Introduction to Neural Networks

Robin Jia USC CSCI 467, Spring 2024 February 8, 2024

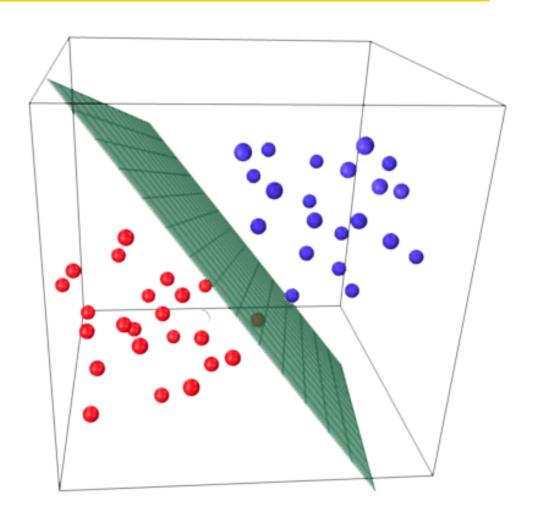
Review: Linear Models

- Examples: Linear regression, logistic regression, softmax regression
- Test time: Make a prediction based on learned parameters
 - E.g., linear regression: $y_{\mathrm{pred}} = w^{\top}x + b$, 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







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Set of building blocks to create complex models

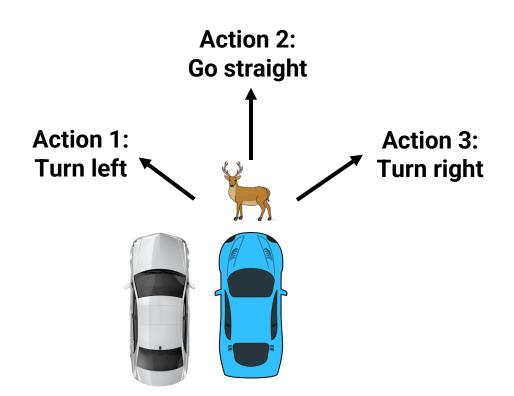
Deep Learning

Machine Learning using Neural Network models



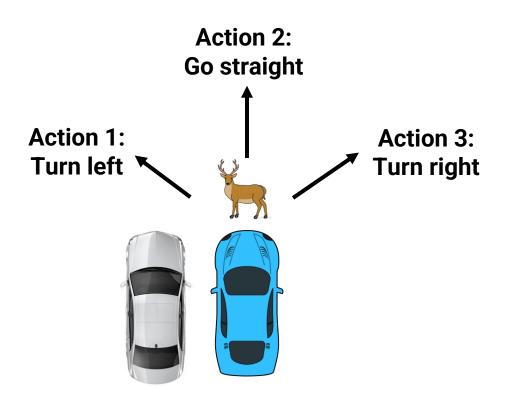
Method for learning features from data

A (toy) self-driving car example



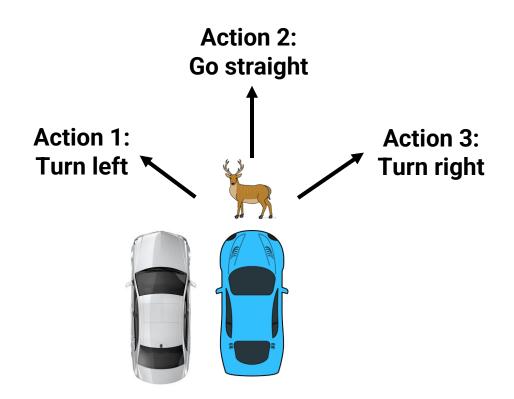
- Three-way classification problem:
 Go left, straight, or right?
- What features are important here?
 - Is front clear?
 - Is left clear?
 - Is right clear?

A (toy) self-driving car example



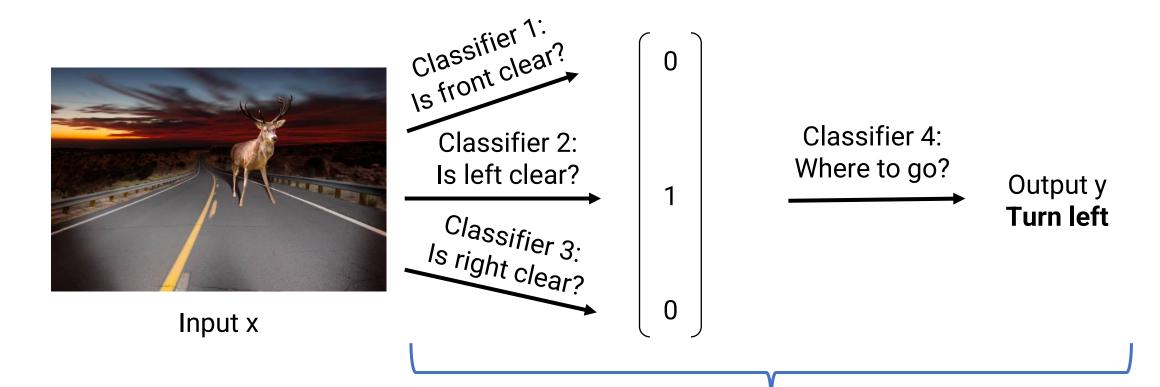
- Suppose we had these features:
 - $z = [z_1, z_2, z_3]$
 - $z_1 = 1$ if front is clear, 0 else
 - $z_2 = 1$ if left is clear, 0 else
 - $z_3 = 1$ if right is clear, 0 else
- With this, we can do softmax regression:
 - Score for "straight": $20 z_1 10$
 - Score for "left": 10 z₂ 10
 - Score for "right": 10z₃ 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



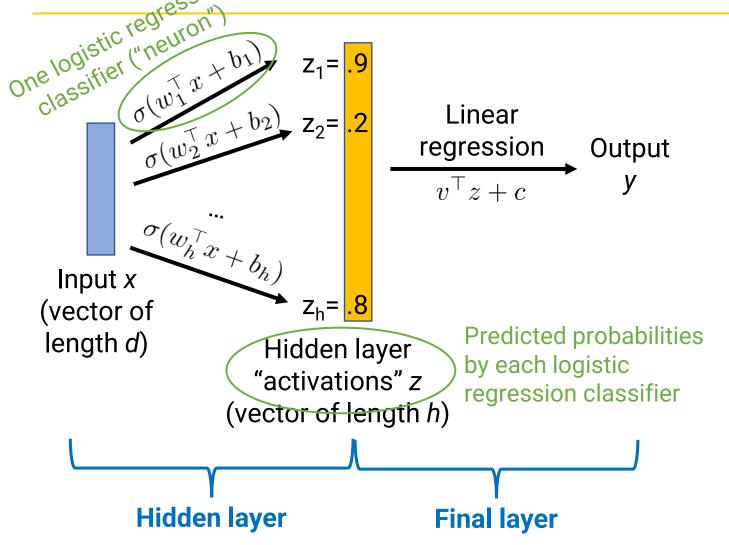
- How can we write the feature "is front clear"?
- Checking if the front is clear is itself a machine learning problem
 - Input = camera image/lidar data,
 Output = whether there is an obstacle
 - Obstacle near or far away?
 - Hard obstacle or a plastic bag?
- Can we make our features the outputs of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

Feature learning



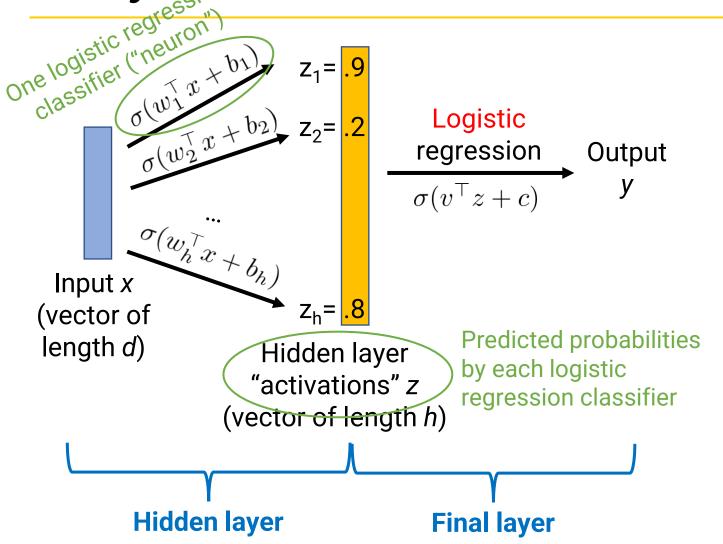
This is a neural network!

2-layer Neural Network, Regression

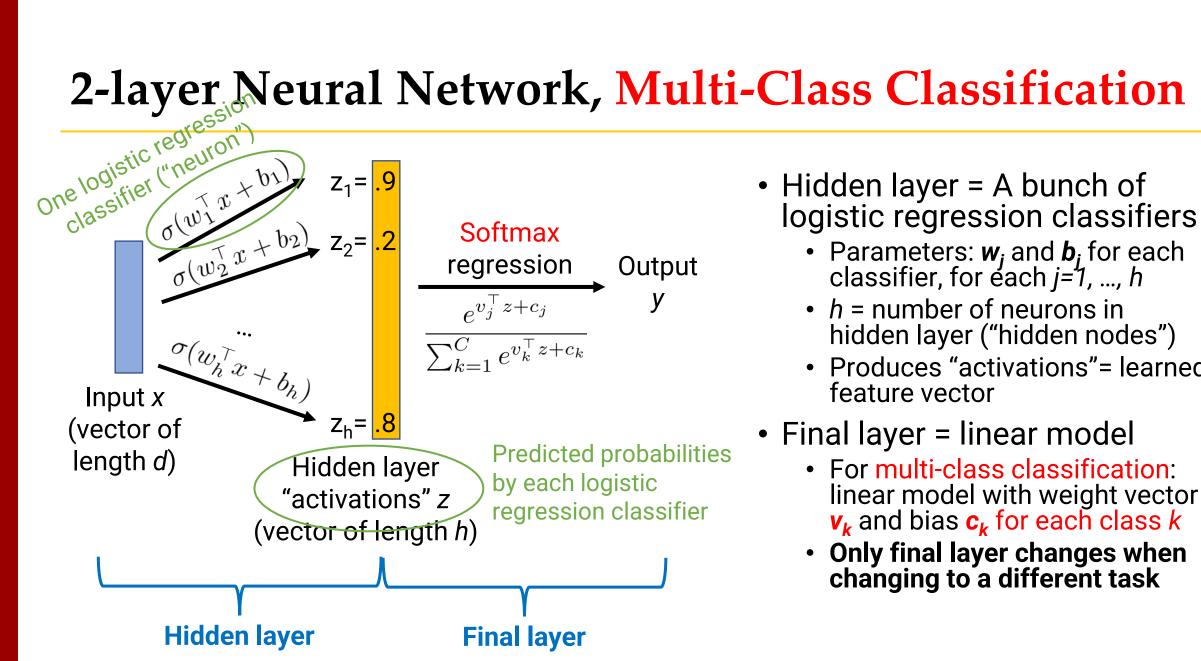


- Hidden layer = A bunch of logistic regression classifiers
 - Parameters: w_j and b_j for each classifier, for each j=1, ..., h
 - h = number of neurons in hidden layer ("hidden nodes")
 - Produces "activations" = learned feature vector
- Final layer = linear model
 - For regression: linear model with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

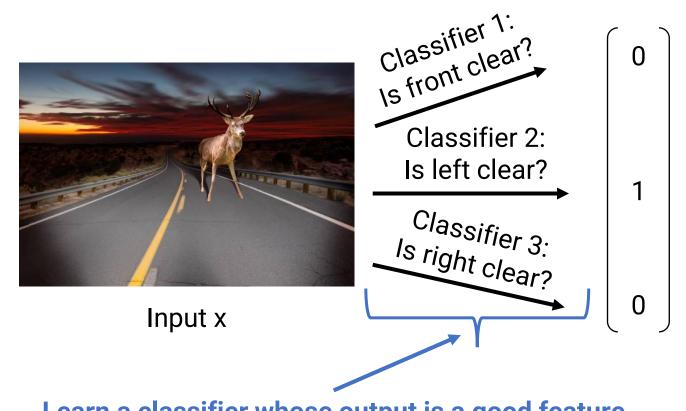
2-layer Neural Network, Binary Classification



- Hidden layer = A bunch of logistic regression classifiers
 - Parameters: \mathbf{w}_{j} and \mathbf{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 binary classification: linear model with weight vector v and bias c
 - Only final layer changes when changing to a different task



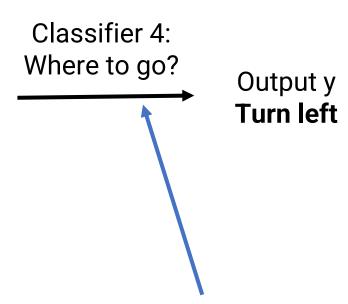
- logistic regression classifiers
 - Parameters: \mathbf{w}_i and \mathbf{b}_i for each classifier, for each *j*=1, ..., *h*
 - *h* = number of neurons in hidden layer ("hidden nodes")
 - Produces "activations" = learned feature vector
- Final layer = linear model
 - For multi-class classification: linear model with weight vector $\mathbf{v}_{\mathbf{k}}$ and bias $\mathbf{c}_{\mathbf{k}}$ for each class k
 - Only final layer changes when changing to a different task



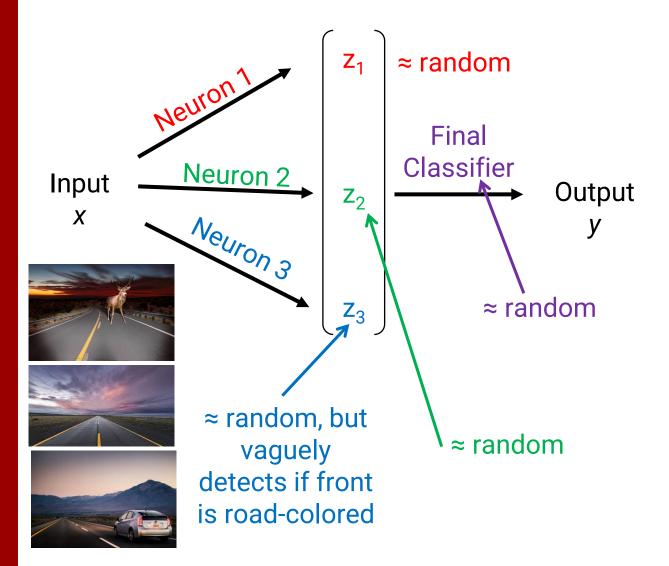
Learn a classifier whose output is a good feature

We don't tell the model what classifier to learn

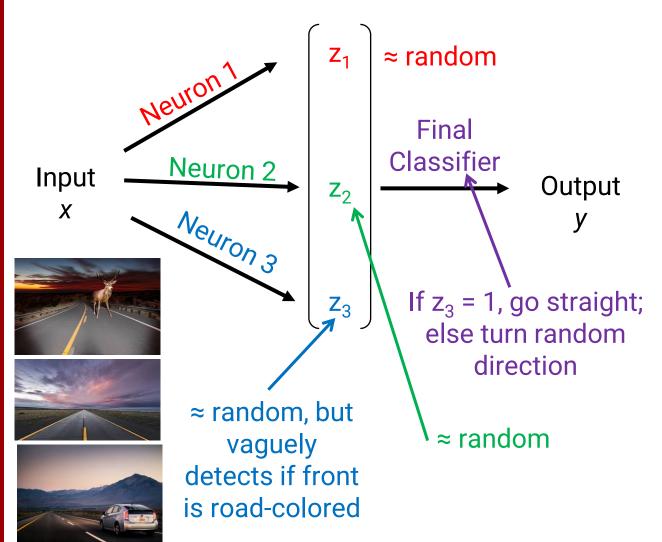
Learn from data that "is front clear" is a useful concept



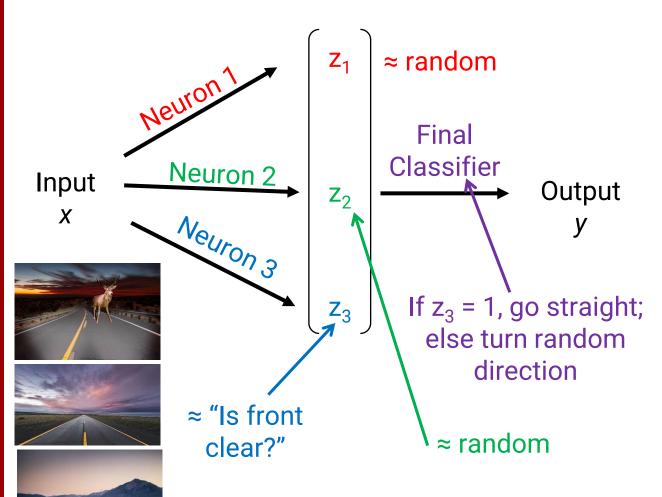
Learn to classify based on features (same as linear model)



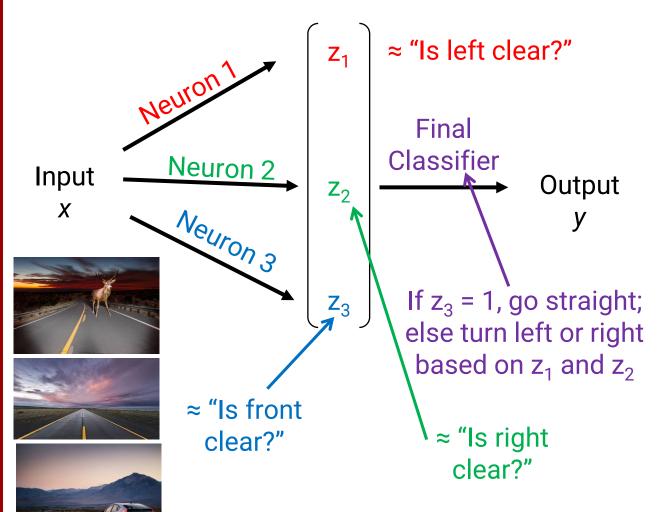
- Plan: Train neural networks to mimic training data via gradient descent
- Initially, each neuron makes random classification "predictions." Some by chance are mildly useful



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- The neurons that get used are incentivized to become better, to improve final accuracy



- 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: Review of linear methods
 - Fill out the poll on piazza!
- Homework 2 released soon, Due February 29

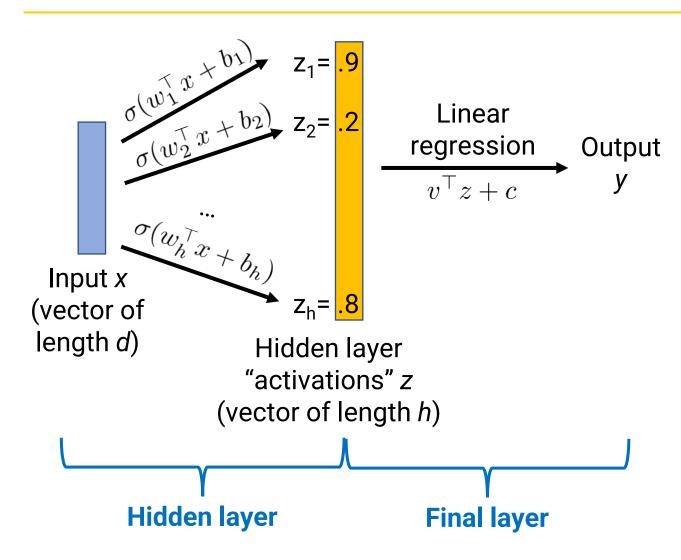


Powerful family of non-linear functions

Neural Networks are Non-linear Functions

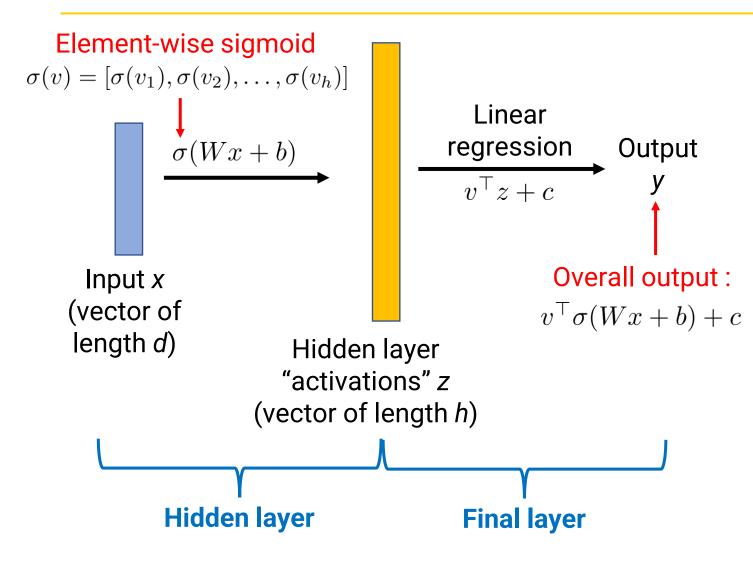
- Second view: Neural networks compute a non-linear function of input to make predictions
 - As a result, neural networks can learn many functions that linear models cannot
- In most other ways, neural networks are very similar to their linear counterparts!
 - E.g., Training is mostly the same

2-layer Neural Network, Regression



- Hidden layer = A bunch of logistic regression classifiers
 - Parameters: w_j and b_j for each classifier, for each j=1, ..., h
 - h = number of neurons in hidden layer ("hidden nodes")
 - Produces "activations" = learned feature vector
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2-layer Neural Network in Matrix Form



- Hidden layer = A bunch of logistic regression classifiers
 - Parameters: \mathbf{w}_{j} and \mathbf{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:
$$\frac{1}{n} \sum_{i=1}^{n} \ell\left(y^{(i)}, g(x^{(i)})\right)$$

How to minimize? Gradient Descent!

$$\theta \leftarrow \theta - \eta \cdot \frac{1}{n} \sum_{i=1}^{n} \nabla_{\theta} \ell \left(y^{(i)}, g(x^{(i)}) \right)$$

Average of per-example gradients

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

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

Importance of "Non-linearities"

With sigmoid, overall output is: $v^{\top}\sigma(Wx+b)+c$

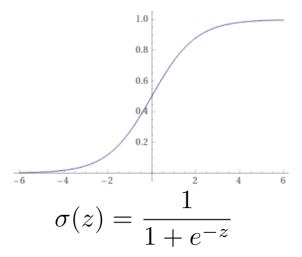
Without sigmoid, overall output is:

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

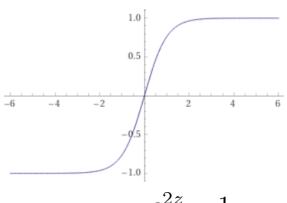
- Having the sigmoid is very important!
- What if we skipped the sigmoid?
- Result: Just another way to write a linear function!
 - New "weight" is v^TW
 - New "bias" is $v^Tb + c$
- Having a simple non-linear function (like sigmoid) between the two linear operations enables us to learn a complex non-linear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

Options for Non-linearities

Sigmoid

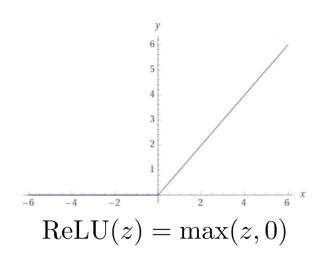


Tanh



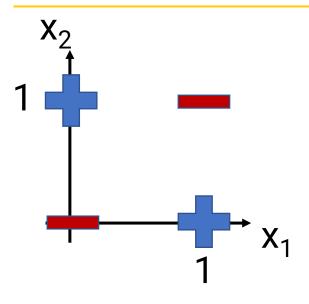
$$\tanh(z) = \frac{e^{2z} - 1}{e^{2z} + 1}$$

ReLU

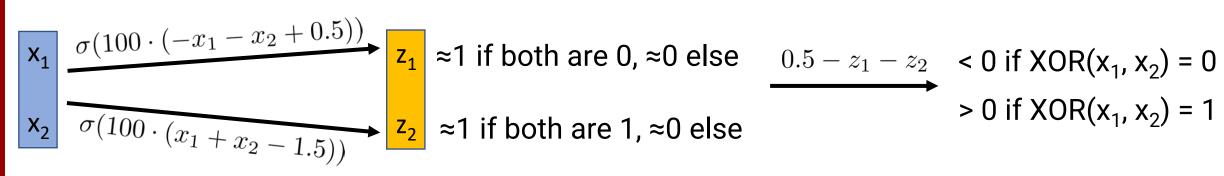


- Many options work, just must be differentiable (for gradient descent)
 - Sometimes called "activation functions" or just "non-linearities"
- In practice: tanh and ReLU often preferred
 - Tanh: Better than sigmoid because outputs centered around zero
 - ReLU: Very fast to compute

Non-linearities make NN's more expressive

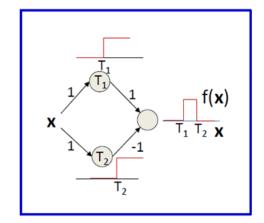


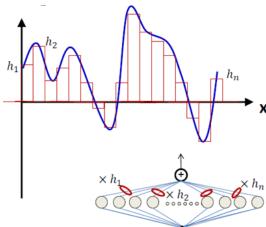
- XOR: Classic binary classification problem that can't be solved by linear classifier
- A 2-layer neural network can solve it!
 - I can choose values for the parameters that lead to perfect classification on this dataset
 - Conclusion: Neural networks are more expressive than linear models



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

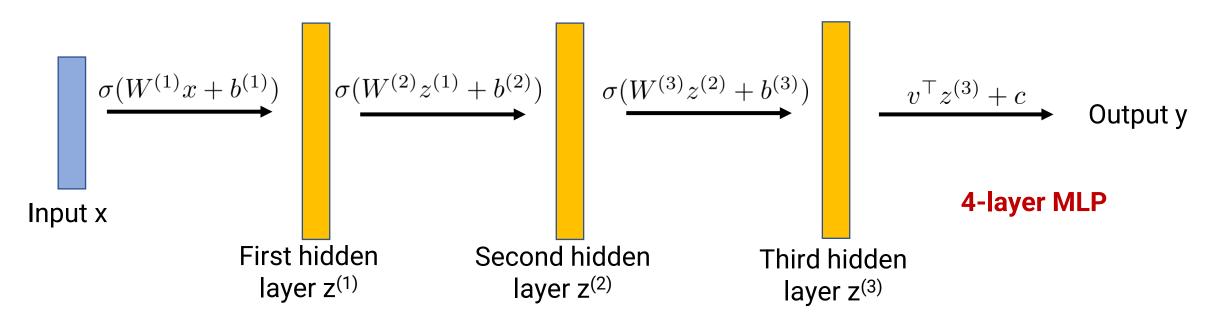




Summary: Neural Networks as Non-linear Functions

- 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

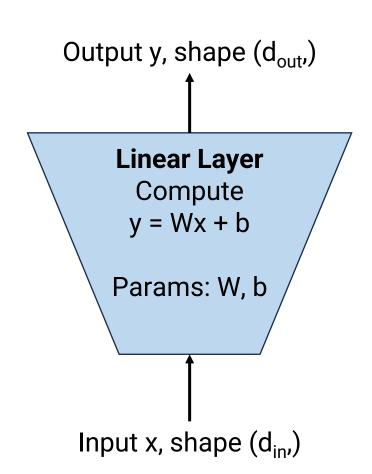
Deep Learning as a Set of Building Blocks

- 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



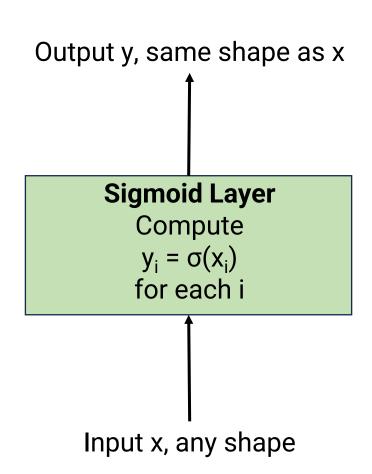
(1) Linear Layer

- 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()



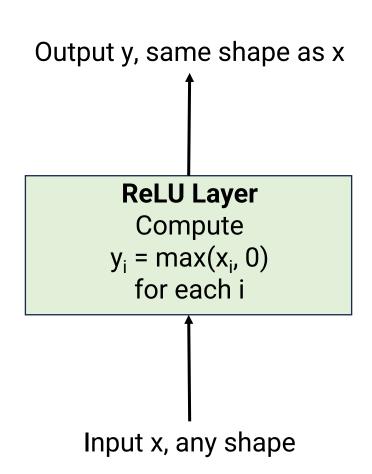
(2) Non-linearity Layer

- 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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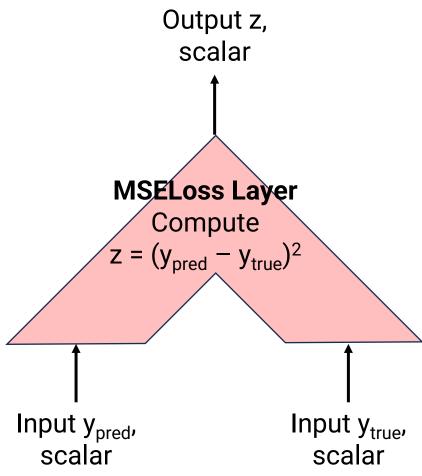


(3) Loss Layer

- 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, $z = (y_{pred} y_{true})^2$

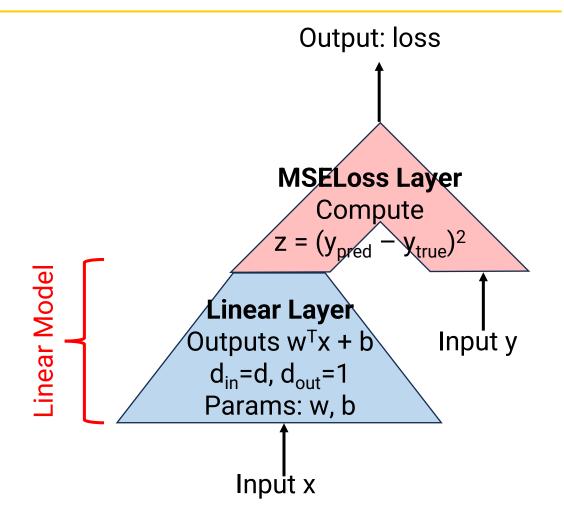
• Softmax regression loss:
$$\mathbf{y}_{\text{pred}}$$
 is vector of length C,
$$z = -\left(y_{\text{pred}}[y_{\text{true}}] - \log \sum_{i=1}^{C} \exp(y_{\text{pred}}[i])\right)$$

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



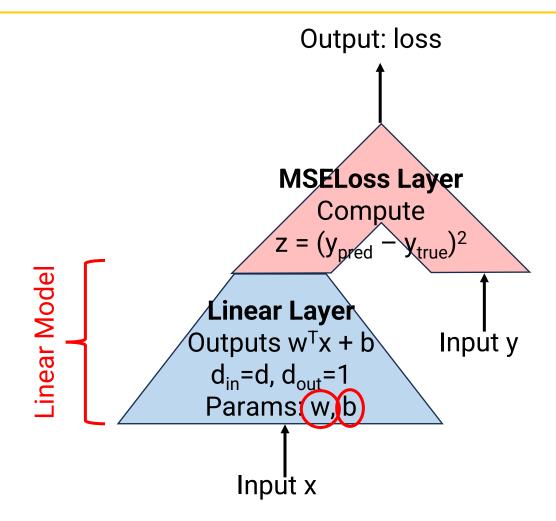
Building Linear Regression Training Loop

- 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



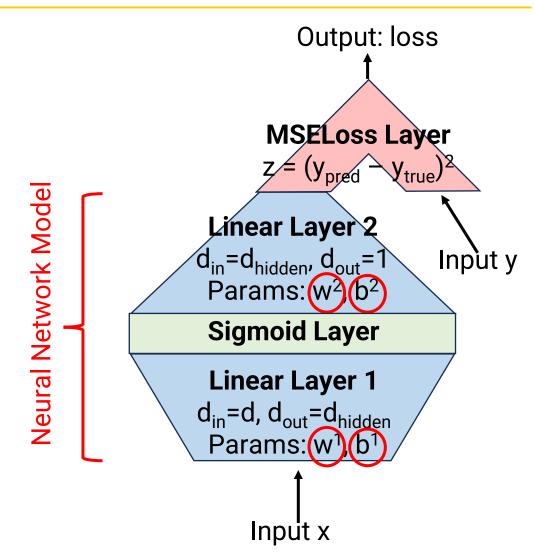
Building Linear Regression Training Loop

- 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









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