HPML Group 11/01/2023

Deep Learning

Introduction Series

Bryan Cardenas
Thomas van Osch

SURF

Prerequisites

Programming

R / Python

Statistics, Calculus

Machine Learning

Parallel Computing

Plan for Today

01.

General Introduction

Machine Learning

02.

Neural Networks

Dense and Convolutions

03.

Language Modelling

Recurrence and Transformers

04.

High Performance

How can I train efficiently?

Machine Learning

High Performance Machine Learning Group

What ML is *not*:

Mimicking human intelligence

Robotics

Deep Learning

What ML is *not*:

Mimicking human intelligence

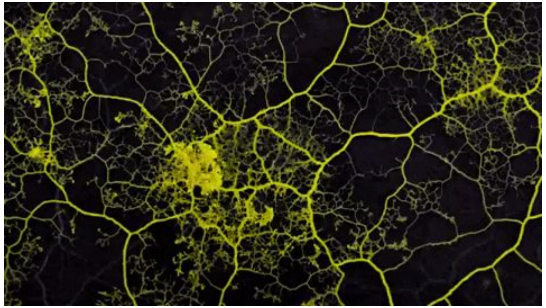
Robotics

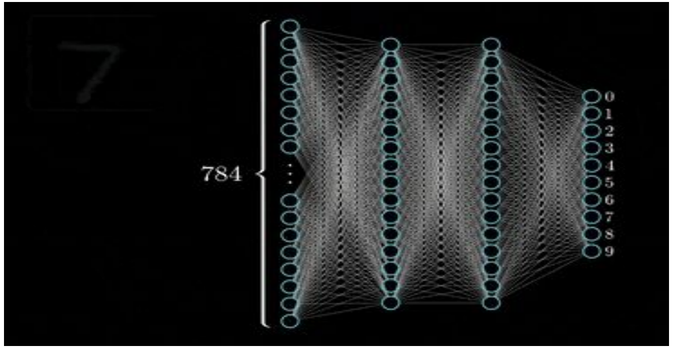
Deep Learning

> “ML is the study of algorithms that can improve through experience and by the use of data. It is seen as part of Artificial Intelligence
>
> ~ Wikipedia

Artificial Intelligence

Having computers to exert Intelligent behaviour



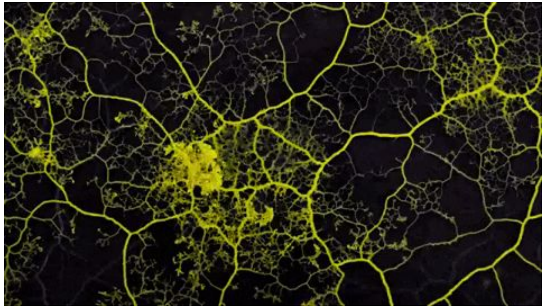


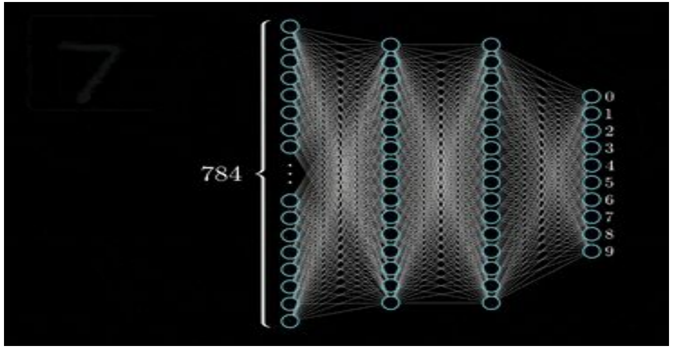
Artificial Intelligence

Having computers to exert Intelligent behaviour

Machine Learning

Perform tasks without Explicitly programmed from data





Artificial Intelligence

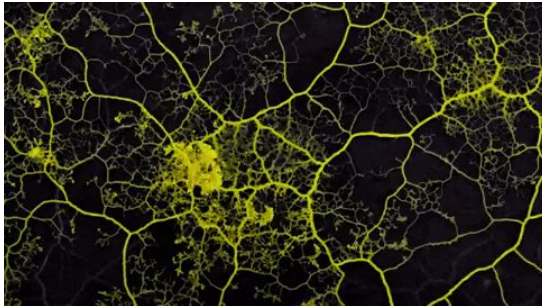
Having computers to exert Intelligent behaviour

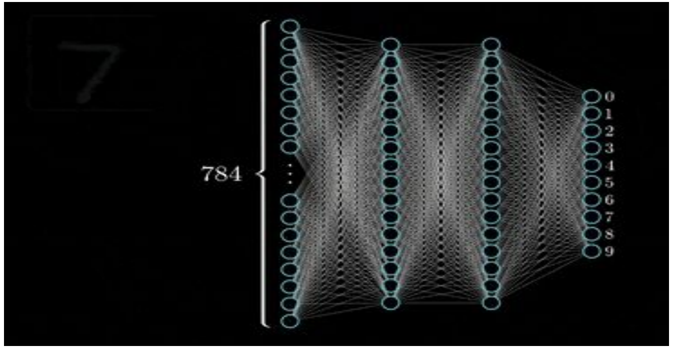
Machine Learning

Perform tasks without Explicitly programmed from data

Deep Learning

Use deep neural networks



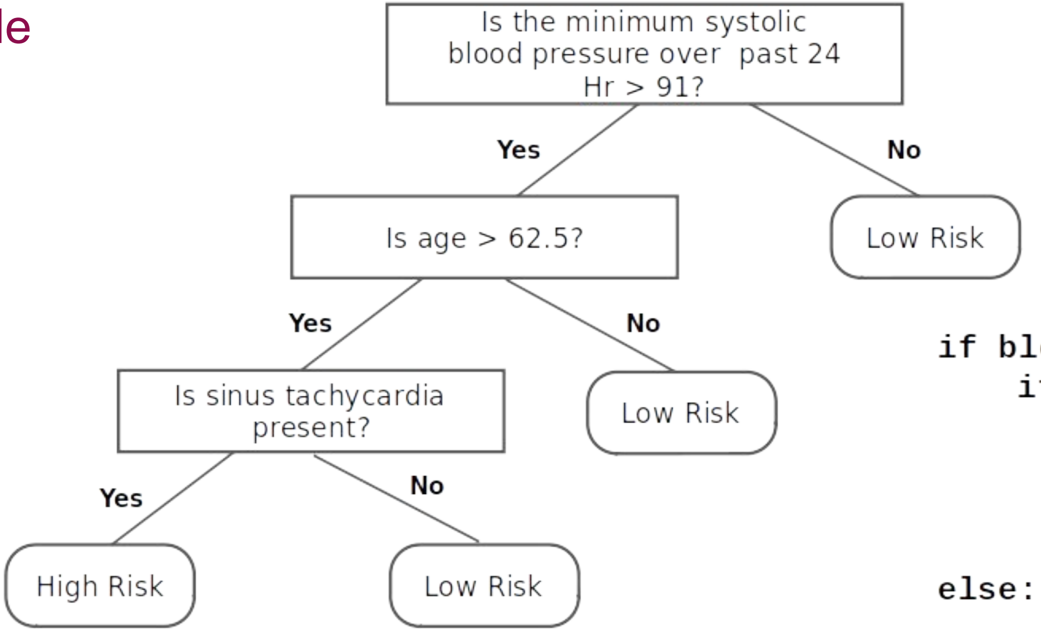


Why Machine Learning?

Think of a simple
decision tree

Why Machine Learning?

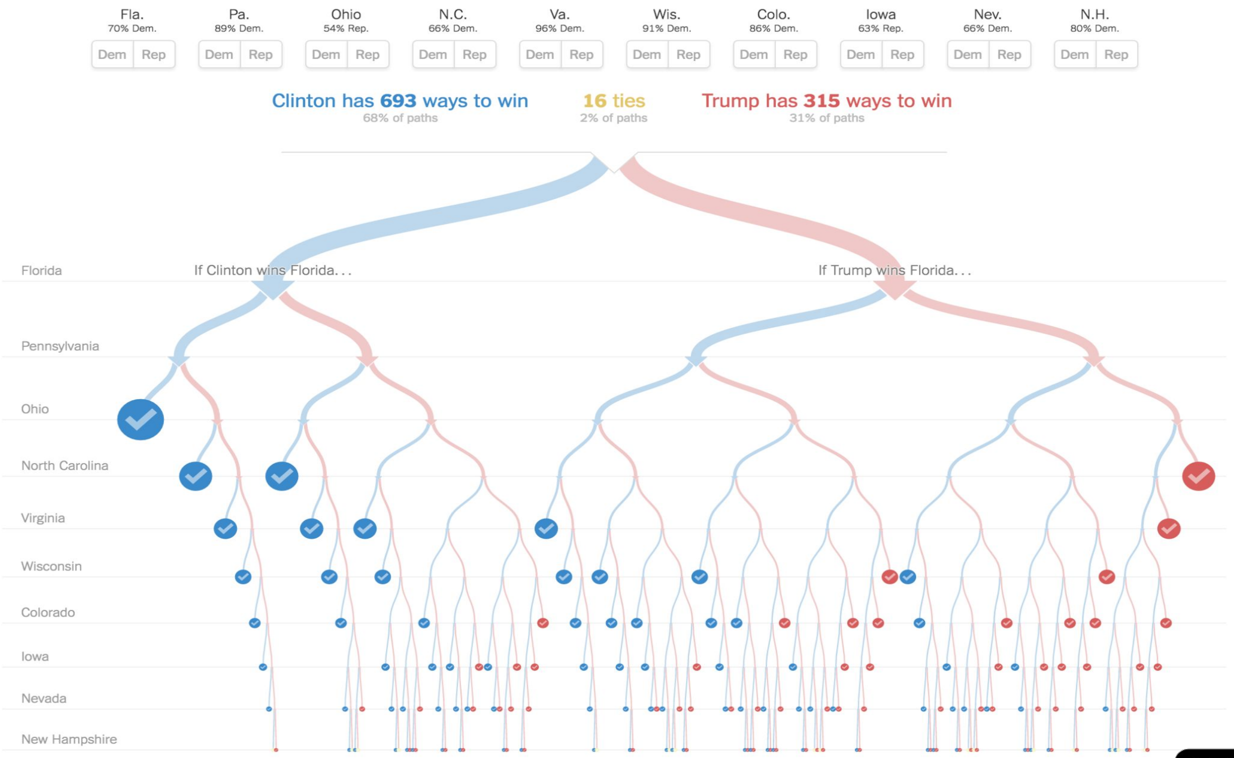
Think of a simple **decision tree**




```
if blood_pressure > 91:
    if age > 62.5:
        if sinus_tach:
            …
        else:
            …
else:
    …
```

Why Machine Learning?

Think of a *hard* **decision tree**

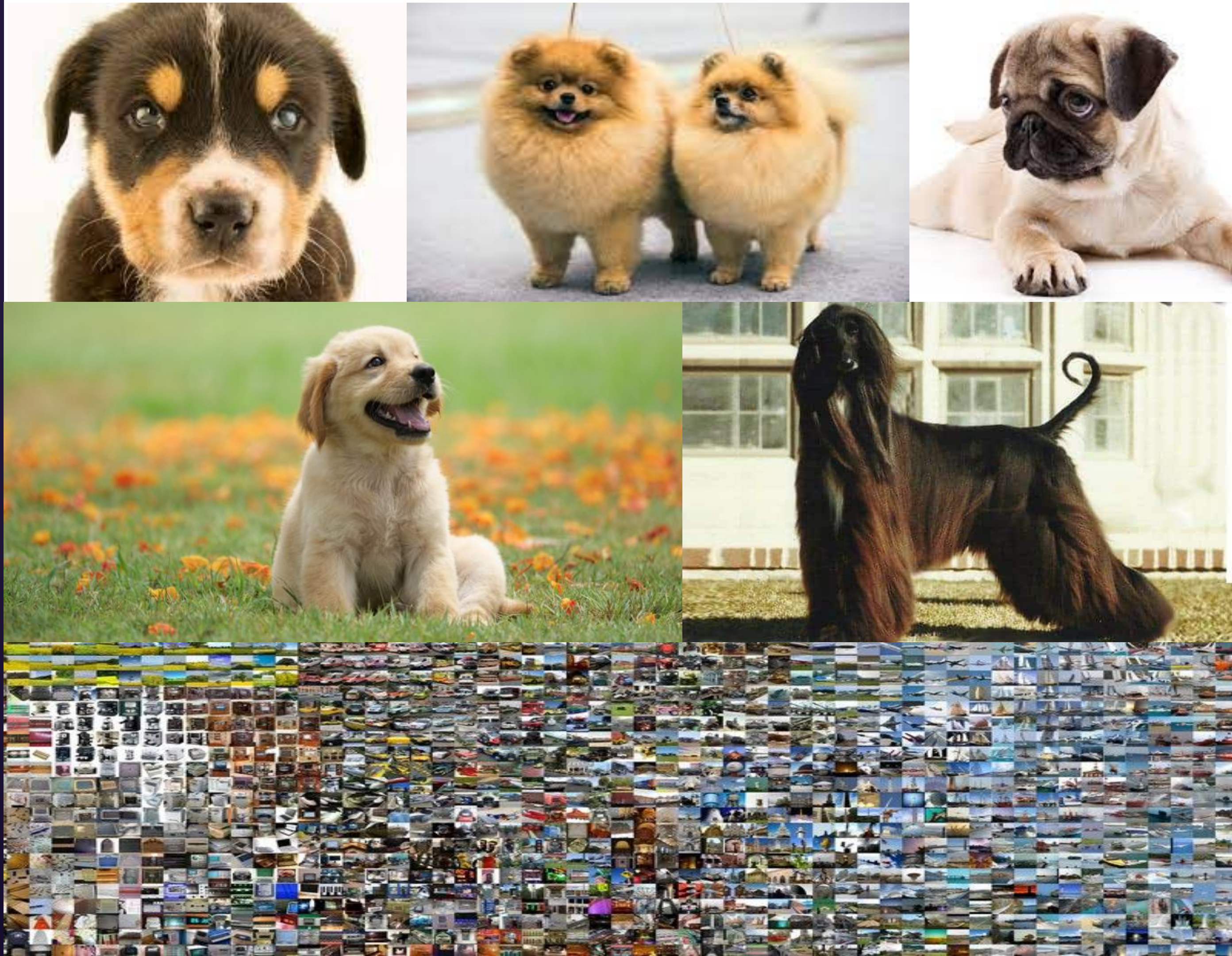


What is a dog?

Uncountable features that define a dog

We want an automatic way of learning these features

Driven by Data



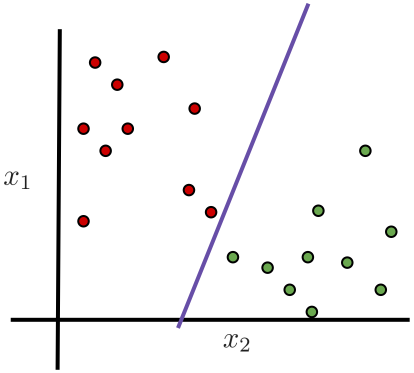
Categories of Machine Learning

01.

Supervised

Learn from labels

Regression, Classification

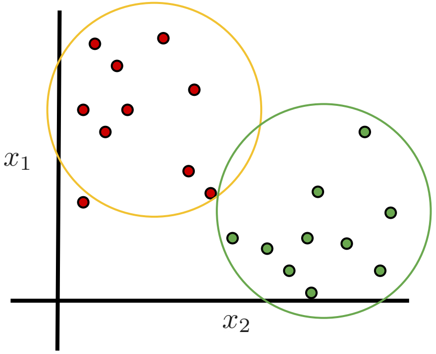


02.

Unsupervised

Detect Patterns in the data

Clustering, Dimensionality Reduction

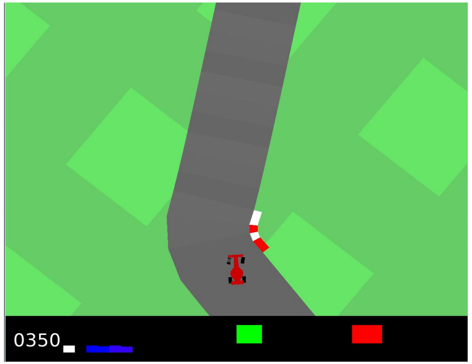


03.

Reinforcement

Learn from the environment

Control, gaming



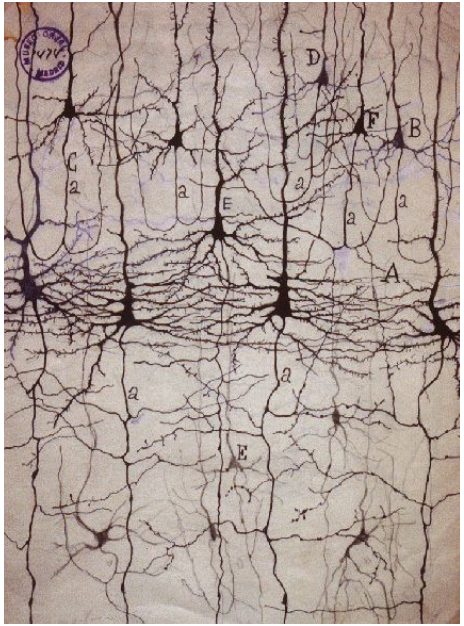
Neural Networks

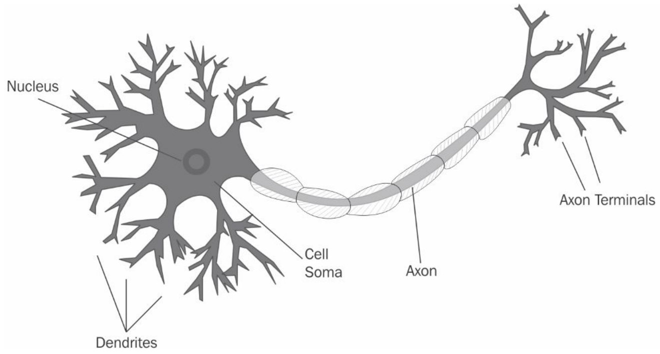
High Performance Machine Learning Group

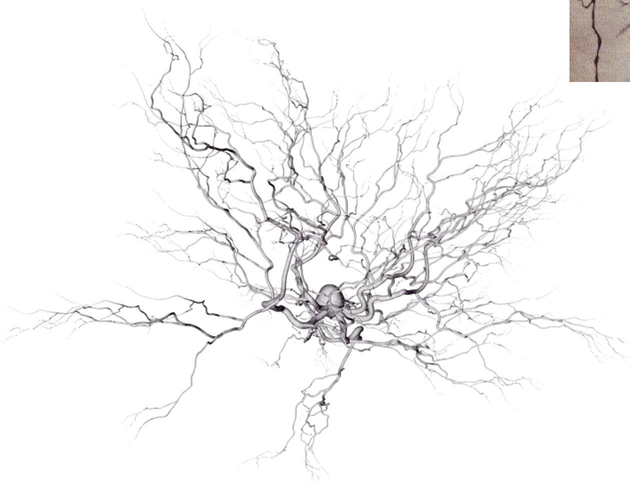
Biological Neuron

A neuron inhibits or excites a signal picked up from its receivers

Only fires if a threshold is reached and is connected to thousands of others.





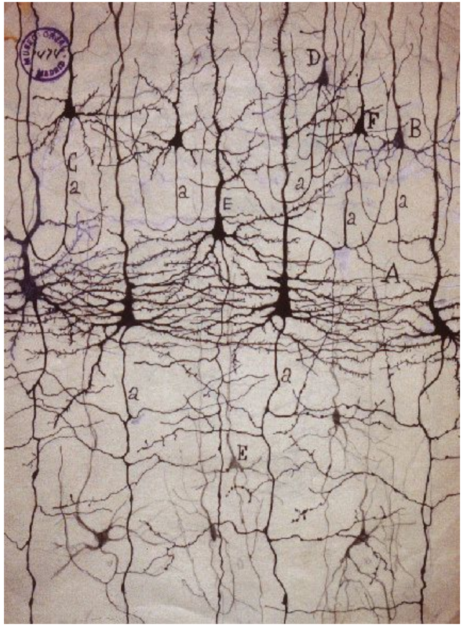


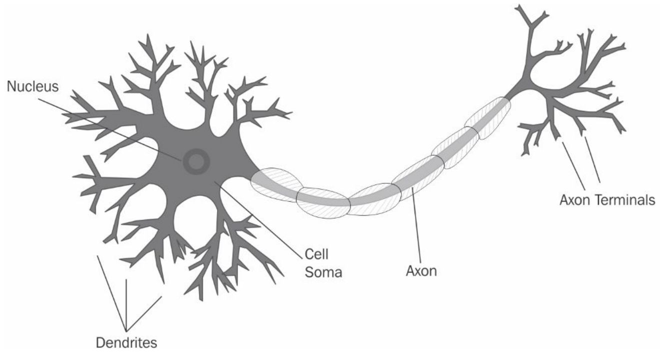
Biological Neuron

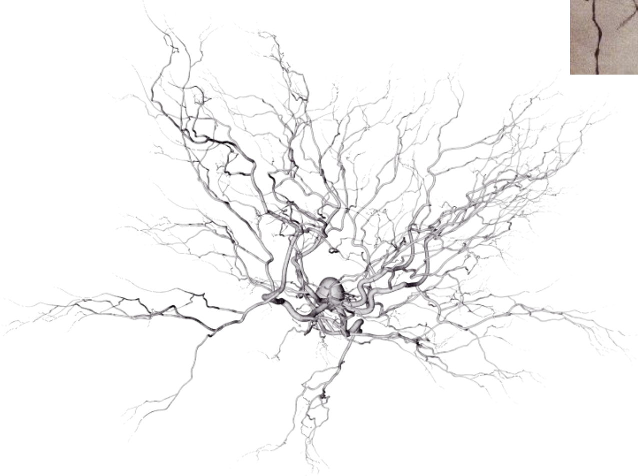
A neuron inhibits or excites a signal picked up from its receivers

Only fires if a threshold is reached and is connected to thousands of others.

Humans have around 80 billion neurons and trillions of connections

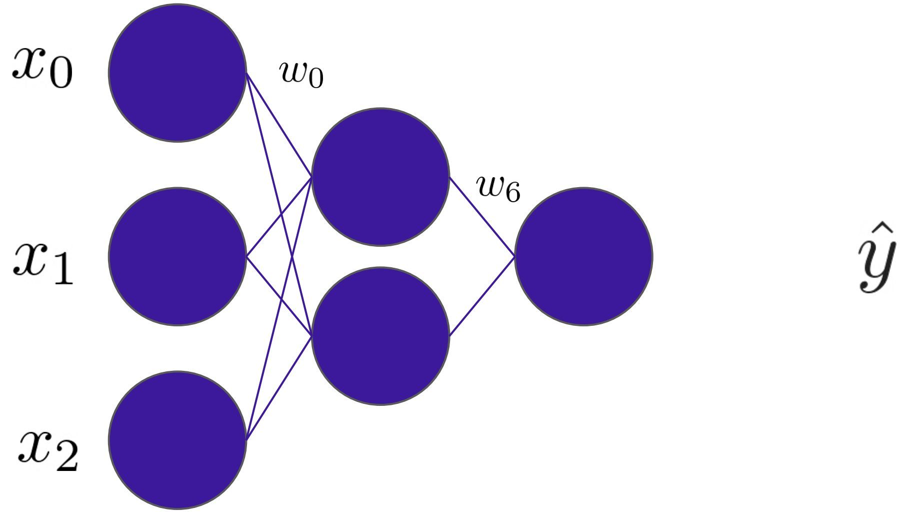






Anatomy of an Artificial Neural Network

Don’t model the biological neuron **precisely**

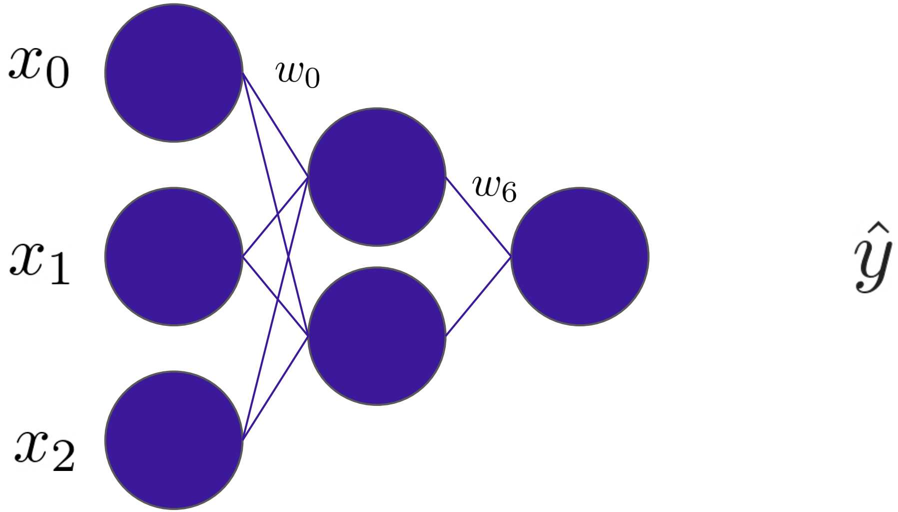


SURF

Anatomy of an Artificial Neural Network

Don’t model the biological neuron **precisely**

- Inputs
- Bias
- Weights
- Dot product
- Non-linear activation

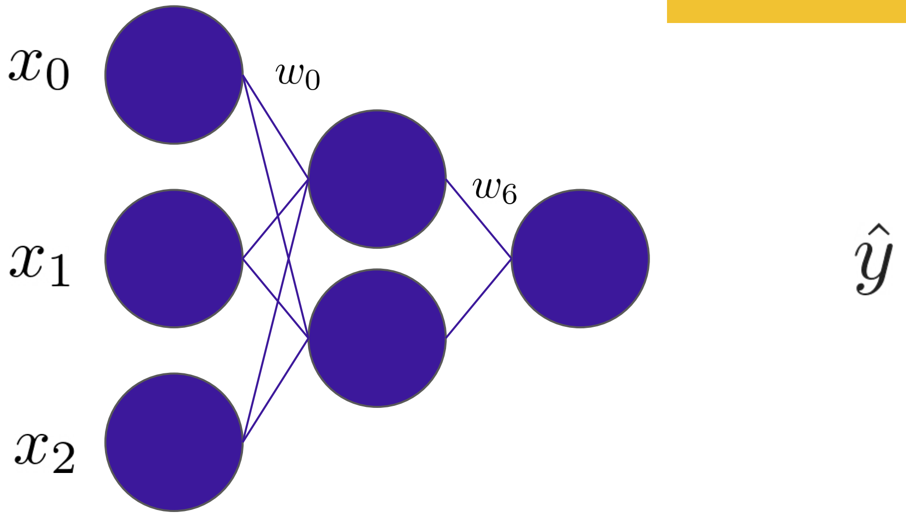


Anatomy of an Artificial Neural Network

Don’t model the biological neuron **precisely**

- Inputs
- Bias
- Weights
- Dot product
- Non-linear activation

Use a (deep) neural network to **approximate** an unknown **function**

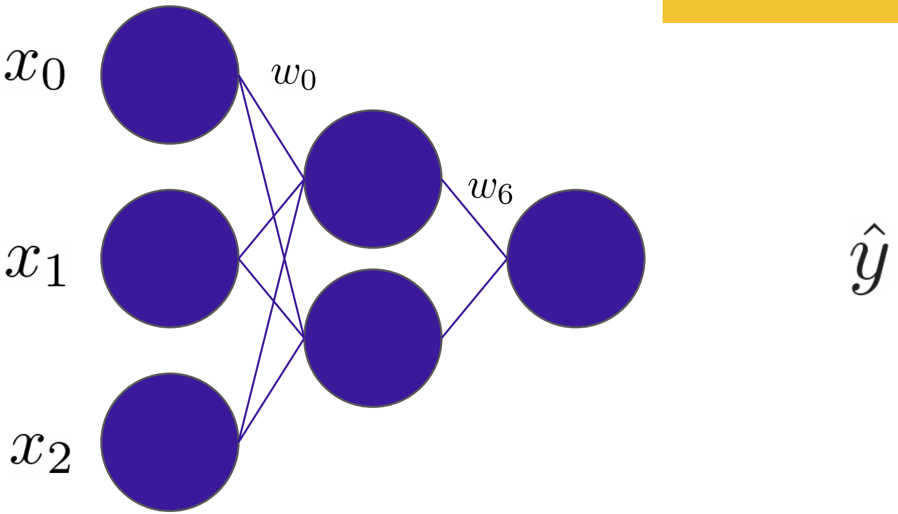


Anatomy of an Artificial Neural Network

Don’t model the biological neuron **precisely**

- Inputs
- Bias
- Weights
- Dot product
- Non-linear activation

Use a (deep) neural network to **approximate** an unknown **function**



$$\sum_{i=1}^{m} w_i x_i + b$$

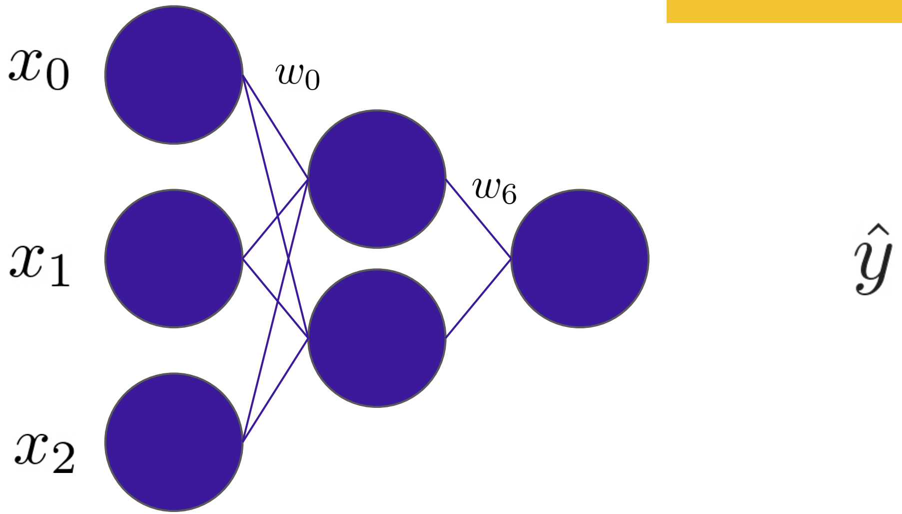
SURF

Anatomy of an Artificial Neural Network

Don't model the biological neuron **precisely**

- Inputs
- Bias
- Weights
- Dot product
- Non-linear activation

Use a (deep) neural network to **approximate** an unknown **function**



$$\sum_{i=1}^{m} w_i x_i + b$$

$$\mathbf{Wx}$$

Anatomy of an Artificial Neural Network

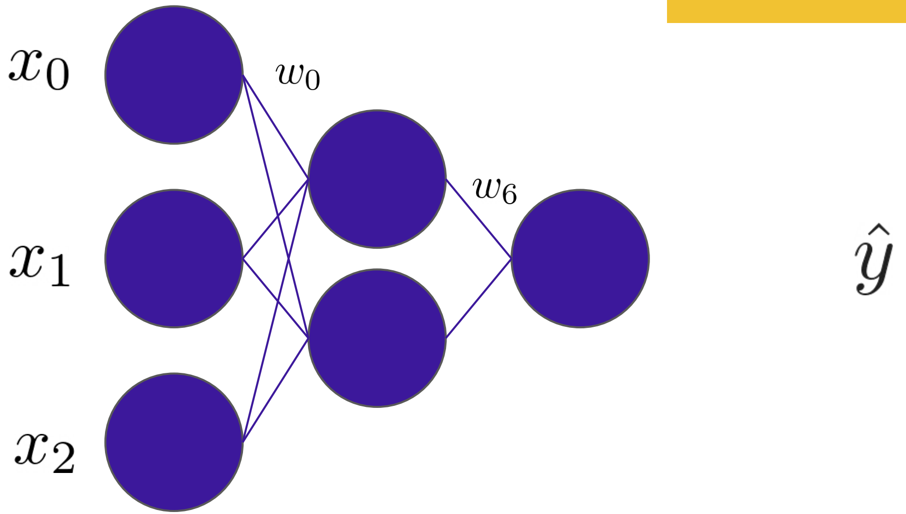
Don't model the biological neuron **precisely**

- Inputs
- Bias
- Weights
- Dot product
- Non-linear activation

❖ Easy to **compose** and easy to **vectorize**

❖ Fits current compute paradigm

Use a (deep) neural network to **approximate** an unknown **function**



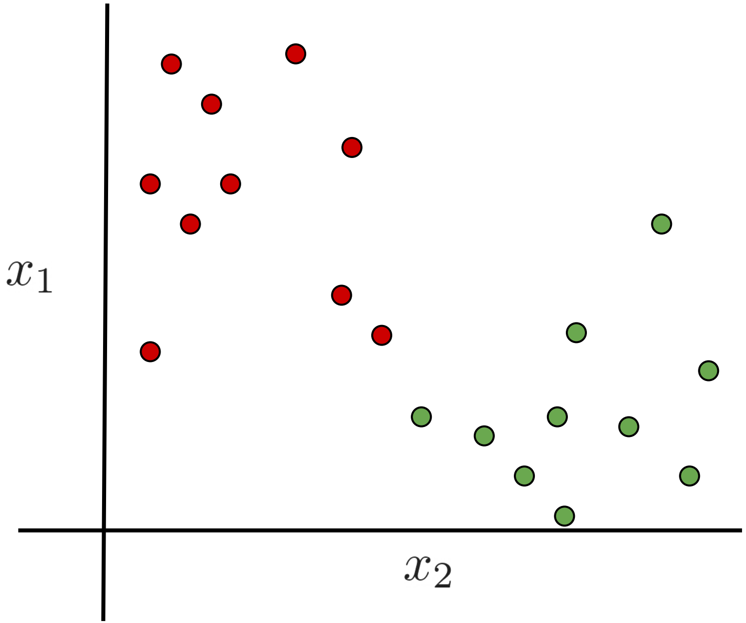
$$\sum_{i=1}^{m} w_i x_i + b$$

$$\mathbf{Wx}$$

SURF

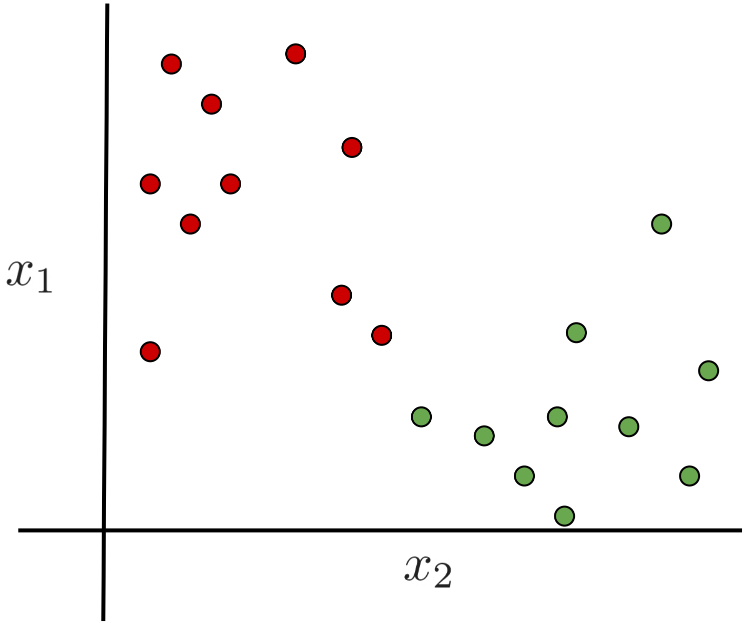
The Perceptron and Activation

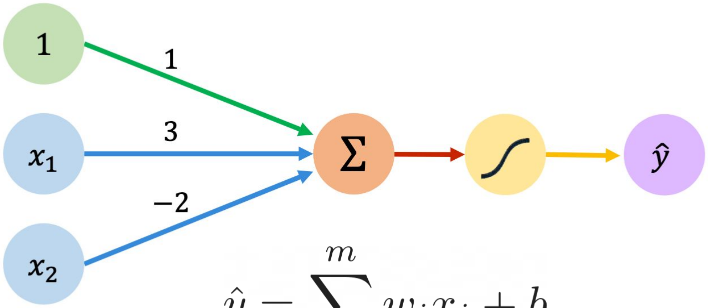
Binary Classification Task



The Perceptron and Activation

Binary Classification Task

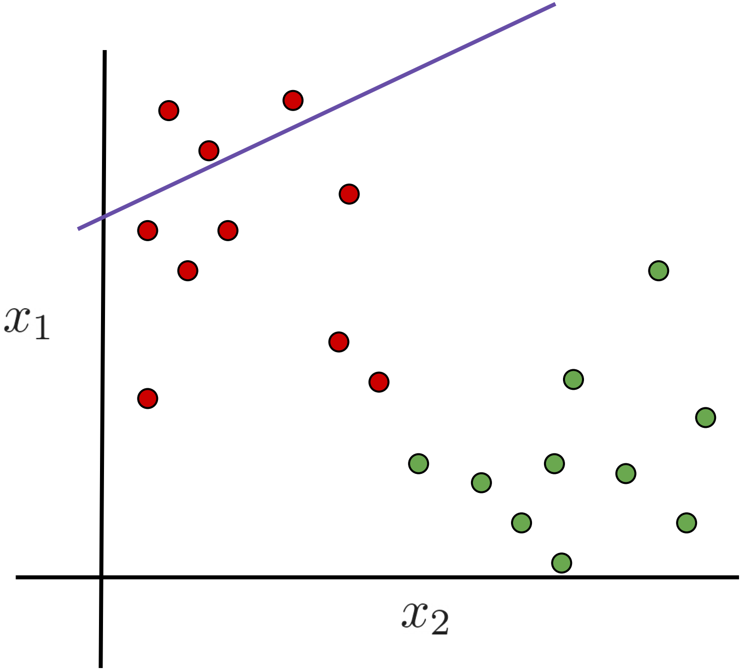


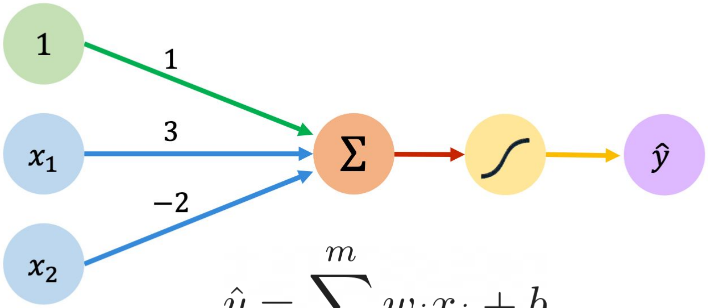


$$\hat{y} = \sum_{i=1}^{m} w_i x_i + b$$

The Perceptron and Activation

Binary Classification Task

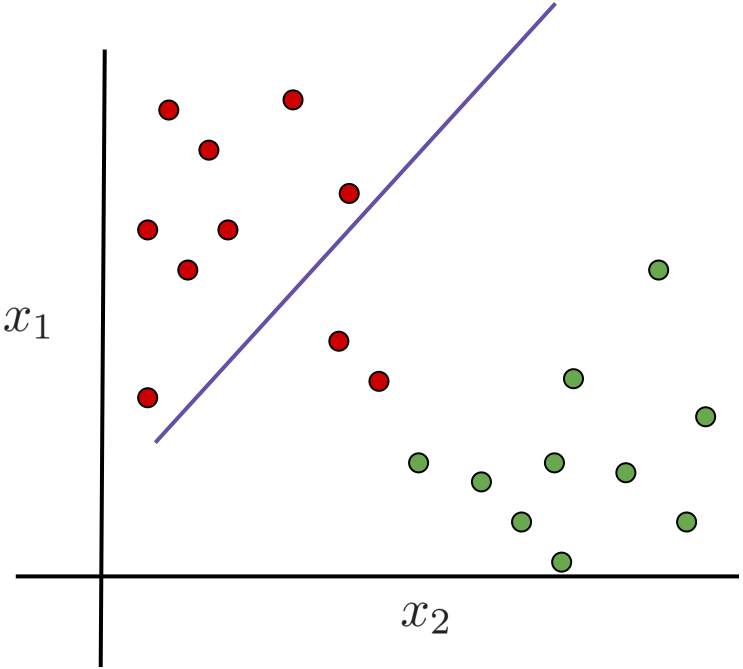


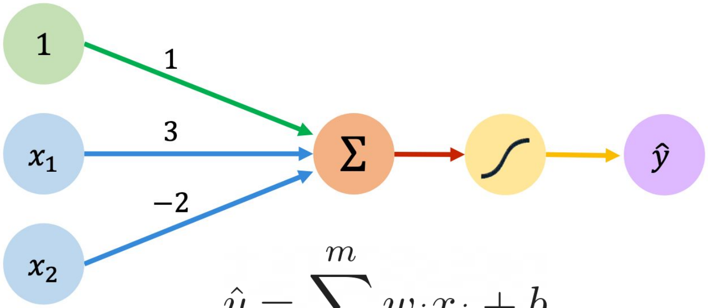


$$\hat{y} = \sum_{i=1}^{m} w_i x_i + b$$

The Perceptron and Activation

Binary Classification Task

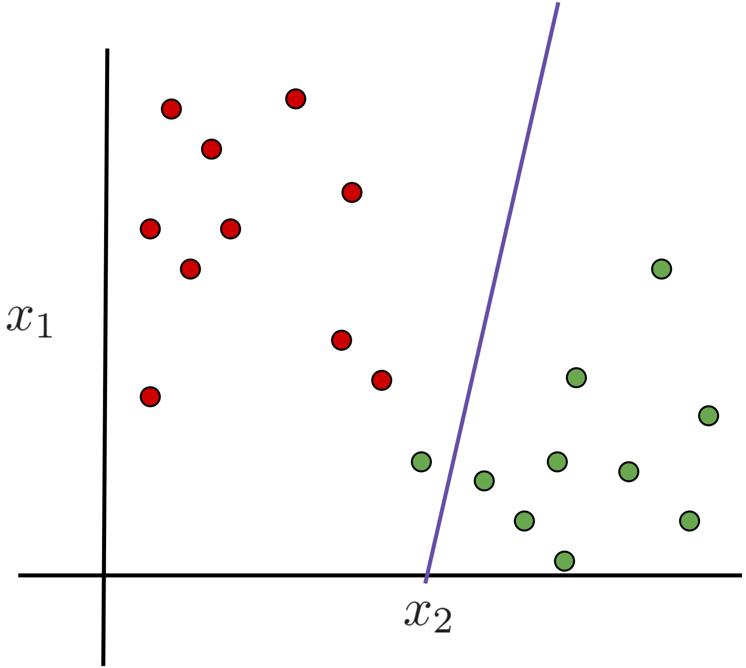


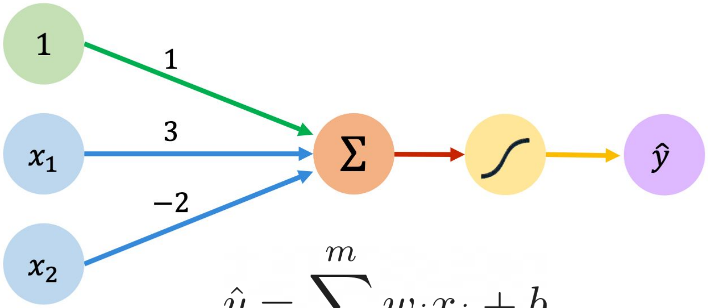


$$\hat{y} = \sum_{i=1}^{m} w_i x_i + b$$

The Perceptron and Activation

Binary Classification Task

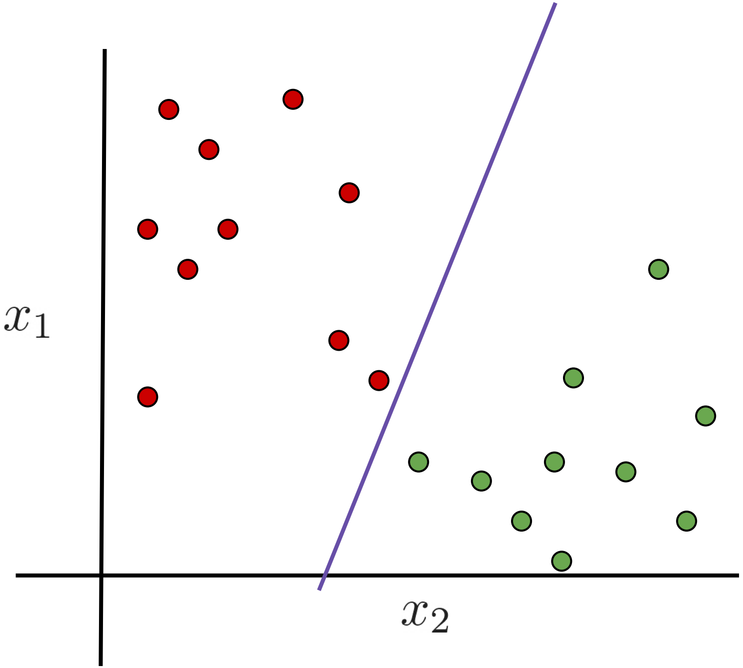


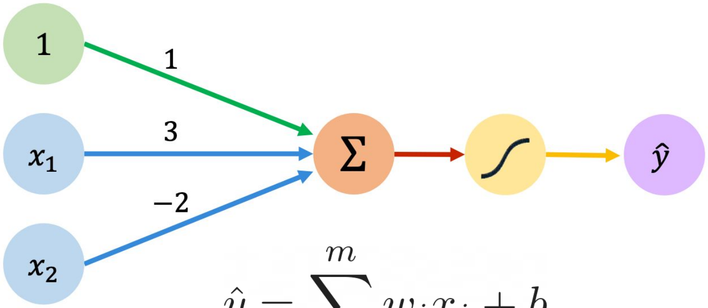


$$\hat{y} = \sum_{i=1}^{m} w_i x_i + b$$

The Perceptron and Activation

Binary Classification Task

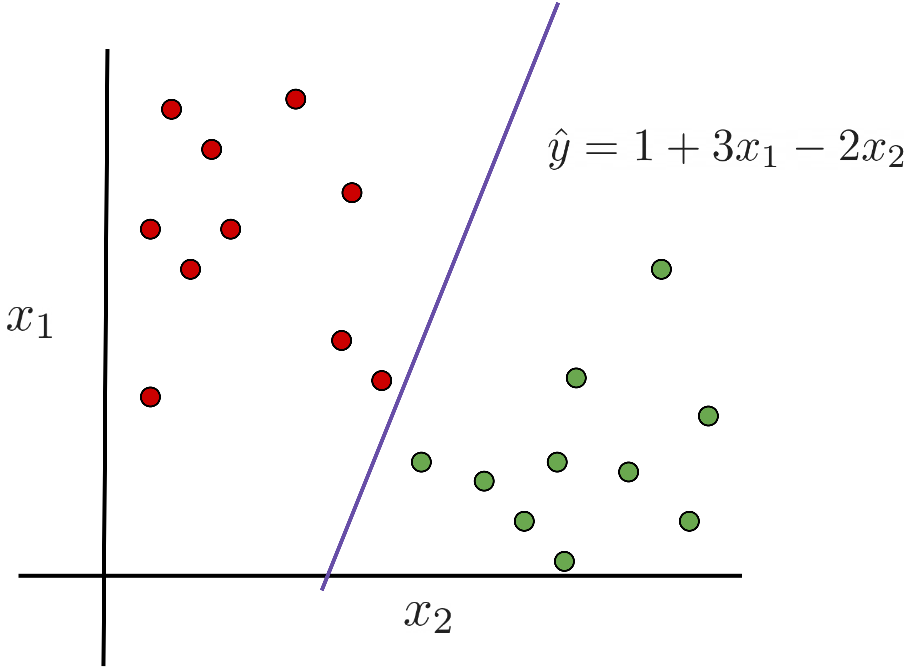


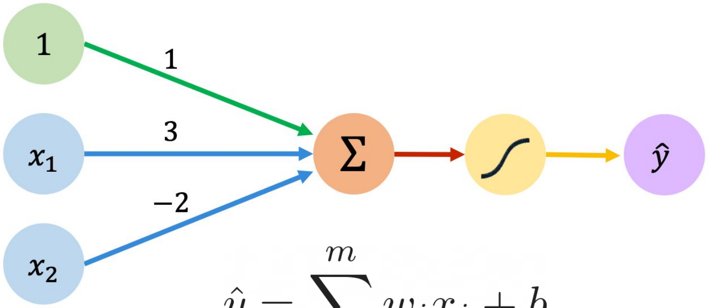


$$\hat{y} = \sum_{i=1}^{m} w_i x_i + b$$

The Perceptron and Activation

Binary Classification Task

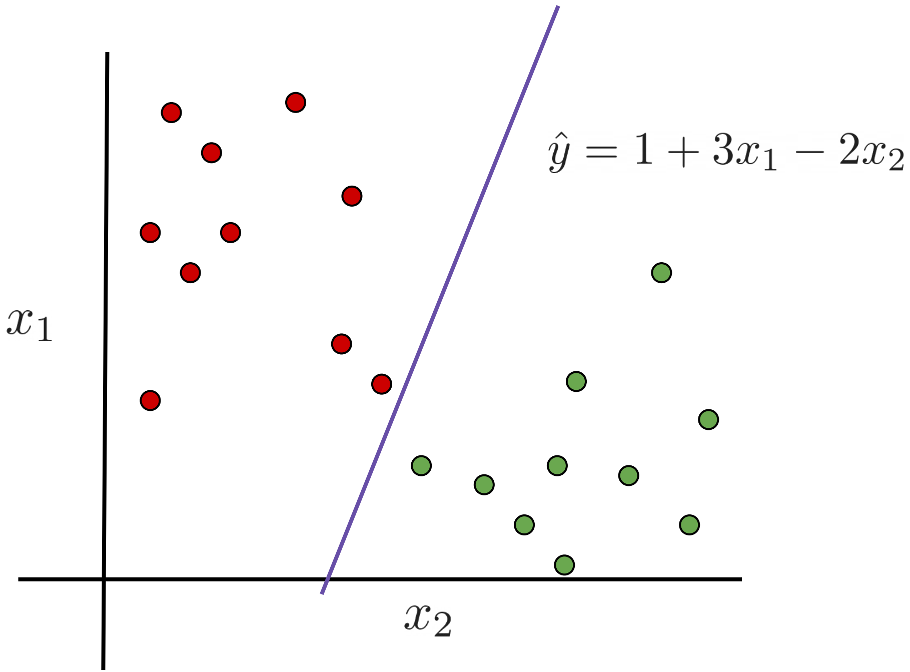




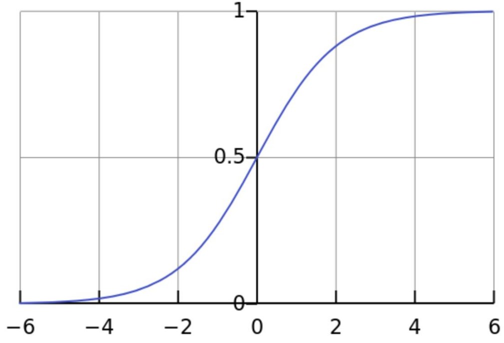
$$\hat{y} = \sum_{i=1}^{m} w_i x_i + b$$

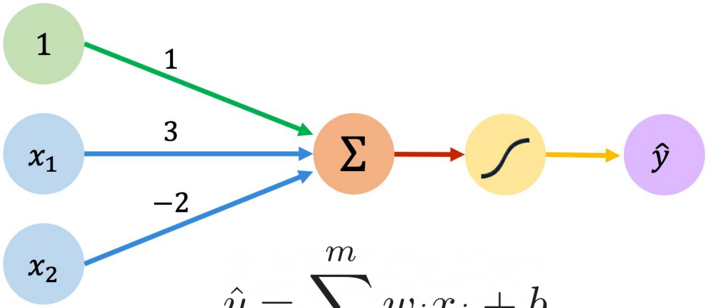
The Perceptron and Activation

Binary Classification Task



Sigmoid

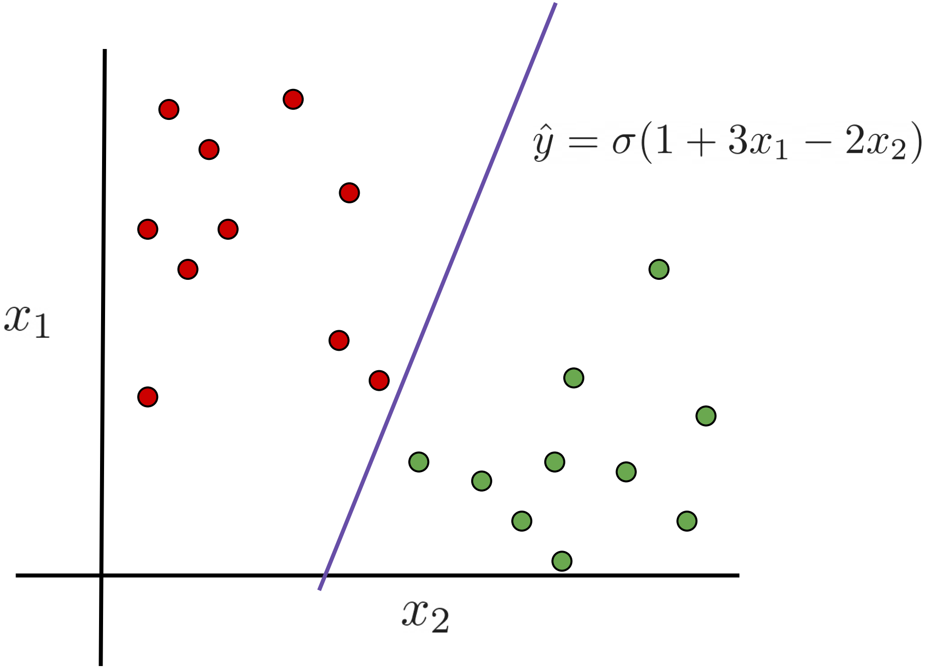




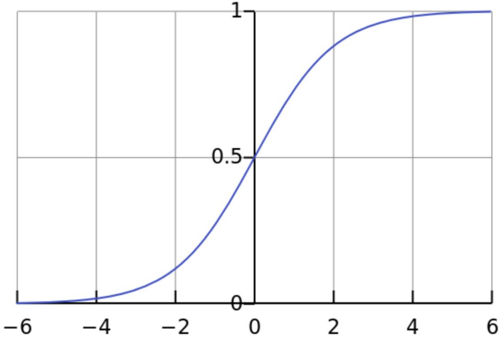
$$\hat{y} = \sum_{i=1}^{m} w_i x_i + b$$

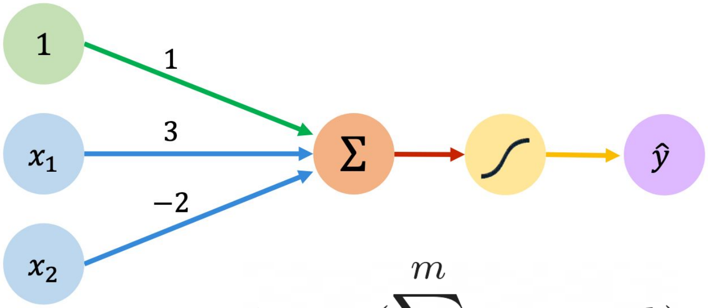
The Perceptron and Activation

Binary Classification Task



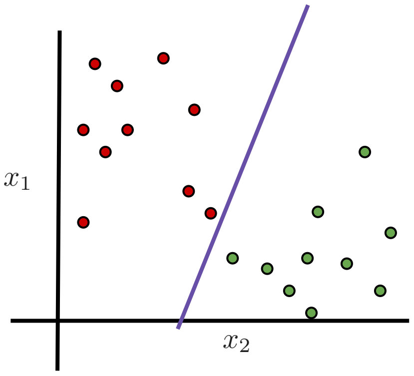
Sigmoid

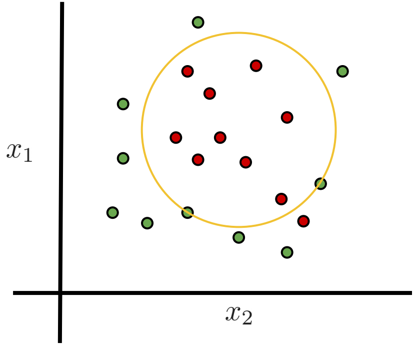


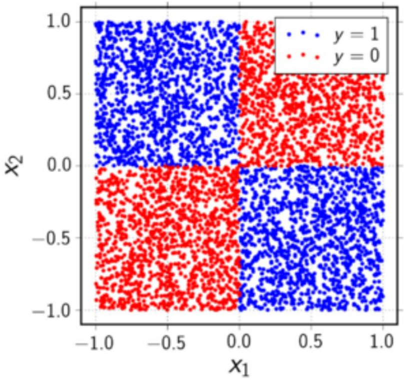


$$\hat{y} = \sigma\left(\sum_{i=1}^{m} w_i x_i + b\right)$$

Limitations of Linear Single Layer Classifiers

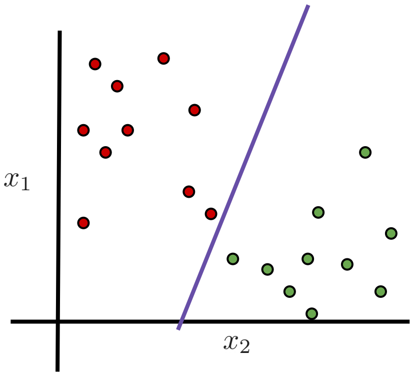


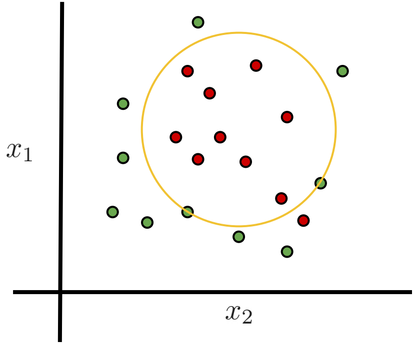


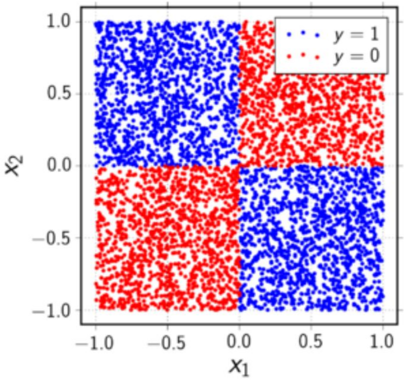


XOR Problem

Limitations of Linear Single Layer Classifiers







XOR Problem

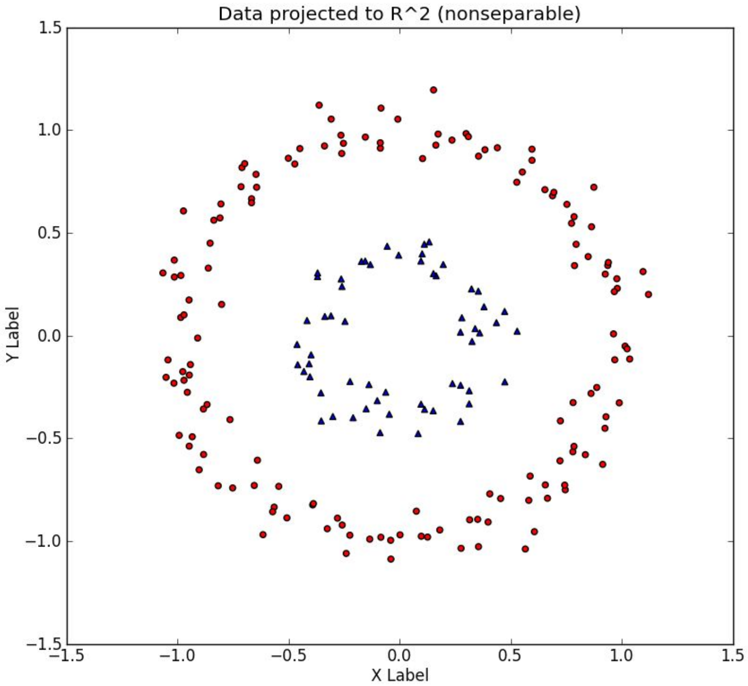
Possible Solutions

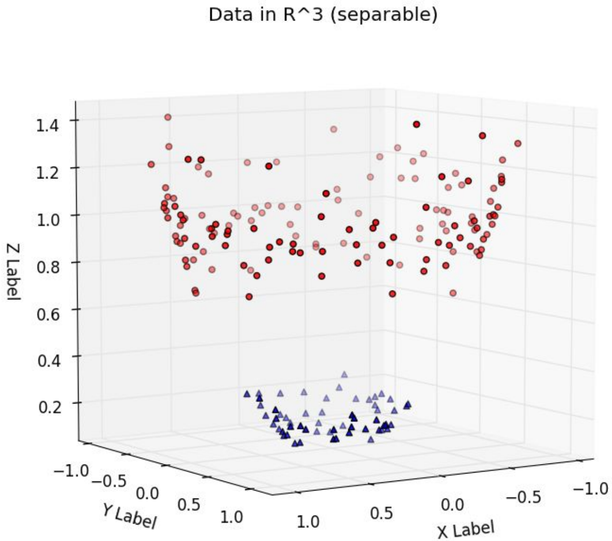
Add more layers (deep learning)

Map into another (higher dimensional) space

We need to be able to automatically extract features

Limitations of Linear Single Layer Classifiers





Universal Approximation Theorem

“

A neural network with a **single hidden layer** of **sufficient size**

Can approximate any continuous function

Universal Approximation Theorem

"

A neural network with a **single hidden layer** of **sufficient size**

Can approximate any continuous function

There exists a true function relating the inputs to the outputs

A neural network can approximate this function to arbitrary precision given sufficient layer size

The required layer size can be extremely large and grow rapidly with the dimensionality of the problem

Universal Approximation Theorem

“

A neural network with a **single hidden layer** of **sufficient size**

Can approximate any continuous function

There exists a true function relating the inputs to the outputs

A neural network can approximate this function to arbitrary precision given sufficient layer size

The required layer size can be extremely large and grow rapidly with the dimensionality of the problem

Use of multiple hidden layers makes the NN vector representation of your problem increasingly more abstract

- How do we train?
- Compute grows (almost) exponentially

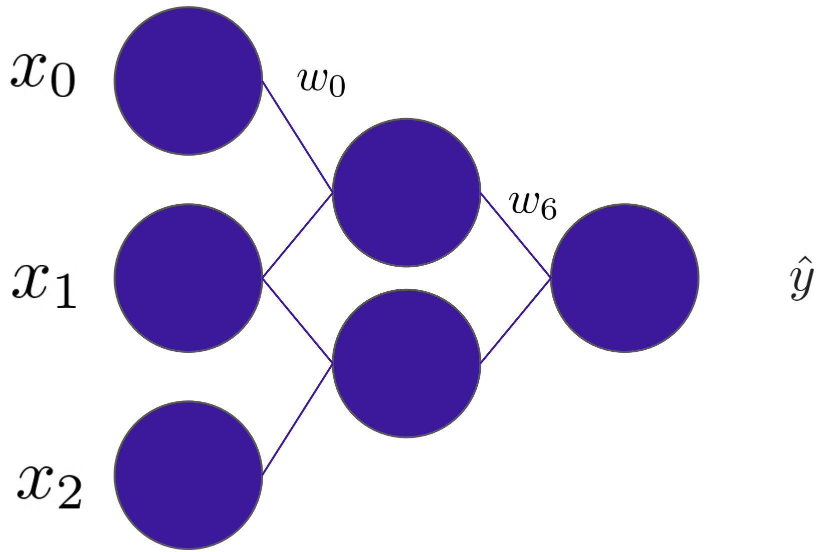
SURF

Predicting Housing Price

During the **optimization** process

The NN learns to **encode** a **representation** that maps

the input to the output

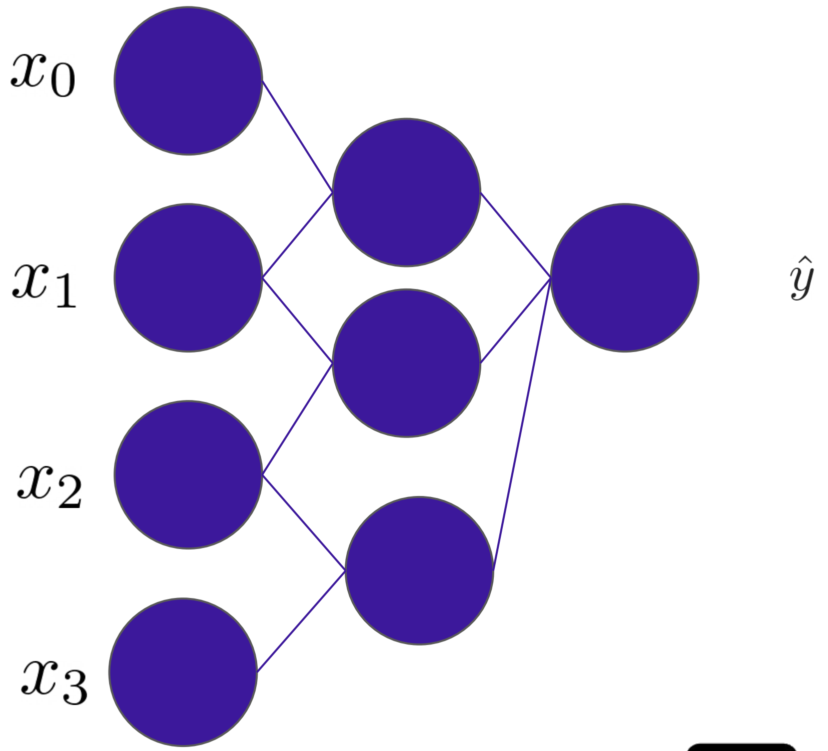


Predicting Housing Price

During the **optimization** process

The NN learns to **encode** a **representation** that maps

the input to the output

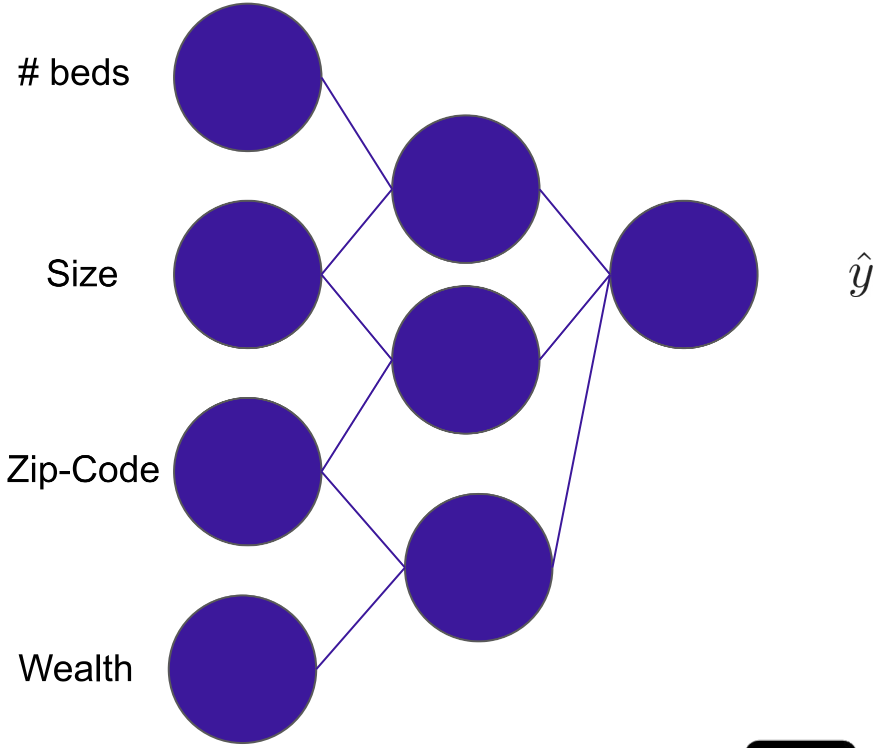


Predicting Housing Price

During the **optimization** process

The NN learns to **encode** a **representation** that maps

the input to the output

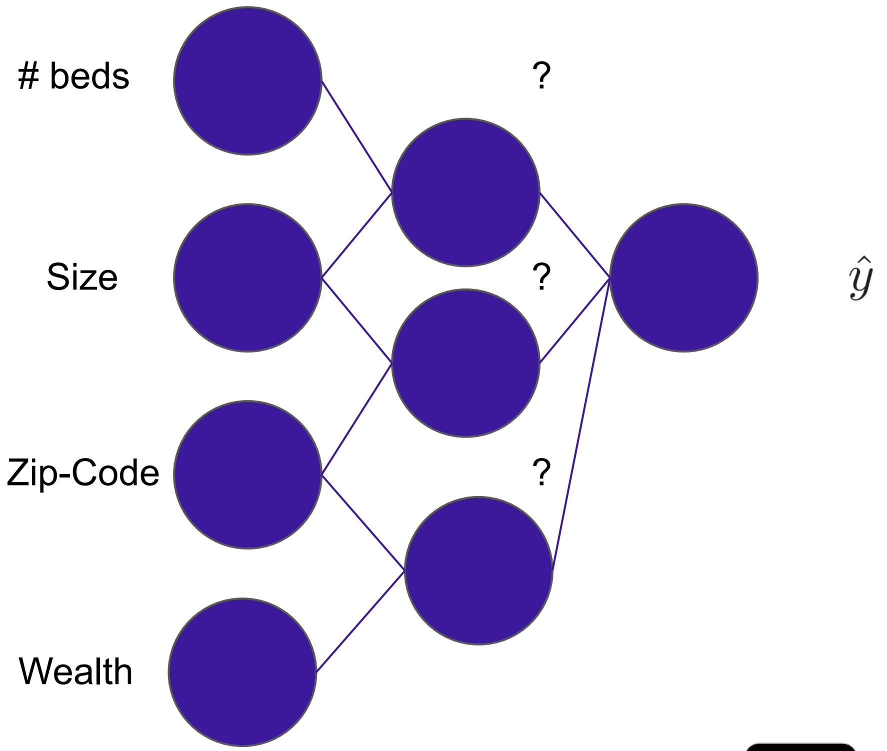


Predicting Housing Price

During the **optimization** process

The NN learns to **encode** a **representation** that maps

the input to the output

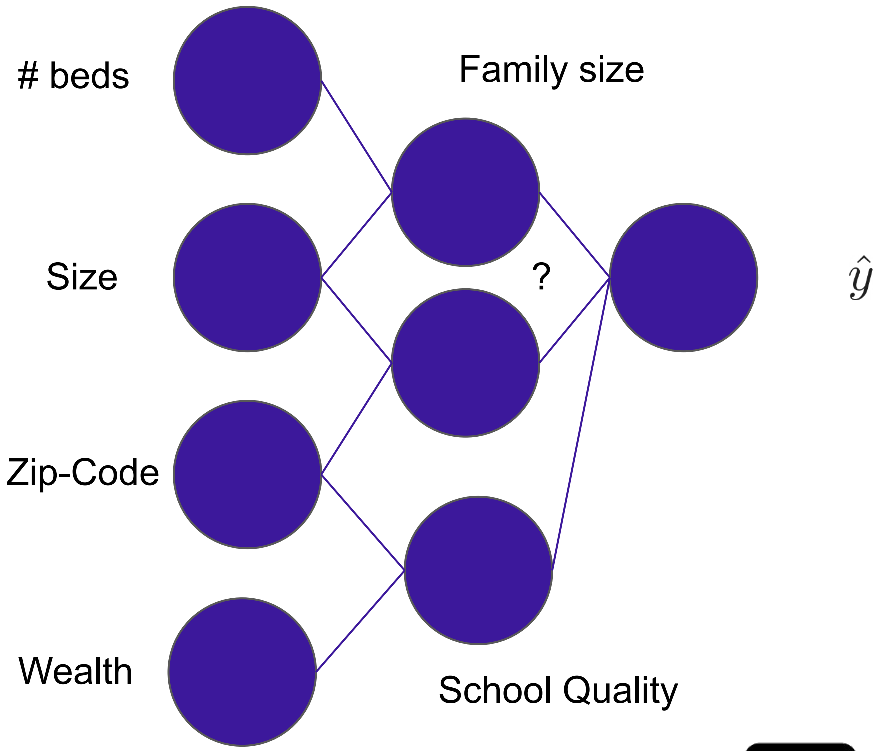


Predicting Housing Price

During the **optimization** process

The NN learns to **encode** a **representation** that maps

the input to the output



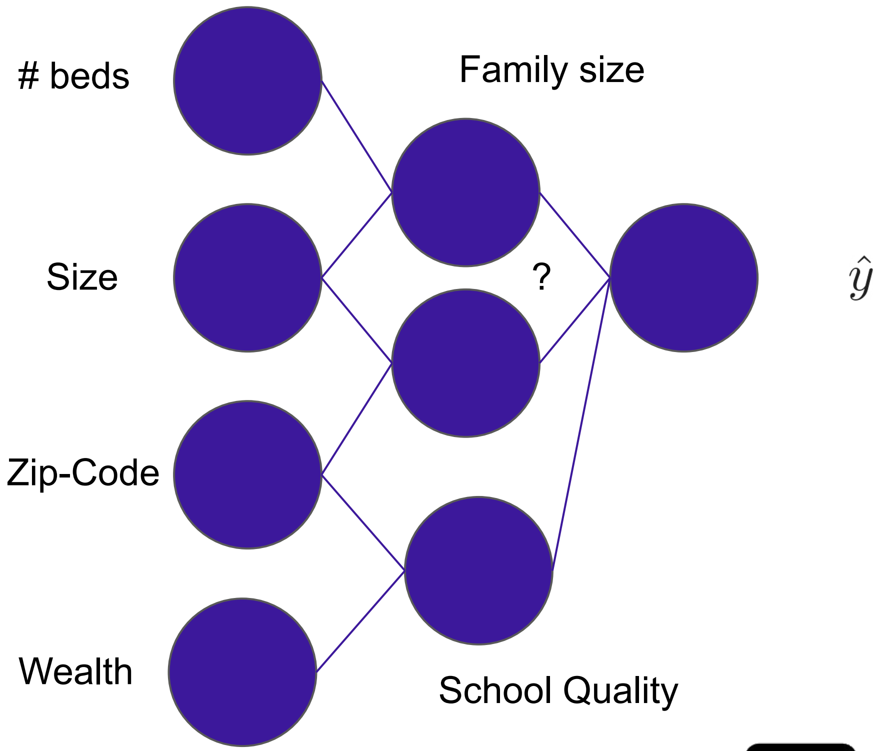
Predicting Housing Price

During the **optimization** process

The NN learns to **encode** a **representation** that maps

the input to the output

Transform the input to a space where we are able to **separate** the features



SURF

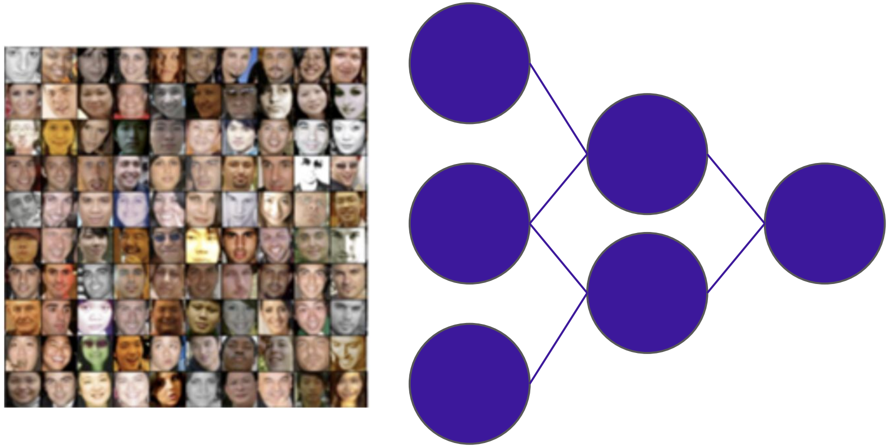
Predicting Faces

During the **optimization** process

The NN learns to **encode** a **representation** that maps

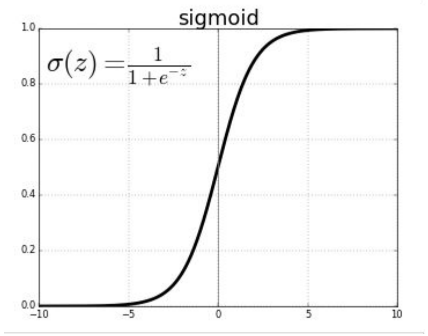
the input to the output

A deep neural network **encodes** the **representation** in an increasingly abstract way



SURF

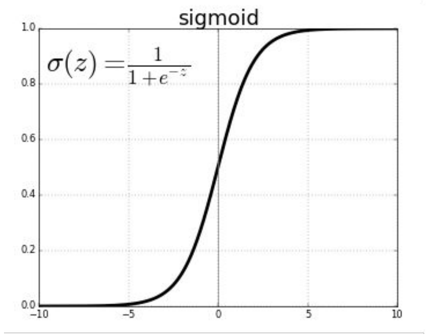
Activation Functions



One of the reasons that enable NNs to encode highly abstract features is the use of **non-linear** activation functions.

Not using non-linearities leads to linear networks

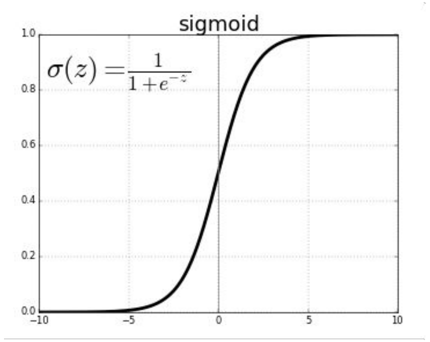
Activation Functions



One of the reasons that enable NNs to encode highly abstract features is the use of **non-linear** activation functions.

Not using non-linearities leads to linear networks

Activation Functions

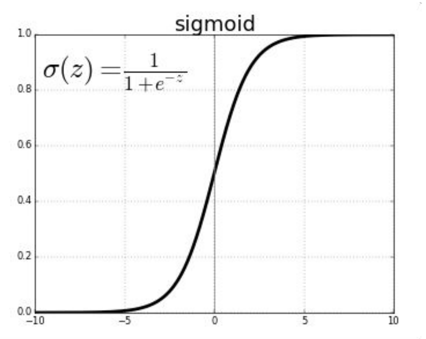


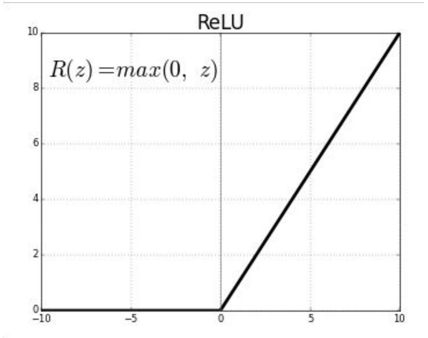
- Probability Estimate
- Continuously differentiable
- Vanishing derivatives due to saturated neurons

One of the reasons that enable NNs to encode highly abstract features is the use of **non-linear** activation functions.

Not using non-linearities leads to linear networks

Activation Functions



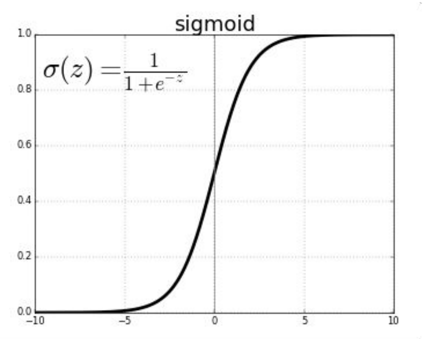


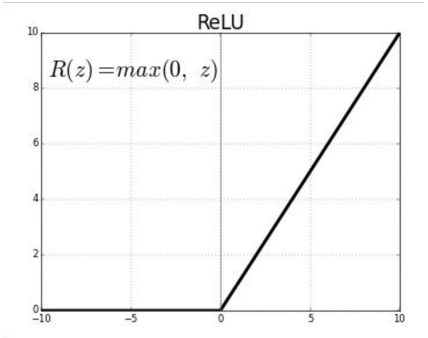
One of the reasons that enable NNs to encode highly abstract features is the use of **non-linear** activation functions.

Not using non-linearities leads to linear networks

- Probability Estimate
- Continuously differentiable
- Vanishing derivatives due to saturated neurons

Activation Functions





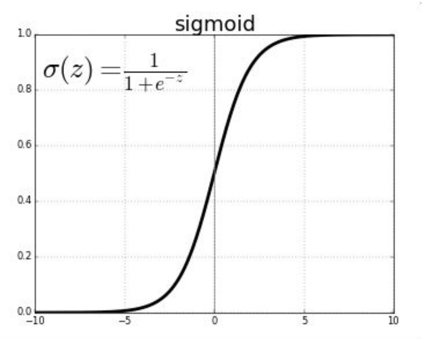
One of the reasons that enable NNs to encode highly abstract features is the use of **non-linear** activation functions.

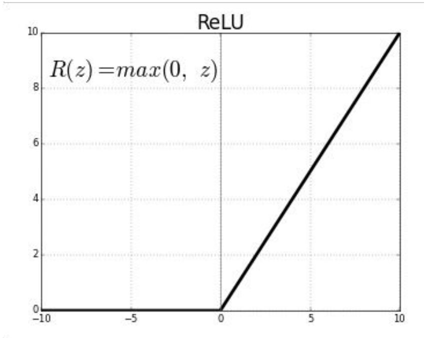
Not using non-linearities leads to linear networks

- ❖ Probability Estimate
- ❖ Continuously differentiable
- ❖ Vanishing derivatives due to saturated neurons

- ❖ Very cheap to compute
- ❖ Piece-wise linear functions
- ❖ Dead neurons
- ❖ Not differentiable at 0

Activation Functions





One of the reasons that enable NNs to encode highly abstract features is the use of **non-linear** activation functions.

Not using non-linearities leads to linear networks

- ❖ Probability Estimate
- ❖ Continuously differentiable
- ❖ Vanishing derivatives due to saturated neurons

- ❖ Very cheap to compute
- ❖ Piece-wise linear functions
- ❖ Dead neurons
- ❖ Not differentiable at 0

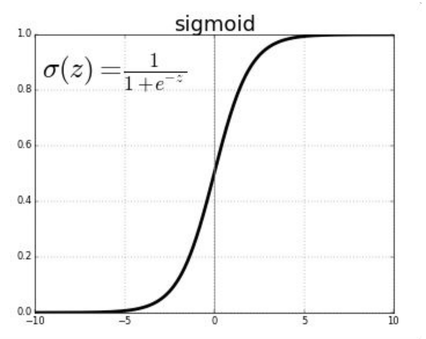
Activation functions are applied to the ou
of each neuron (point-wise)

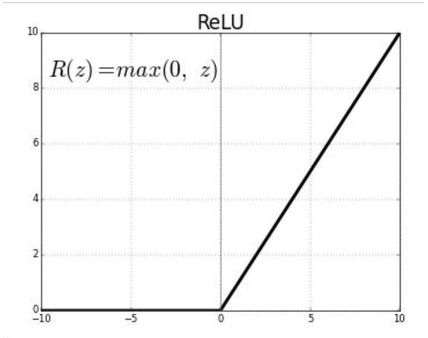
Simple derivative

Non-linear behaviour

SURF

Activation Functions





One of the reasons that enable NNs to encode highly abstract features is the use of **non-linear** activation functions.

Not using non-linearities leads to linear networks

- ❖ Probability Estimate
- ❖ Continuously differentiable
- ❖ Vanishing derivatives due to saturated neurons

- ❖ Very cheap to compute
- ❖ Piece-wise linear functions
- ❖ Dead neurons
- ❖ Not differentiable at 0

Activation functions are applied to the ou of each neuron (point-wise)

Simple derivative

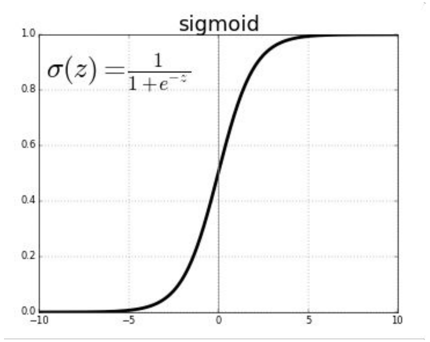
Non-linear behaviour

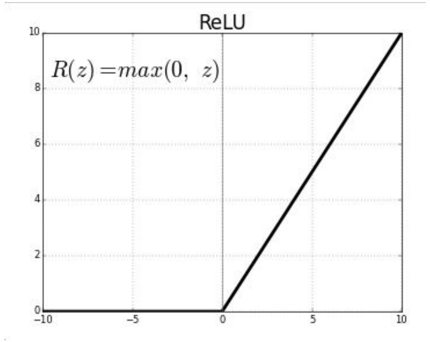
ReLU made our lives much easier and faster

Most commonly used activation

SURF

Activation Functions





One of the reasons that enable NNs to encode highly abstract features is the use of **non-linear** activation functions.

Not using non-linearities leads to linear networks

- Probability Estimate
- Continuously differentiable
- Vanishing derivatives due to saturated neurons

- Very cheap to compute
- Piece-wise linear functions
- Dead neurons
- Not differentiable at 0

Activation functions are applied to the ou of each neuron (point-wise)

Simple derivative

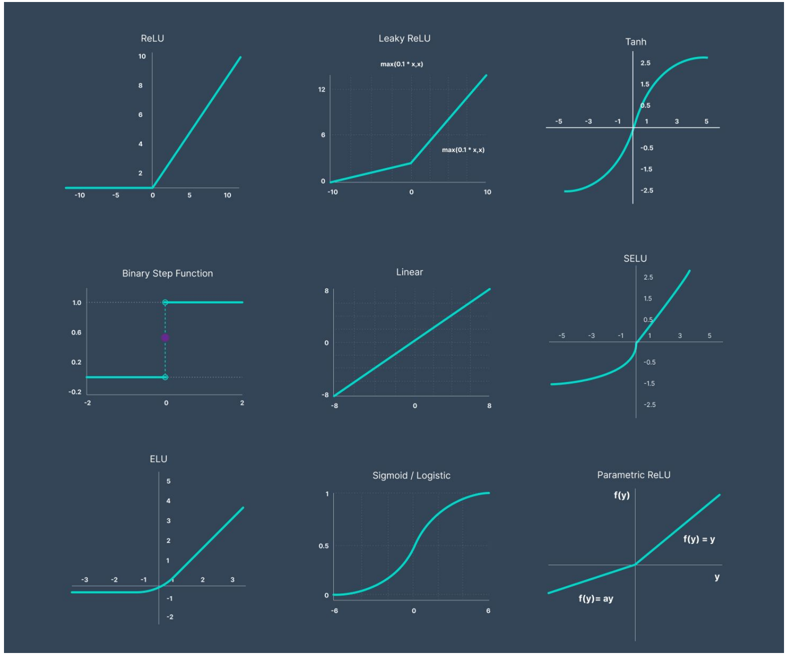
Non-linear behaviour

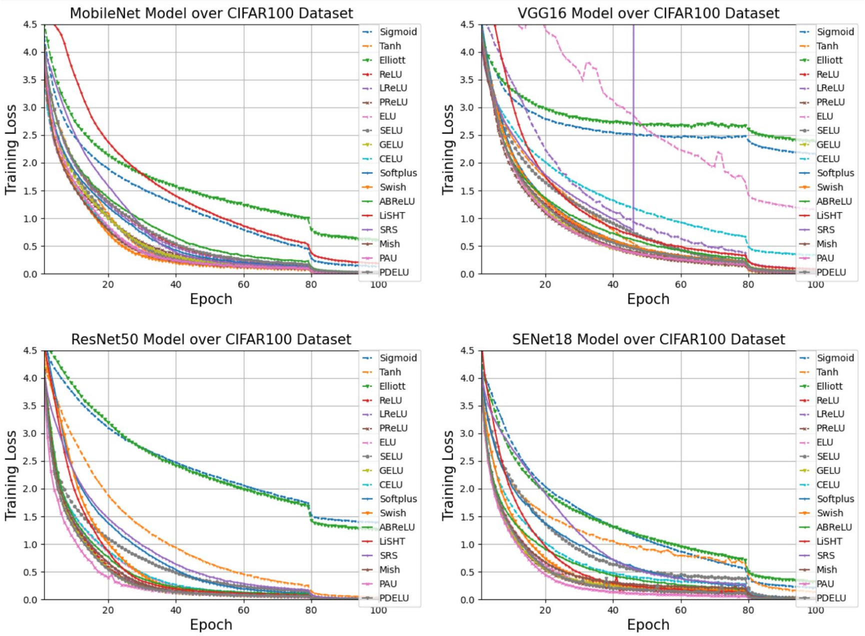
ReLU made our lives much easier and faster

Most commonly used activation

Many more! We can design our own!

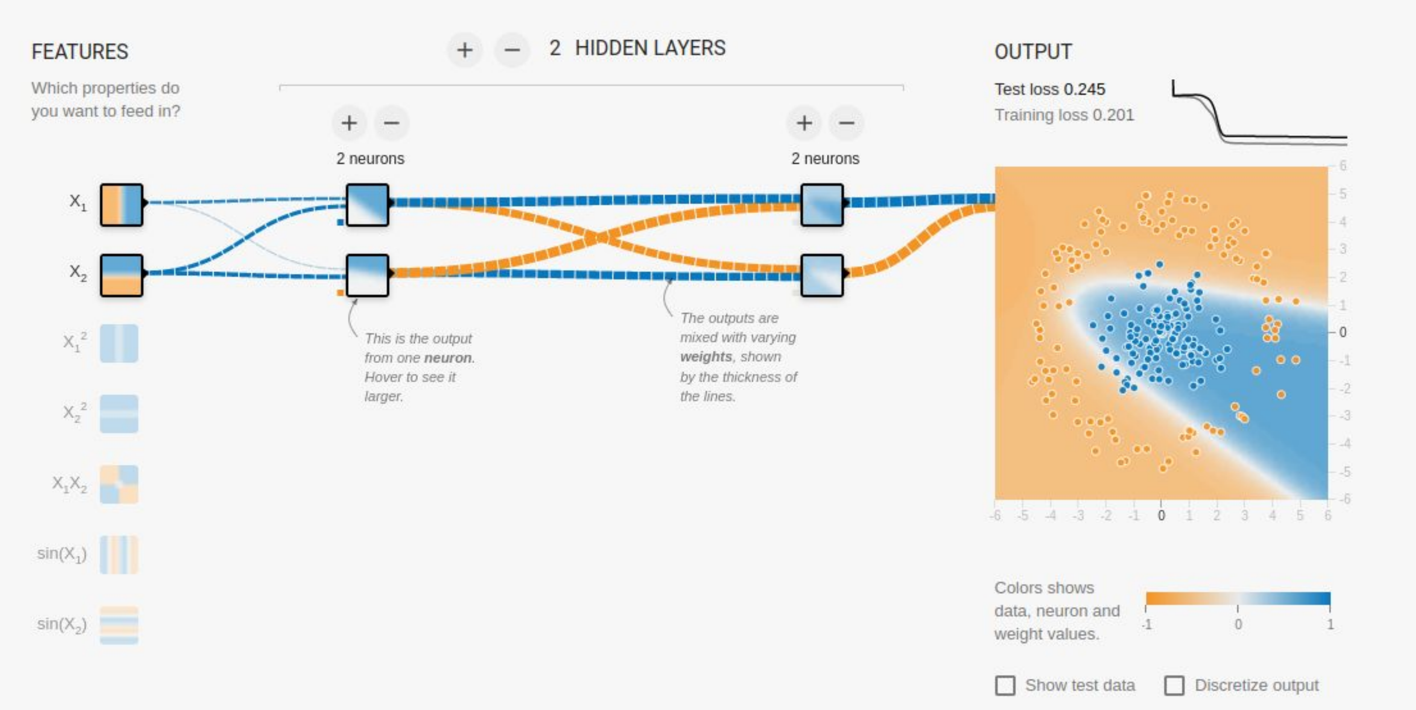
Activation Functions





Many more! We can design our own!

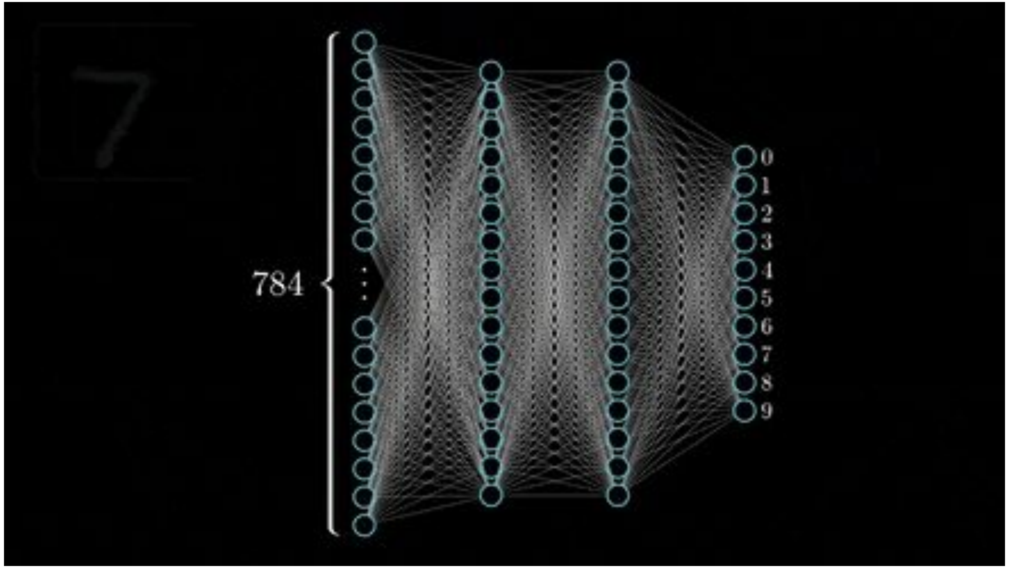
Neural Network Demo



https://playground.tensorflow.org/

Neural Network

- The output of previous layer is used as an input to the next layer
- The input layer is data input and the output is a prediction
- Anything in between is **hidden**
- Layers are represented as vectors
- Edges are matrices
- We train the weights



Neural Network Training

High Performance Machine Learning Group

Recipe for Training

01.

Process your data

Define the data to be used
Do we have labels?

02.

Define the Model

Define the layers and
The forward propagation

03.

What function to optimize?

Define the function to approximate
your desired solution

04.

How to evaluate the model?

Which metrics are going to tell us how well we are doing on unseen data?

SURF

Recipe for Training

01.

$$(x_1, \ldots, x_m), y$$

Recipe for Training

01.

$$(x_1, \ldots, x_m), y$$

02.

$$f_{NN}(x_1, x_2, \ldots, x_n)$$

Recipe for Training

01.

$$(x_1, \ldots, x_m), y$$

02.

$$f_{NN}(x_1, x_2, \ldots, x_n)$$

03.

MSE $$\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

SURF

Recipe for Training

01.

$$(x_1, \ldots, x_m), y$$

02.

$$f_{NN}(x_1, x_2, \ldots, x_n)$$

03.

MSE $$\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

CE $$-\sum_{i=1}^{\substack{\text{output}\\\text{size}}} y_i \cdot \log \hat{y}_i$$

Recipe for Training

01.

$$(x_1, \ldots, x_m), y$$

02.

$$f_{NN}(x_1, x_2, \ldots, x_n)$$

03.

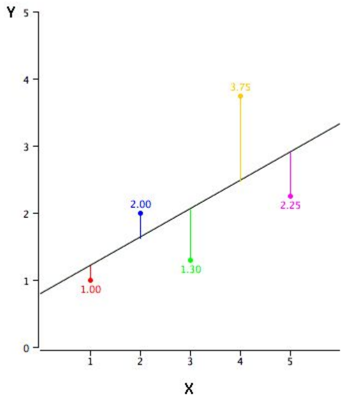
MSE $$\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

CE $$-\sum_{i=1}^{\substack{\text{output}\\\text{size}}} y_i \cdot \log \hat{y}_i$$

04.

Accuracy, F1-score, precision, recall

Loss Functions

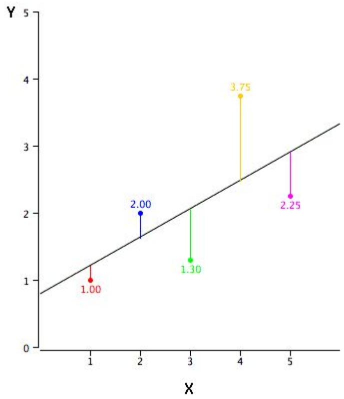


$$\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

The loss function is used to bridge the gap between your neural network predictions and the true value

We optimize (minimize) the loss to tune the weights
In the direction of biggest positive change

Loss Functions



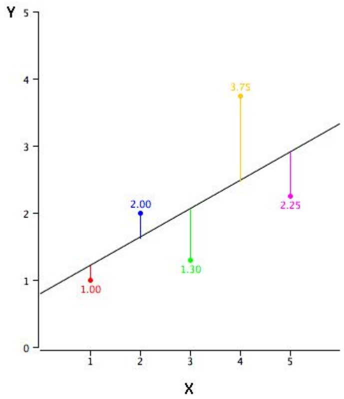
$$\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

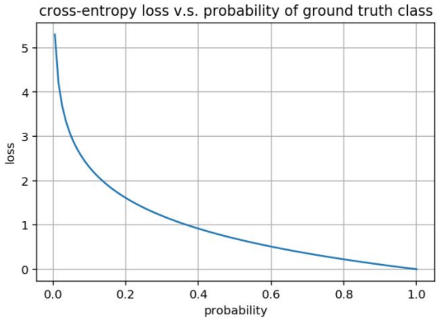
- Distance/statistical metric assumes a Gaussian prior
- Easy to understand, easy to Compute
- Prone to outliers
- Not suitable for classification problems

The loss function is used to bridge the gap between your neural network predictions and the true value

We optimize (minimize) the loss to tune the weights
In the direction of biggest positive change

Loss Functions





The loss function is used to bridge the gap between your neural network predictions and the true value

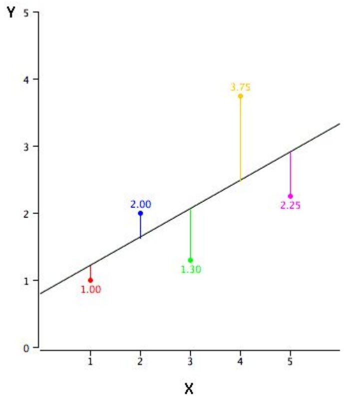
We optimize (minimize) the loss to tune the weights
In the direction of biggest positive change

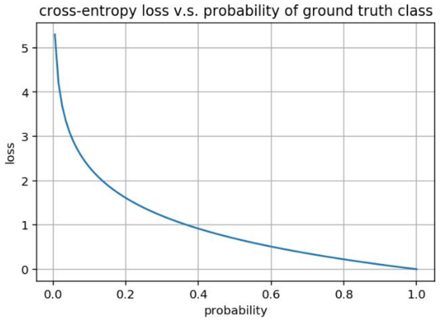
$$\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

- ❖ Distance/statistical metric assumes a Gaussian prior
- ❖ Easy to understand, easy to Compute
- ❖ Prone to outliers
- ❖ Not suitable for classification problems

SURF

Loss Functions





The loss function is used to bridge the gap between your neural network predictions and the true value

We optimize (minimize) the loss to tune the weights
In the direction of biggest positive change

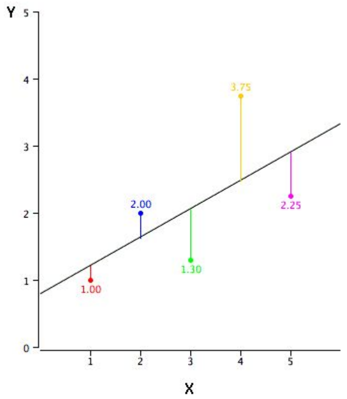
$$\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

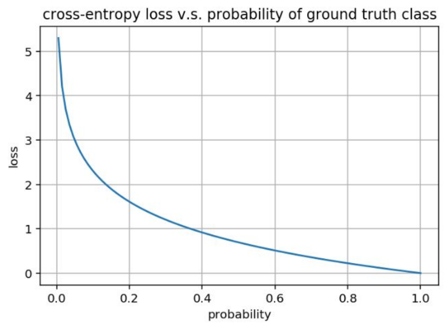
- Distance/statistical metric assumes a Gaussian prior
- Easy to understand, easy to Compute
- Prone to outliers
- Not suitable for classification problems

$$-\sum_{i=1}^{\substack{\text{output}\\\text{size}}} y_i \cdot \log \hat{y}_i$$

- Suitable for multi-class problems
- Information theory foundation
- Not exactly the most stable loss

Loss Functions





The loss function is used to bridge the gap between your neural network predictions and the true value

We optimize (minimize) the loss to tune the weights In the direction of biggest positive change

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

- Distance/statistical metric assumes a Gaussian prior
- Easy to understand, easy to Compute
- Prone to outliers
- Not suitable for classification problems

$$-\sum_{i=1}^{\text{output size}} y_i \cdot \log \hat{y}_i$$

- Suitable for multi-class problems
- Information theory foundation
- Not exactly the most stable loss

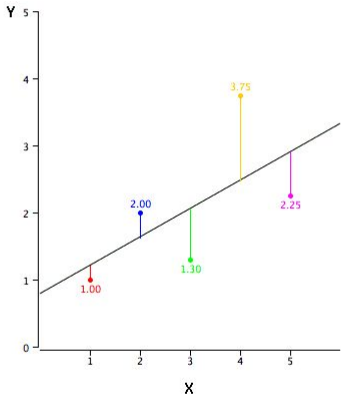
CE is easily composed with sigmoid Or Softmax activations!

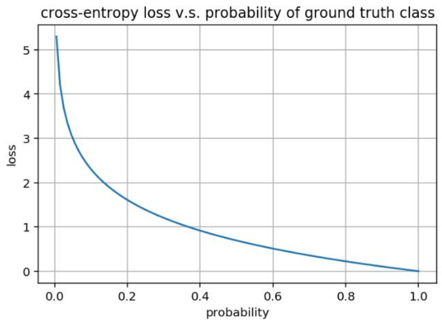
CE and Softmax has better behaved gradients.

Non-linear behaviour

SURF

Loss Functions





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

- Distance/statistical metric assumes a Gaussian prior
- Easy to understand, easy to Compute
- Prone to outliers
- Not suitable for classification problems

$$-\sum_{i=1}^{\substack{\text{output}\\\text{size}}} y_i \cdot \log \hat{y}_i$$

- Suitable for multi-class problems
- Information theory foundation
- Not exactly the most stable loss

The loss function is used to bridge the gap between your neural network predictions and the true value

We optimize (minimize) the loss to tune the weights
In the direction of biggest positive change

CE is easily composed with sigmoid
Or Softmax activations!

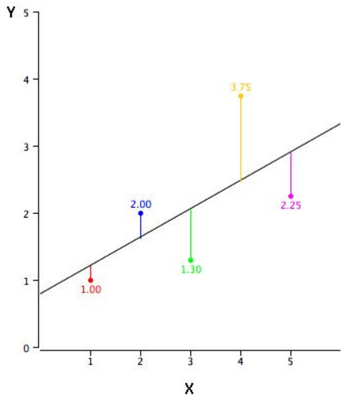
CE and Softmax has better behaved gradients.

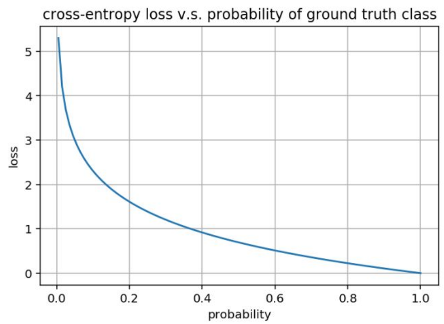
Non-linear behaviour

CE is the negative log-likelihood

Most commonly used activation for classification

Loss Functions





The loss function is used to bridge the gap between your neural network predictions and the true value

We optimize (minimize) the loss to tune the weights
In the direction of biggest positive change

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

- Distance/statistical metric assumes a Gaussian prior
- Easy to understand, easy to Compute
- Prone to outliers
- Not suitable for classification problems

$$-\sum_{i=1}^{\substack{\text{output}\\\text{size}}} y_i \cdot \log \hat{y}_i$$

- Suitable for multi-class problems
- Information theory foundation
- Not exactly the most stable loss

CE is easily composed with sigmoid
Or Softmax activations!

CE and Softmax has better behaved gradients.

Non-linear behaviour

CE is the negative log-likelihood

Most commonly used activation for classification

Many more! We can design our own!

Stochastic Gradient Descent

01. $$L(y,\hat{y}) = L(W,b) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

Stochastic Gradient Descent

01. $$L(y, \hat{y}) = L(W, b) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

02. $$\nabla L(\mathbf{w}_j, b)$$

Stochastic Gradient Descent

01. $$L(y, \hat{y}) = L(W, b) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

02. $$\nabla L(\mathbf{w}_j, b)$$

03. Create batches of ***N*** examples to propagate and compute $\nabla L(\mathbf{w}_j, b)$

Stochastic Gradient Descent

01. $$L(y, \hat{y}) = L(W, b) = \frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

02. $$\nabla L(\mathbf{w}_j, b)$$

03. Create batches of ***N*** examples to propagate and compute $\nabla L(\mathbf{w}_j, b)$

04. $$\mathbf{w}_{j+1} = \mathbf{w}_j - \alpha \nabla L(\mathbf{w}_j, b)$$

Stochastic Gradient Descent

01. $$L(y, \hat{y}) = L(W, b) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

02. $$\nabla L(\mathbf{w}_j, b)$$

03. Create batches of ***N*** examples to propagate and compute $\nabla L(\mathbf{w}_j, b)$

04. $$\mathbf{w}_{j+1} = \mathbf{w}_j - \alpha \nabla L(\mathbf{w}_j, b)$$

Learning Rate

Choice of learning rate critical
SGD is the main engine behind training
Many variations exist

Stochastic Gradient Descent

01. $$L(y, \hat{y}) = L(W, b) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

02. $$\nabla L(\mathbf{w}_j, b)$$

03. Create batches of ***N*** examples to propagate and compute $\nabla L(\mathbf{w}_j, b)$

04. $$\mathbf{w}_{j+1} = \mathbf{w}_j - \alpha \nabla L(\mathbf{w}_j, b)$$

Learning Rate

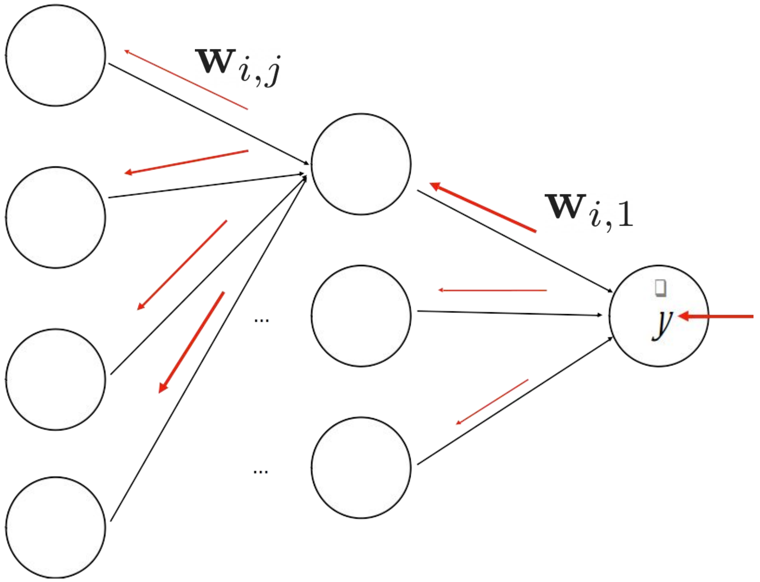
Choice of learning rate critical
SGD is the main engine behind training
Many variations exist

- Can be used with loss function that are not differentiable
- No Guarantee that we find the global optimum

Backpropagation

$$\hat{y} = g(\mathbf{W}_0 f(\mathbf{W}_1 \mathbf{x}))$$

A (deep) neural network is a deeply **nested functions**

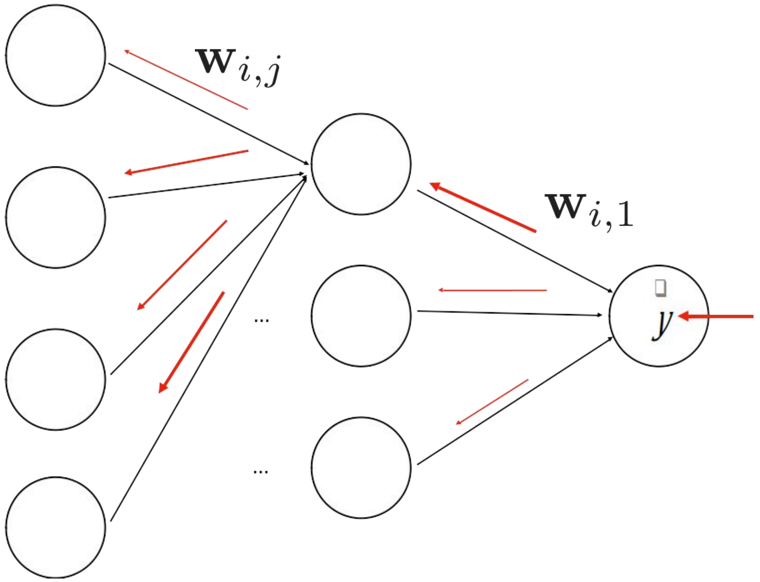


Backpropagation

$$\hat{y} = g(\mathbf{W}_0 f(\mathbf{W}_1 \mathbf{x}))$$

A (deep) neural network is a deeply **nested functions**:

- We need to compute the gradient for each layer
- Apply the chain rule
- This is **backpropagation**

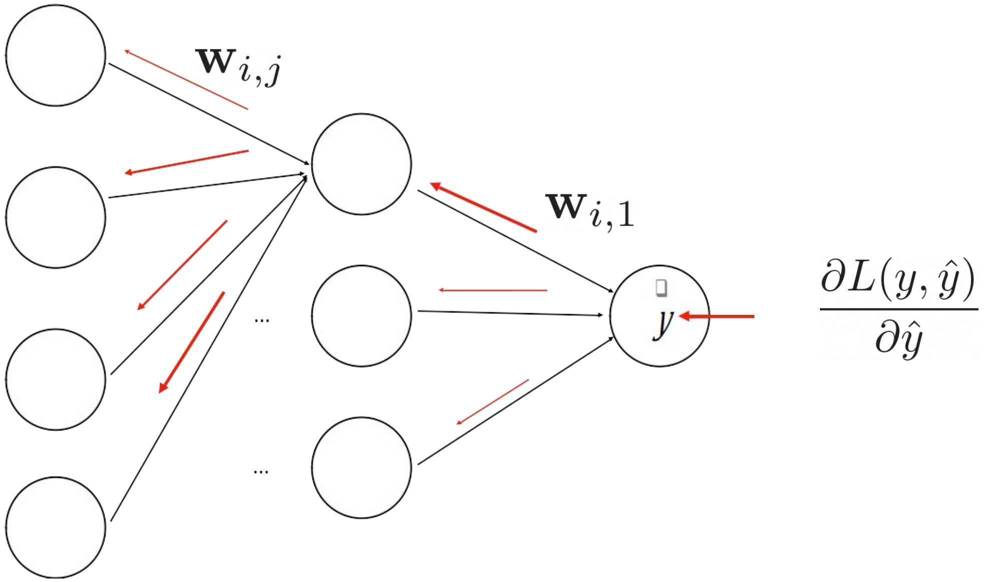


Backpropagation

$$\hat{y} = g(\mathbf{W}_0 f(\mathbf{W}_1 \mathbf{x}))$$

A (deep) neural network is a deeply **nested functions**:

- We need to compute the gradient for each layer
- Apply the **chain rule**
- This is **backpropagation**

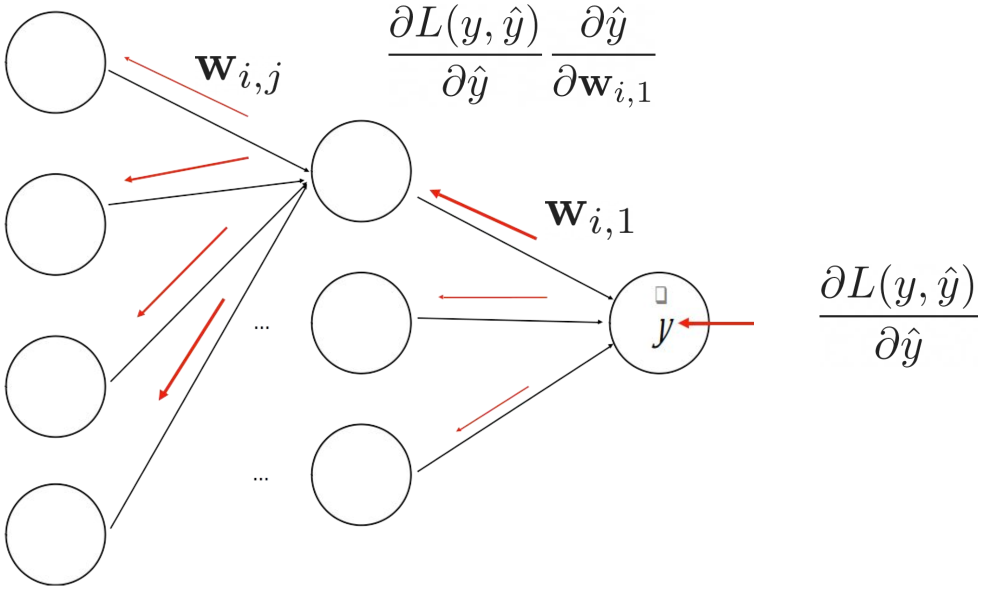


Backpropagation

$$\hat{y} = g(\mathbf{W}_0 f(\mathbf{W}_1 \mathbf{x}))$$

A (deep) neural network is a deeply **nested functions**:

- We need to compute the gradient for each layer
- Apply the **chain rule**
- This is **backpropagation**

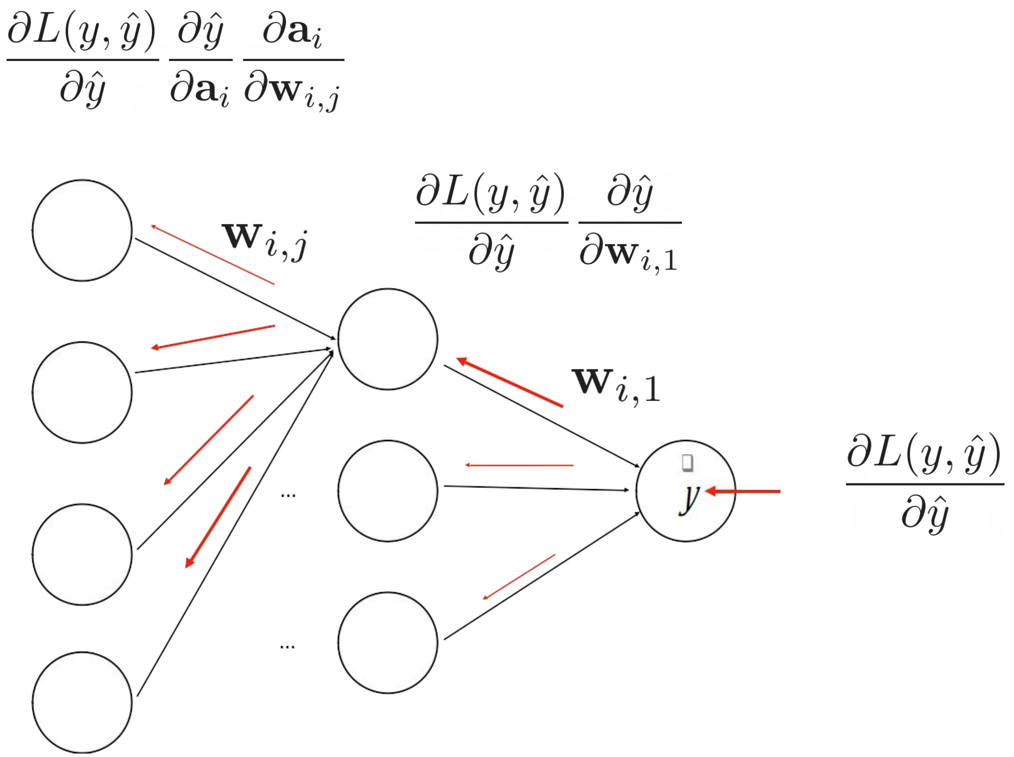


Backpropagation

$$\hat{y} = g(\mathbf{W}_0 f(\mathbf{W}_1 \mathbf{x}))$$

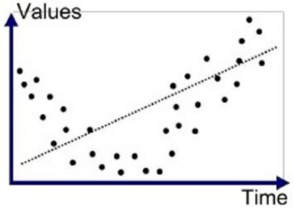
A (deep) neural network is a deeply **nested functions**:

- We need to compute the gradient for each layer
- Apply the **chain rule**
- This is **backpropagation**

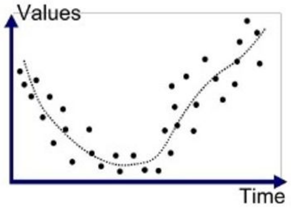


SURF

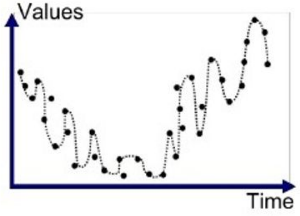
Combatting Overfitting



Underfitted

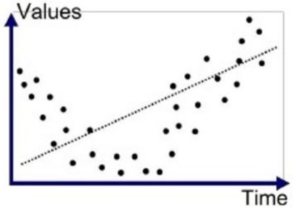


Good Fit/Robust

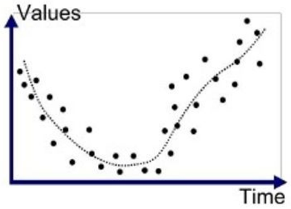


Overfitted

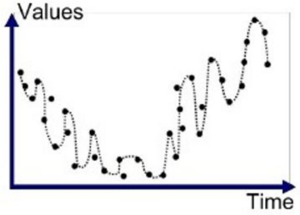
Combatting Overfitting



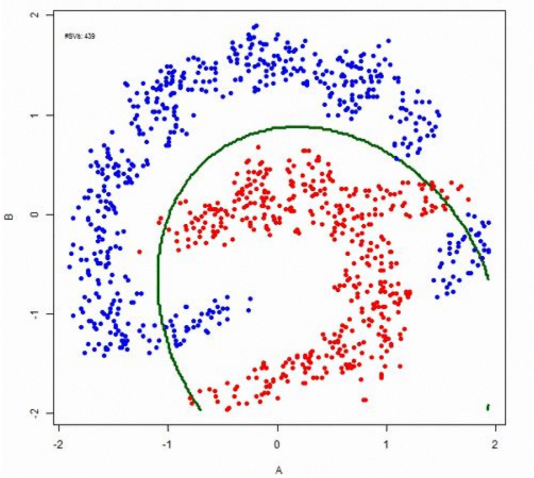
Underfitted



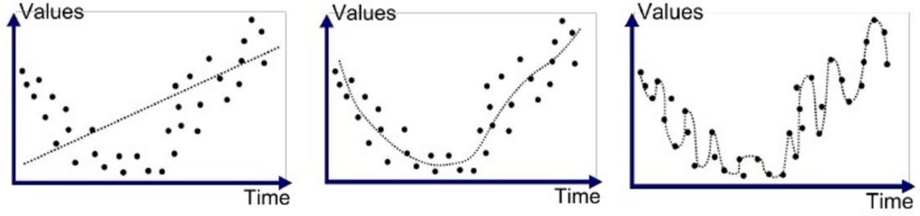
Good Fit/Robust



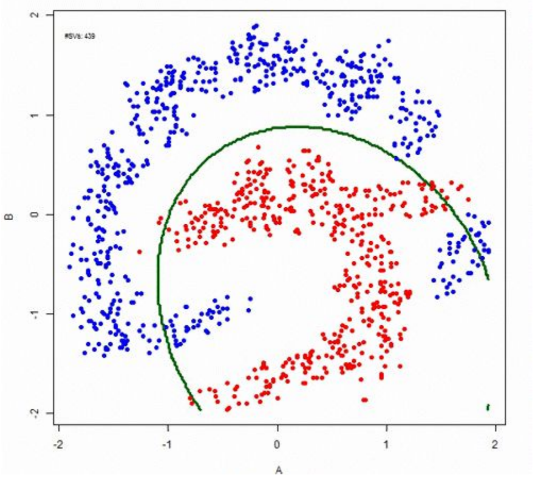
Overfitted



Combatting Overfitting



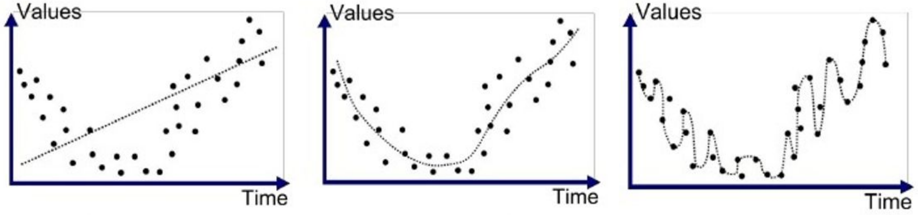
Underfitted   Good Fit/Robust   Overfitted



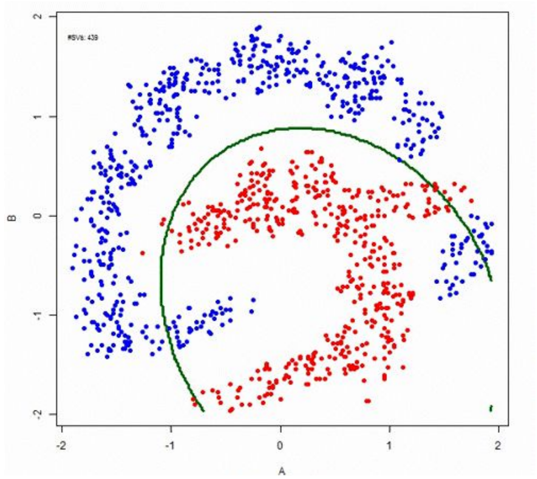
- Dropout prior
- Weight decay
- Early stopping
- Batch Normalization

SURF

Combatting Overfitting



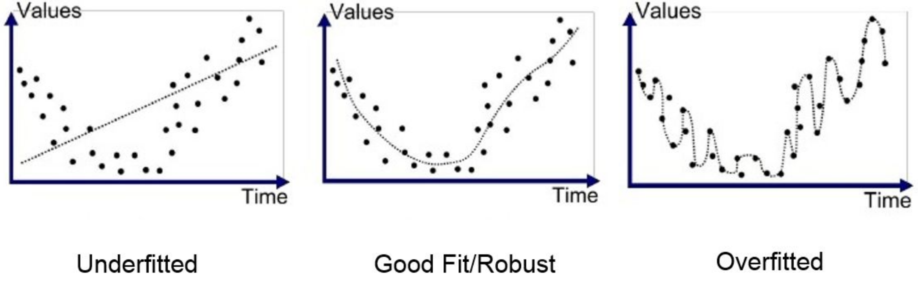
Underfitted Good Fit/Robust Overfitted

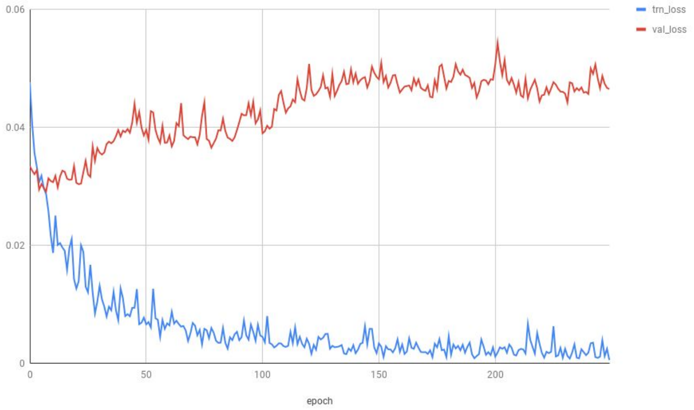


- Dropout prior
- Weight decay
- Early stopping
- Batch Normalization

The more weights we need to train, the more complex the model becomes and the sooner it starts to memorize, if we don’t have enough data

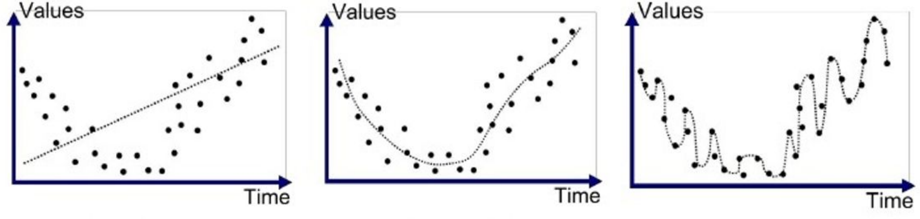
Combatting Overfitting





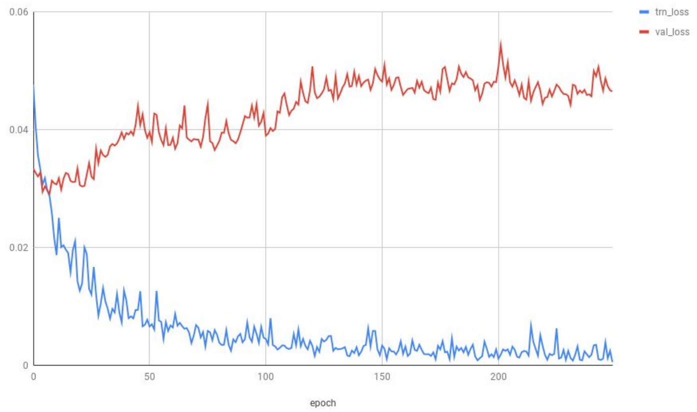
- Dropout prior
- Weight decay
- Early stopping
- Batch Normalization

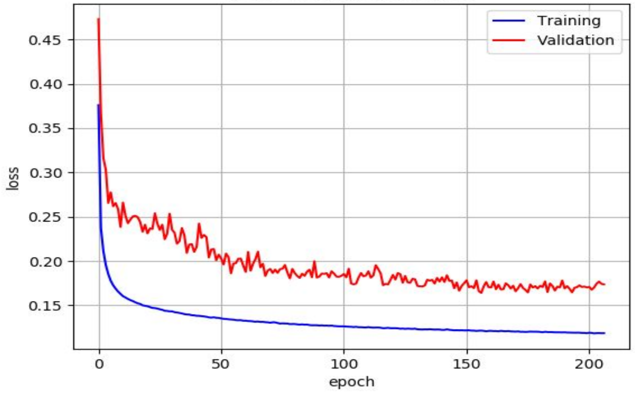
Combatting Overfitting



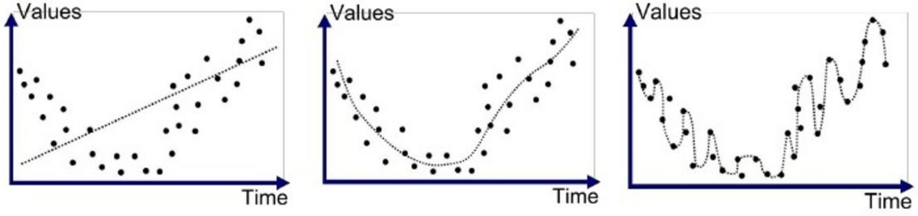
Underfitted | Good Fit/Robust | Overfitted

- Dropout prior
- Weight decay
- Early stopping
- Batch Normalization



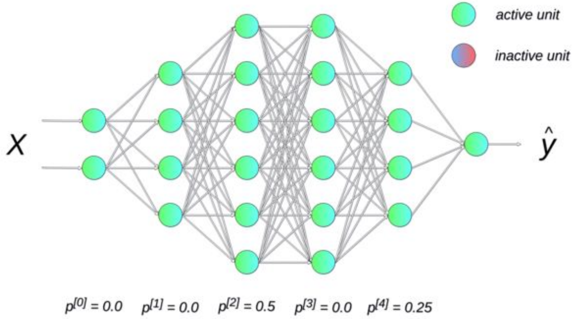


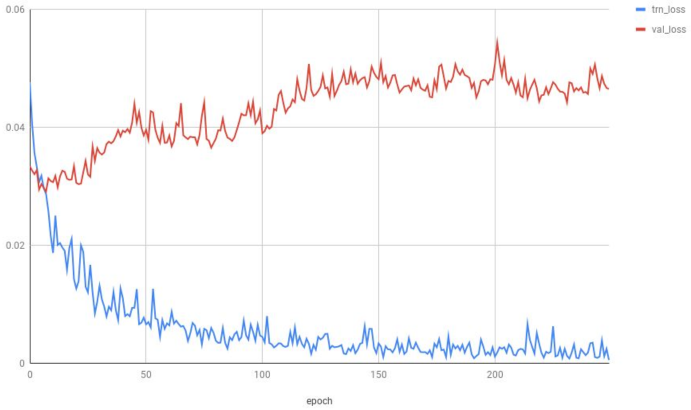
Combatting Overfitting

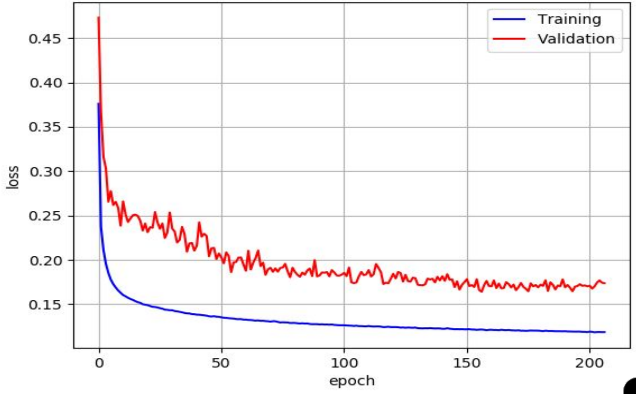


Underfitted   Good Fit/Robust   Overfitted

- Dropout prior
- Weight decay
- Early stopping
- Batch Normalization

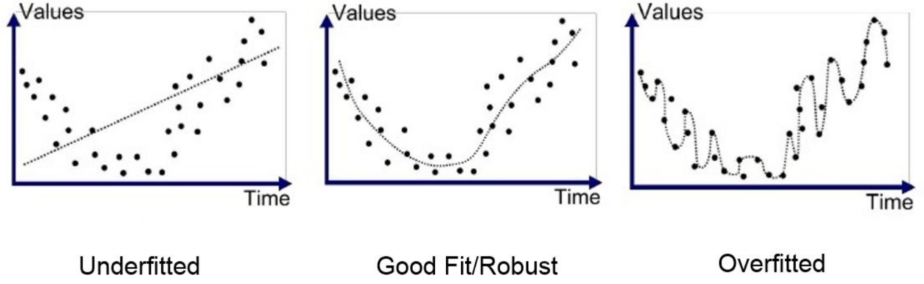


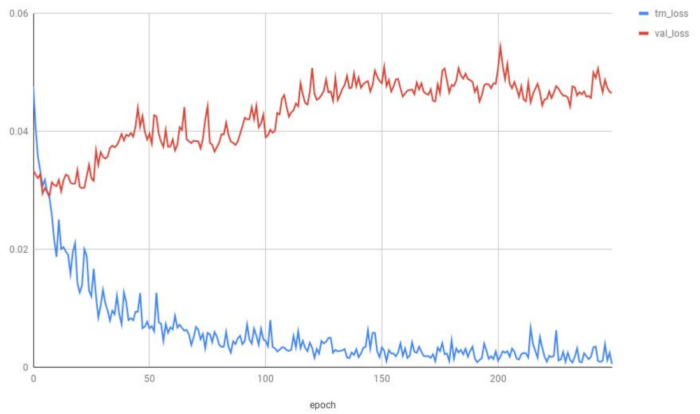




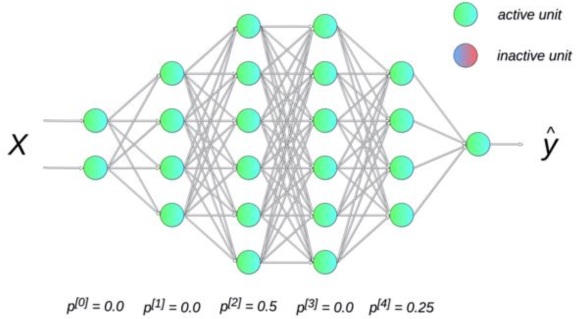
SURF

Combatting Overfitting





- Dropout prior
- Weight decay
- Early stopping
- Batch Normalization

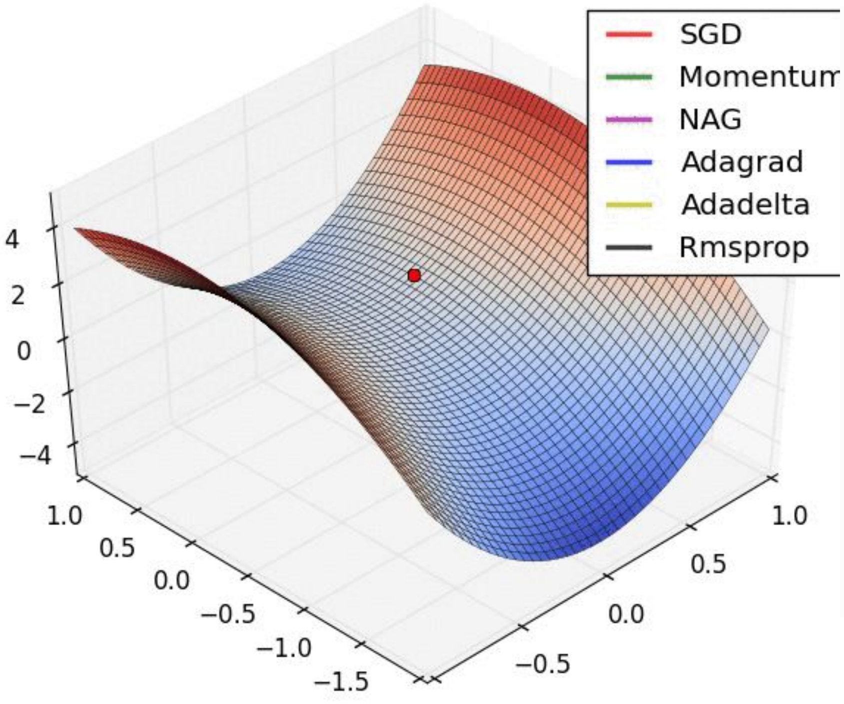


Models always need regularization no matter how big

Not entirely understood how all these tricks amount to a more complex separating hyperplane

Optimizers

In what way should we change the weights?



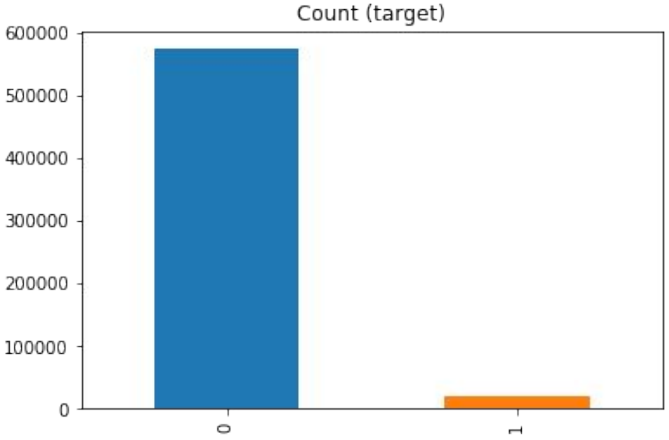
11/01/2023

ML Workflow

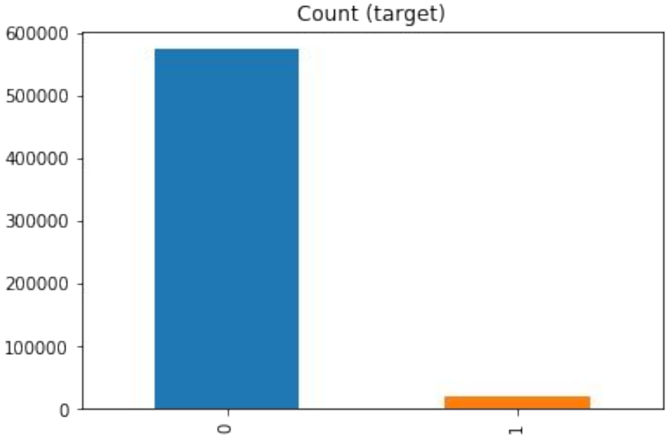
Artificial Intelligence still heavily relies on human intelligence

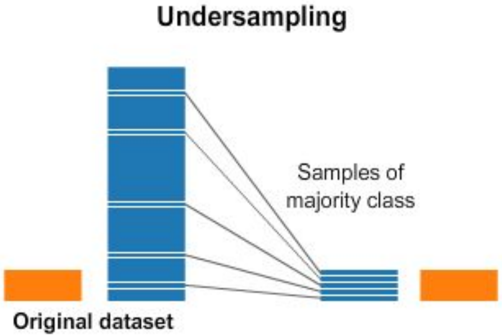
High Performance Machine Learning Group

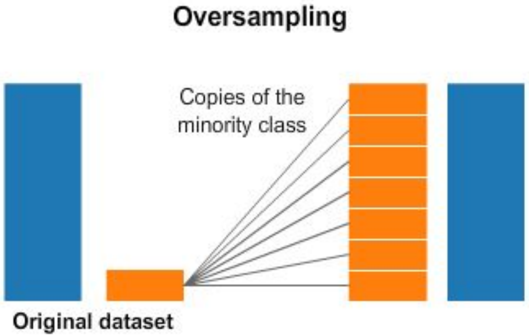
Imbalanced Training set



Imbalanced Training set

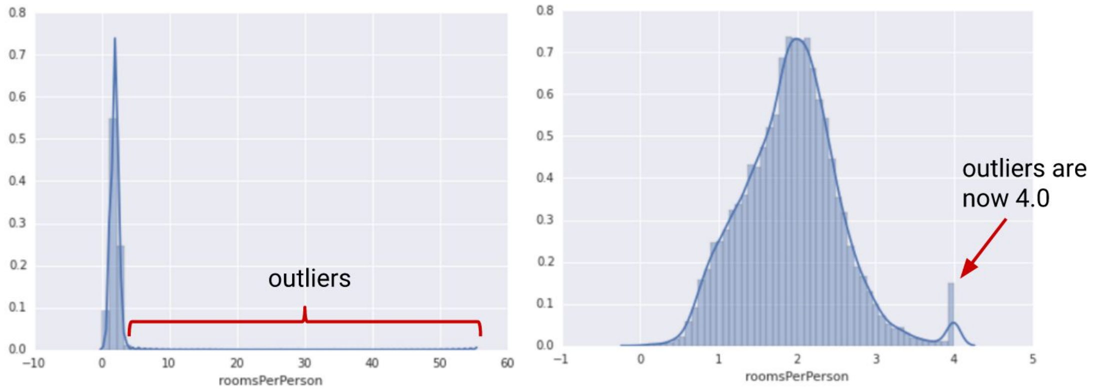


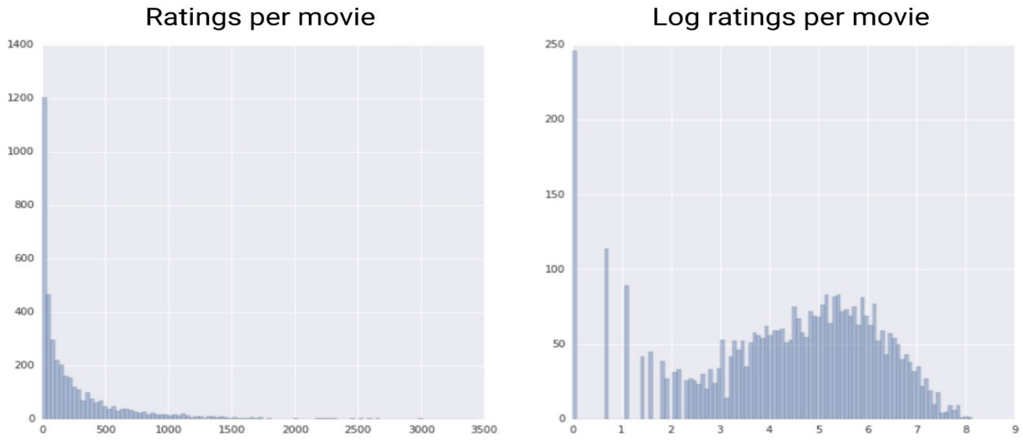




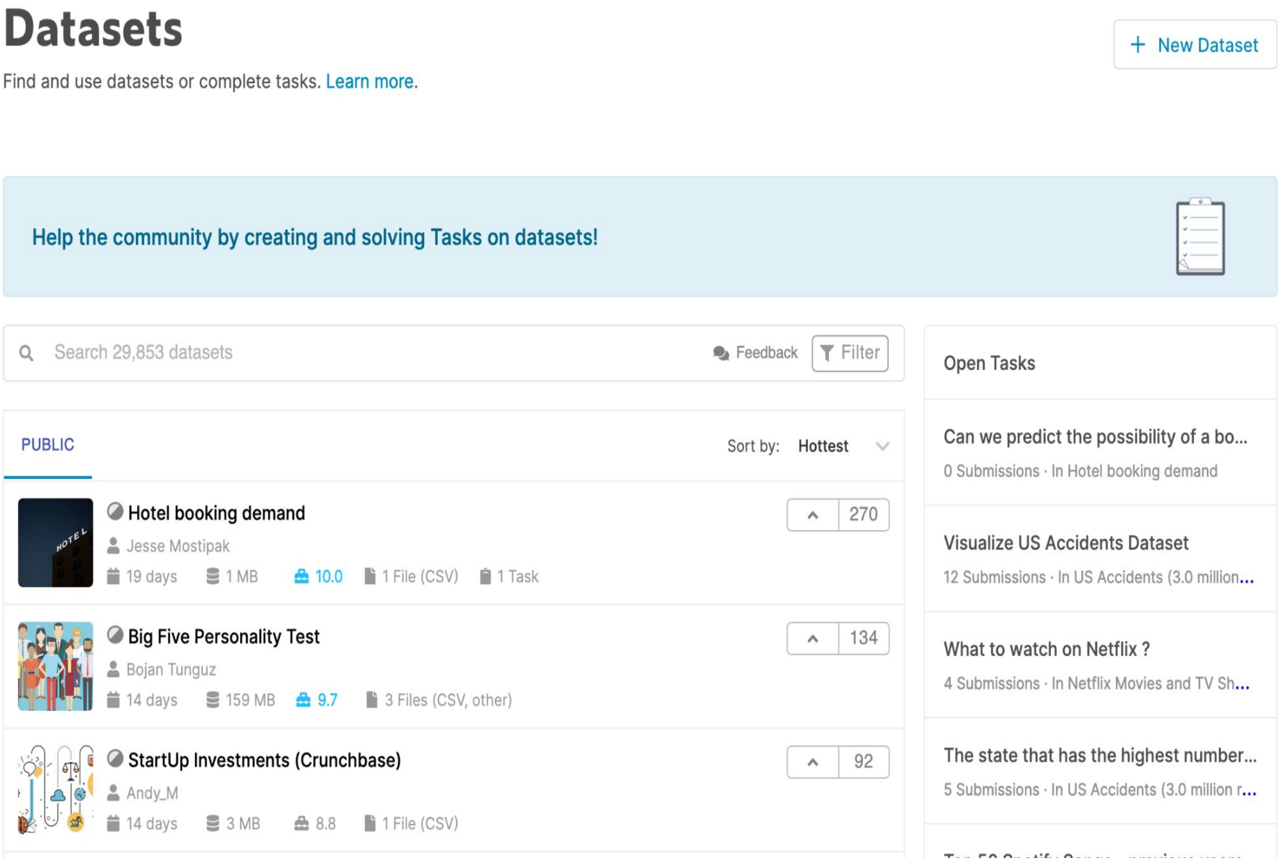
Data normalization

A process to transform the input **data** in a **well-behaved** form





Open Datasets



Processed, balanced, well-behaved and labelled datasets

tensorflow.org/datasets

kaggle.com/datasets

topepo.github.io/caret/data-sets.html

github.com/awesomedata/awesome-public-datasets

Dataset Splitting

Training set

Model training

Best model parameters
Weights

70%

Validation set

Model selection

Best hyperparameters
Learning rate
#neurons
#layers

20%

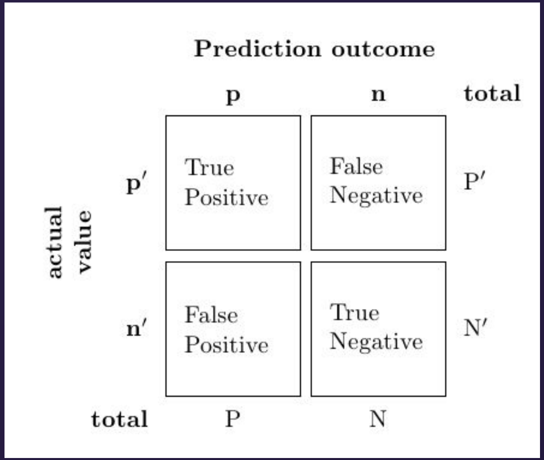
Test set

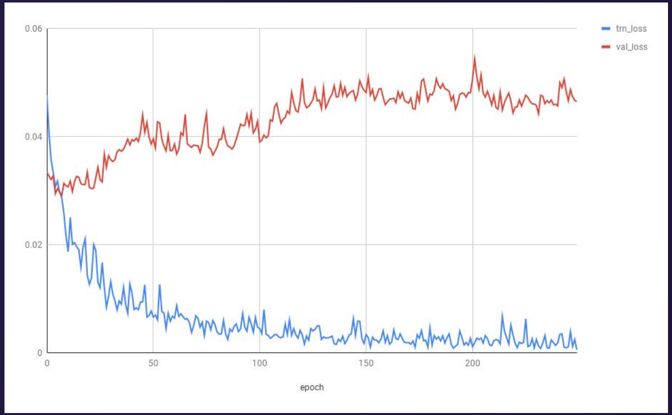
Model testing

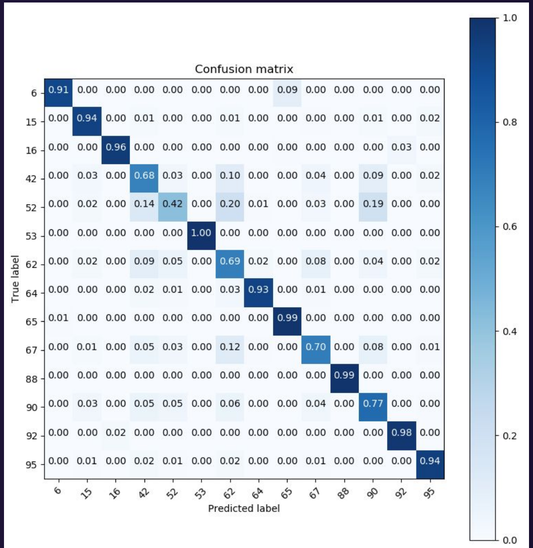
Final model
Accuracy
Sensitivity/
specificity

10%

Network Evaluation







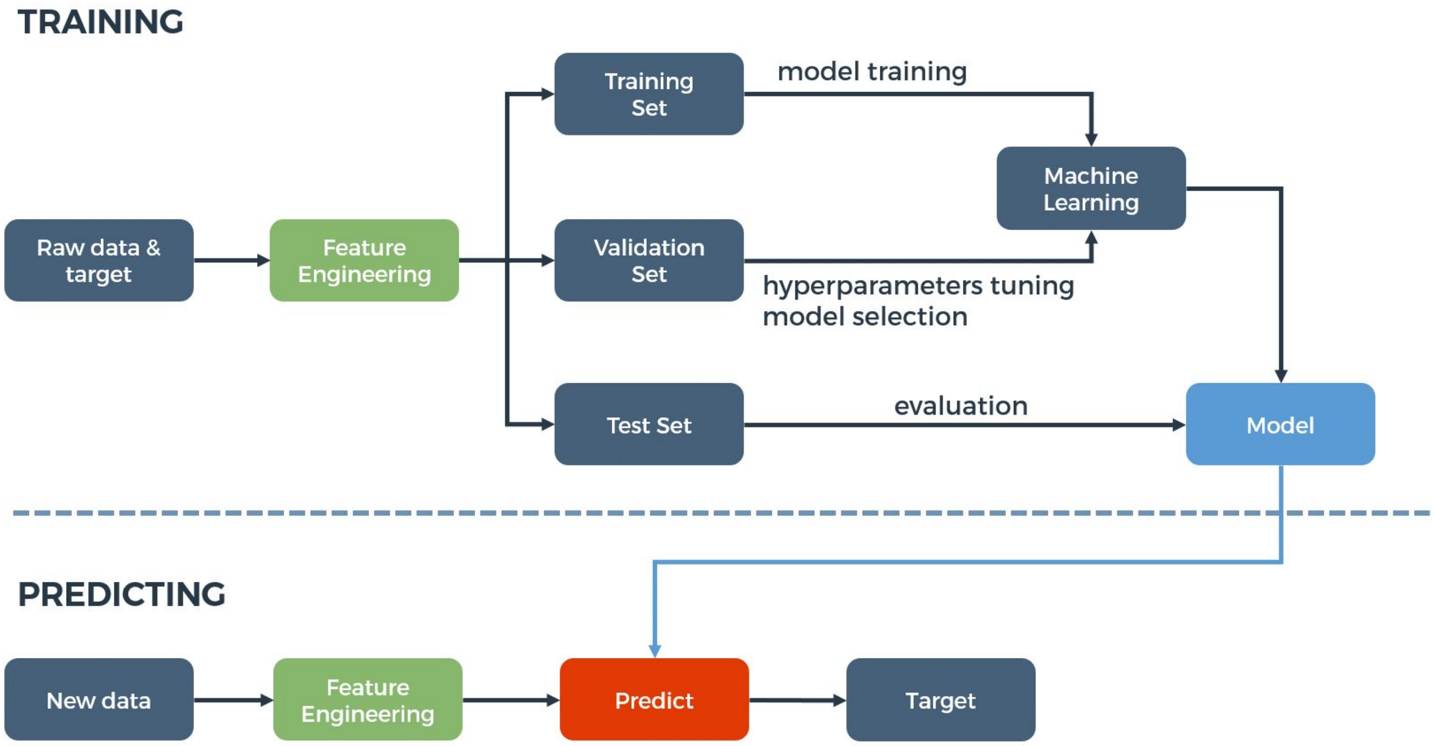
Choose an appropriate metric for your own problem

Always sanity check your model, is it better than a baseline?

An almost perfect classification score is always sketchy

Keep questioning the model, never trust it

Workflow


TRAINING
Raw data & target
Feature Engineering
Training Set
Validation Set
Test Set
model training
Machine Learning
hyperparameters tuning
model selection
evaluation
Model
PREDICTING
New data
Feature Engineering
Predict
Target

11/01/2023

DL Frameworks

Do not compute your own gradients

High Performance Machine Learning Group

How to train your NN

- Define neurons and layers
- Define loss function
- Forward propagate and compute loss
- Compute gradient
- Propagate backward
- Update weights

Keras

theano

TensorFlow

Microsoft Cognitive Toolkit

PyTorch

PyTorch and Modularity

PyTorch

Three Levels of Abstraction

01. **Tensor:** imperative ndarray, possible to run on GPU/TPU

02. (node) **Variable:** Node in the built computational graph; data, gradient storage

03. (NN) **Module:** A neural network layer, store the state and the weights of the neural network

PyTorch

Three Levels of Abstraction

01. Tensor: imperative ndarray, possible to run on GPU/TPU

02. (node) **Variable:** Node in the built computational graph; data, gradient storage

03. (NN) **Module:** A neural network layer, store the state and the weights of the neural network

SURF

PyTorch

Three Levels of Abstraction

01. **Tensor**: imperative ndarray, possible to run on GPU/TPU

02. (node) **Variable**: Node in the built computational graph; data, gradient storage

03. (NN) **Module:** A neural network layer, store the state and the weights of the neural network

SURF

PyTorch

Three Levels of Abstraction

01. **Tensor**: imperative ndarray, possible to run on GPU/TPU

02. (node) **Variable**: Node in the built computational graph; data, gradient storage

03. (NN) **Module**: A neural network layer, store the state and the weights of the neural network

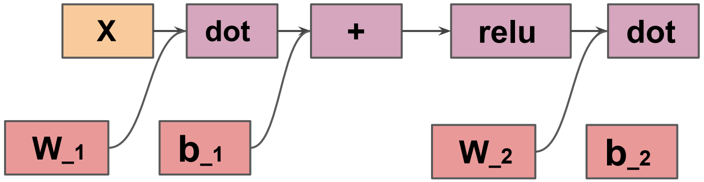
PyTorch

Three Levels of Abstraction

01. **Tensor**: imperative ndarray, possible to run on GPU/TPU

02. (node) **Variable**: Node in the built computational graph; data, gradient storage

03. (NN) **Module**: A neural network layer, store the state and the weights of the neural network



SURF

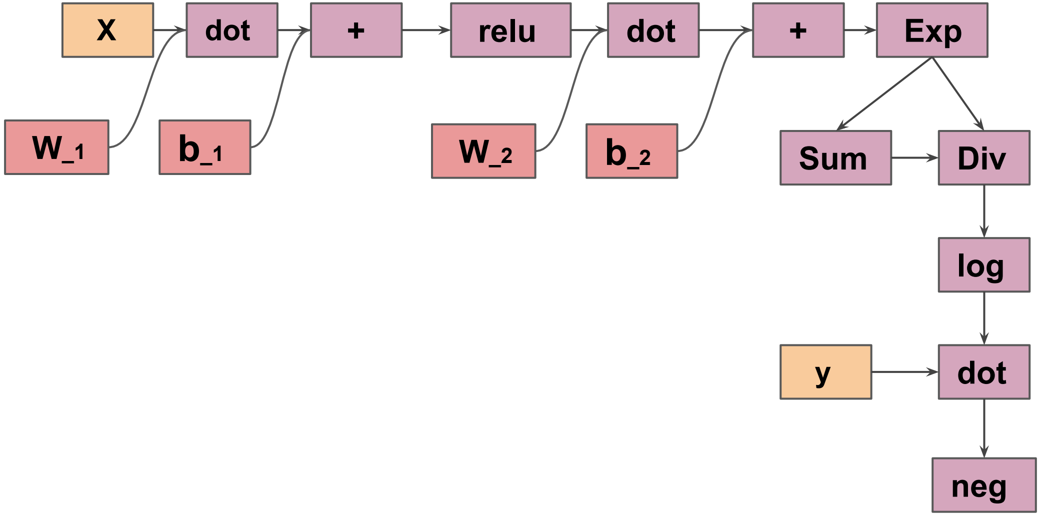
PyTorch

Three Levels of Abstraction

01. **Tensor**: imperative ndarray, possible to run on GPU/TPU

02. (node) **Variable**: Node in the built computational graph; data, gradient storage

03. (NN) **Module**: A neural network layer, store the state and the weights of the neural network



SURF

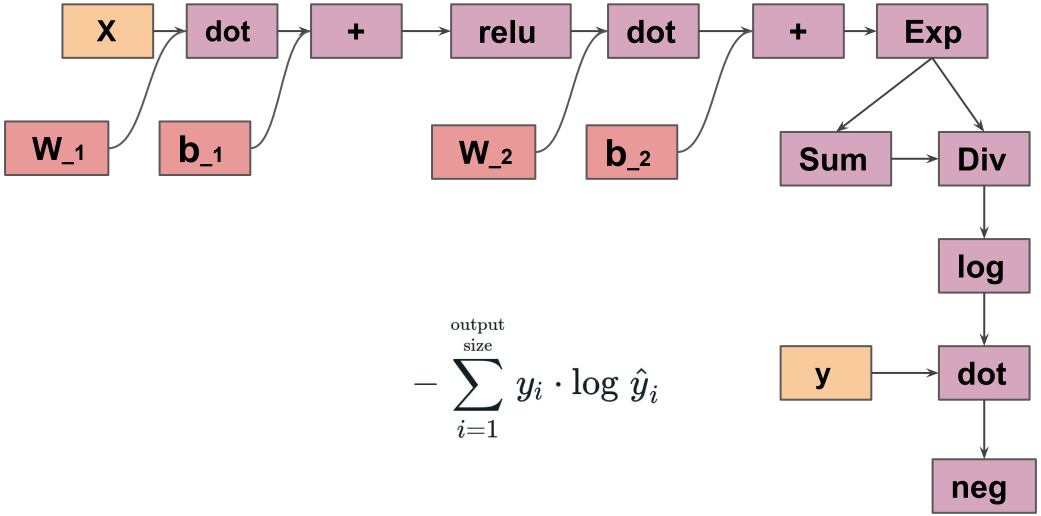
PyTorch

Three Levels of Abstraction

01. **Tensor**: imperative ndarray, possible to run on GPU/TPU

02. (node) **Variable**: Node in the built computational graph; data, gradient storage

03. (NN) **Module**: A neural network layer, store the state and the weights of the neural network



$$-\sum_{i=1}^{\text{output size}} y_i \cdot \log \hat{y}_i$$

SURF

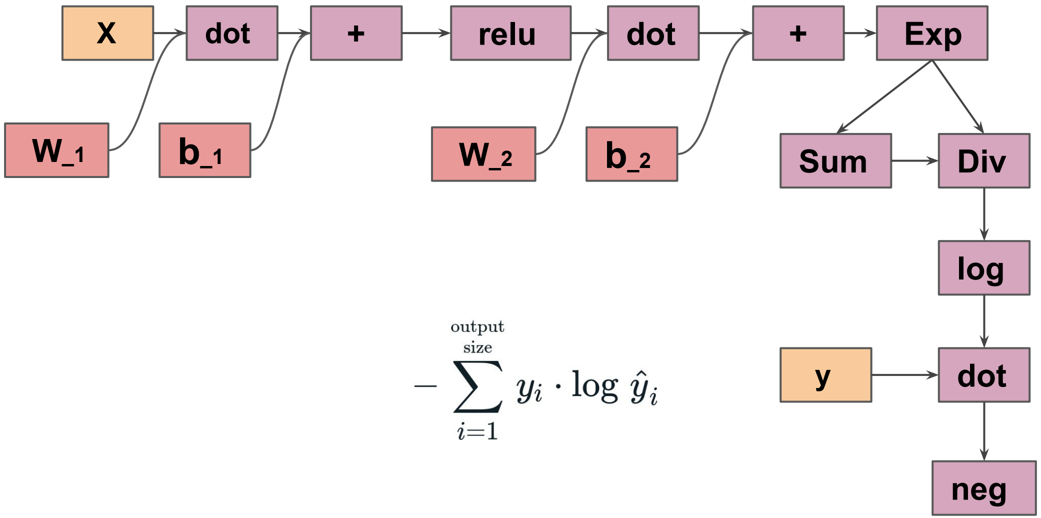
PyTorch

Three Levels of Abstraction

01. **Tensor**: imperative ndarray, possible to run on GPU/TPU

02. (node) **Variable**: Node in the built computational graph; data, gradient storage

03. (NN) **Module**: A neural network layer, store the state and the weights of the neural network



$$-\sum_{i=1}^{\text{output size}} y_i \cdot \log \hat{y}_i$$

PyTorch

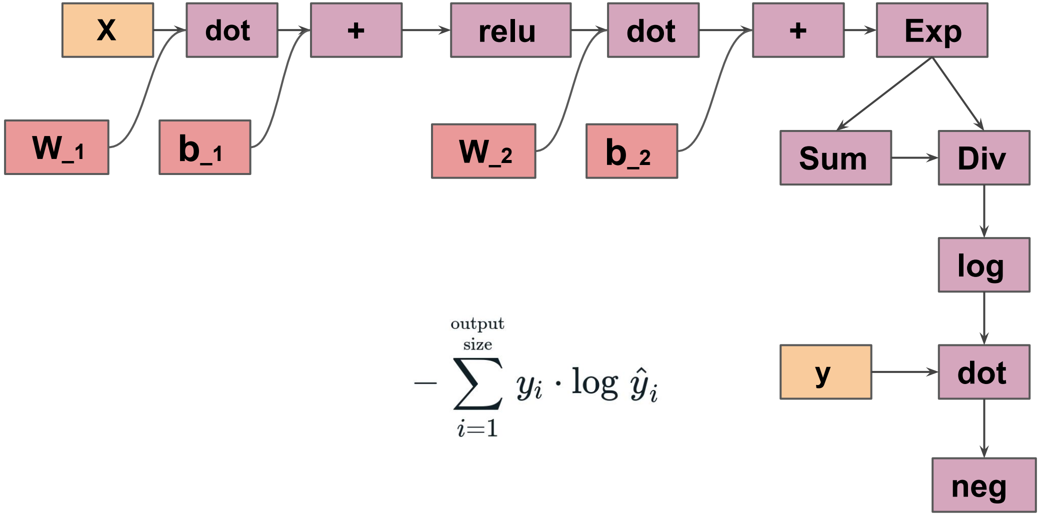
Three Levels of Abstraction

01. **Tensor**: imperative ndarray, possible to run on GPU/TPU

02. (node) **Variable**: Node in the built computational graph; data, gradient storage

03. (NN) **Module**: A neural network layer, store the state and the weights of the neural network

$$\hat{y} = g(\mathbf{W}_0 f(\mathbf{W}_1 \mathbf{x}))$$



$$-\sum_{i=1}^{\text{output size}} y_i \cdot \log \hat{y}_i$$

SURF

PyTorch

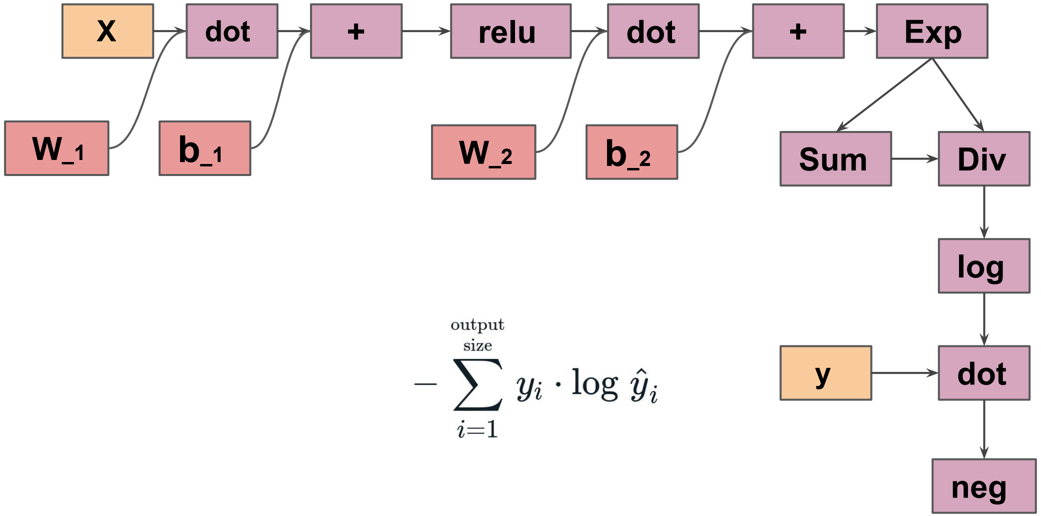
Three Levels of Abstraction

01. **Tensor**: imperative ndarray, possible to run on GPU/TPU

02. (node) **Variable**: Node in the built computational graph; data, gradient storage

03. (NN) **Module**: A neural network layer, store the state and the weights of the neural network

$$\hat{y} = g(\mathbf{W}_0 f(\mathbf{W}_1 \mathbf{x}))$$



$$-\sum_{i=1}^{\substack{\text{output}\\\text{size}}} y_i \cdot \log \hat{y}_i$$

Pytorch will helps us with

- Defining a dataset
- Automatic Gradient Computation
- Defining Neural Networks
- Optimization
- Scheduling
- Distributing

TORCH.NN

These are the basic building blocks for graphs:

torch.nn

- Containers
- Convolution Layers
- Pooling layers
- Padding Layers
- Non-linear Activations (weighted sum, nonlinearity)
- Non-linear Activations (other)
- Normalization Layers
- Recurrent Layers
- Transformer Layers
- Linear Layers
- Dropout Layers
- Sparse Layers
- Distance Functions
- Loss Functions
- Vision Layers
- Shuffle Layers
- DataParallel Layers (multi-GPU, distributed)
- Utilities
- Quantized Functions
- Lazy Modules Initialization

https://pytorch.org/docs/stable/

PyTorch

General Training Structure

data loader
model
optimizer
loss function

PyTorch

General Training Structure

data loader
model
optimizer
loss function
For every datapoint, y in **data_loader**

SURF

PyTorch

General Training Structure

data loader
model
optimizer
loss function
For every datapoint, y in **data_loader**
        optimizer.zero_grad()

PyTorch

General Training Structure

data loader
model
optimizer
loss function

```
For every datapoint, y in data_loader
        optimizer.zero_grad()
        prediction = model(datapoint)
```

SURF

PyTorch

General Training Structure

data loader
model
optimizer
loss function

```
For every datapoint, y in data_loader
        optimizer.zero_grad()
        prediction = model(datapoint)
        loss = loss_function(prediction, y)
```

SURF

PyTorch

General Training Structure

```
data loader
model
optimizer
loss function
For every datapoint, y in data_loader
        optimizer.zero_grad()
        prediction = model(datapoint)
        loss = loss_function(prediction, y)
        loss.backward()
```

PyTorch

General Training Structure

data loader
model
optimizer
loss function

```
For every datapoint, y in data_loader
        optimizer.zero_grad()
        prediction = model(datapoint)
        loss = loss_function(prediction, y)
        loss.backward()
        optimizer.step()
```

$$\mathbf{w}_{j+1} = \mathbf{w}_j - \alpha \nabla L(\mathbf{w}_j, b)$$

SURF

PyTorch

General Training Structure

data loader
model
optimizer
loss function

For every datapoint, y in **data_loader**

    optimizer.zero_grad()
    prediction = model(datapoint)
    loss = loss_function(prediction, y)
    loss.backward()
    optimizer.step()

$$\mathbf{w}_{j+1} = \mathbf{w}_j - \alpha \nabla L(\mathbf{w}_j, b)$$

```python
for batch_idx, (data, target) in enumerate(train_loader):
    data, target = data.to(device), target.to(device)

    optimizer.zero_grad()
    output = model(data)
    loss = F.nll_loss(output, target)
    loss.backward()
    optimizer.step()
```

PyTorch

Data:

d_1 = [0.9, -0.2], y = 0
d_2 = [0.75, 0.6],y = 1

Define Neural Network

Input size of 2
One hidden layer of 8 nodes
1 output node (binary)

PyTorch

Data:

d_1 = [0.9, -0.2], y = 0
d_2 = [0.75, 0.6],y = 1

Define Neural Network

Input size of 2
One hidden layer of 8 nodes
1 output node (binary)

Learning rate = 0.01
Optimizer = Stochastic Gradient Descent
Loss = Binary Cross Entropy

PyTorch

Data:

d_1 = [0.9, -0.2], y = 0
d_2 = [0.75, 0.6],y = 1

Define Neural Network

Input size of 2
One hidden layer of 8 nodes
1 output node (binary)

Learning rate = 0.01
Optimizer = Stochastic Gradient Descent
Loss = Binary Cross Entropy

$$\text{Loss} = -\sum_{i=1}^{\substack{\text{output}\\ \text{size}}} y_i \cdot \log \hat{y}_i$$

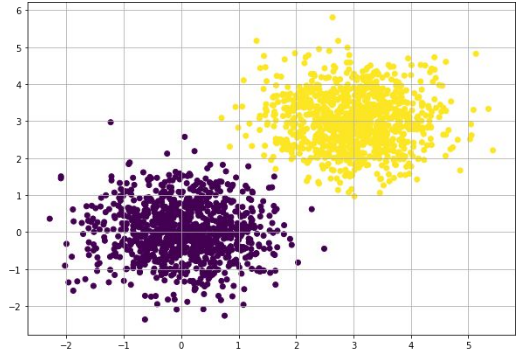
PyTorch

Data:

d_1 = [0.9, -0.2], y = 0
d_2 = [0.75, 0.6],y = 1

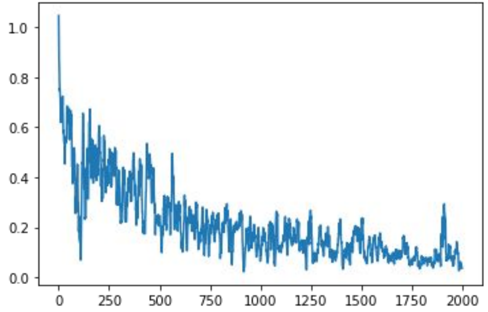
Define Neural Network

Input size of 2
One hidden layer of 8 nodes
1 output node (binary)



Learning rate = 0.01
Optimizer = Stochastic Gradient Descent
Loss = Binary Cross Entropy

$$\text{Loss} = -\sum_{i=1}^{\substack{\text{output}\\\text{size}}} y_i \cdot \log \hat{y}_i$$



Fin

Introduction Series

Bryan Cardenas
Thomas van Osch