Argonne Intro to HPC Bootcamp

An Introduction to Linear Regression with Applications to AI

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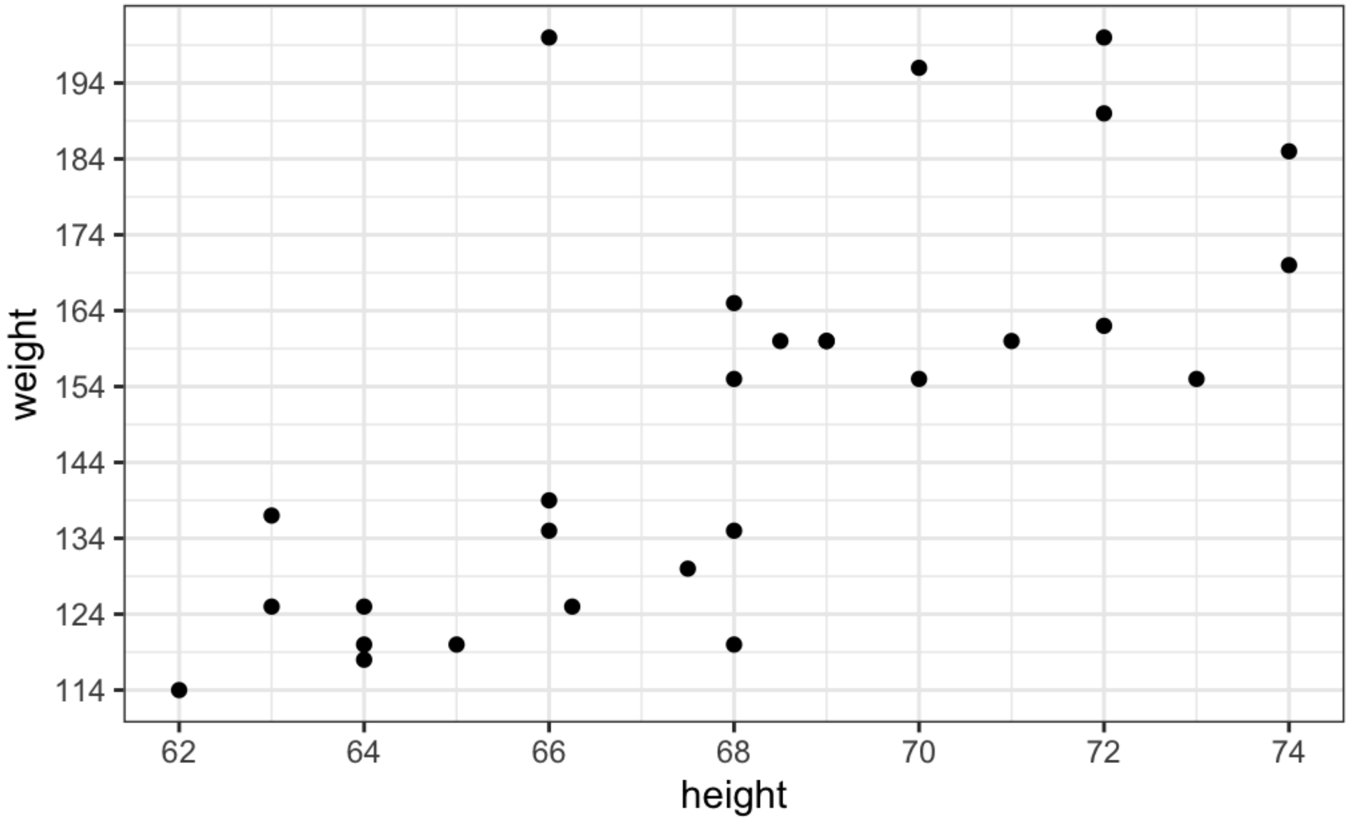
Motivation for Linear Regression

- Allows us to investigate the relationship between two or more variables statistically
- Basic introduction to supervised learning
- Can be thought of as a building block of artificial neural networks (many perceptrons)
- Learning Objectives

    1. Fit a SLR model to data and interpret model coefficients (parameters)
    2. Build a Perceptron to solve a regression problem
    3. Build and train a deep neural network using Keras

Simple Linear Regression: Model Definition

- The goal for SLR is to investigate the relationship between the ***response*** (***Y***) and the ***predictor*** (***X***) variables
- Recall from high school algebra: $\boldsymbol{y = b + mx}$
  - —Where ***m*** is the slope and ***b*** is the y-intercept



Simple Linear Regression: Model Definition

- The general form of the SLR model closely resembles the algebraic equation ($\boldsymbol{y = b + mx}$):

$$Y = \beta_0 + \beta_1 X + \epsilon$$

- For an individual observation (x_i, y_i), the regression equation becomes:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

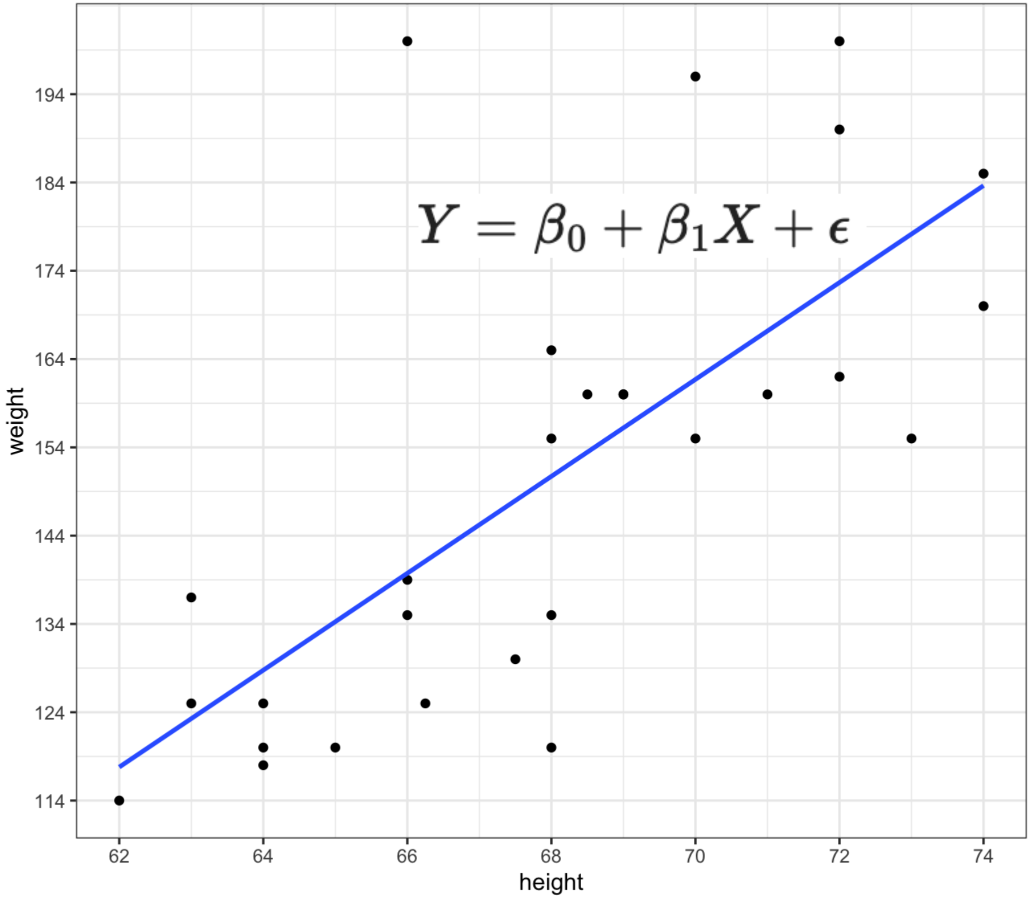
- Where
  - — β_0 is the is the population y-intercept,
  - — β_1 is the population slope
  - — ϵ_i is the error or deviation of an observation from regression line

- Together, β_0 and β_1 are the (unknown) population model ***coefficients*** or ***parameters***

- The goal of regression is to estimate parameters ($\hat{\beta}$) to describe the relationship between ***Y*** and ***X***

- We estimate $\hat{\beta}$ using the method of Ordinary Least Squares (OLS)

Simple Linear Regression: Errors (Loss)



- Predicted value ($\hat{y}_i$) based on the $\hat{x}_i$ is obtained by

$$fit_i = \hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

- An error is defined by

$$res_i = \epsilon_i = y_i - \hat{y}_i$$

- We quantify the total error (loss)

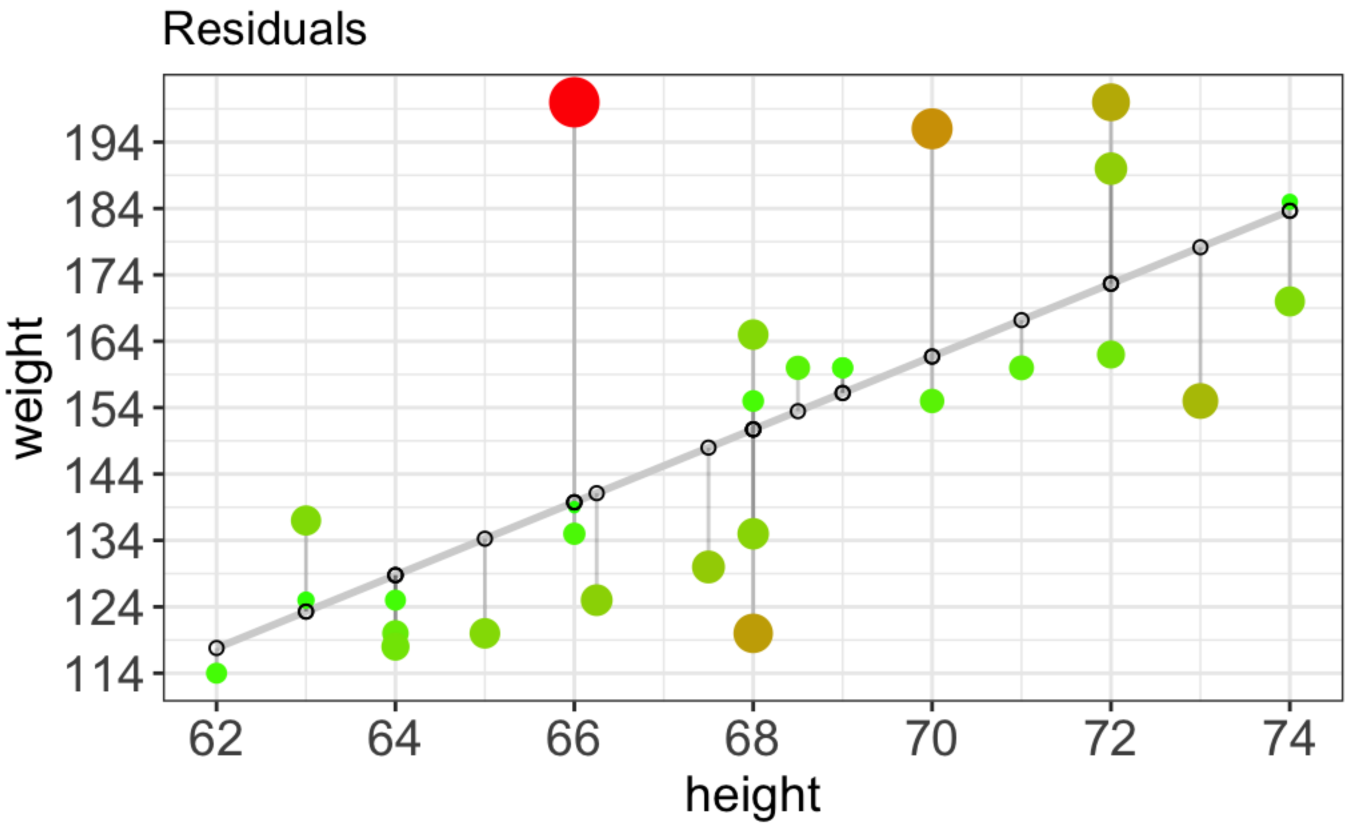
$$RSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

$$MSE = \frac{1}{n} \sum_{i=1}^{n} \left(\hat{y}^{(i)} - y^{(i)}\right)^2$$

- Goal: obtain least squares estimates of β to minimize MSE

Simple Linear Regression: Errors (Loss)

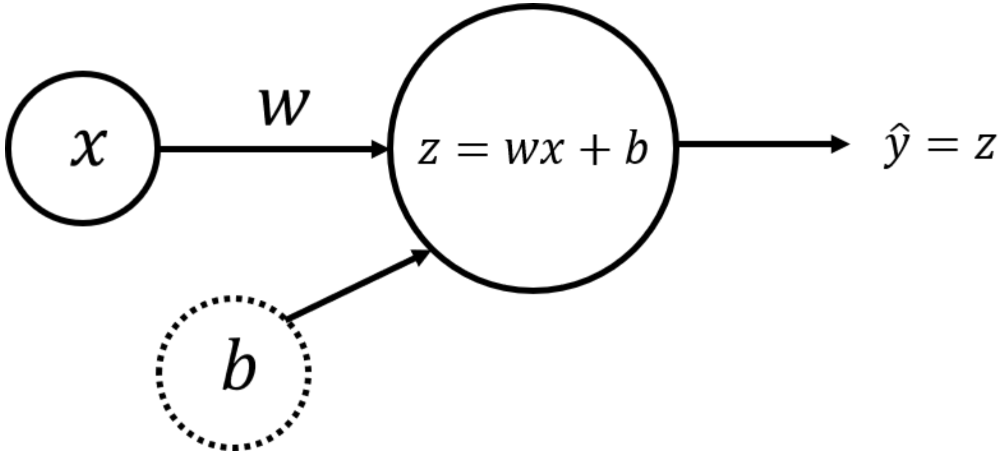
Errors, visualized



Hands-On!

SLR with Perceptron

- We will construct a ‘neuron’ corresponding to a SLR model, and train with **gradient descent**

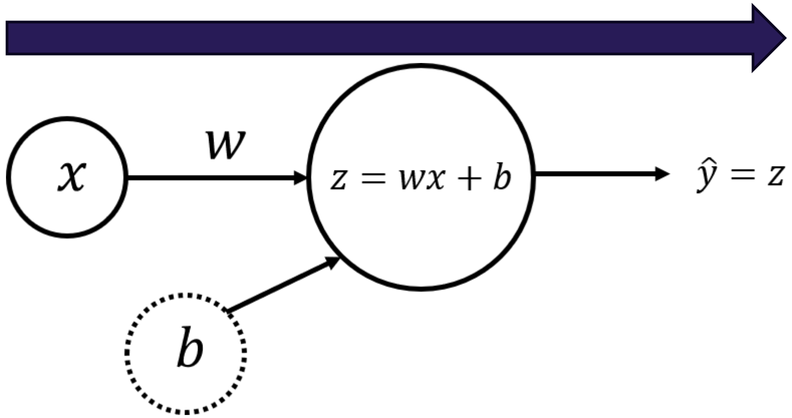


$$\hat{y} = wx + b$$

- **Weight** (*w*) and **bias** (*b*) are the parameters that will get updated when you **train** the model
- As in the previous SLR model, the goal is to identify parameters that minimize the average loss function: **cost function**

$$\mathcal{L}(w, b) = \frac{1}{2m} \sum_{i=1}^{m} \left(\hat{y}_i - y_i\right)^2$$

Training the model



- After defining the model structure,
  - — initialize parameters to some random values (or set to 0) and
  - — **update** as the training progresses
- For each training example (x_i, yi), predict $\hat{y}_i$:

$$z_i = wx_i + b,$$

$$\hat{y}_i = z_i,$$

where $i = 1, \ldots, m$

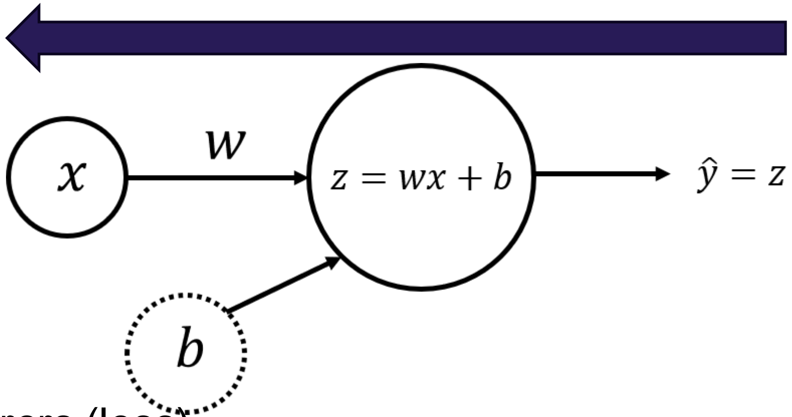
- Training examples are a vector $\boldsymbol{X}$ of size $(1 \times m)$
- Perform scalar multiplication of $\boldsymbol{X}$ by a scalar $\boldsymbol{w}$, adding $\boldsymbol{b}$.

$$Z = wX + b,$$

$$\hat{Y} = Z,$$

- This set of calculations is called **forward propagation**

Training the model

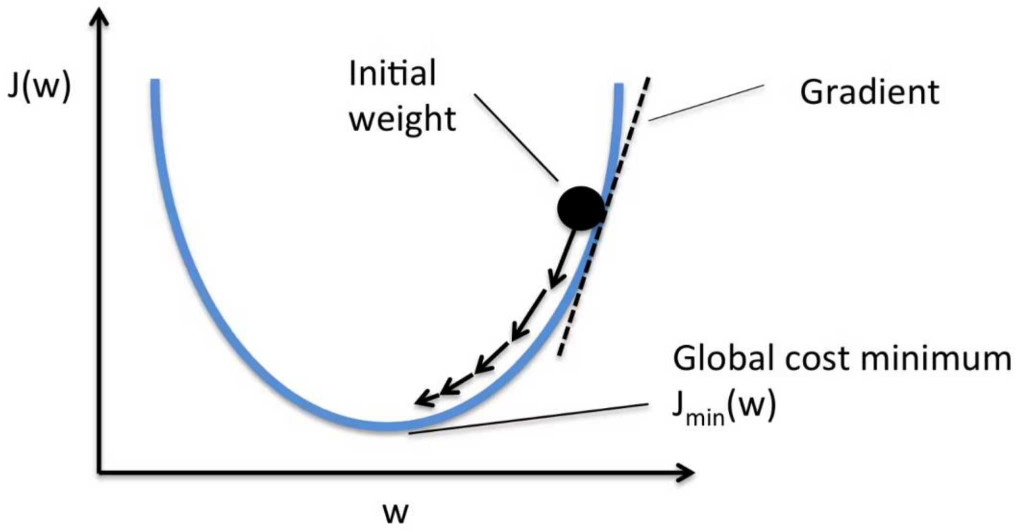


- Given $\hat{Y}$, calculate the cost function

$$\mathcal{L}(w, b) = \frac{1}{2m} \sum_{i=1}^{m} \left(\hat{y}_i - y_i\right)^2$$

  — Aim is to optimize the cost function during training, hence minimize the errors (loss)

- We minimize the cost function by use of an optimization algorithm, like **gradient descent**
  — Attempt to identify parameter values that minimize the cost function by taking partial derivatives of the cost function



We calculate partial derivatives as:

$$\frac{\partial \mathcal{L}}{\partial w} = \frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}_i - y_i\right) x_i,$$

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}_i - y_i\right)$$

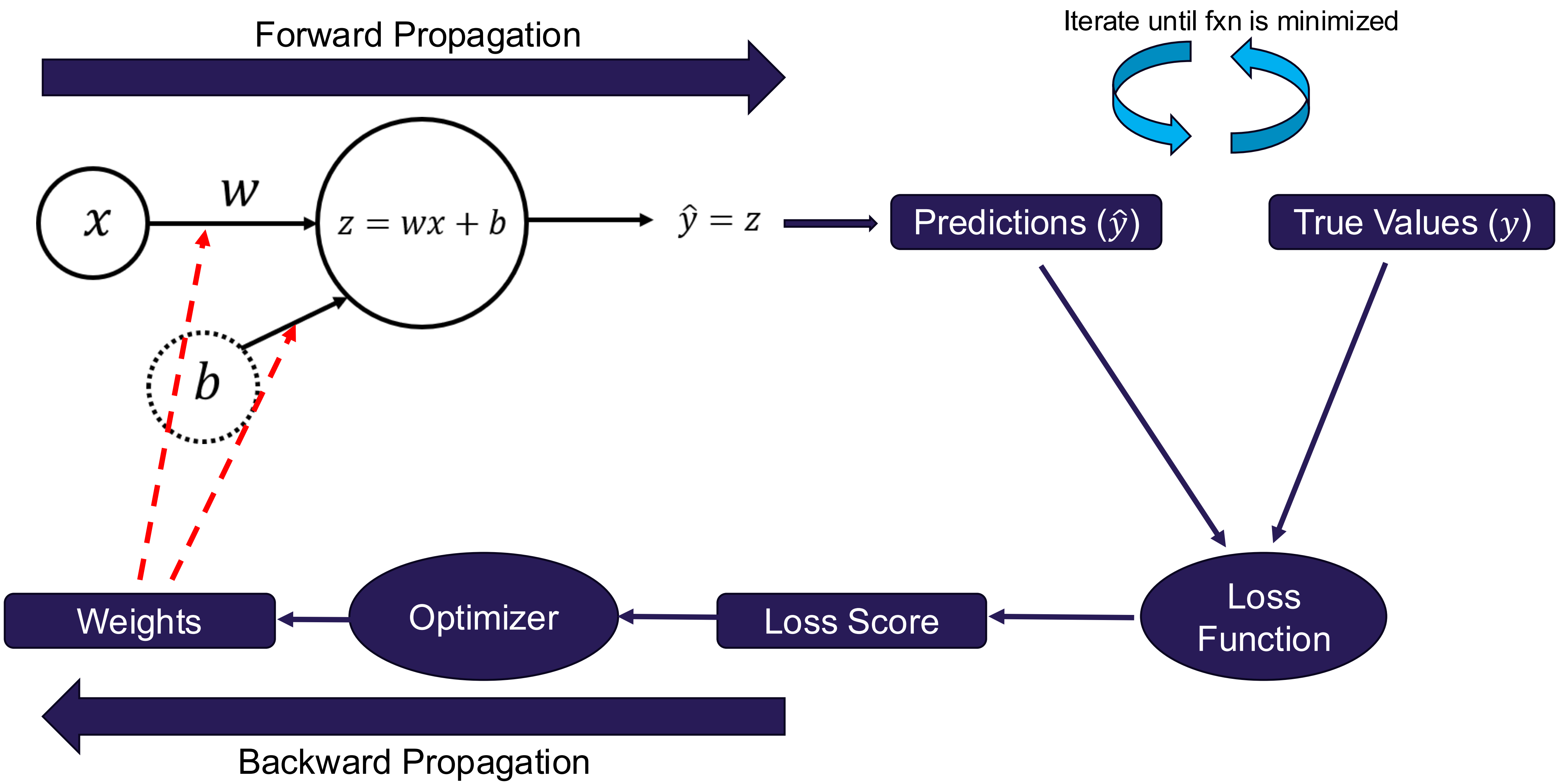
We then update the parameters iteratively using the expressions:

$$w = w - \alpha \frac{\partial \mathcal{L}}{\partial w},$$

$$b = b - \alpha \frac{\partial \mathcal{L}}{\partial b},$$ where α is the learning rate

- This set of calculations is called **backward propagation**

Training the model



Methodology to build a neural network

- Define the neural network structure (# of input units, # of hidden units, etc)

- Initialize the model's parameters

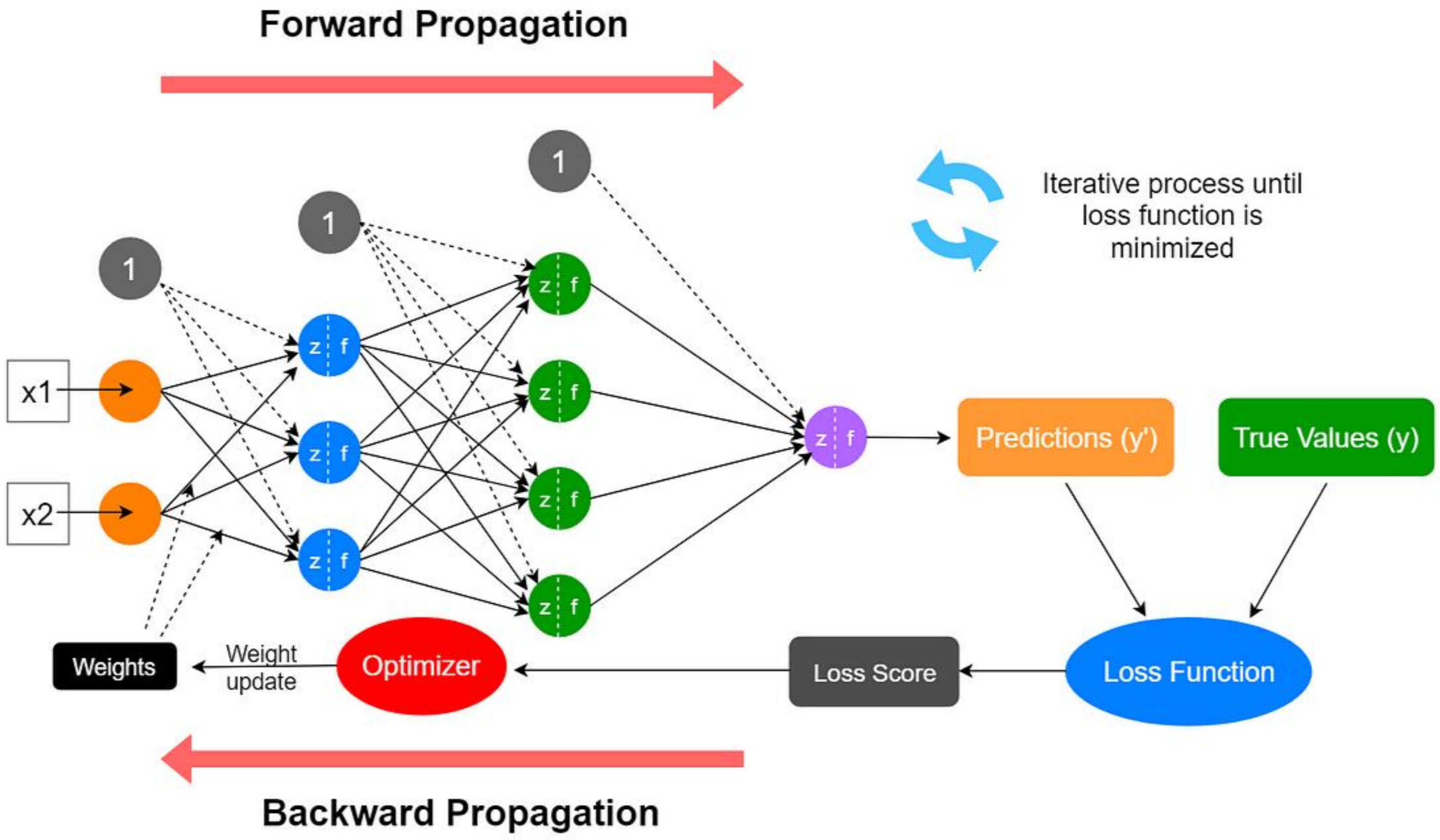
- Loop (iterate)
  - — Implement forward propagation (calculate the perceptron output)
  - — Implement backward propagation (to get the required corrections for the parameters)
  - — Update parameters

- Make predictions with “best” parameters

Hands-On!

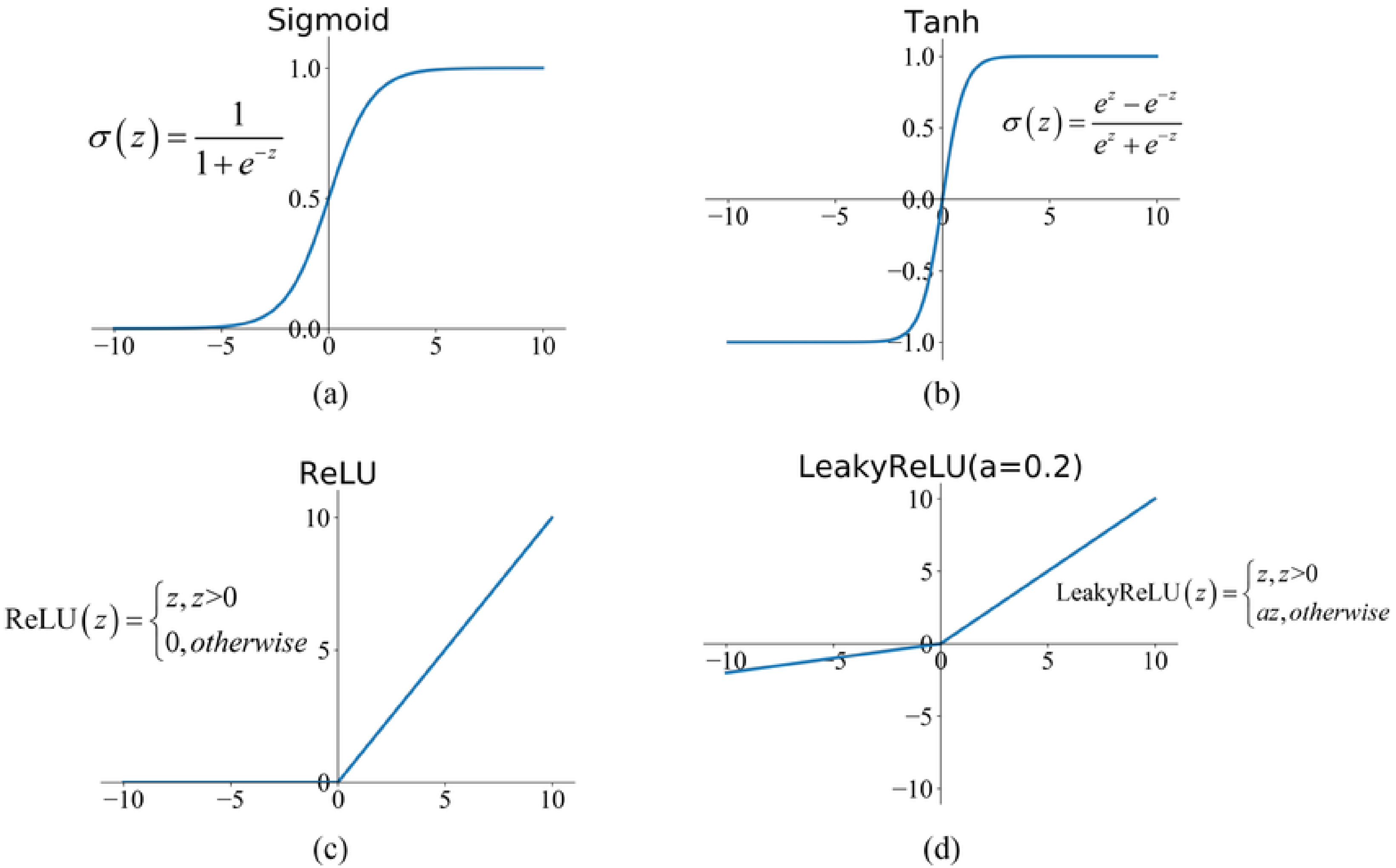
Let's Dive Deep! An Introduction to Deep Learning

The ***deep*** in deep learning: successive layers of data representation



Let's Dive Deep! An Introduction to Deep Learning

Commonly used activation functions



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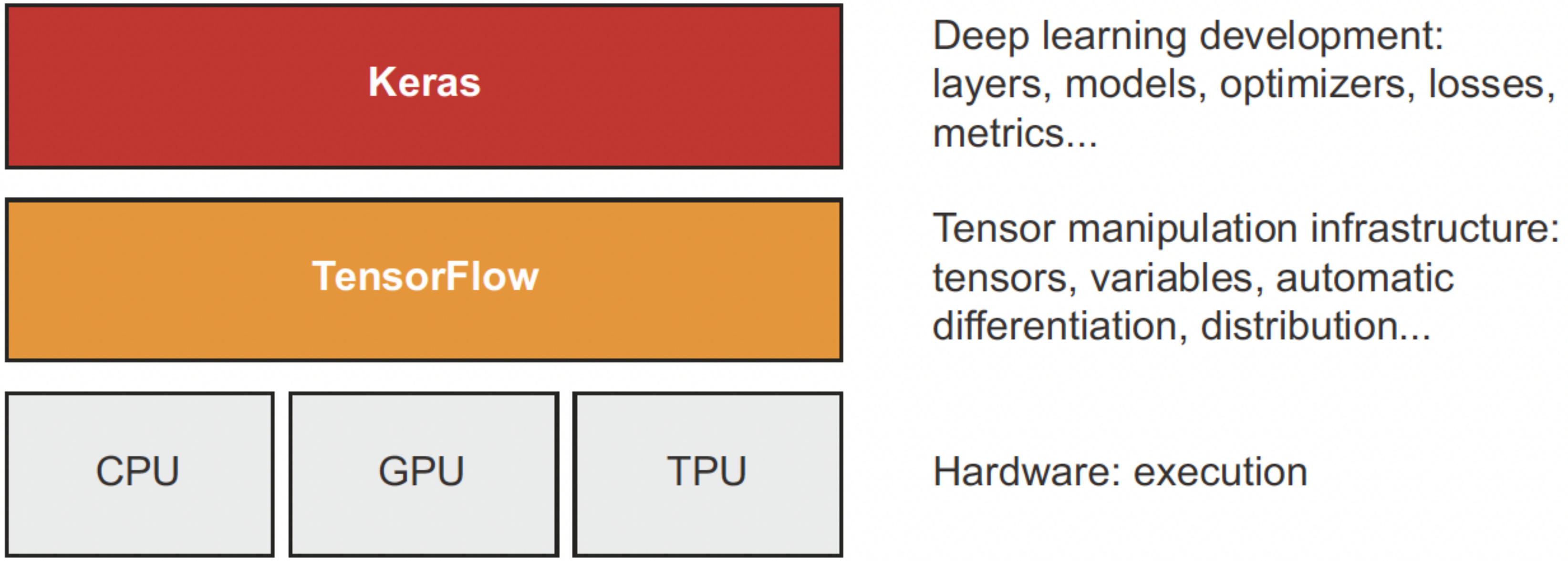
Let's Dive Deep! An Introduction to Deep Learning

You don’t have to build neural nets from scratch — somebody already did this for you!



Hands-On!

Questions?