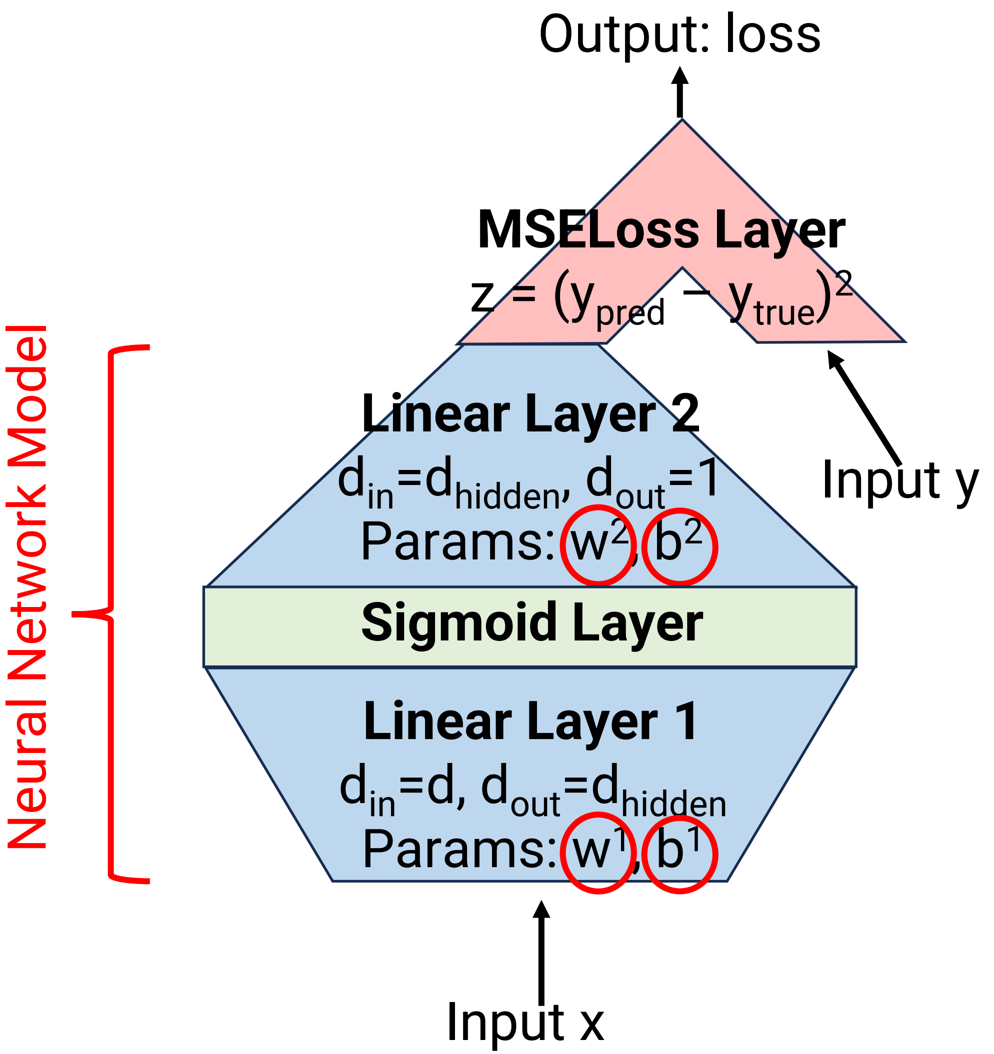
- Step 2: Compute gradient of loss with respect to all parameters
- Step 3: Update all parameters with gradient descent update rule



Building a 2-layer MLP for Regression

- **Steps for training are exactly the same!**
- Step 1: Compute the loss on one example at a time
  - Training example is (x, y)
  - x is vector of length d, y is scalar
- Step 2: Compute gradient of loss with respect to all parameters
  - **Next class: Compute gradient automatically with backpropagation. Easy if each building block is differentiable!**
- Step 3: Update all parameters with gradient descent update rule



Summary: Deep Learning as Building Blocks

- Power of deep learning: You can **stack building blocks together any way you want**
  - No “right” or “wrong” architecture, just different design decisions
  - Best architecture choice depends on the task and data
  - Endless possibilities for new architectures

Method for learning features from data

Powerful family of non-linear functions

Set of building blocks to create complex models