THE UNIVERSITY of TENNESSEE KNOXVILLE

Lecture 29: Introduction to Deep Learning

Given by Mani Valleti

Instructor: Sergei V. Kalinin

What are Neural Nets?

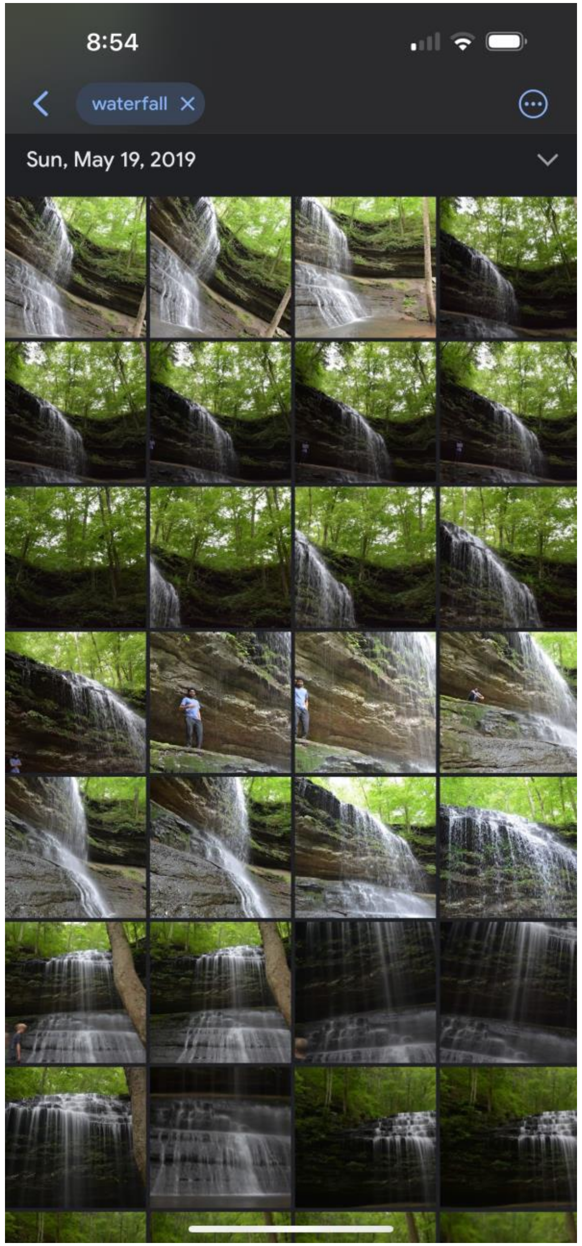
- Neural Networks are "glorified function fitters"
  - Suppose, you have an input set (X) and the corresponding outputs (y)
  - The neural nets approximate the function that maps X to y
    f: X→y
- How do they do that?
  - They have trainable parameters ranging from 100s to billions (175 billion in ChatGPT-3)
  - Given X and y, we tune the parameters such that the function approximation gets better
- Important terms that you need to know to understand how any neural net works:
  - Input-output pairs and how they are constructed
  - Neural network and it's architecture
  - Loss function to evaluate our predictions
  - Optimization algorithm (tuning) and its hyper-parameters

Applications: Image classification

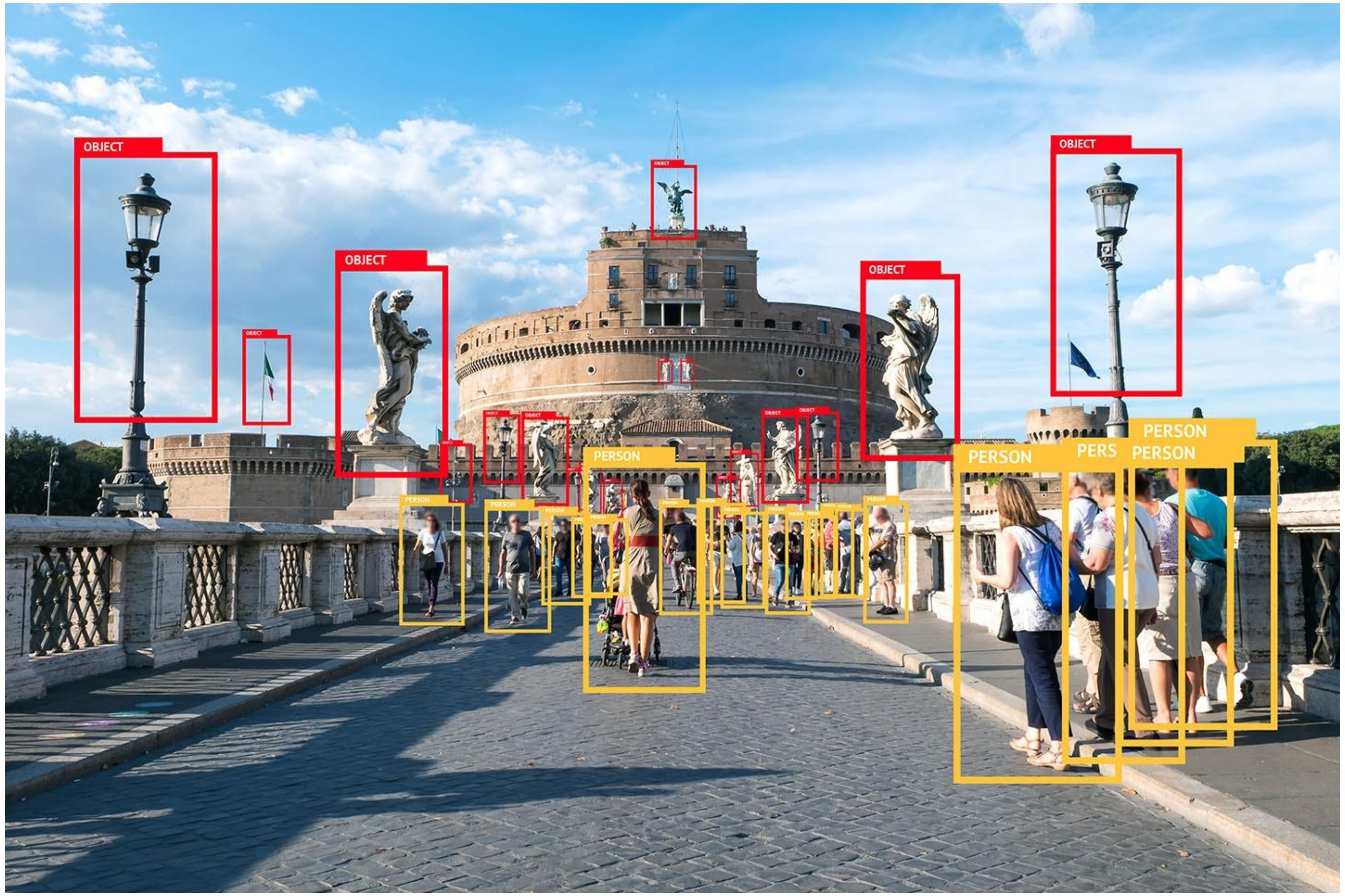
Dog

Dog

Cat

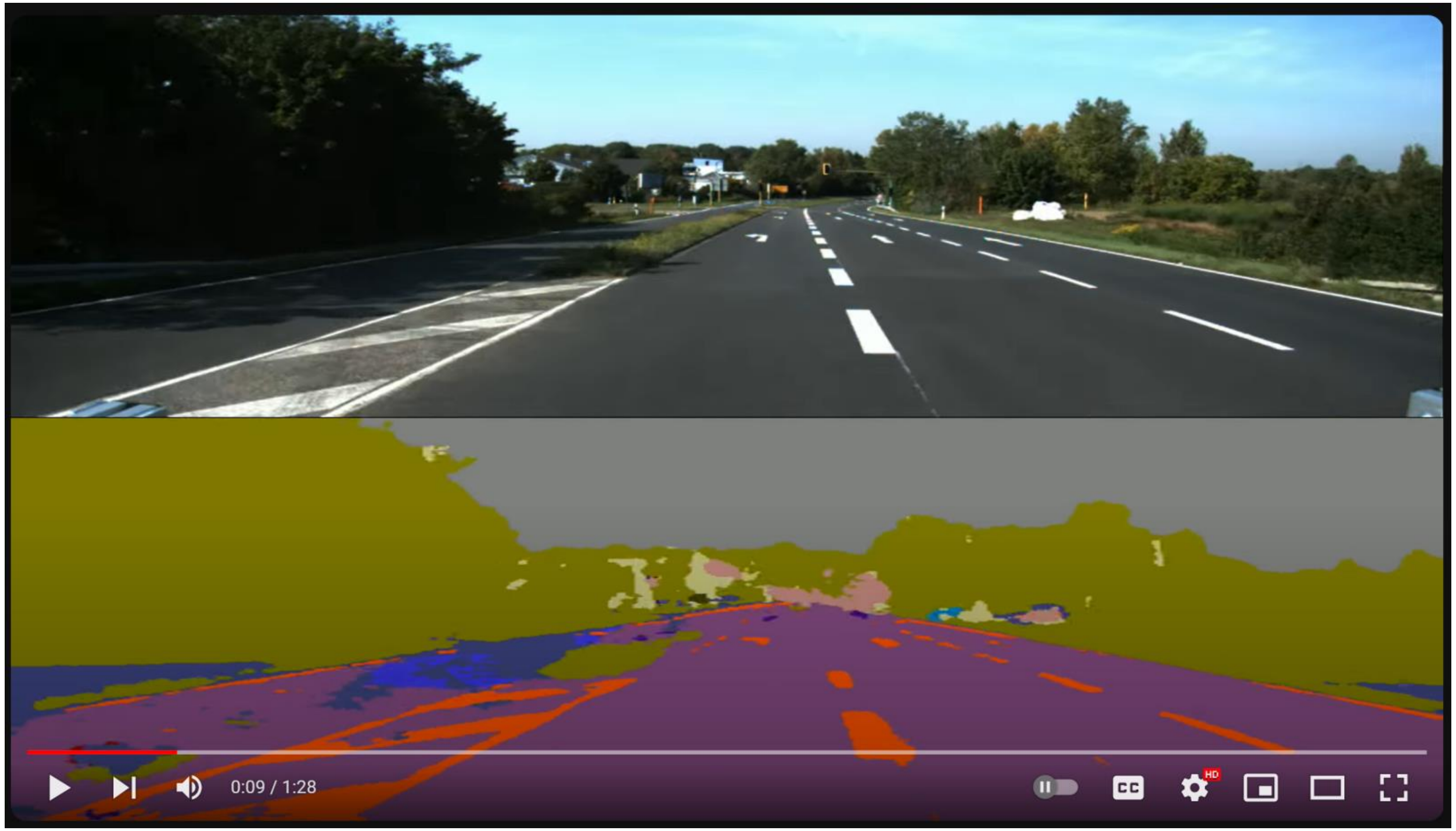


Applications: Object Detection



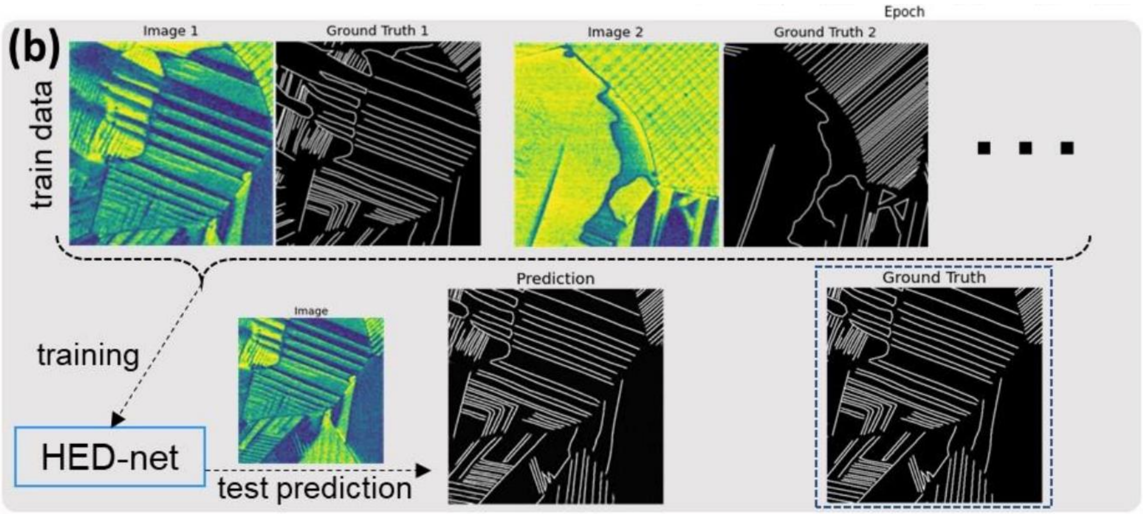
https://www.augmentedstartups.com/blog/how-to-implement-object-detection-using-deep-learning-a-step-by-step-guide

Applications: Semantic segmentation



https://youtu.be/e9bHTlYFwhg?t=9

Semantic segmentation continued…



Domain wall prediction from PFM images using ResHedNet, doi: https://doi.org/10.1002/adma.202103680

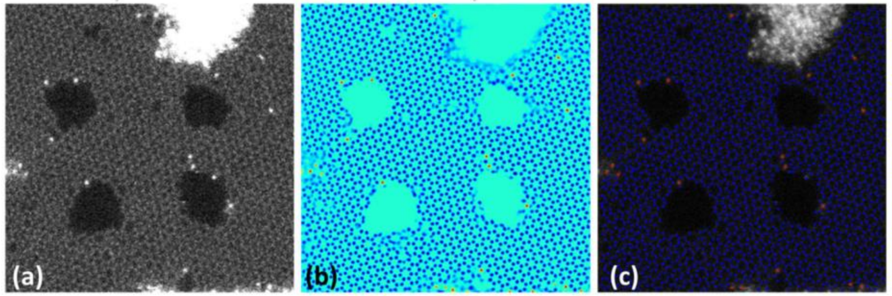


Figure 2. Experimental and deep learning-processed data. (a) Single image from dynamic STEM dataset corresponding to 10^{th} frame. (b) DCNN analysis of image in (a) illustrating pixel probability density corresponding to carbon (blue) and silicon (red) atoms. (c) Atomic coordinates of C and Si. Note that amorphous region (same as holes) remain unrecognized by the DCNN. Image size is 16 nm.

Getting atomic coordinates from STEM images. Doi: https://doi.org/10.1126/sciadv.abd5084

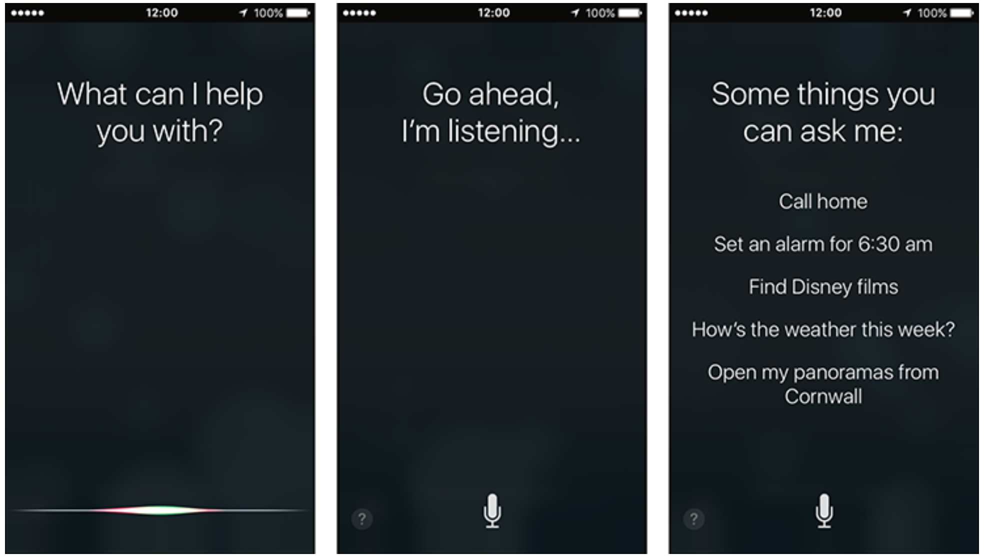
From the eyes of a Tesla

https://www.youtube.com/watch?v=fKXztwtXaGo

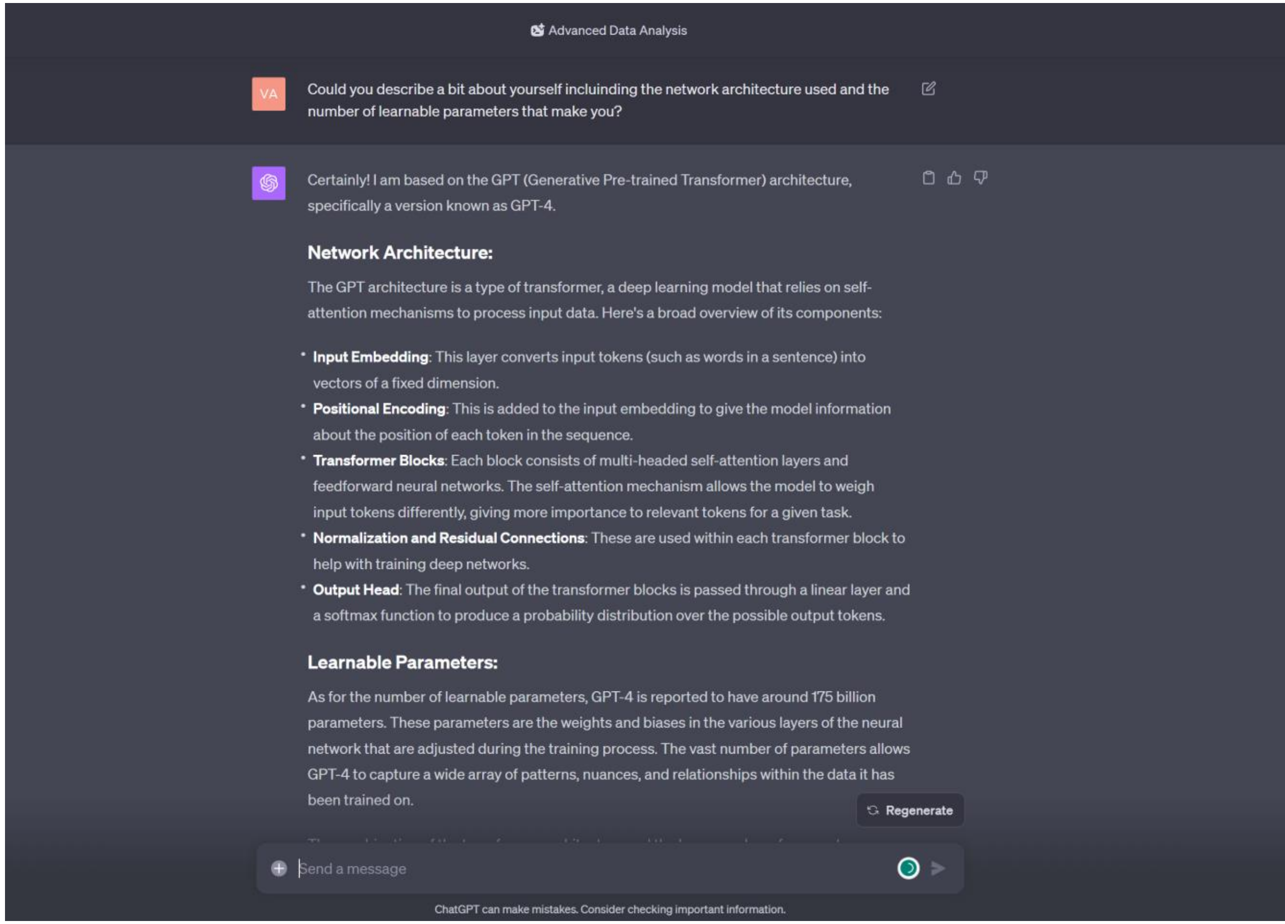
Applications: Activity recognition

https://youtu.be/qrzQ_AB1DZk?t=5

Applications: Language models



Hey Siri! Image from: https://accessibility.baesystems.com/siri-iphoneipadipod-touch

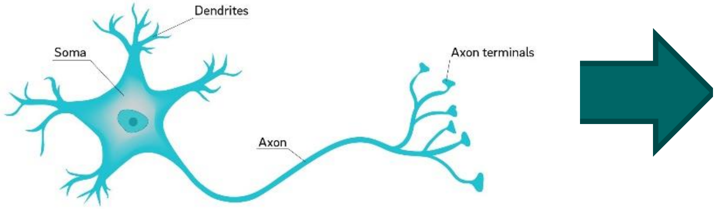


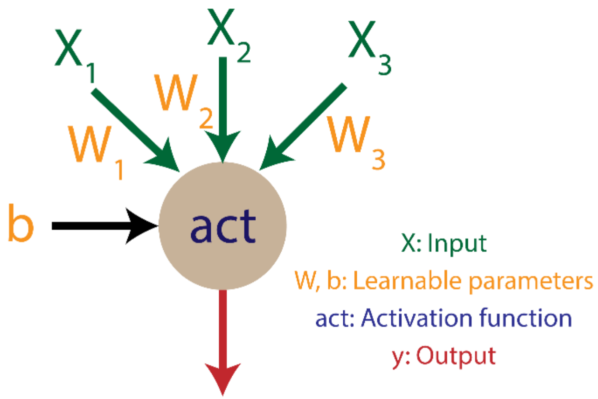
ChatGPT

You can find a plethora of other examples from various disciplines like science, robotics, art, medical imaging.

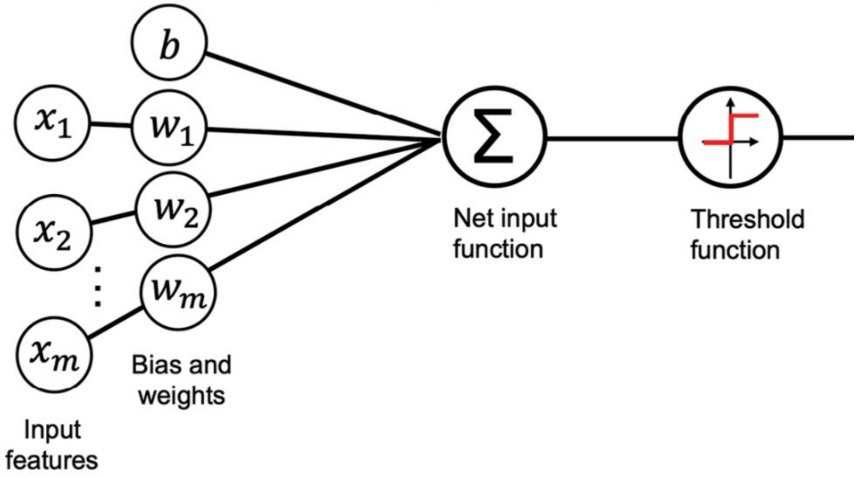
“Neuron”

- Artificial neuron is weakly inspired from the biological neuron
- Biological neuron receives its inputs from dendrites, decides whether to fire, and communicates its output *via*., axon terminals
- Artificial neuron works on the same principle as you have seen from the previous lectures



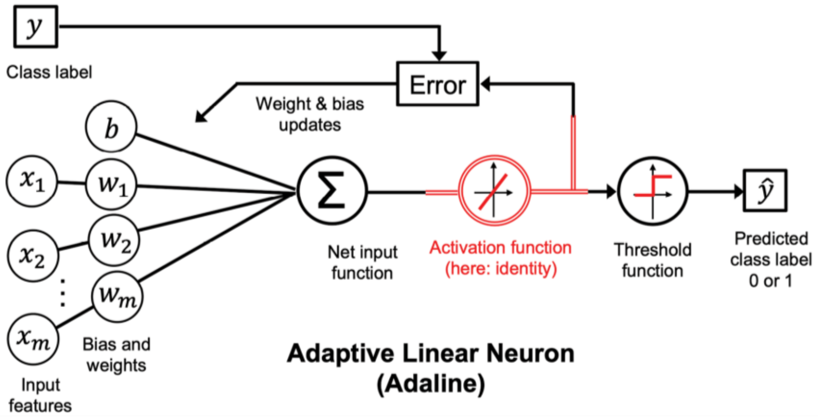


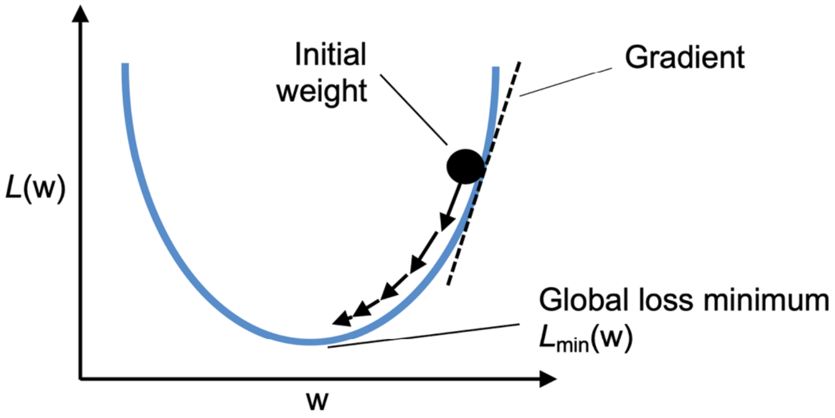
$$y = act(W_1X_1 + W_2X_2 + W_3X_3 + b)$$



Linear Neuron from Lecture-06

Quick review into Adaline





Loss function:

$$L(\boldsymbol{w}, b) = \frac{1}{n}\sum_{i=1}^{n}\left(y^{(i)} - \sigma(z^{(i)})\right)^2$$

Weights update:

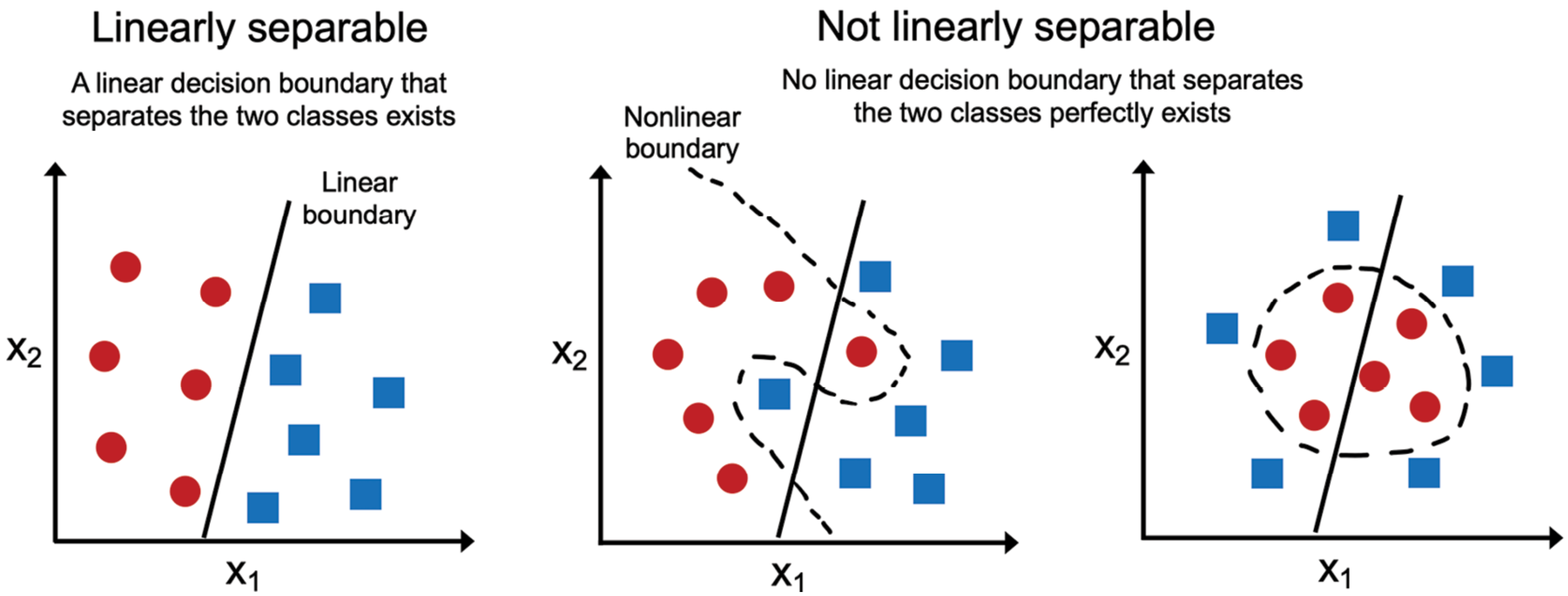
$$\boldsymbol{w} := \boldsymbol{w} + \Delta\boldsymbol{w}, \quad b := b + \Delta b$$

Learning rule:

$$\Delta\boldsymbol{w} = -\eta\nabla_{w}L(\boldsymbol{w}, b), \quad \Delta b = -\eta\nabla_{b}L(\boldsymbol{w}, b$$

Issues with Adaline

- Linear Decision Boundaries: It can only draw straight-line (linear) decision boundaries.
  - Many real-world problems are not linearly separable.
- Limited feature interactions: It does not account for feature interactions.
  - Real-world data often contains features that influence predictions in a non-linear and interdependent way



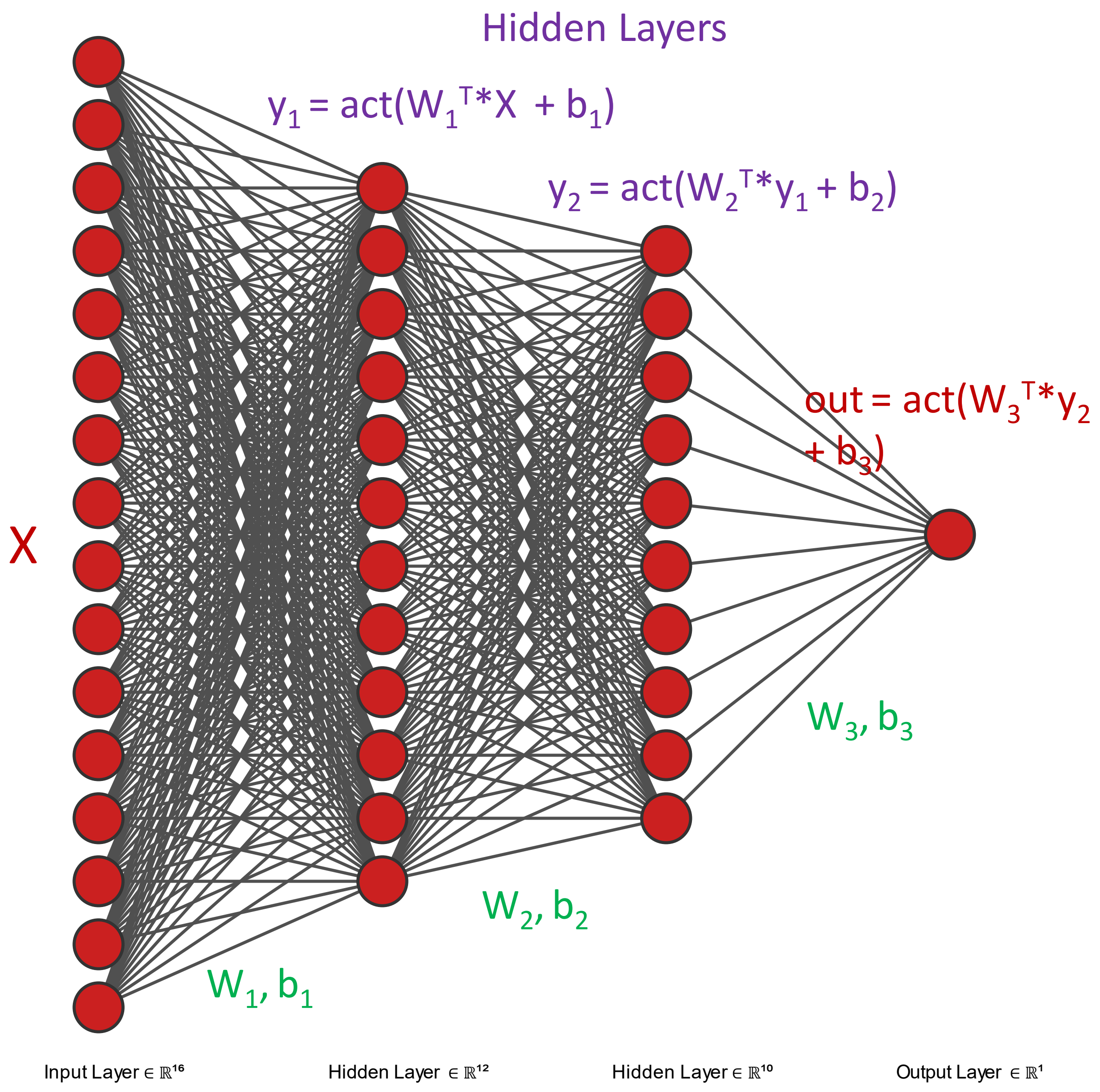
Enter the realm of Deep Neural networks

- Composed of multiple layers of artificial neurons, mirroring the complexity of a human brain.

- Each layer processes inputs received, applies a transformation (weights, biases, activation function), and passes the output to the next layer.

- Training a DNN involves adjusting weights and biases using backpropagation and a chosen optimization algorithm.

- The deep architecture enable the network to learn complex and abstract patterns in data.

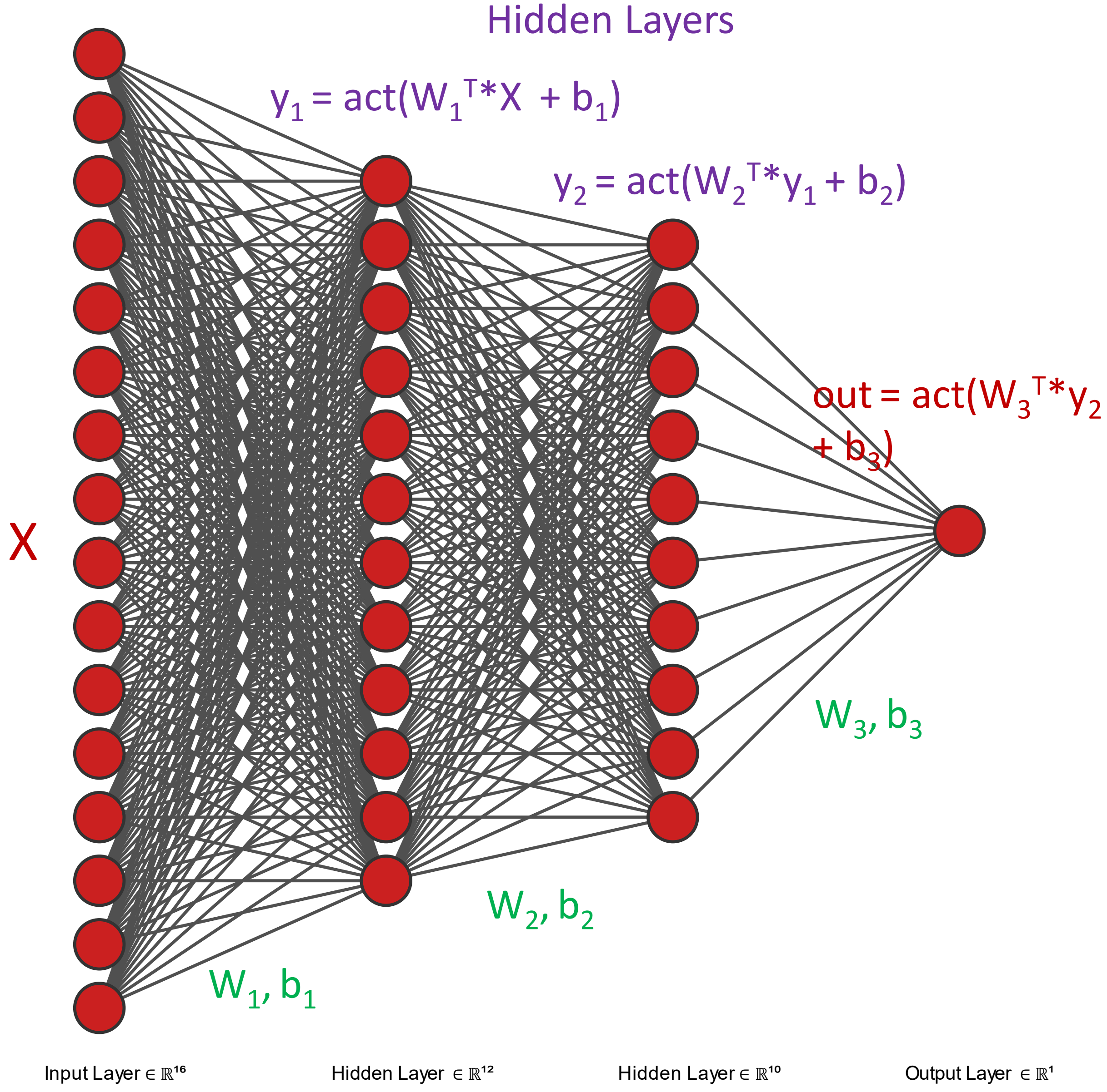


Delving deep: Layers

- Each layer processes inputs received, applies a transformation (weights, biases, activation function), and passes the output to the next layer.

- The next layer then takes the output of the previous layer and does the same.
    - The keyword ‘DEEP’ arises from this process

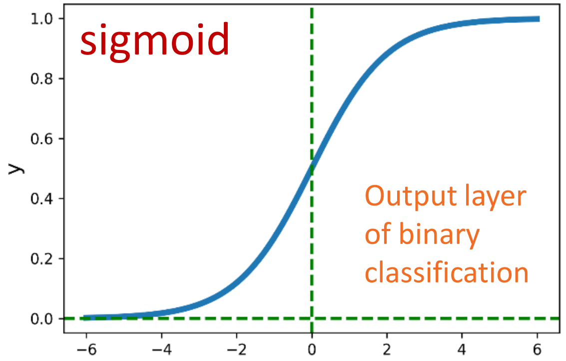
- Lower-level features can be combined and recombined in subsequent layers, allowing the network to build up a representation of feature interactions in a data-driven way.

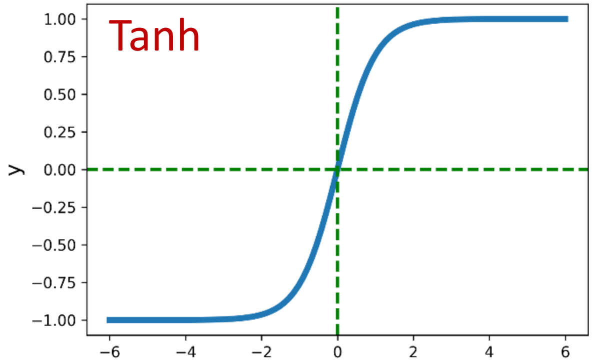


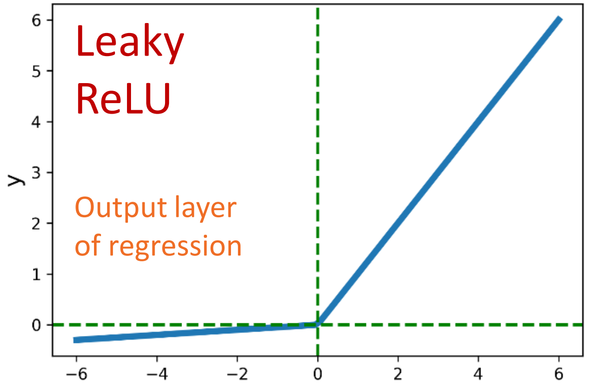
Delving deep: Activation functions (Non-linearity)

- Activation functions introduce non-linearity to the neuron's output.

- Without them, the whole neural network can be replaced by a simple linear regression.







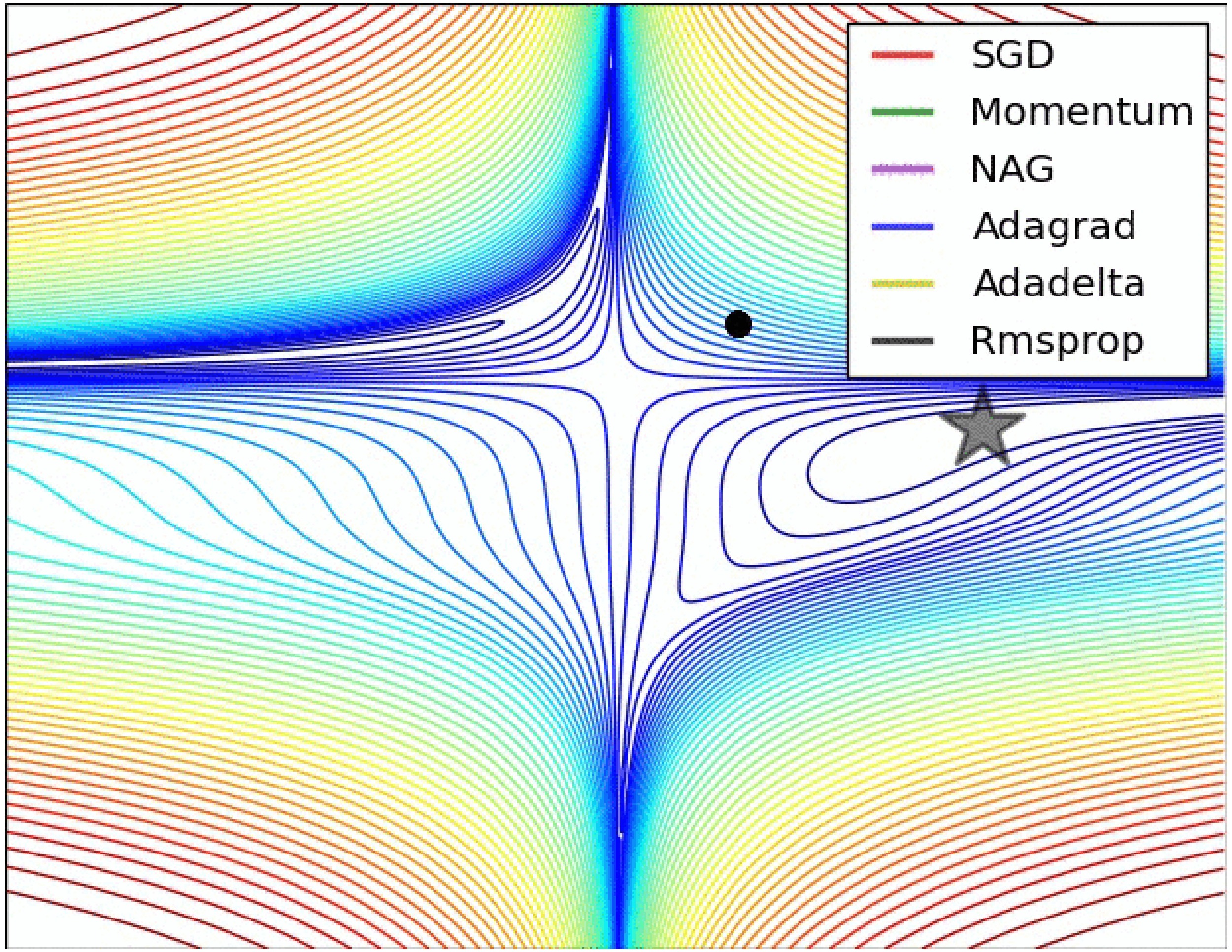
- Softmax activation function is another widely used activation function
- Usually, in the last layer of multi-class classification problem

Delving deep: Learning

- The error in our predictions is back-propagated through the network.
- This is done using gradient-descent algorithms.
- Gradient of the error with respect to the weights is calculated and the weights are updated using the learning equation:

$$\boldsymbol{w} := \boldsymbol{w} + \Delta\boldsymbol{w}, \quad b := b + \Delta b$$

$$\Delta\boldsymbol{w} = -\eta\nabla_{w}L(\boldsymbol{w}, b), \quad \Delta b = -\eta\nabla_{b}L(\boldsymbol{w}, b)$$



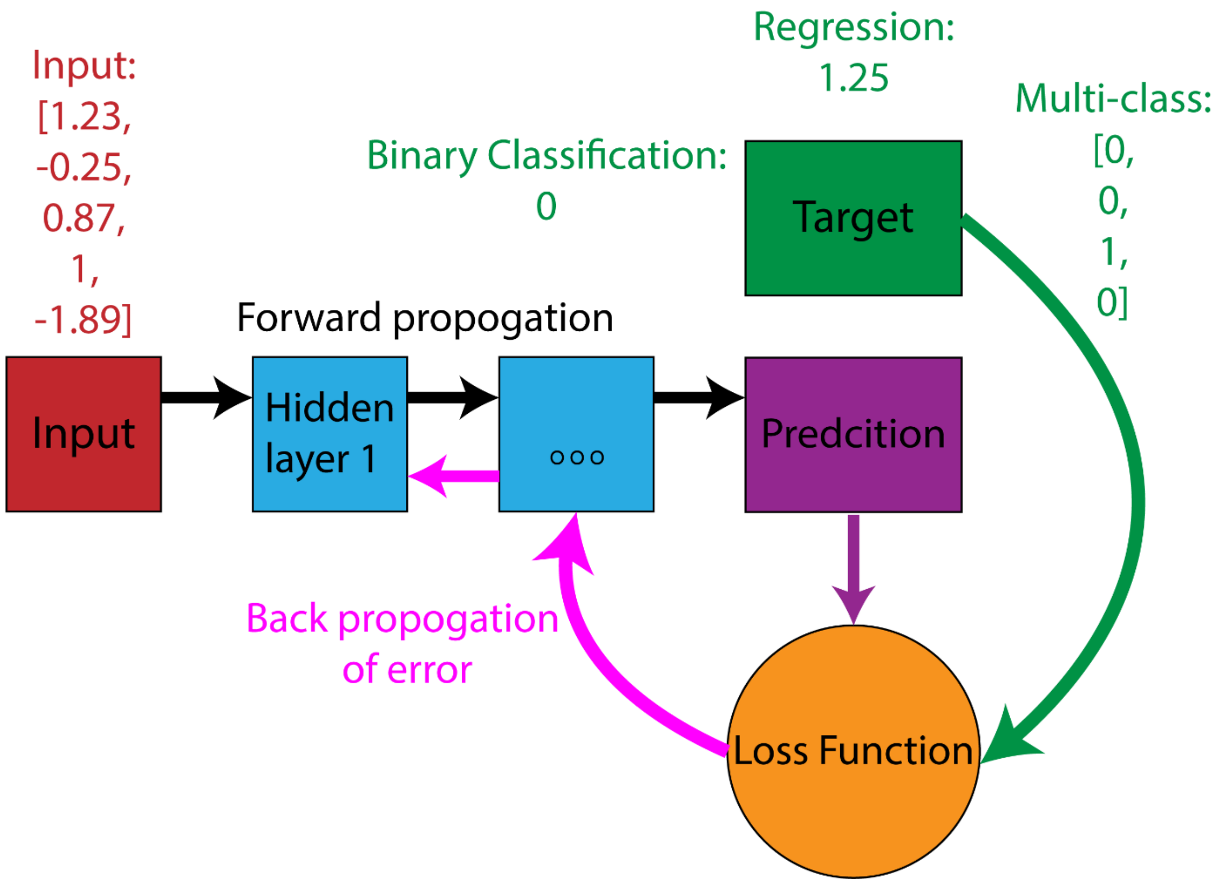
https://www.analyticsvidhya.com/blog/2021/10/a-comprehensive-guide-on-deep-learning-optimizers/

Hyperparameter tuning

- Hyperparameters are the configuration settings used to structure the neural network and guide the learning process.
- Unlike weights, hyperparameters are not learned from the data but set prior to the training process.
    - Number of Layers and Neurons: Too few may lead to underfitting, while too many can cause overfitting and increased computational cost.
    - Learning Rate: If it's too high, the model may overshoot minima; if too low, training may be slow or get stuck in local minima.
    - Batch size: Influences the accuracy of the gradient estimation and can affect both the speed of convergence and the stability of the learning process.
- How do we do it?
    - Grid Search
    - Random Search
    - Bayesian Optimization
    - Leveraging Experience: One can use their knowledge from previous projects to choose a good starting point for hyperparameter settings. This intuition, built from empirical evidence of what has worked in the past, can significantly reduce the search space and lead to faster convergence on optimal or near-optimal configurations.

Overview on ML tasks

- **Input:**
  - Typical input to a FCNN is a column vector of features that describe a datum.
  - The features are spatially independent of each other.
  - Advanced network architectures deal with spatially correlated data (CNN), temporal data (RNN), and graph data(GNN).



- **Regression**
  - **Target:** Continuously varying quantity
  - **Loss Functions:** Root mean squared error (RMSE), Mean absolute error (MAE)

- **Classification**
  - **Target:** Divided into classes
    - 0 or 1 for a binary class classification
    - One-hot encoded vector for multi-class classification
  - **Loss Functions:** Binary cross entropy loss (BCE) for binary classification and cross-entropy loss (CE) for multi-class classification

Convolutional Neural Network (CNN)

• Convolutional Neural Networks (CNNs) are a class of deep learning models, applied to analyzing visual imagery.
•CNNs are invariant to object position and distortion in the scene.
•CNNs use fewer parameters than fully connected networks, which makes them computationally efficient.

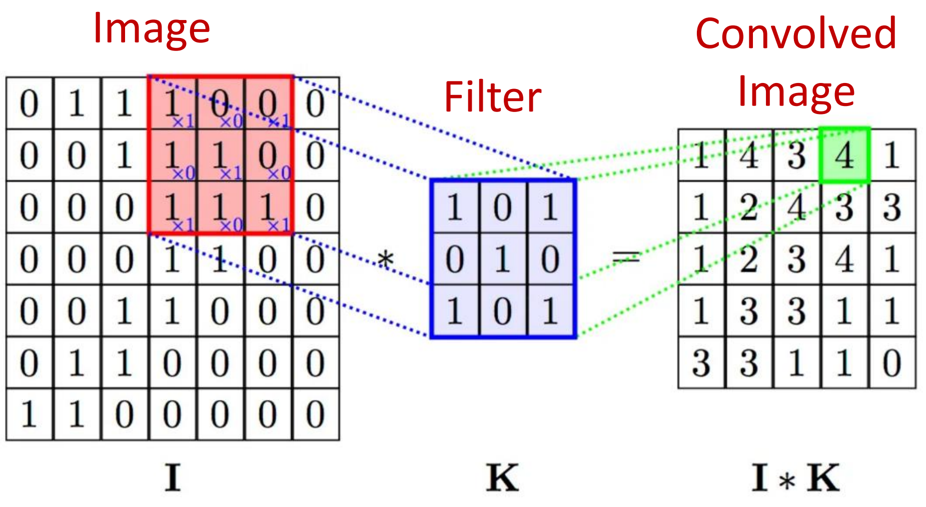
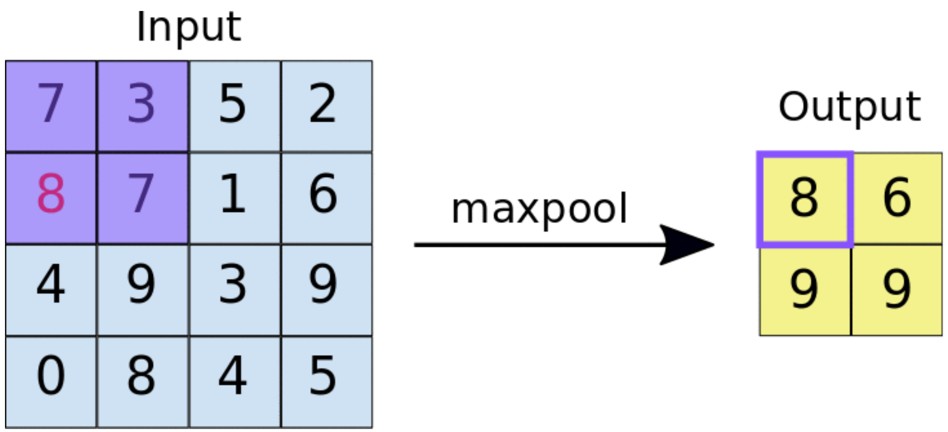


Image convolution

Two major components of CNN:

- Convolutions (kernel size, stride, and padding):
  - Filter or "kernel“ (learnable parameters is passed over the input data
  - Performs element-wise multiplication and sums up the results to produce a transformed version of the input (feature map)
- Pooling (subsampling or downsampling):
  - Used to reduce the dimensionality of the feature map
  - Min, max, and mean are the most commonly used.



Max pooling layer

Developing intuition (If time permits)

https://colab.research.google.com/drive/1jvKJlQSRBsaIiqAQbzdkE7gWRknQjqpW#scrollTo=KTf9s58dWP6F