09/11/2022

Deep Learning

Introduction Series

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Robert Jan Schlimbach
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High Performance Machine Learning Group

Prerequisites

Programming

R / Python

Statistics, Calculus

Machine Learning / Deep Learning

Parallel Computing

Plan for Today

01.

General Introduction to ML

Neural Network

Convolutional Neural Networks

02.

Profiling your Neural Networks

High Performance

Plan until Lunch

01. DL Introduction — Pytorch Intro

02. Hands-on: Fully connected

03. Recap — Coffee Break

04. CNN Theory — Hands-on: CNNs

LUNCH

SURF

01. Machine Learning

SURF

What ML is *not*:

Mimicking human intelligence

Robotics

Deep Learning

SURF

What ML is *not*:

Mimicking human intelligence

Robotics

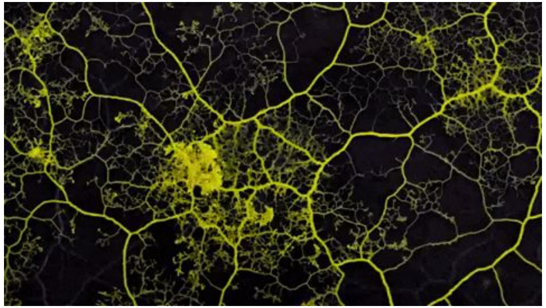
Deep Learning

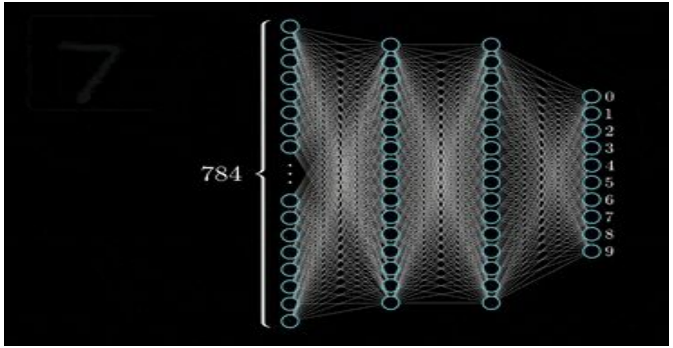
> “ML is the study of algorithms that can improve through experience and by the use of data. It is seen as part of Artificial Intelligence
>
> ~ Wikipedia

SURF

Artificial Intelligence

Having computers to exert Intelligent behaviour





Artificial Intelligence

Having computers to exert
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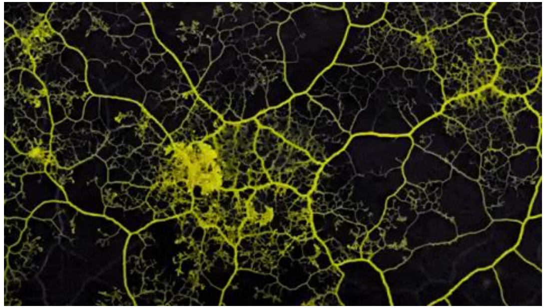
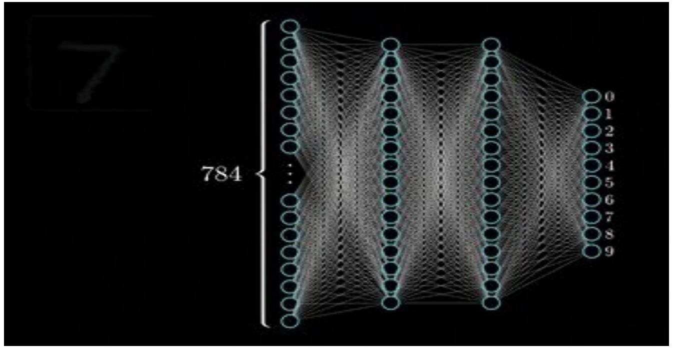
Machine Learning

Perform tasks without
Explicitly programmed
from data





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Artificial Intelligence

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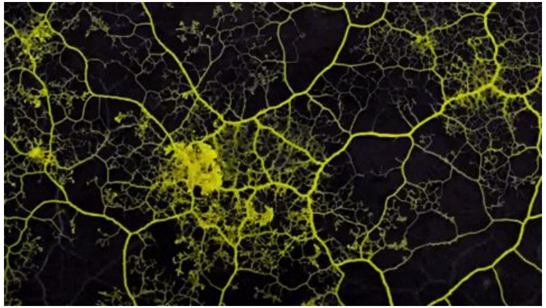
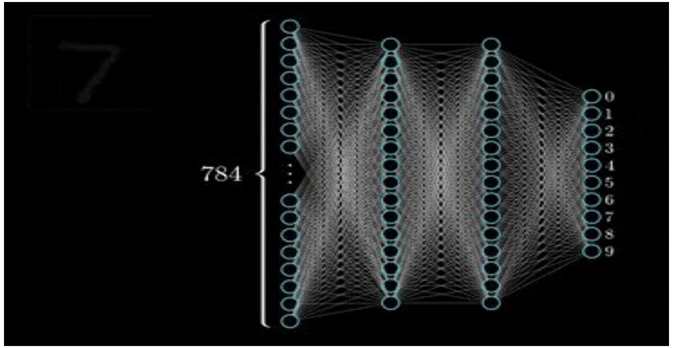
Machine Learning

Perform tasks without Explicitly programmed from data

Deep Learning

Use deep neural networks





Why Machine Learning?

Think of a simple
decision tree

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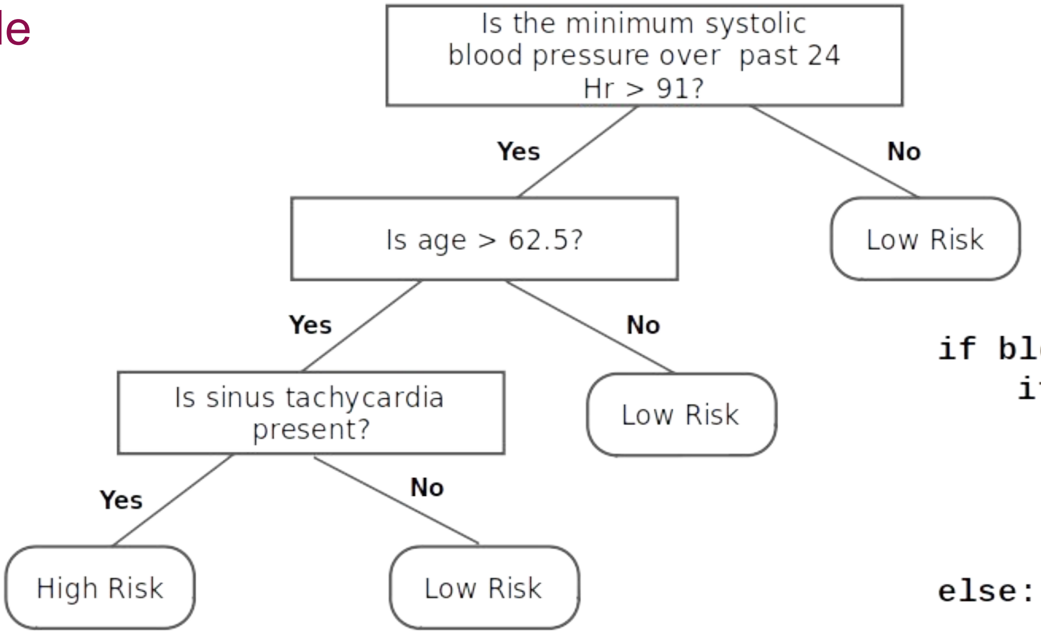
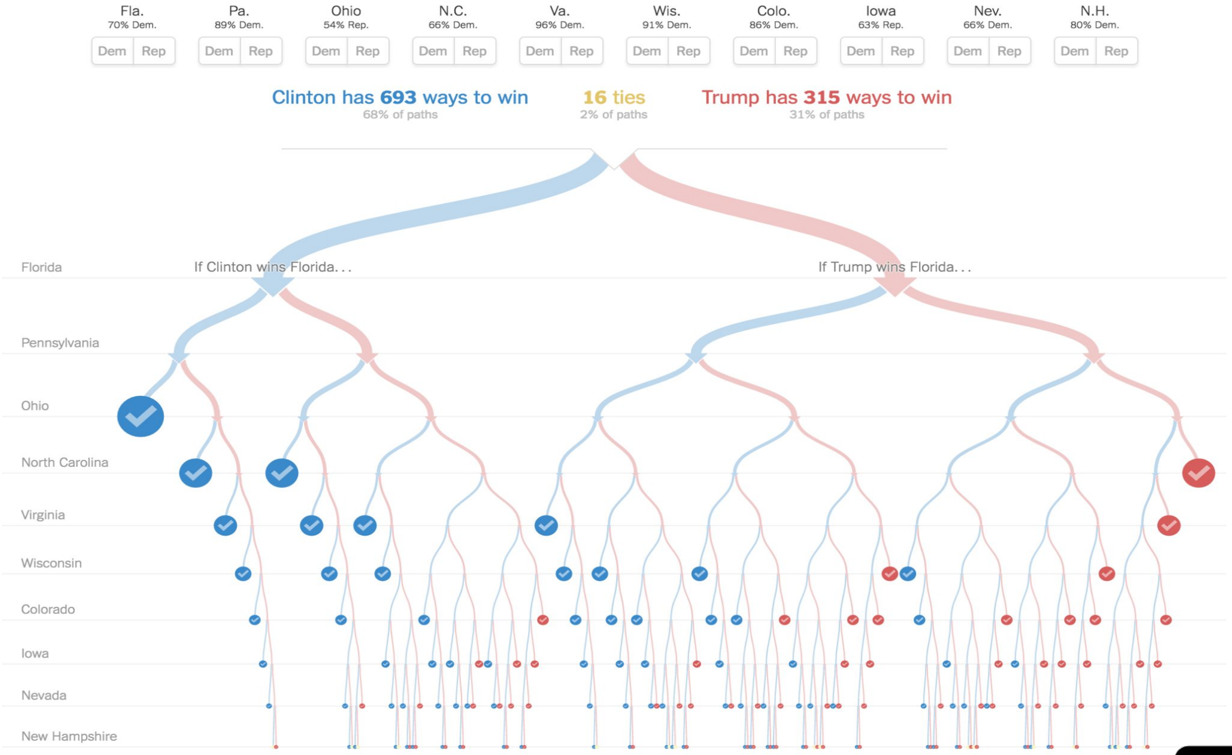
Think of a simple **decision tree**




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

Why Machine Learning?

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

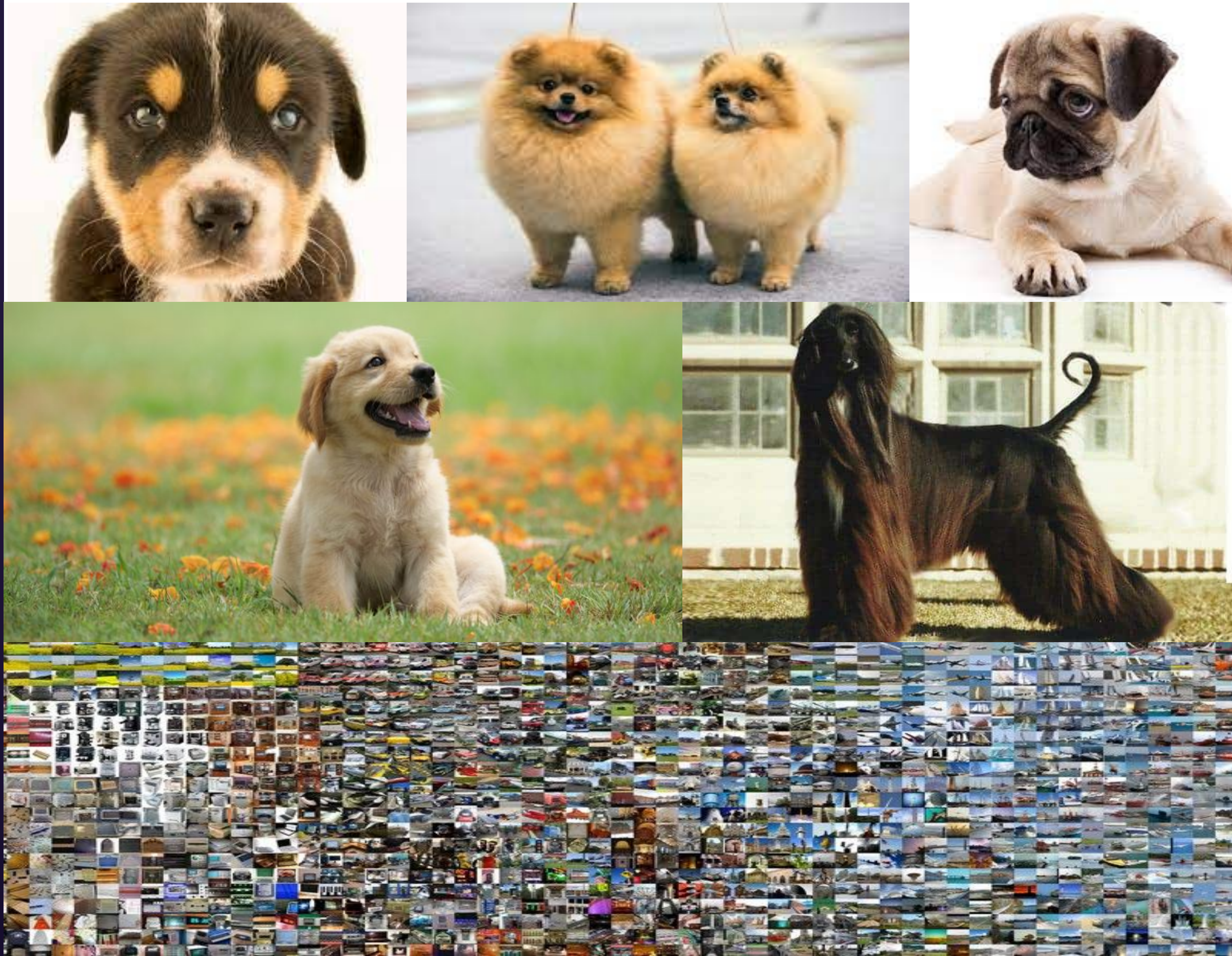


What is a dog?

Uncountable features that define a dog

We want an automatic way of learning these features

Driven by Data



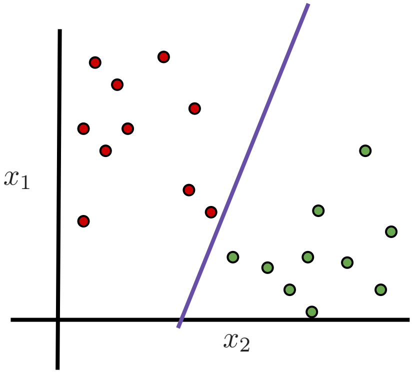
Categories of Machine Learning

01.

Supervised

Learn from labels

Regression, Classification

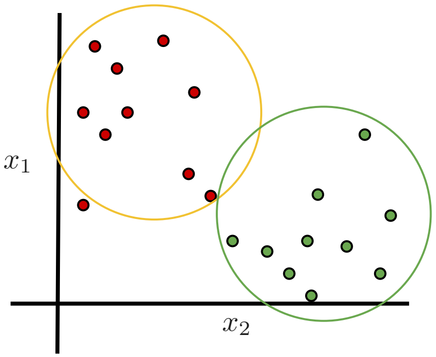


02.

Unsupervised

Detect Patterns in the data

Clustering, Dimensionality Reduction

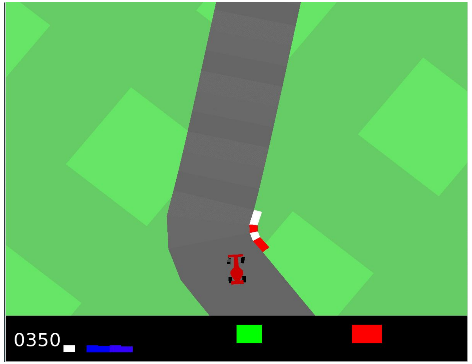


03.

Reinforcement

Learn from the environment

Control, gaming



SURF

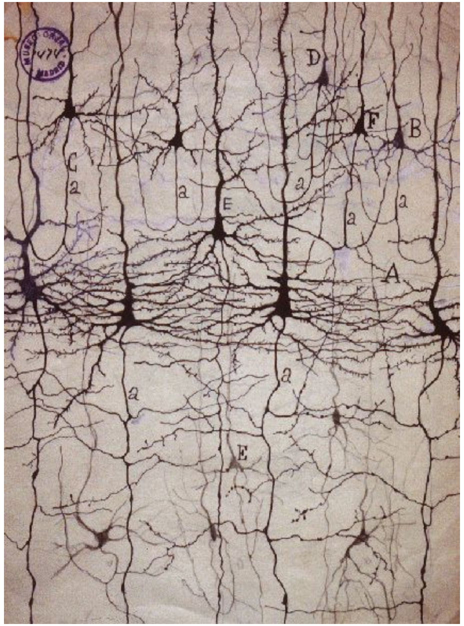
02. Neural Networks

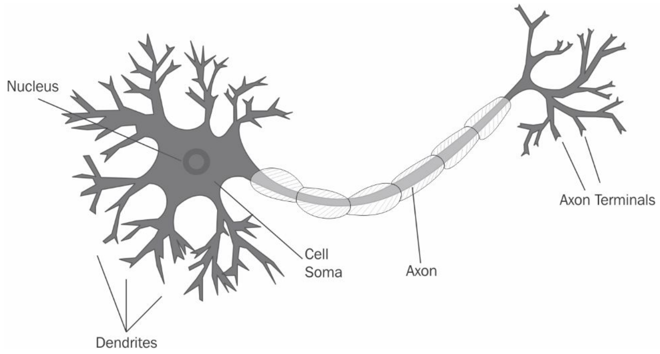
SURF

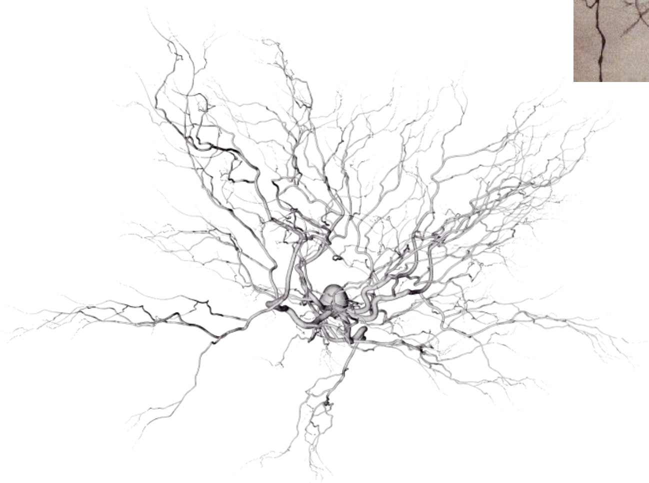
Biological Neuron

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

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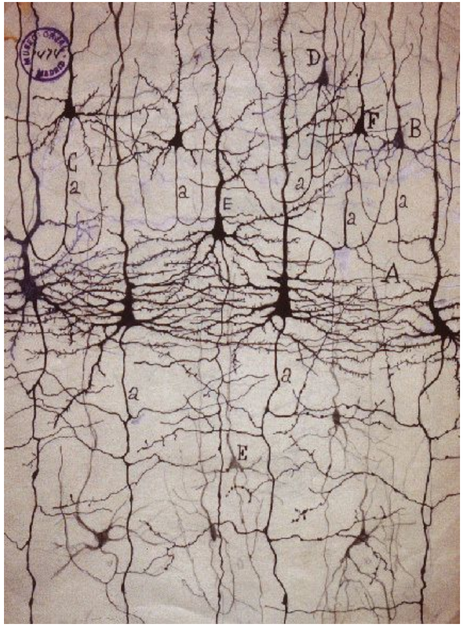
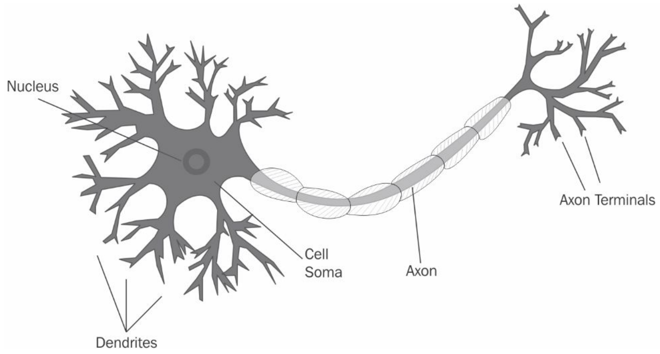
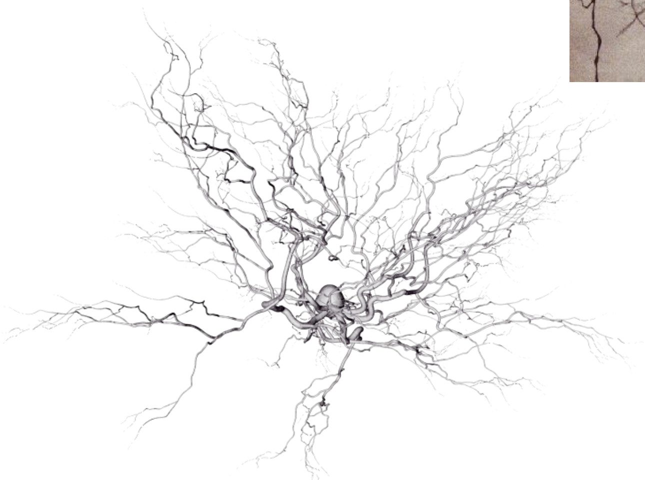
Humans have around 80 billion neurons and trillions of connections



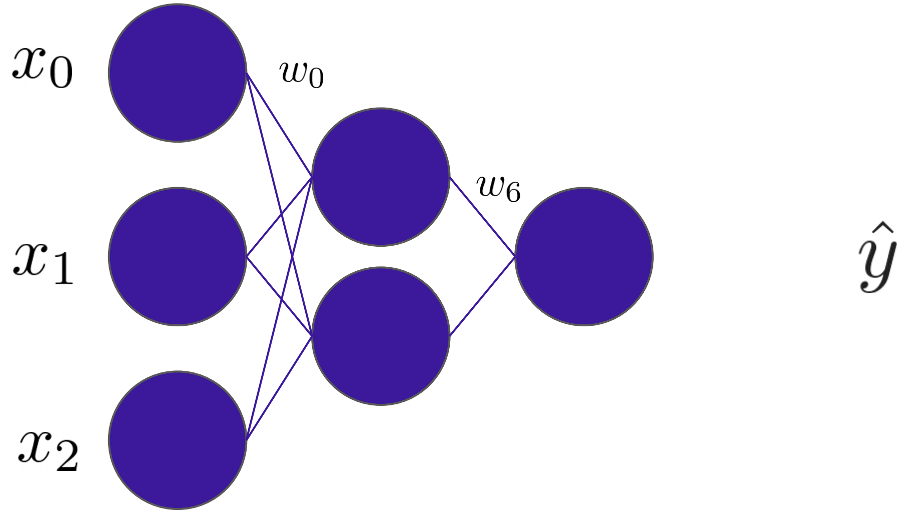




SURF

Anatomy of an Artificial Neural Network

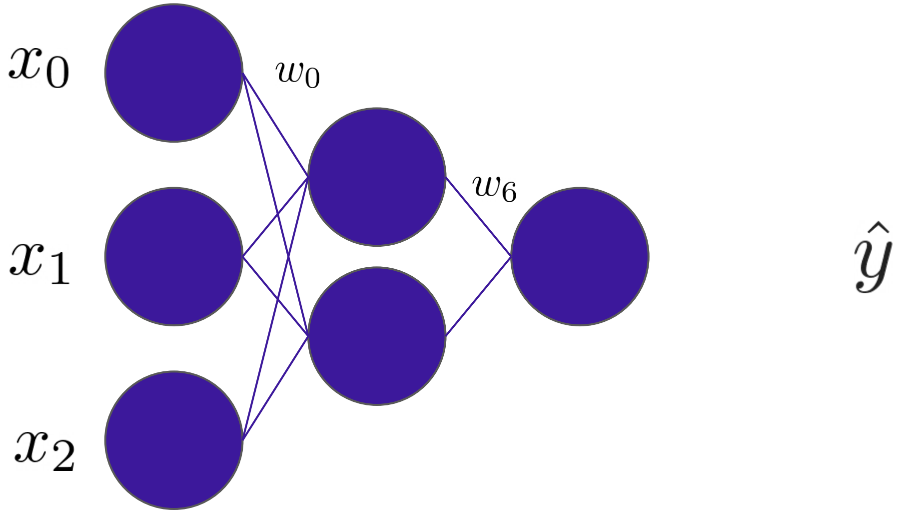
Don't model the biological neuron **precisely**



Anatomy of an Artificial Neural Network

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

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



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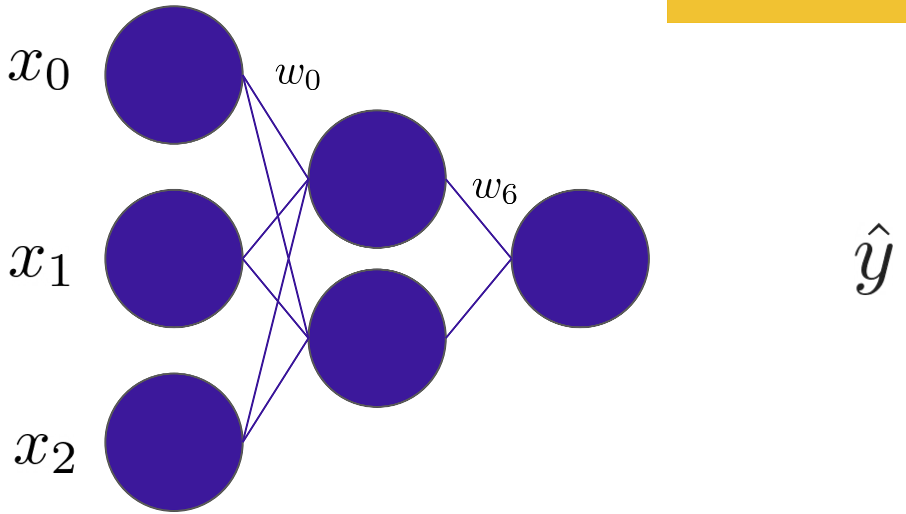
Use a (deep) neural network to **approximate** an unknown **function**



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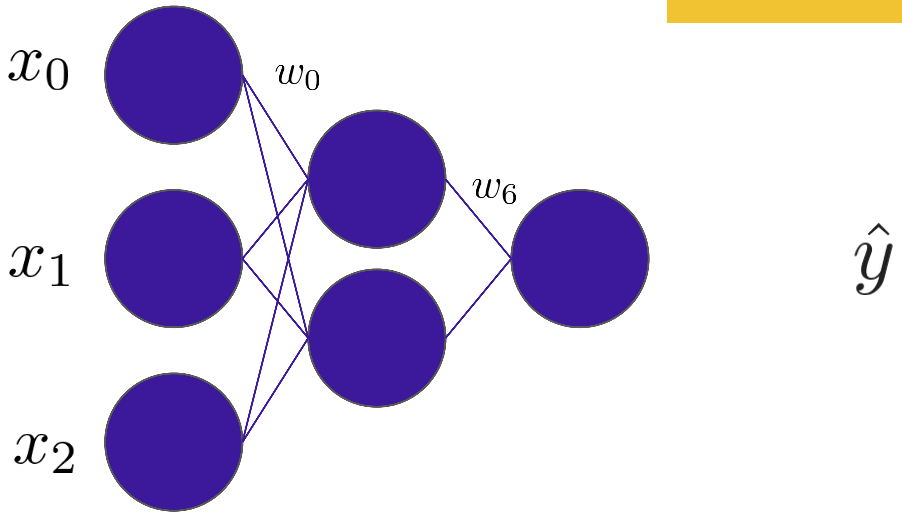

$$\sum_{i=1}^{m} w_i x_i + b$$

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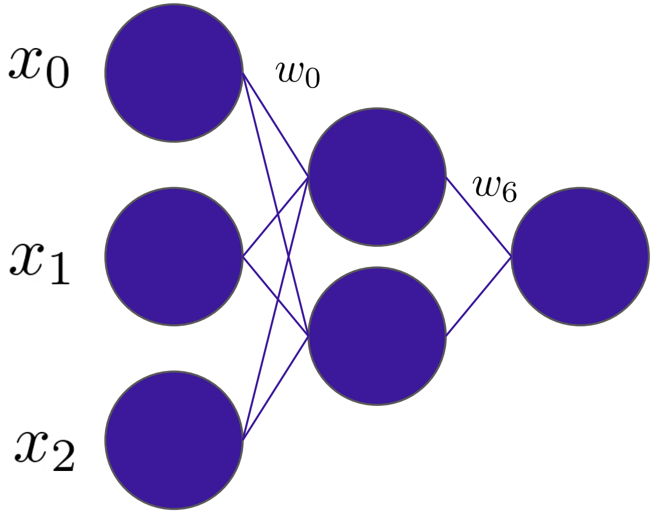

$\hat{y}$

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

$$\mathbf{Wx}$$

Anatomy of an Artificial Neural Network

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

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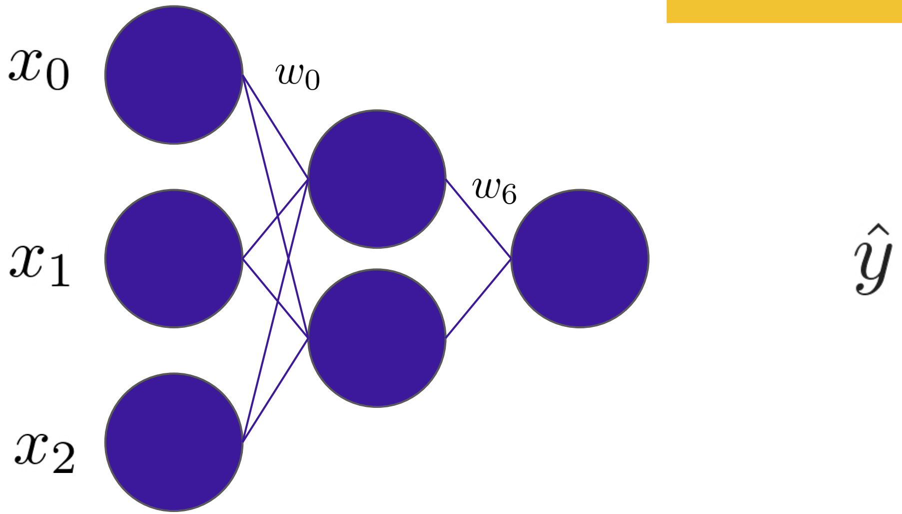
❖ Easy to **compose** and easy to **vectorize**

❖ Fits current compute paradigm

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



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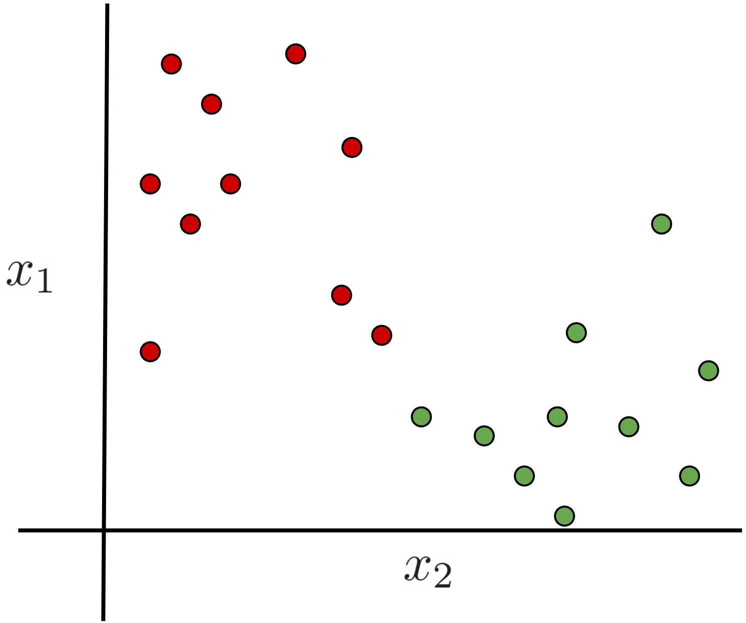
SURF

The Perceptron and Activation

Binary Classification Task



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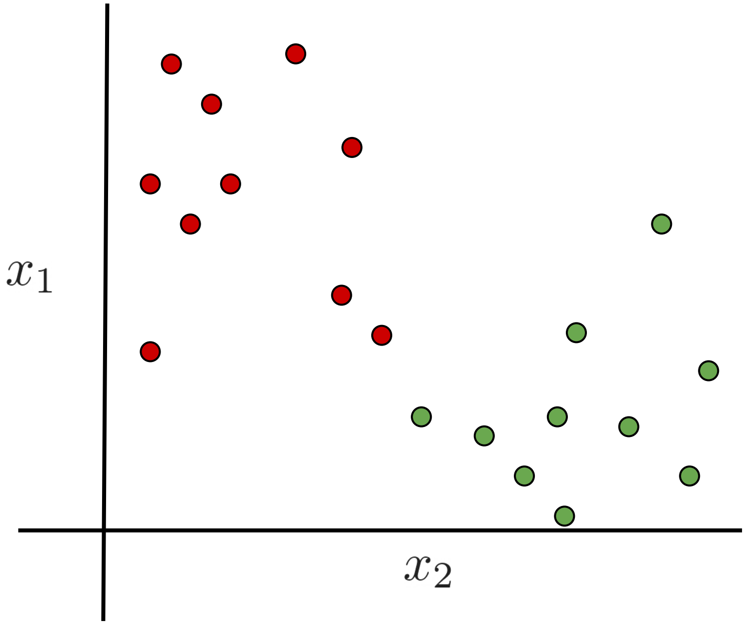

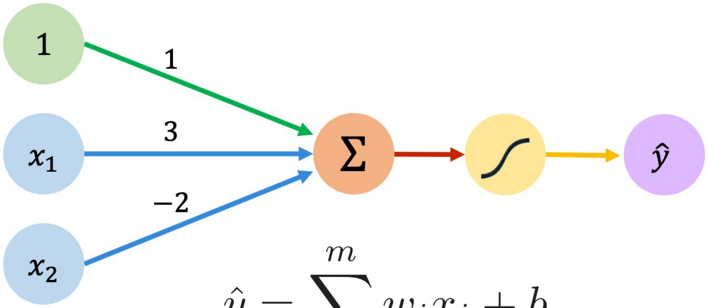

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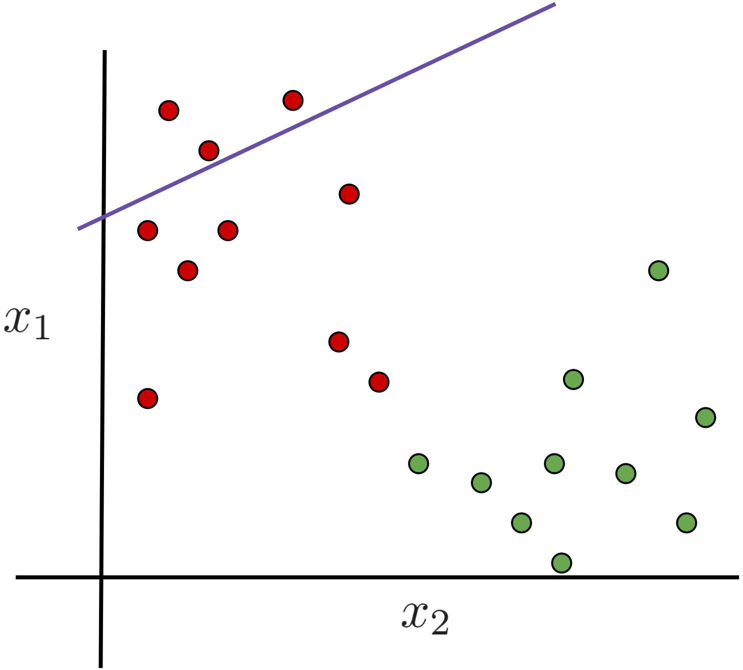

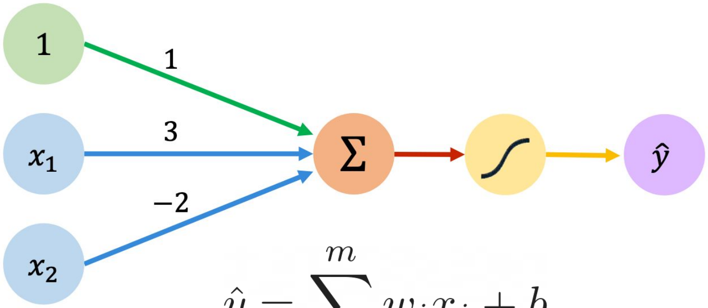

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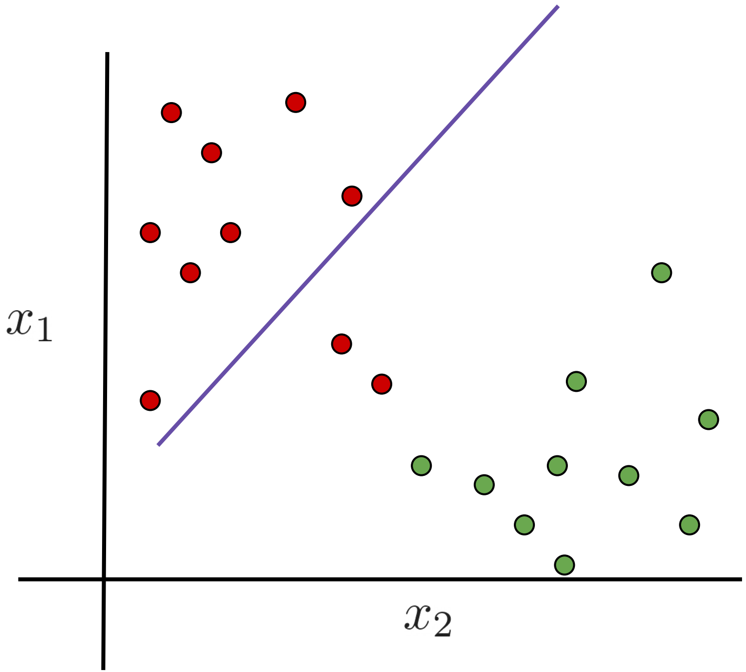

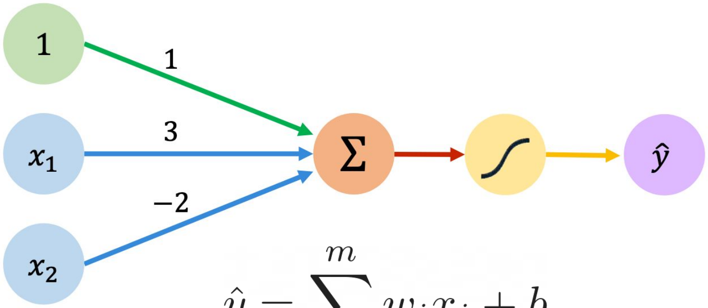

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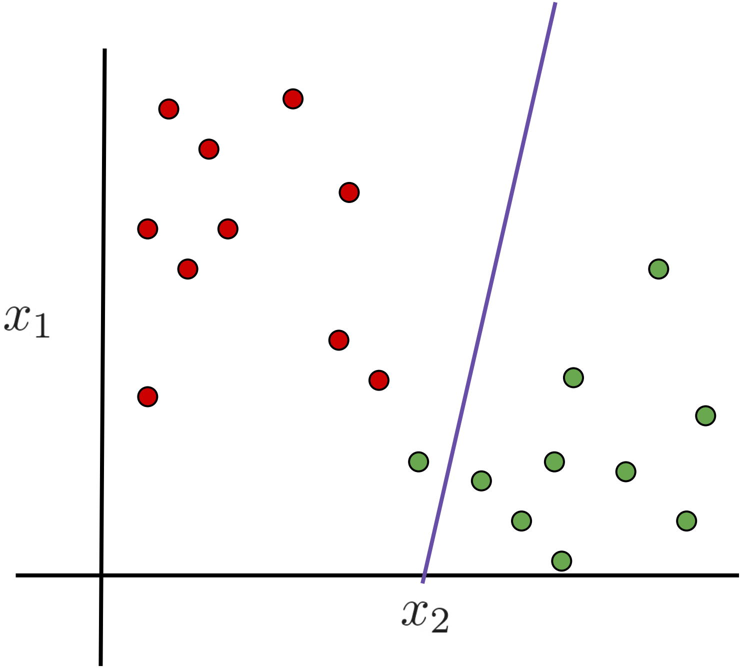

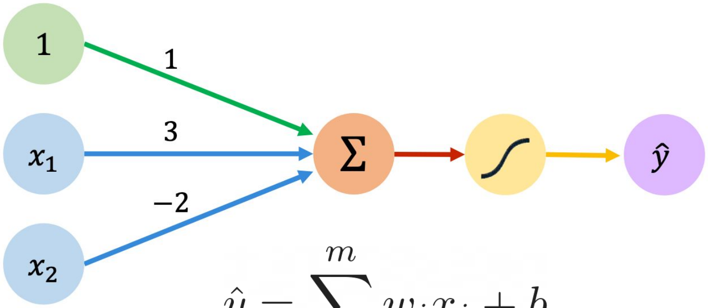

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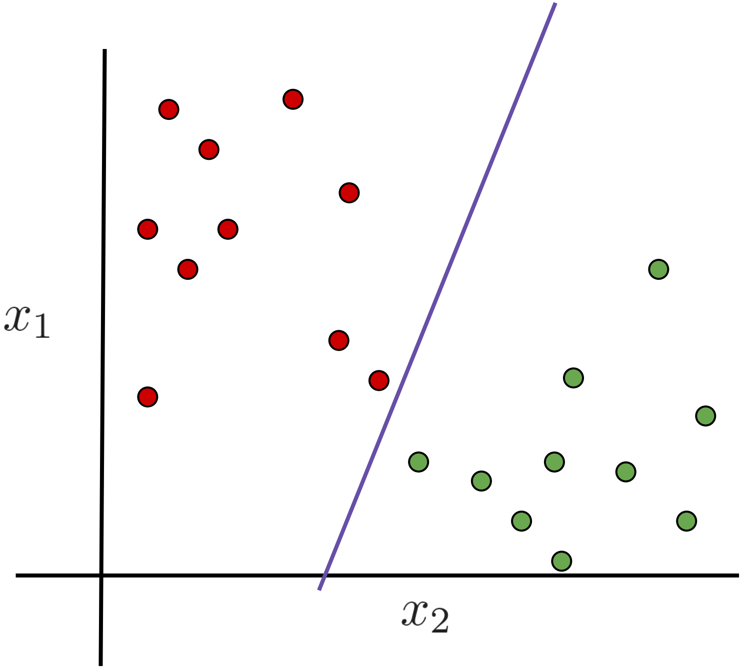

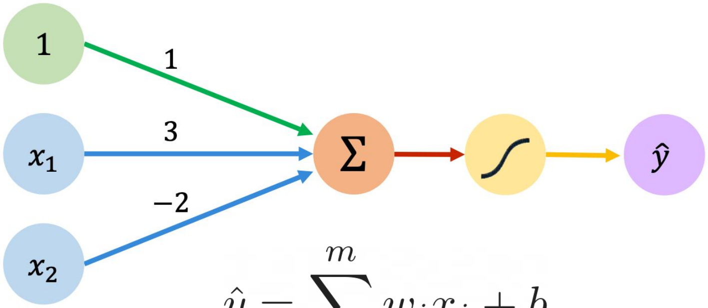

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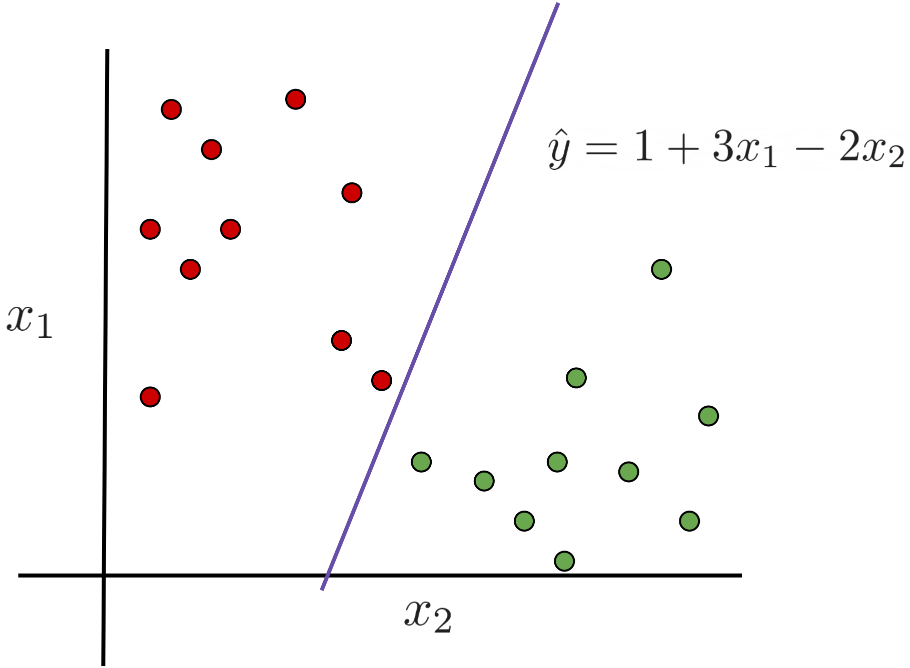

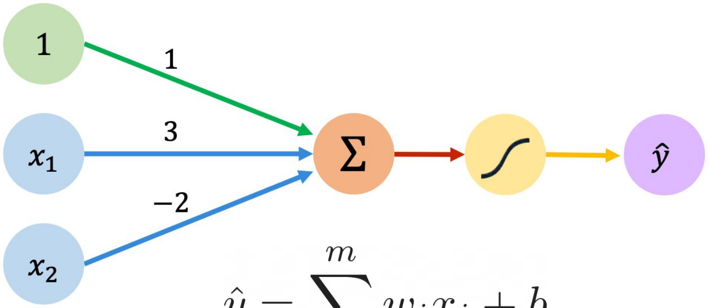

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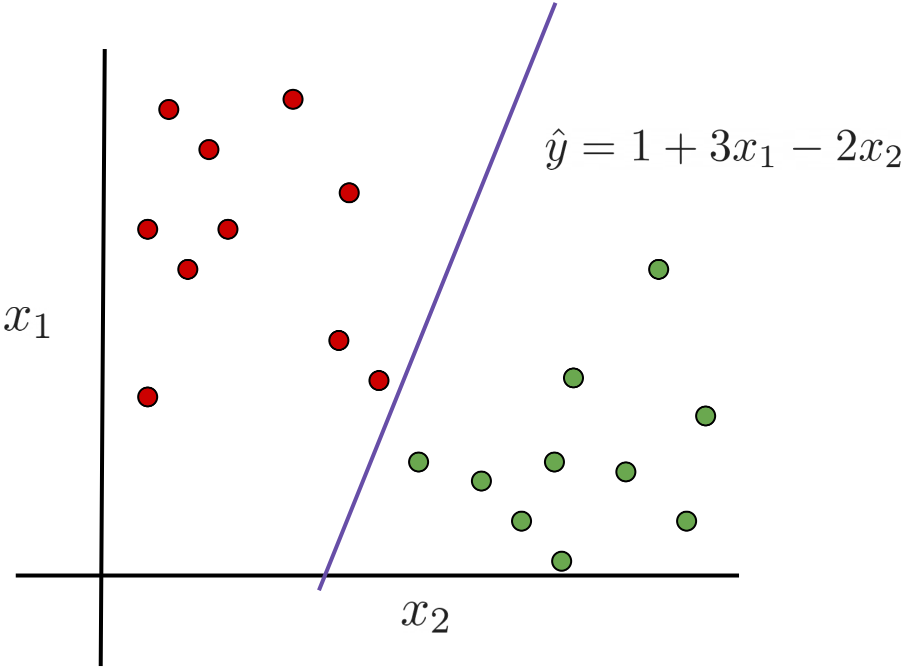
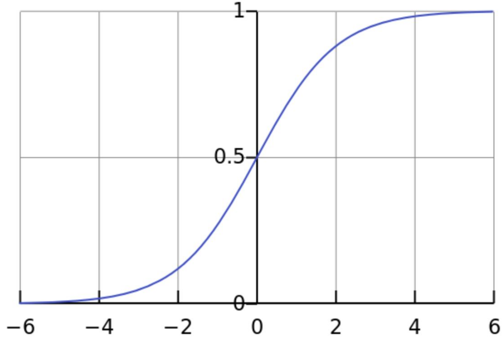
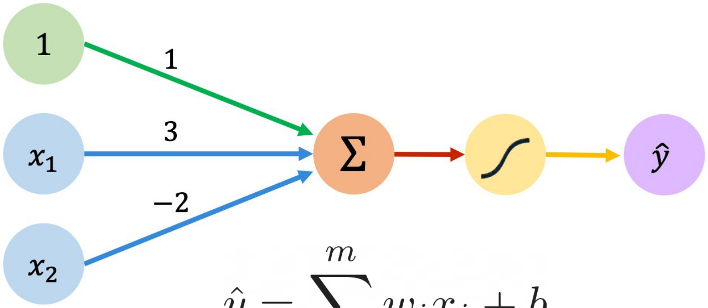


Sigmoid





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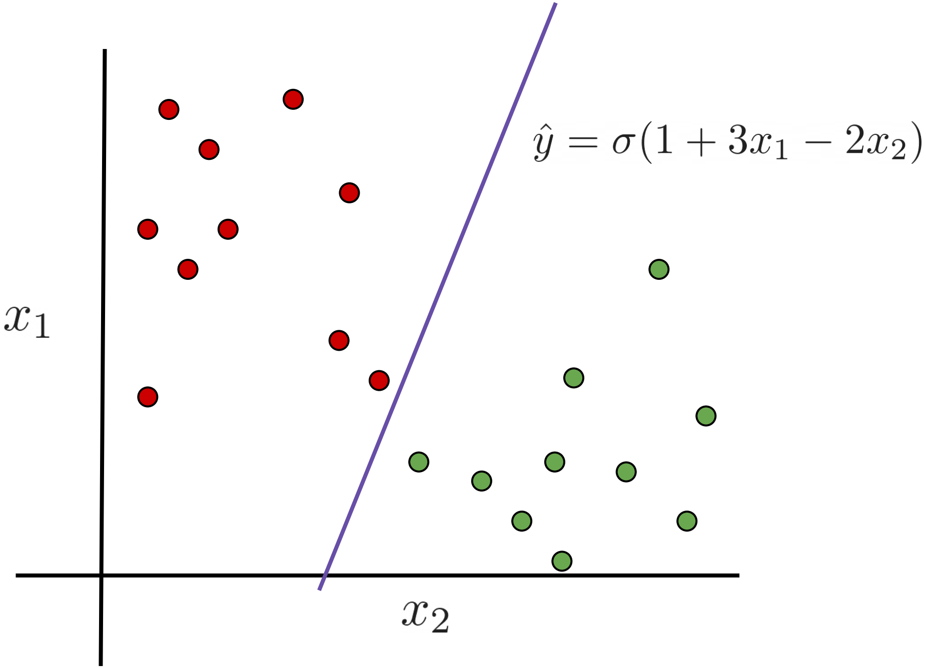

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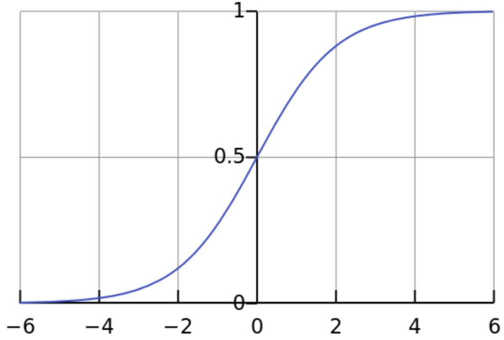
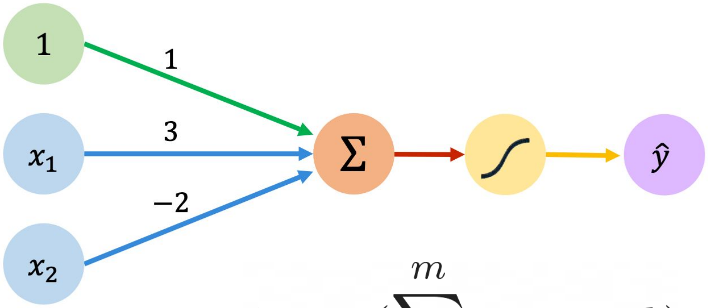
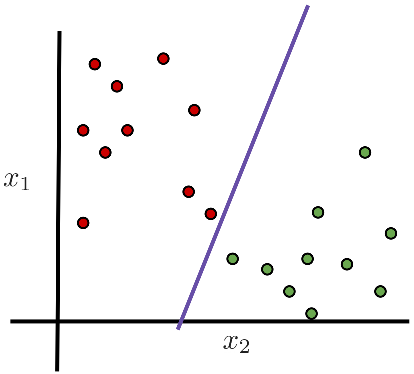
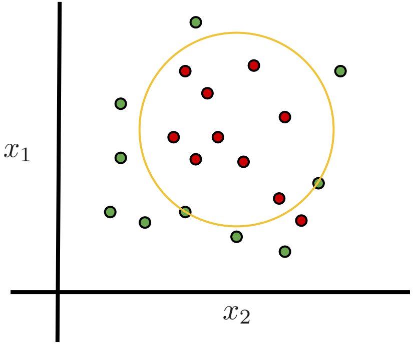


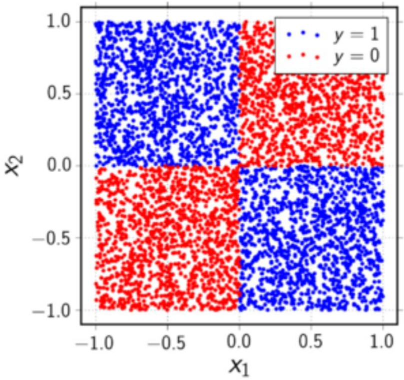


$$\hat{y} = \sigma\left(\sum_{i=1}^{m} w_i x_i + b\right)$$

Limitations of Linear Single Layer Classifiers







XOR Problem

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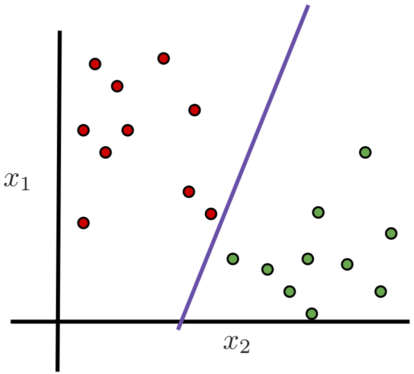
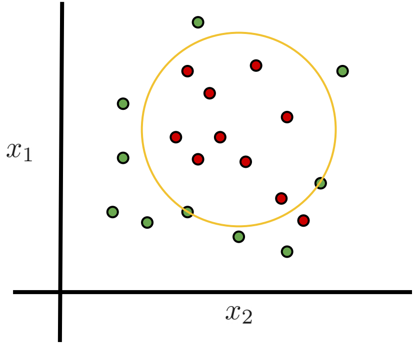
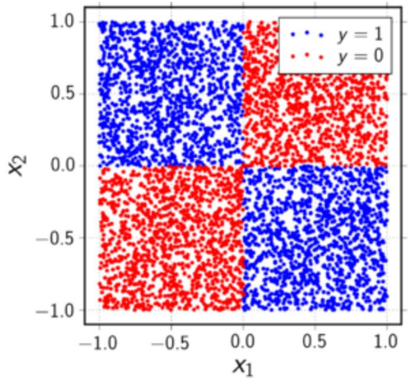
Limitations of Linear Single Layer Classifiers







XOR Problem

Possible Solutions

Add more layers (deep learning)

Map into another (higher dimensional) space

We need to be able to automatically extract features

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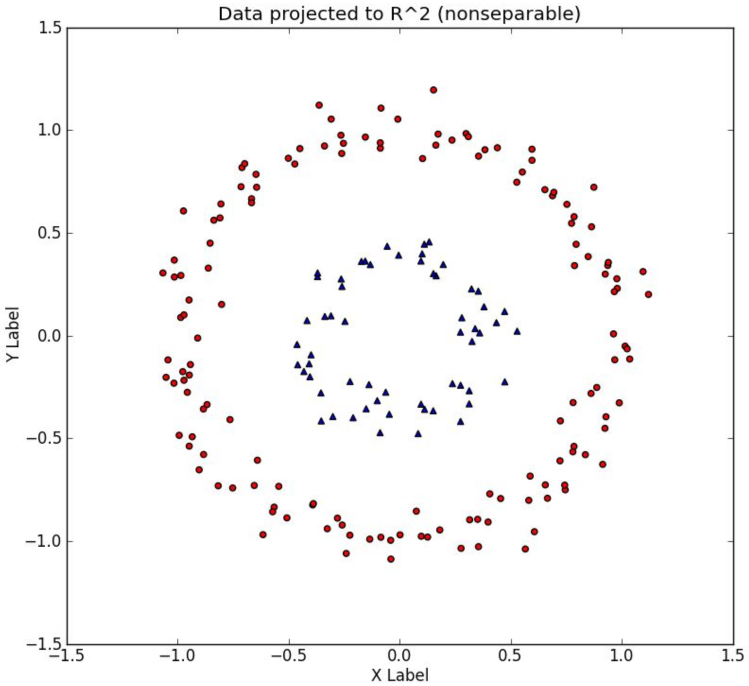
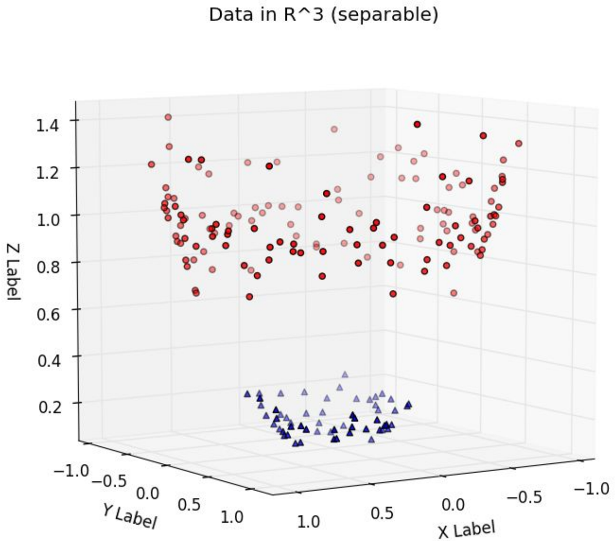
Limitations of Linear Single Layer Classifiers





Universal Approximation Theorem

“

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

Can approximate any continuous function

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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

SURF

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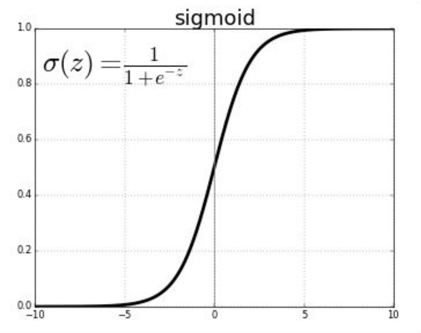
Use of multiple hidden layers makes the NN vector representation of your problem increasingly more abstract

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

SURF

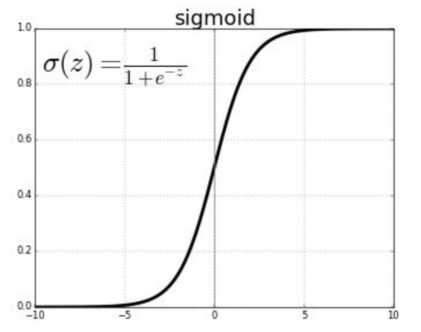
Activation Functions



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



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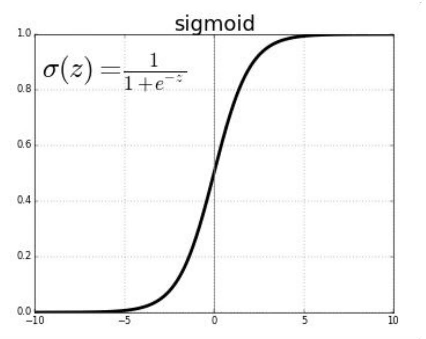

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- Probability Estimate
- Continuously differentiable
- Vanishing derivatives due to saturated neurons

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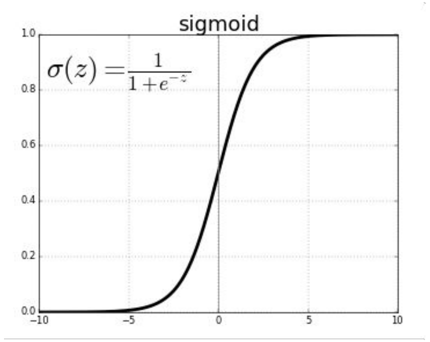

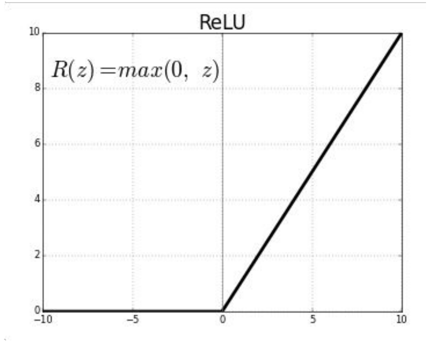

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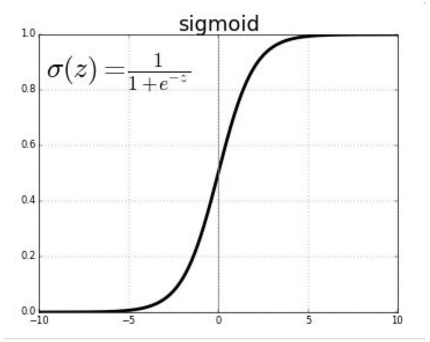

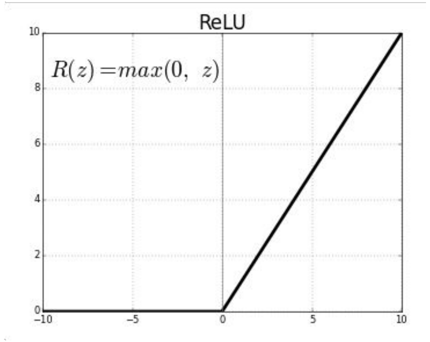

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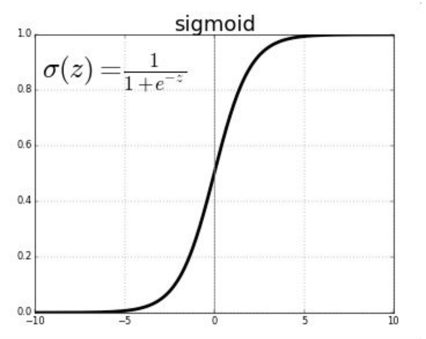
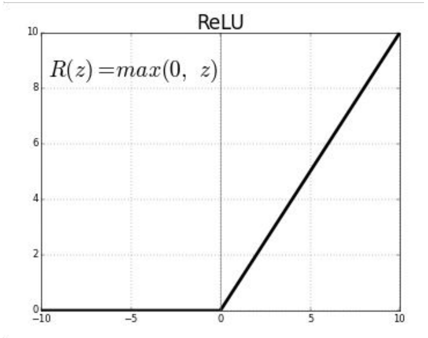
- Continuously differentiable
- Vanishing derivatives due to saturated neurons

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

Activation Functions





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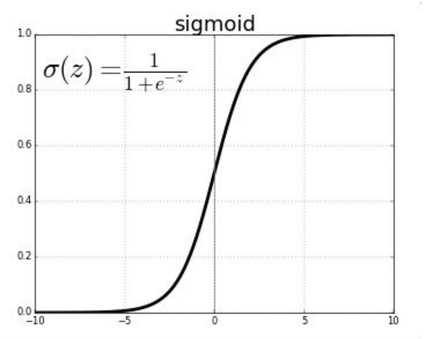
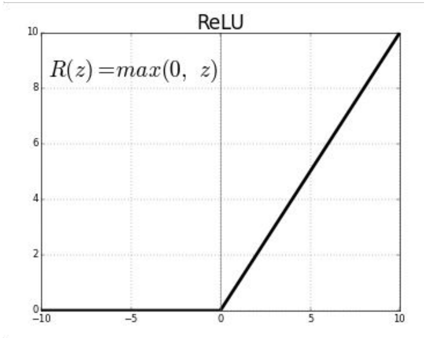
Simple derivative

Non-linear behaviour

SURF

Activation Functions





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SURF

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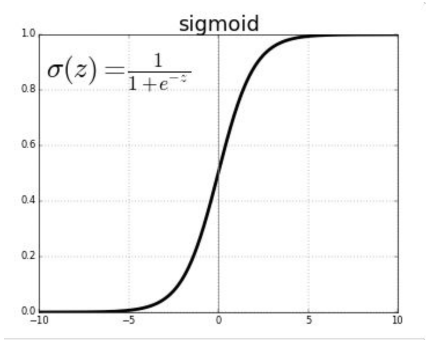

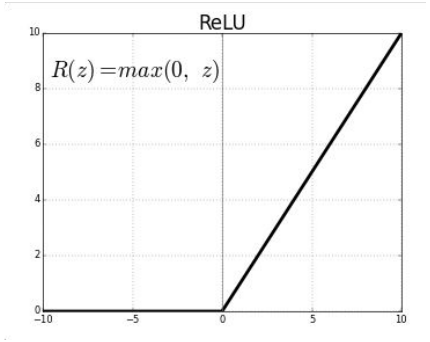

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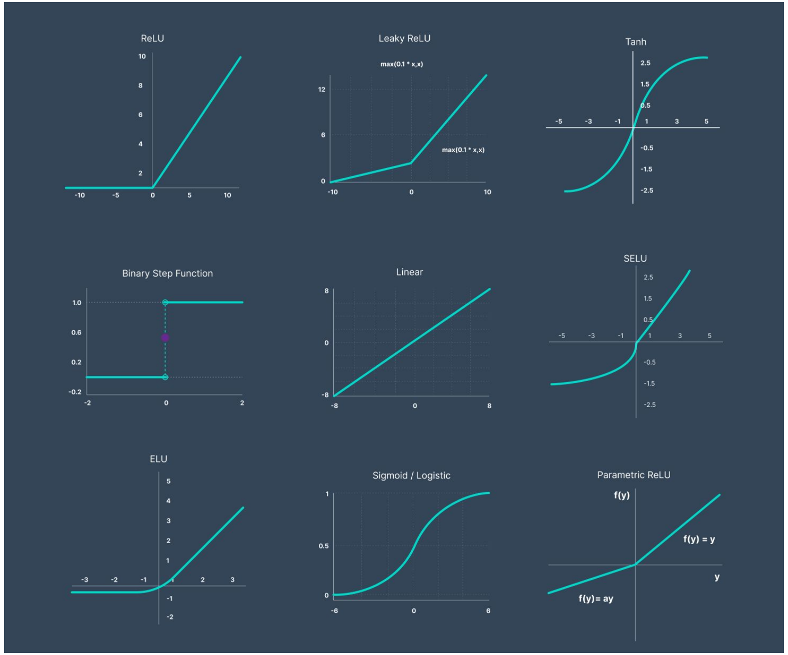

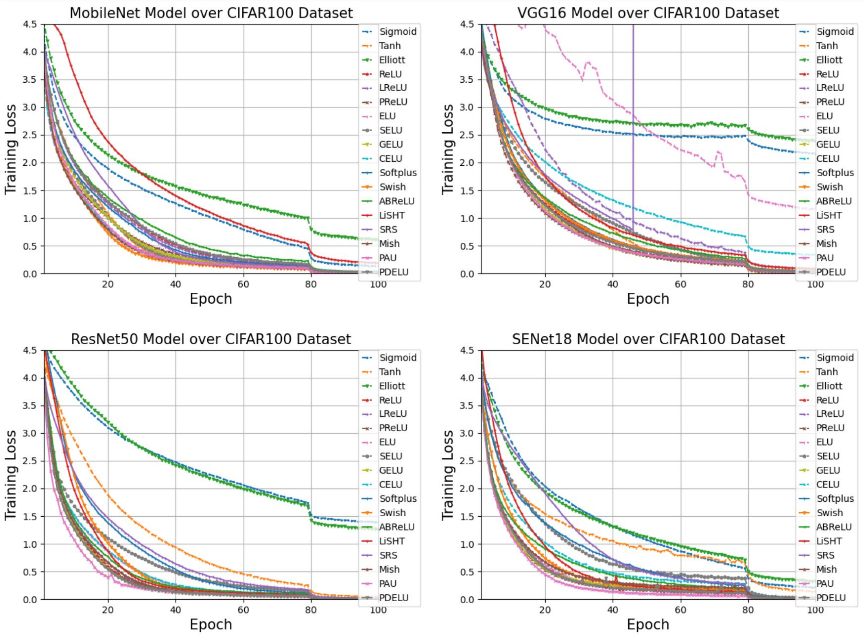

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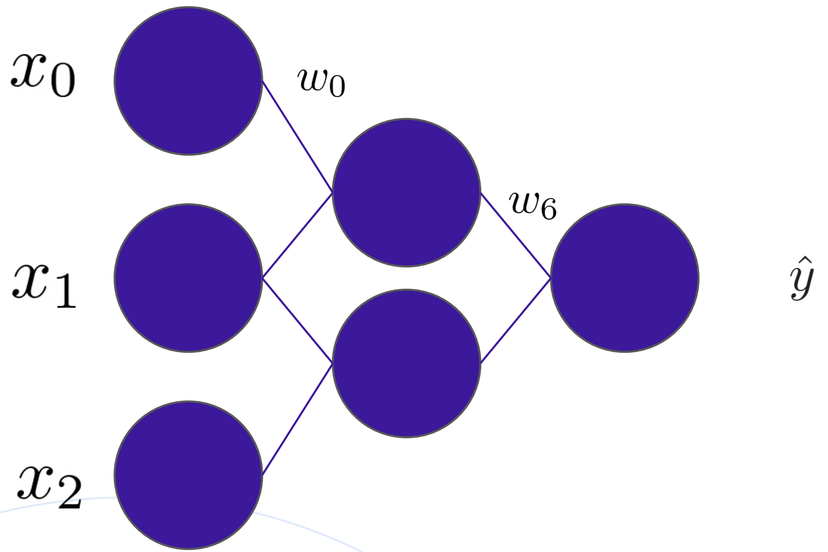
Predicting Housing Price

During the **optimization** process

The NN learns to **encode** a **representation** that maps the input to the output



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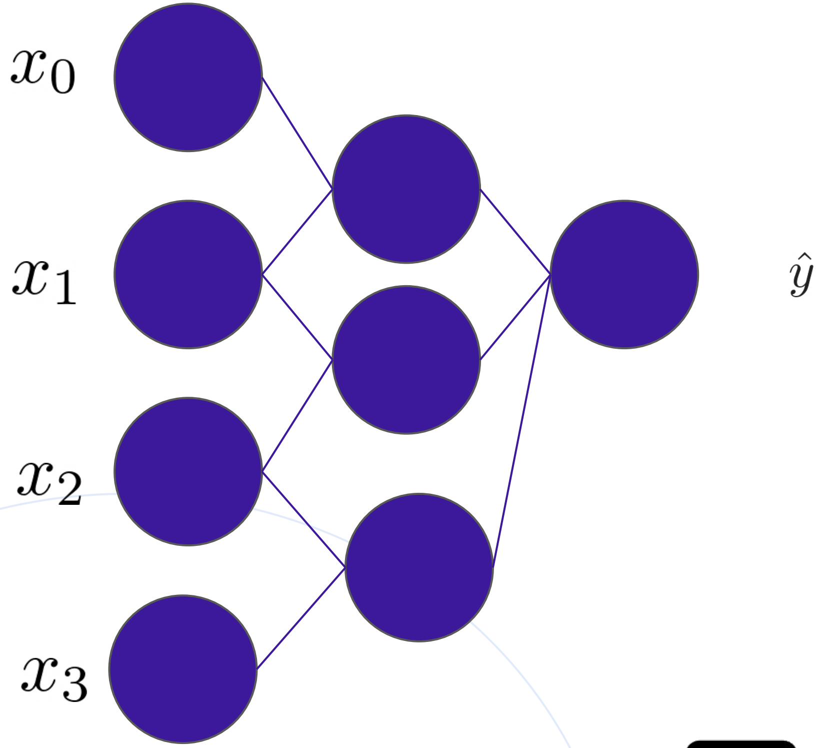

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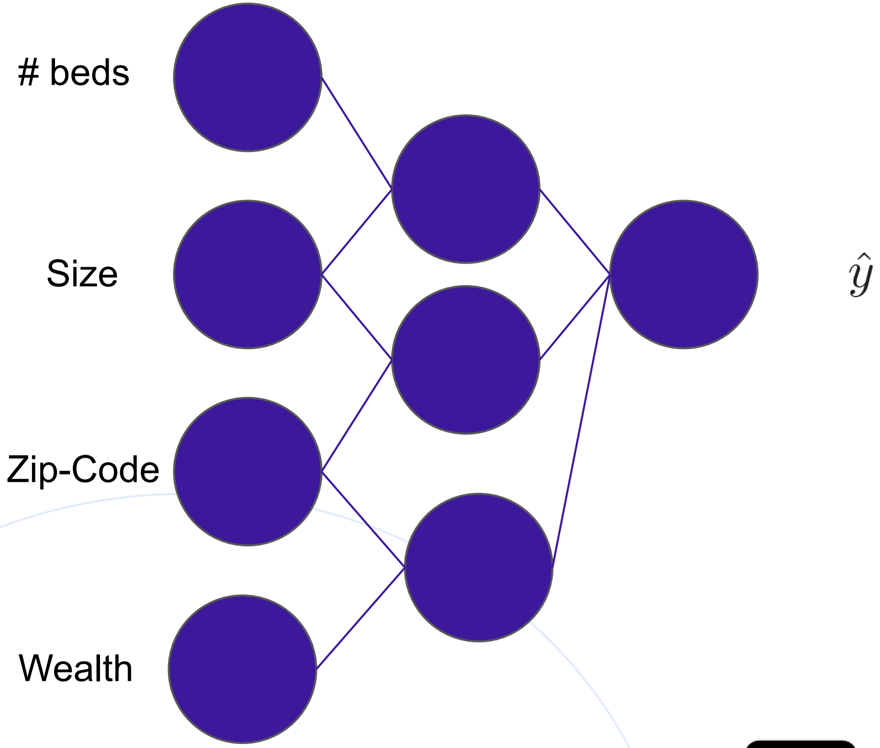

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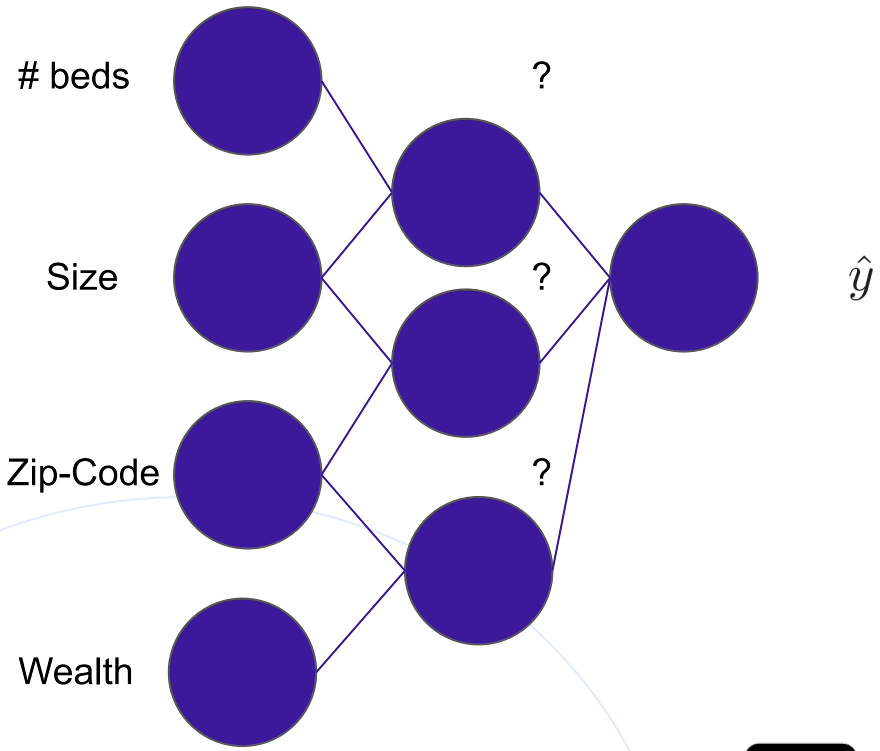

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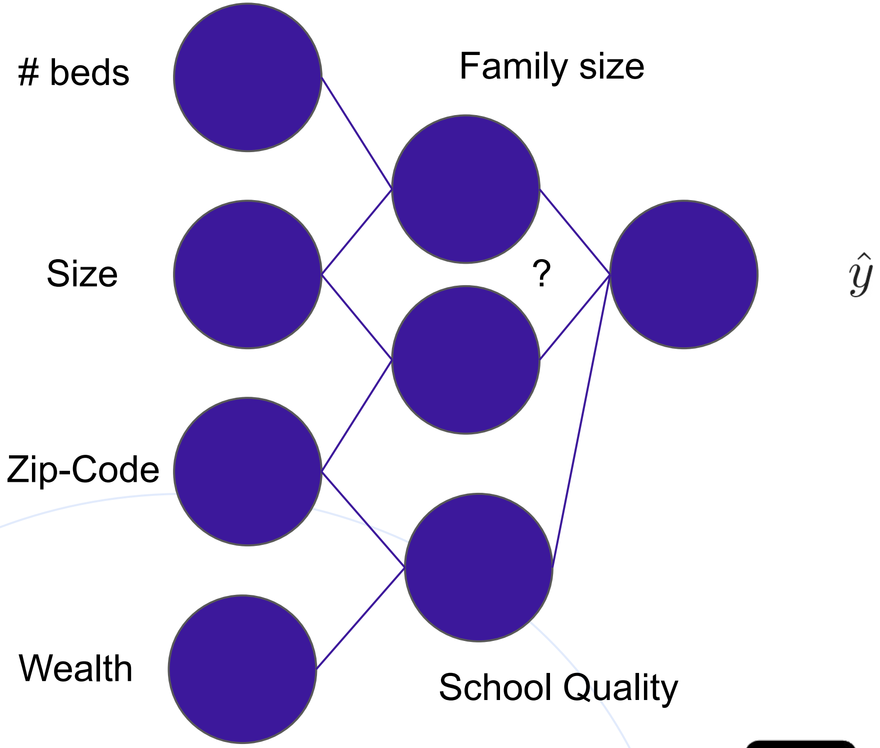

Predicting Housing Price

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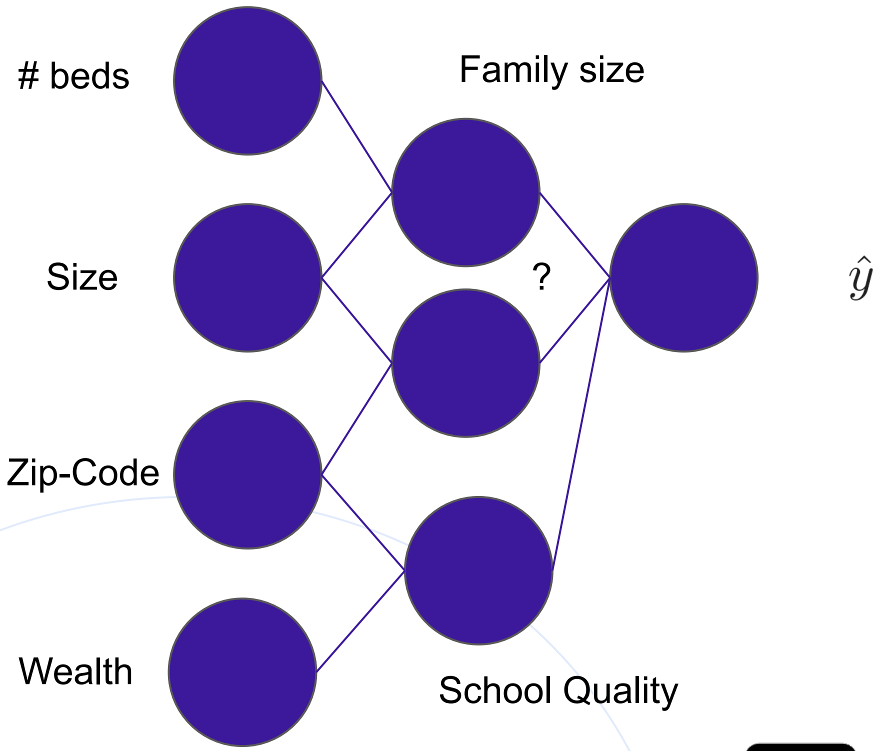
Transform the input to a space where we are able to **separate** the features



Predicting Faces

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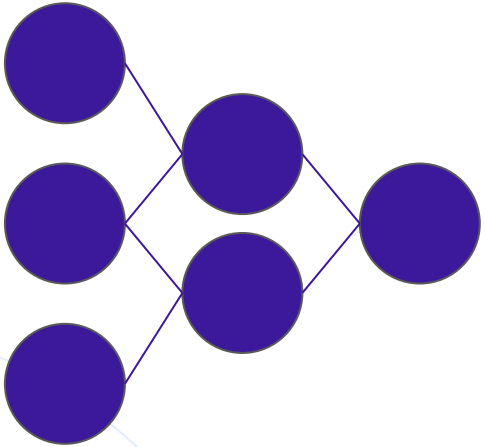
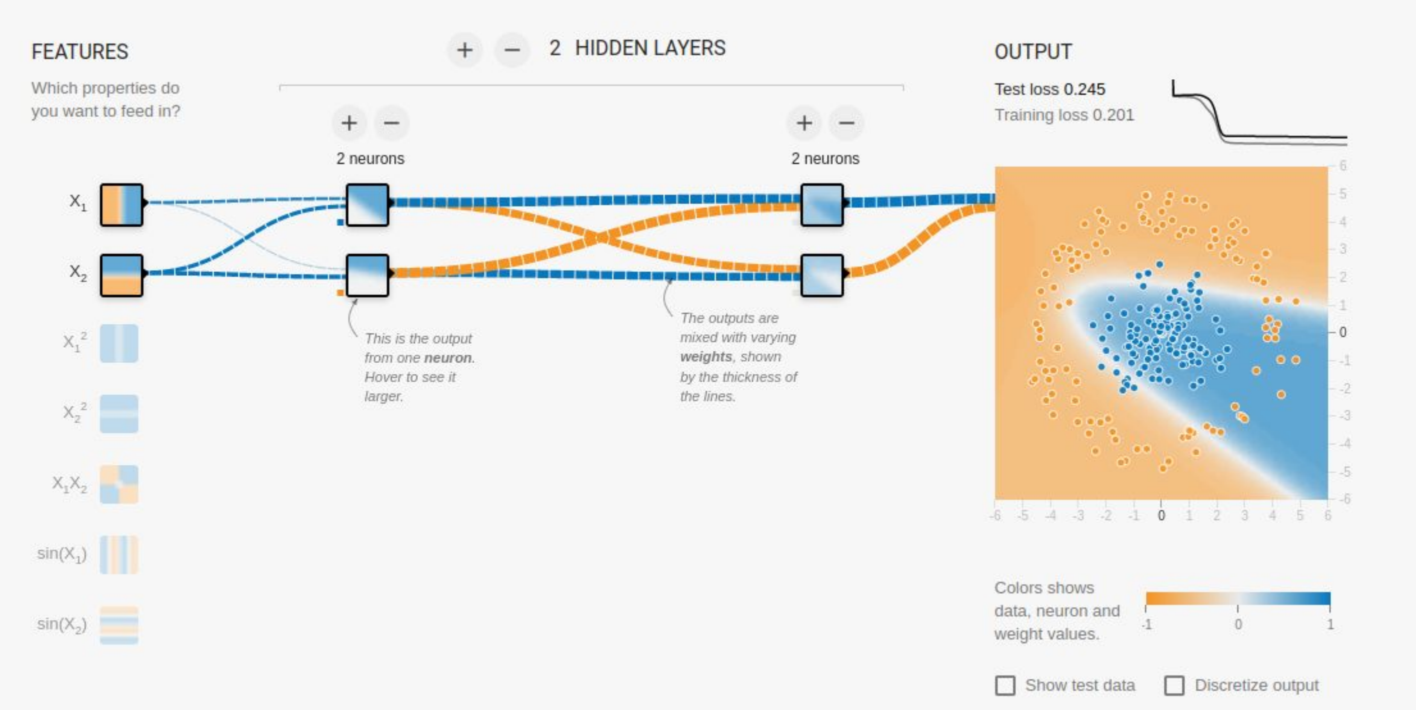


A deep neural network **encodes** the **representation** in an increasingly abstract way

Neural Network Demo



https://playground.tensorflow.org/

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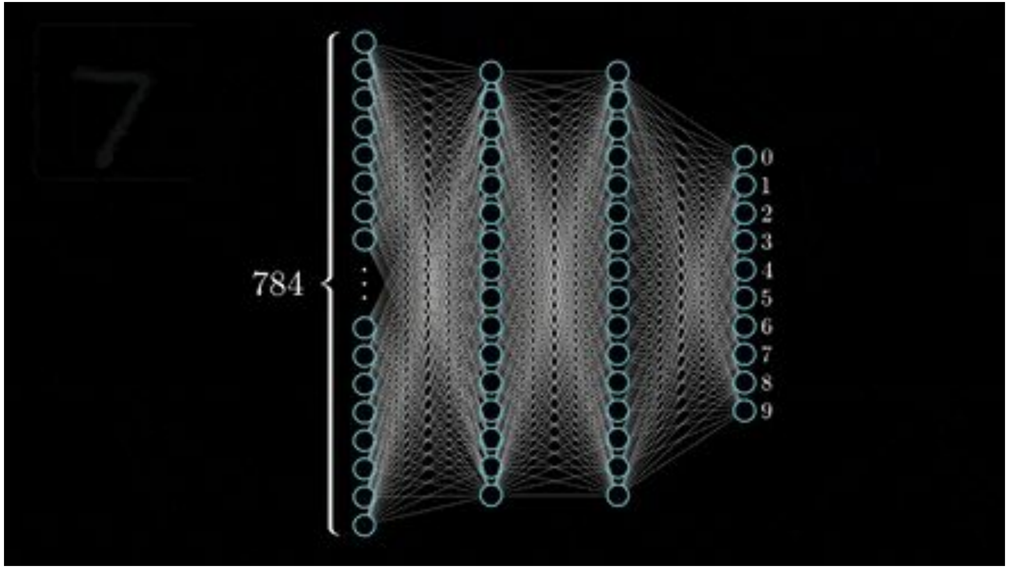
Neural Network

- 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

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?

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Recipe for Training

01.

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

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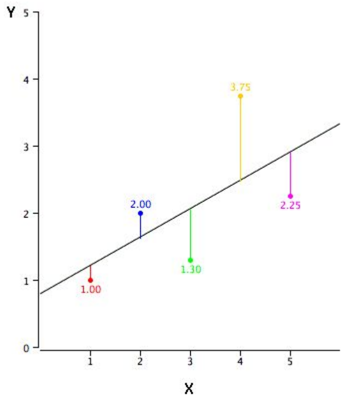
04.

Accuracy, F1-score, precision, recall

Loss Functions



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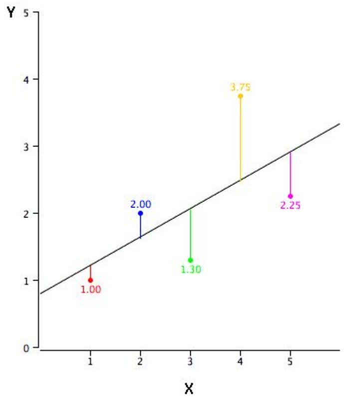
The loss function is used to bridge the gap between your neural network predictions and the true value

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

Loss Functions



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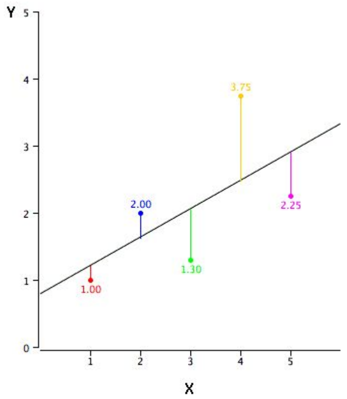

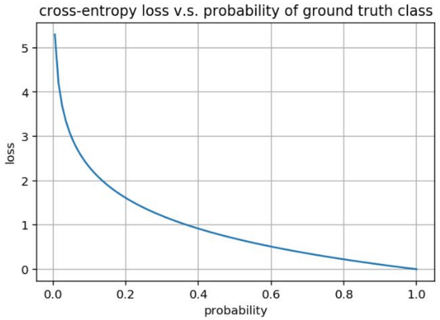

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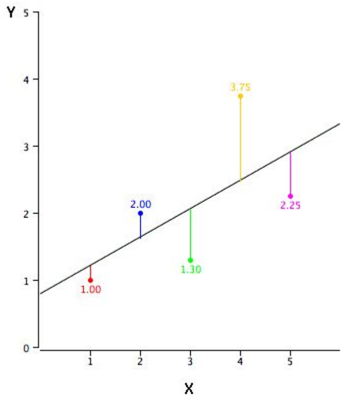

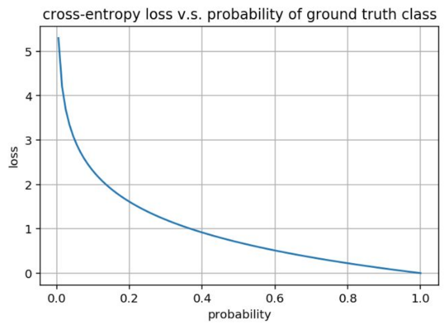

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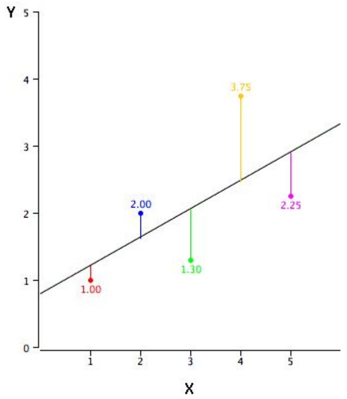

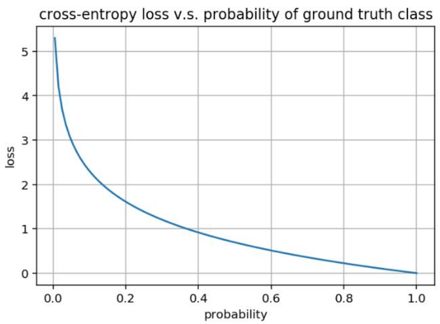

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CE and Softmax has better behaved gradients.

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SURF

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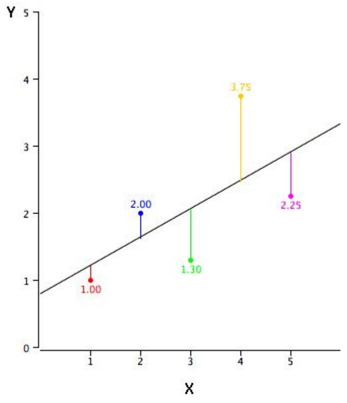

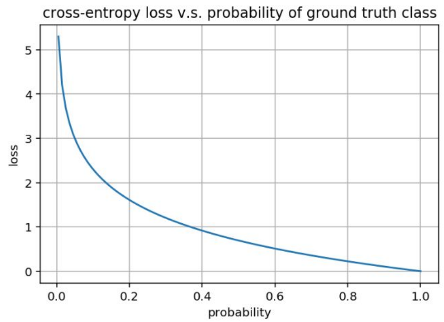

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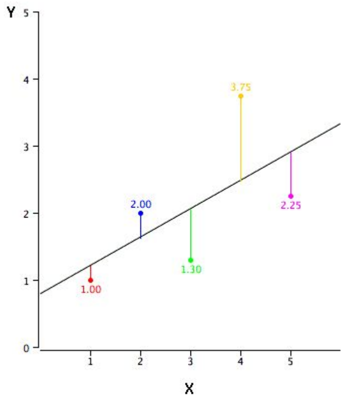

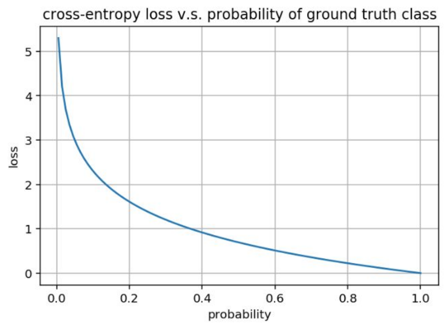

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SGD is the main engine behind training
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- ❖ Can be used with loss function that are not differentiable
- ❖ No Guarantee that we find the global optimum

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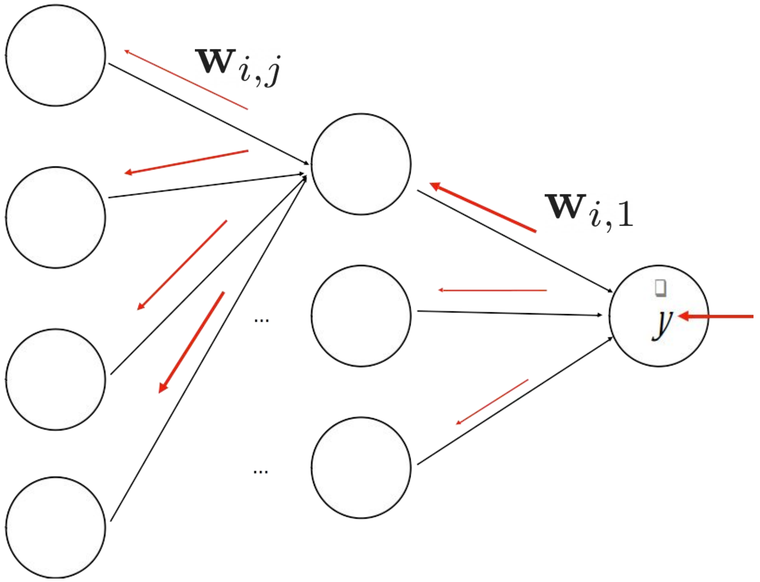

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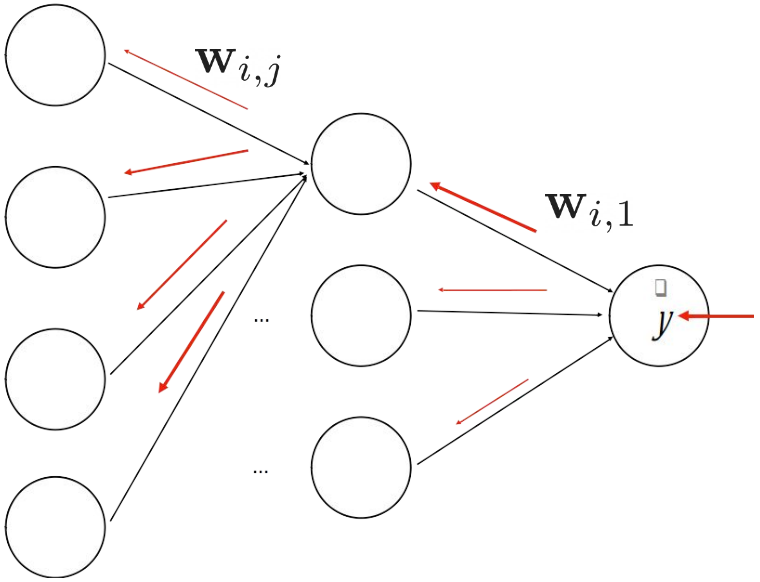

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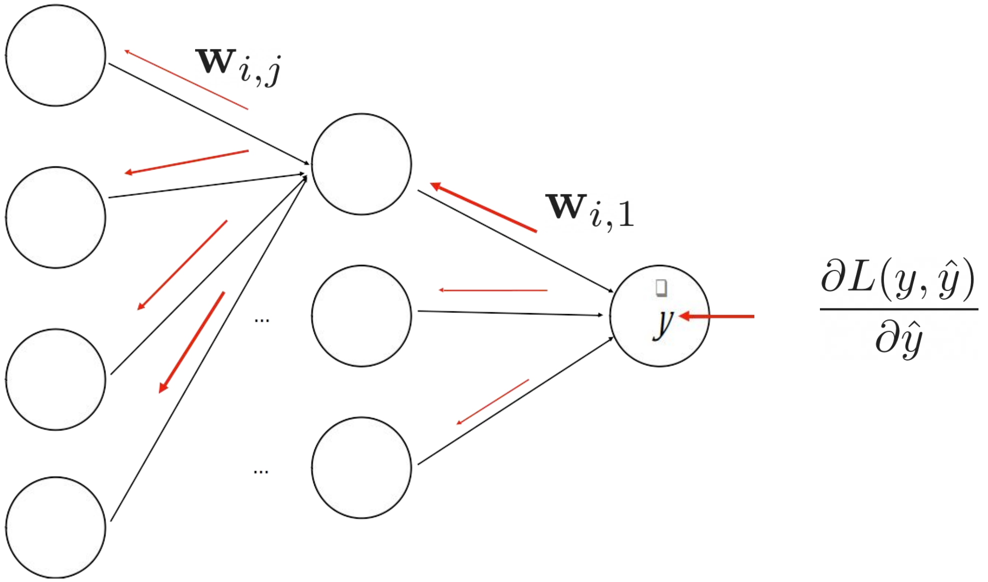

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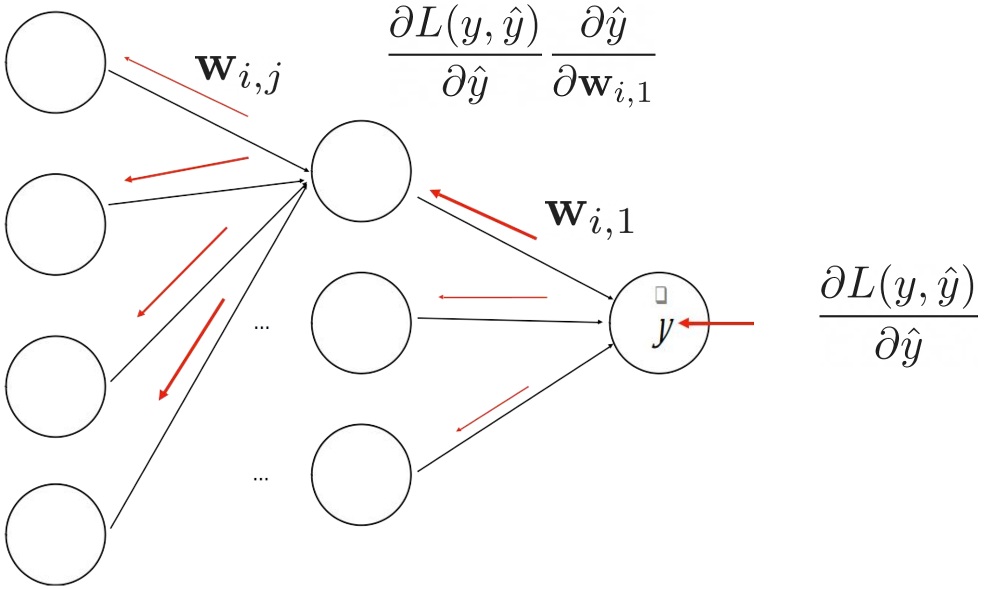

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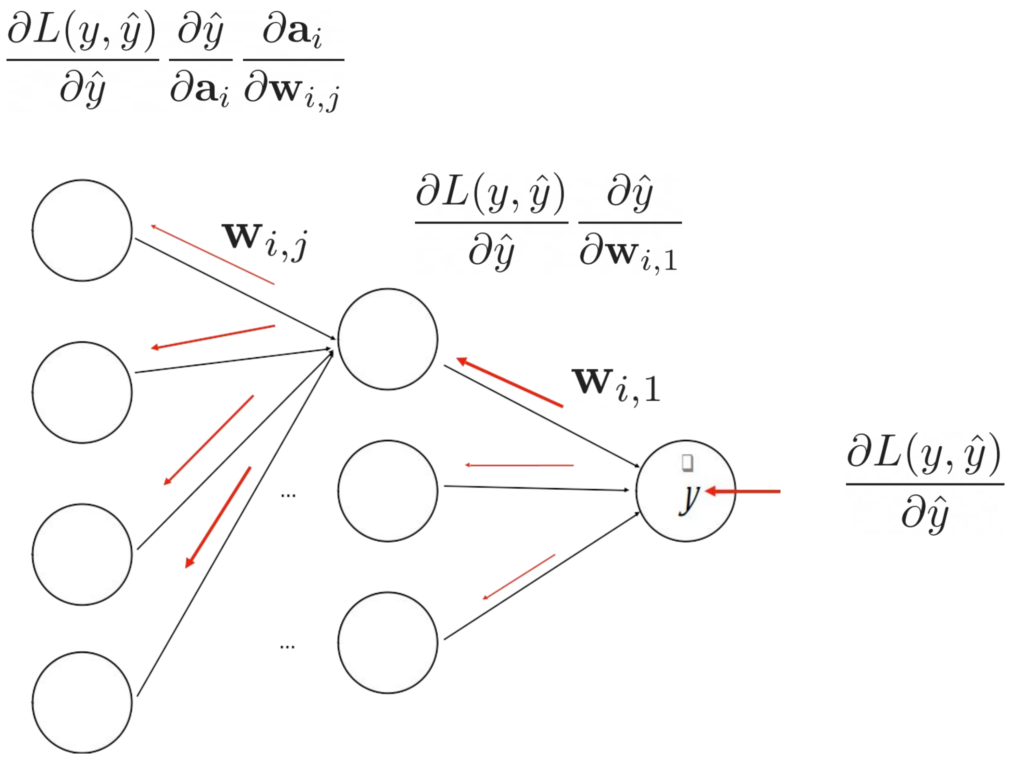
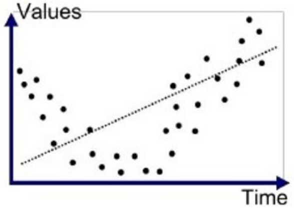
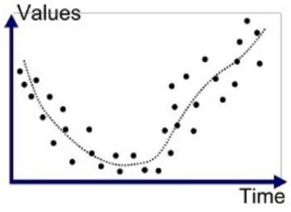


Combatting Overfitting



Underfitted



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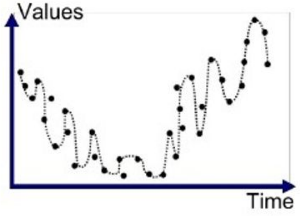

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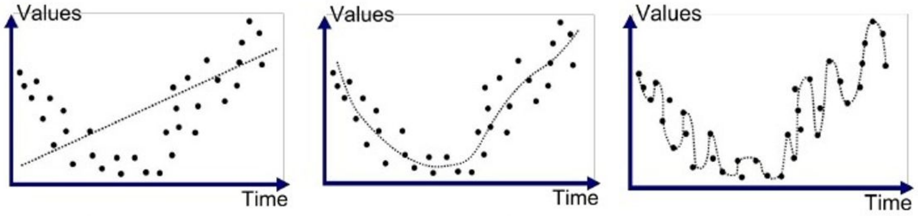

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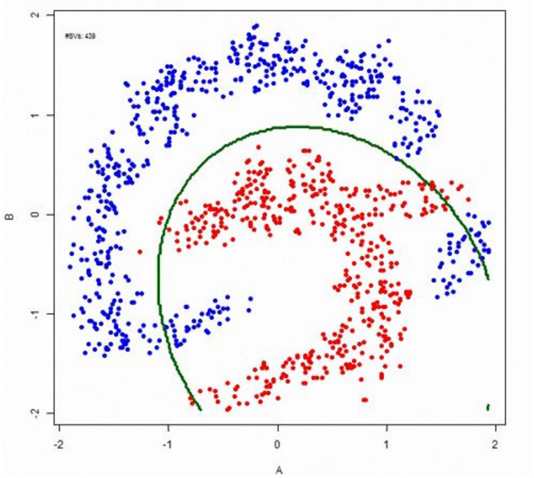

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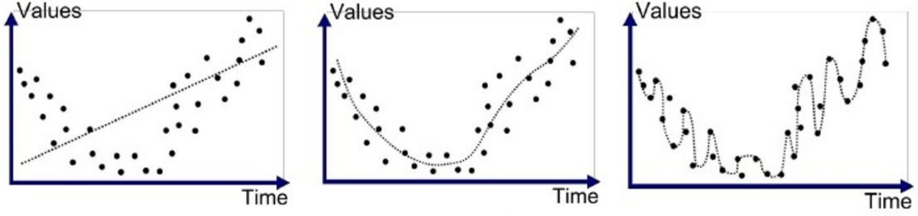

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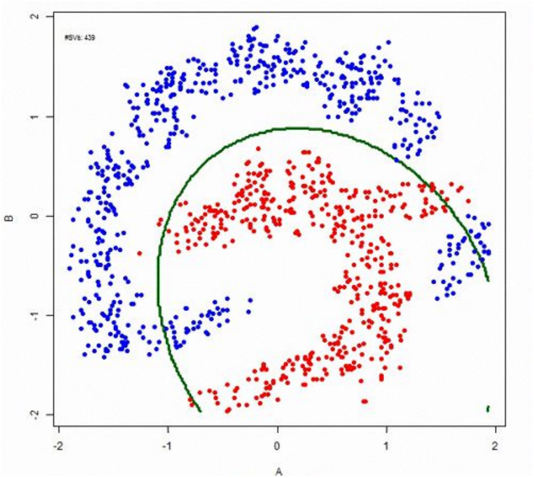
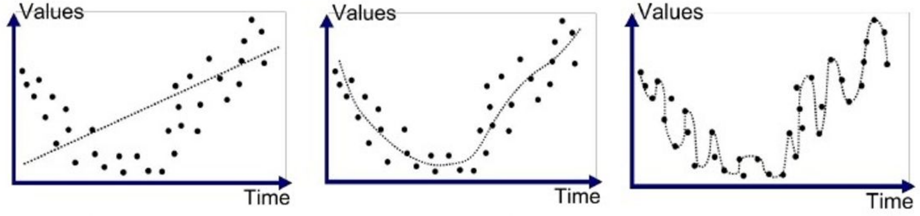
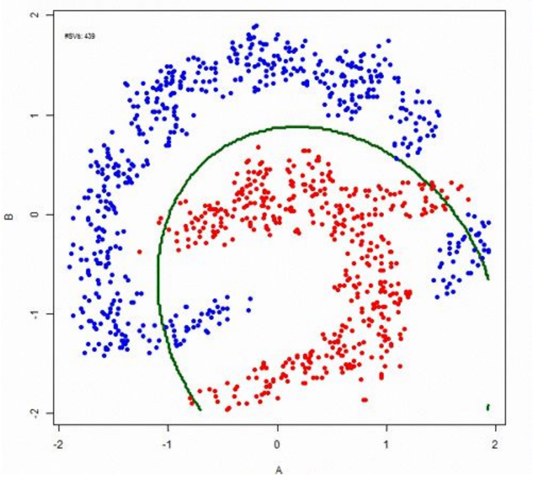


- Dropout prior
- Weight decay
- Early stopping
- Batch Normalization

Combatting Overfitting



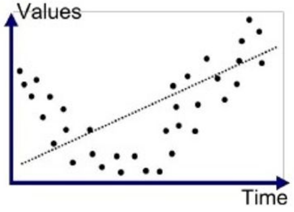
Underfitted | Good Fit/Robust | Overfitted



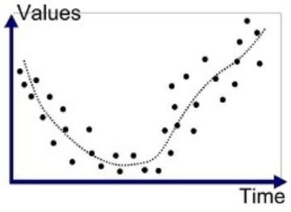
- Dropout prior
- Weight decay
- Early stopping
- Batch Normalization

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

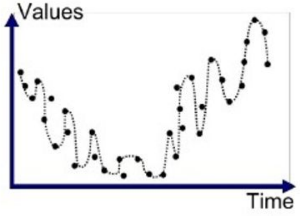
Combatting Overfitting



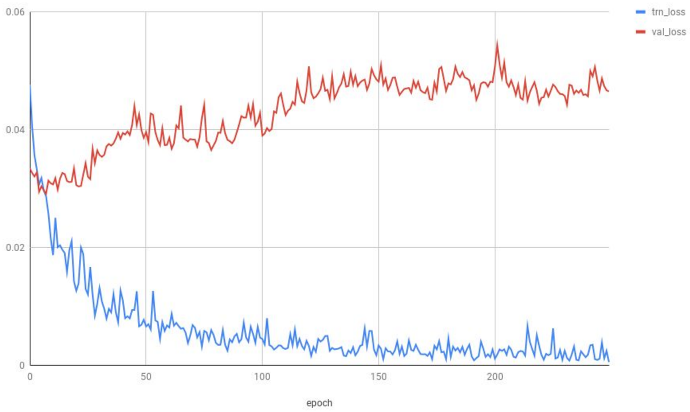
Underfitted



Good Fit/Robust



Overfitted



- Dropout prior
- Weight decay
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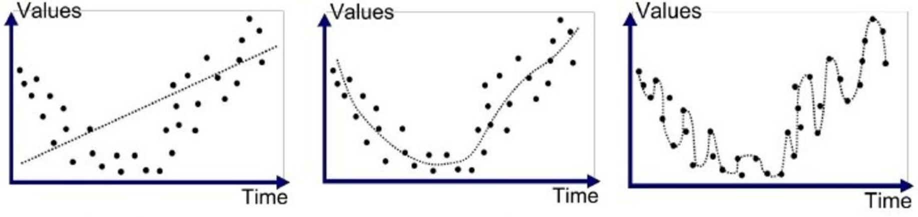
- Batch Normalization

Combatting Overfitting

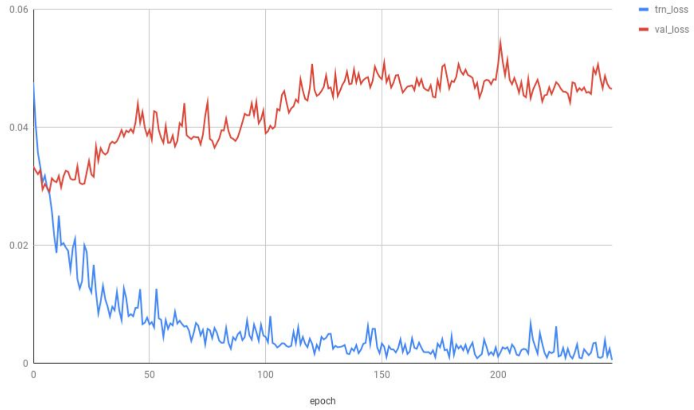


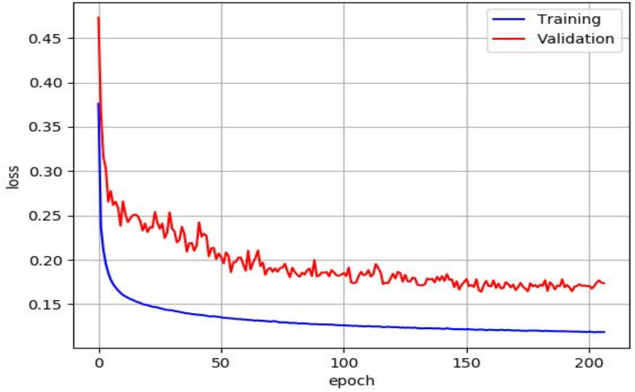
Underfitted

Good Fit/Robust

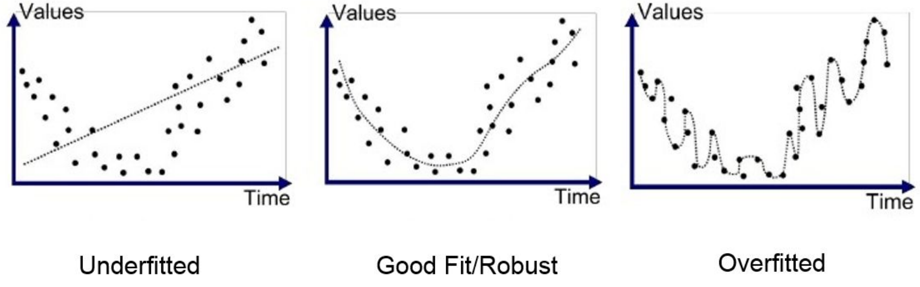
Overfitted

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





Combatting Overfitting



- Dropout prior
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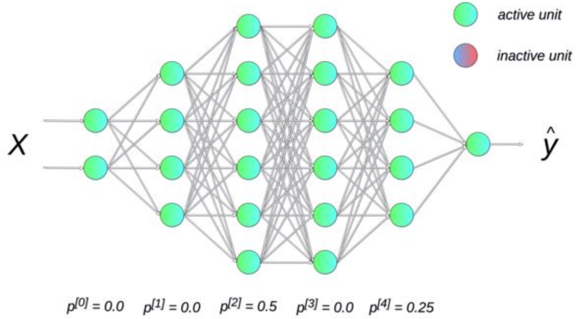

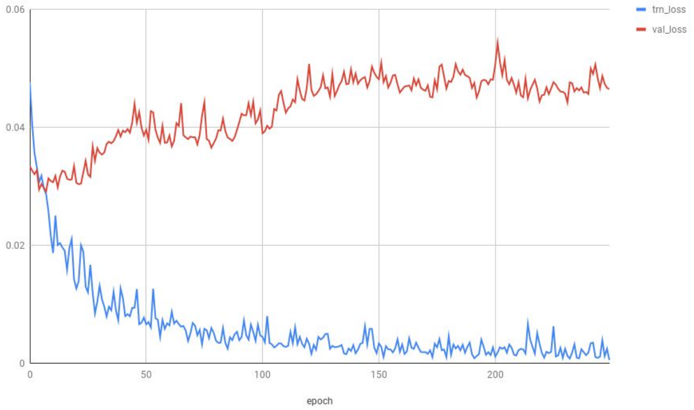

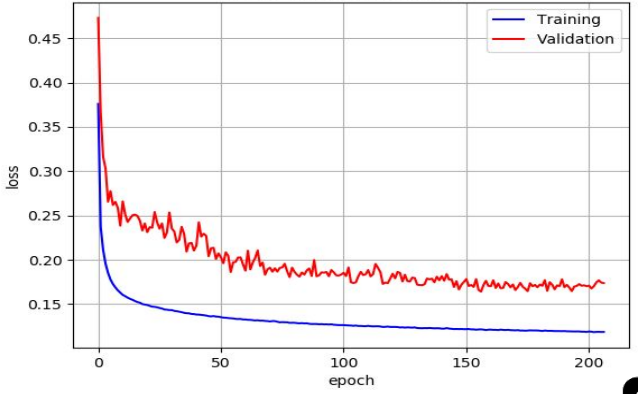

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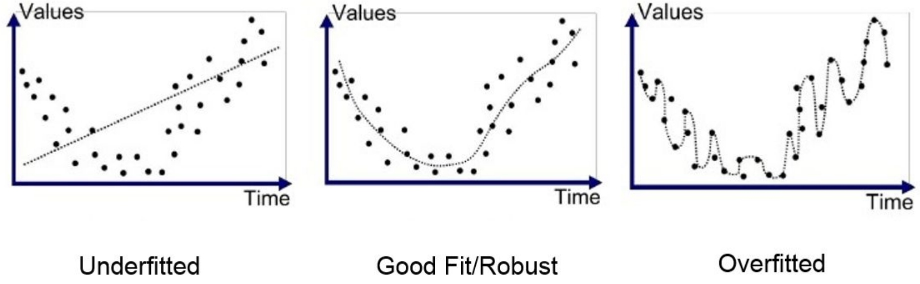
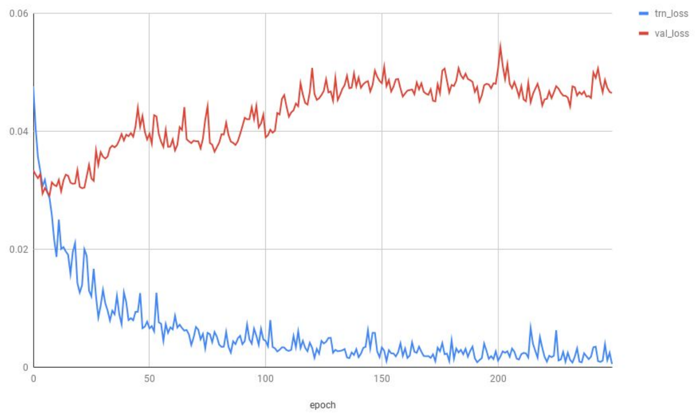
Combatting Overfitting





- Dropout prior
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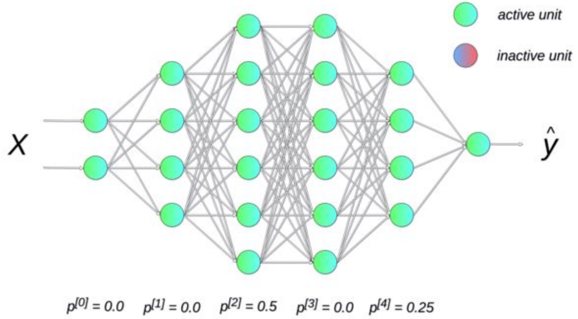
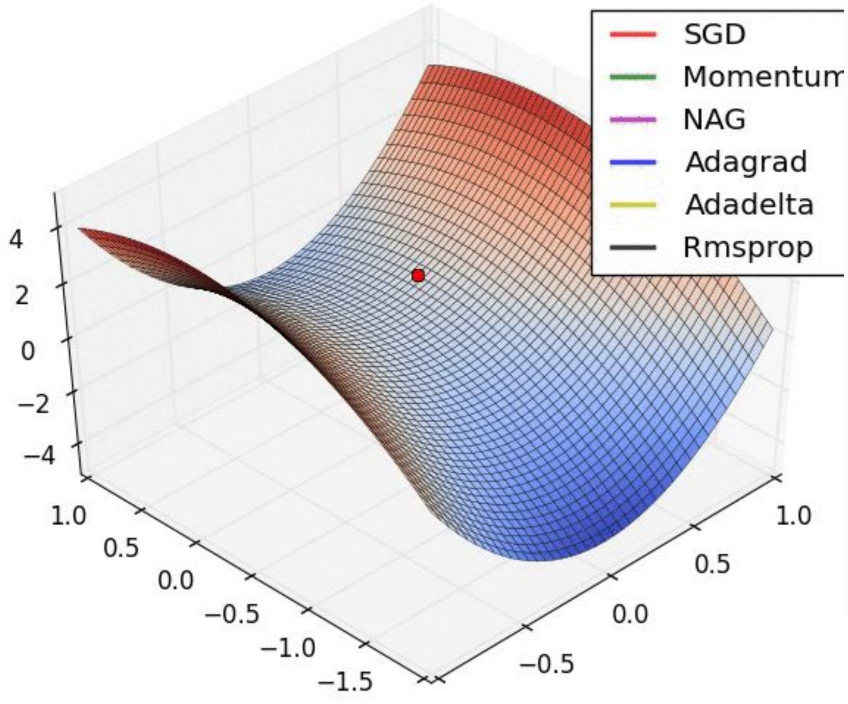


Models always need regularization no matter how big

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

Optimizers

In what way should we change the weights?

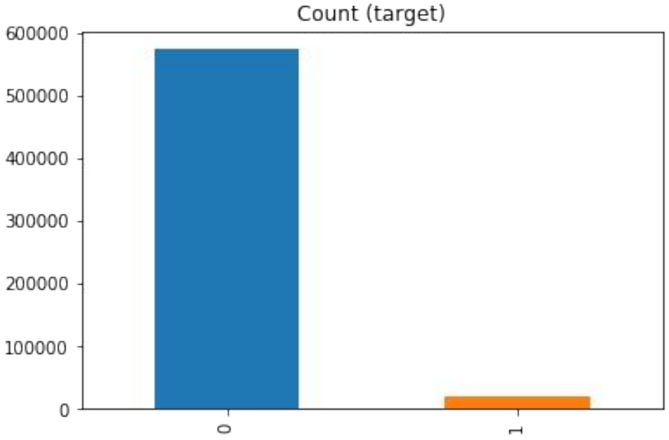


03. ML Workflow

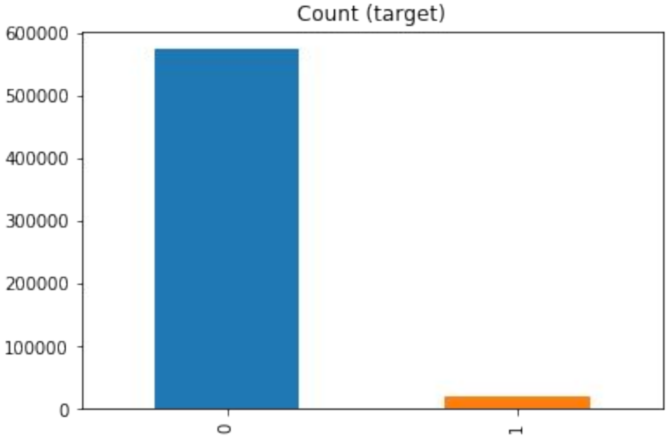
You need to know your data and your models well

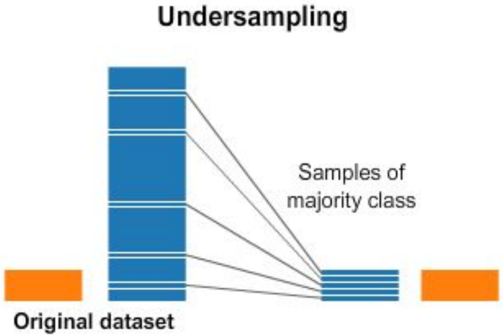
Artificial Intelligence still heavily relies on human intelligence

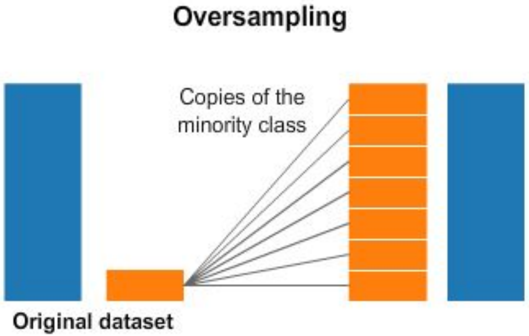
Imbalanced Training set



Imbalanced Training set

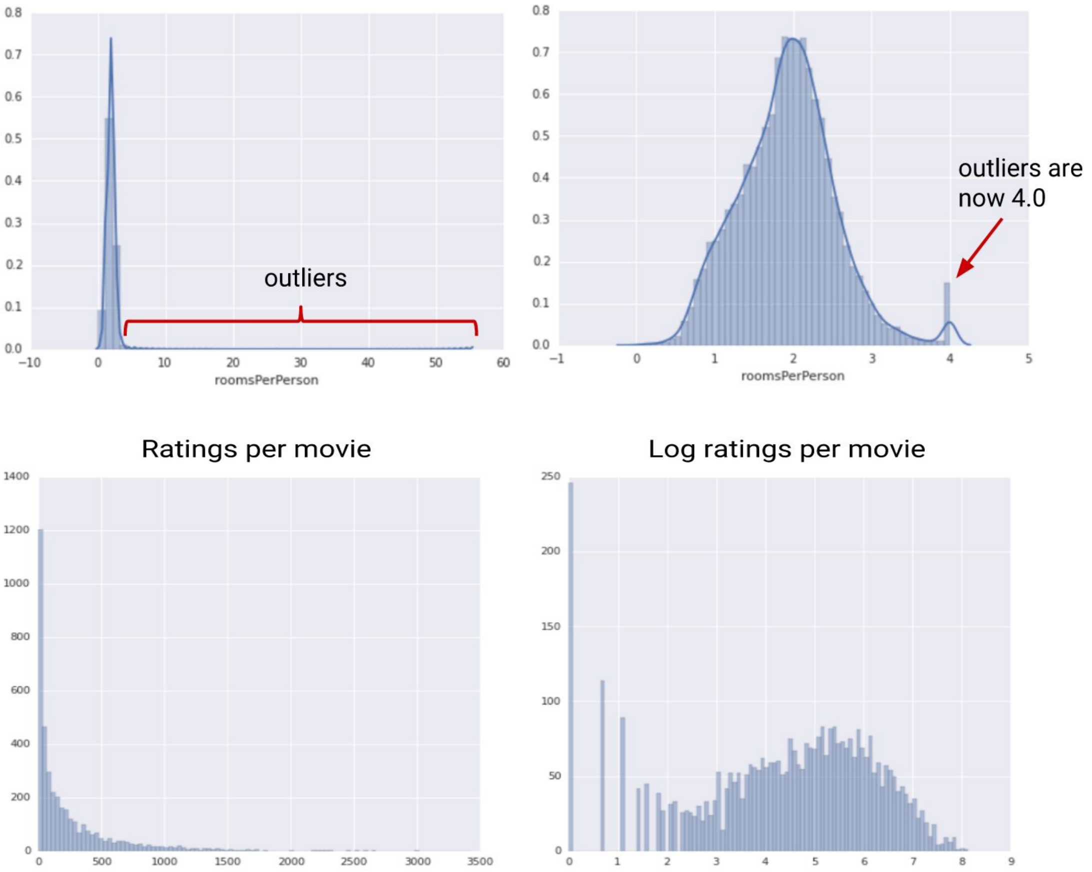




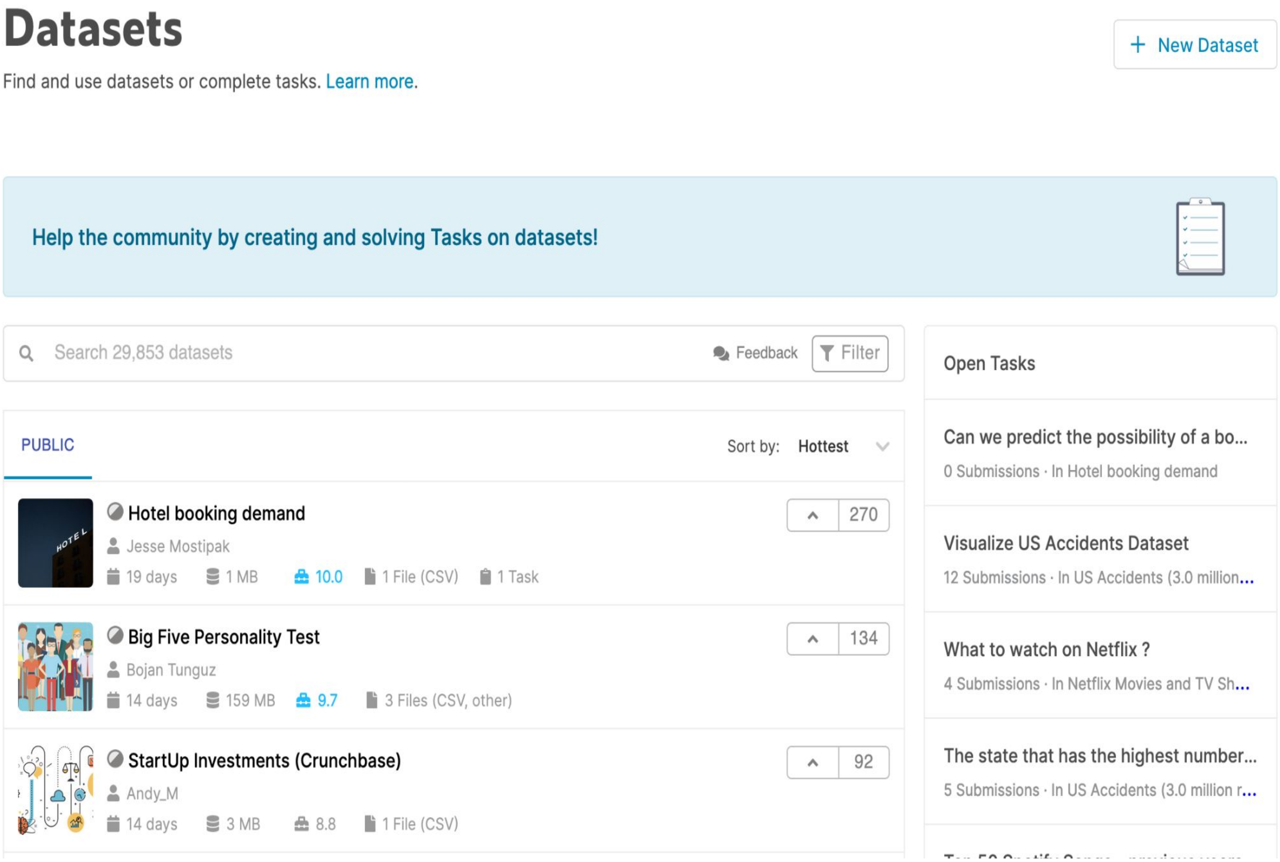


Data normalization

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	Validation set	Test set
Model training	Model selection	Model testing
Best model parameters Weights	**Best hyperparameters** Learning rate #neurons #layers	**Final model** Accuracy Sensitivity/ specificity
70%	20%	10%

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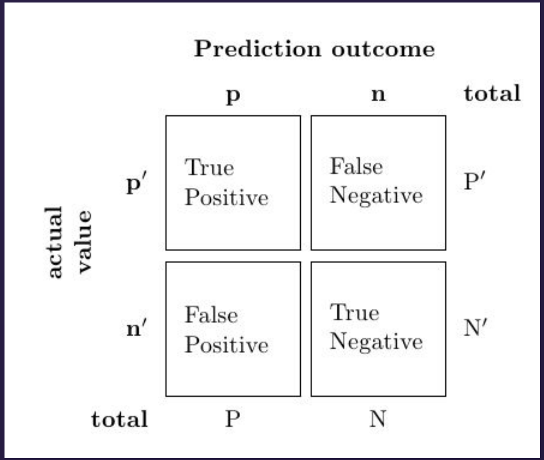
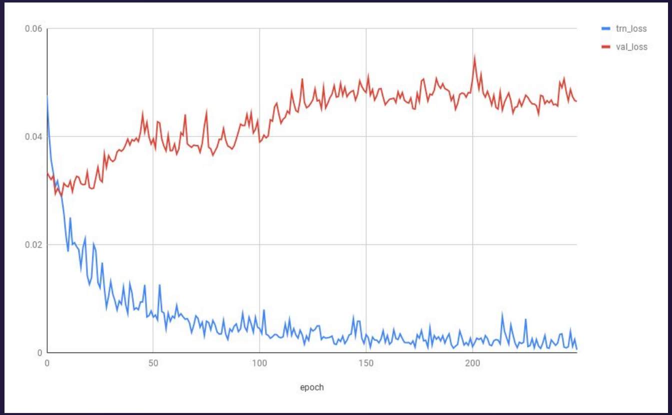
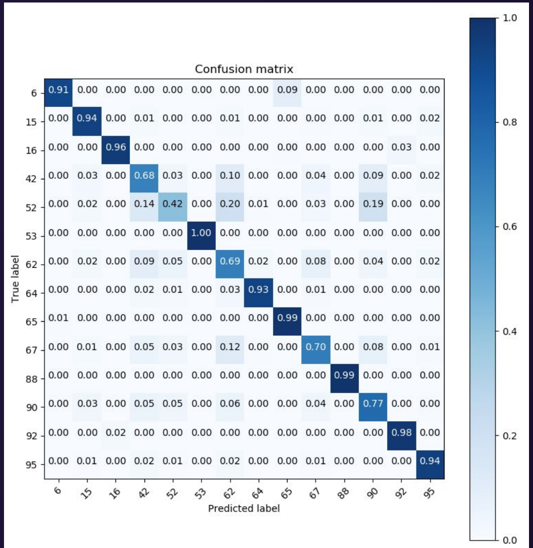
Network Evaluation

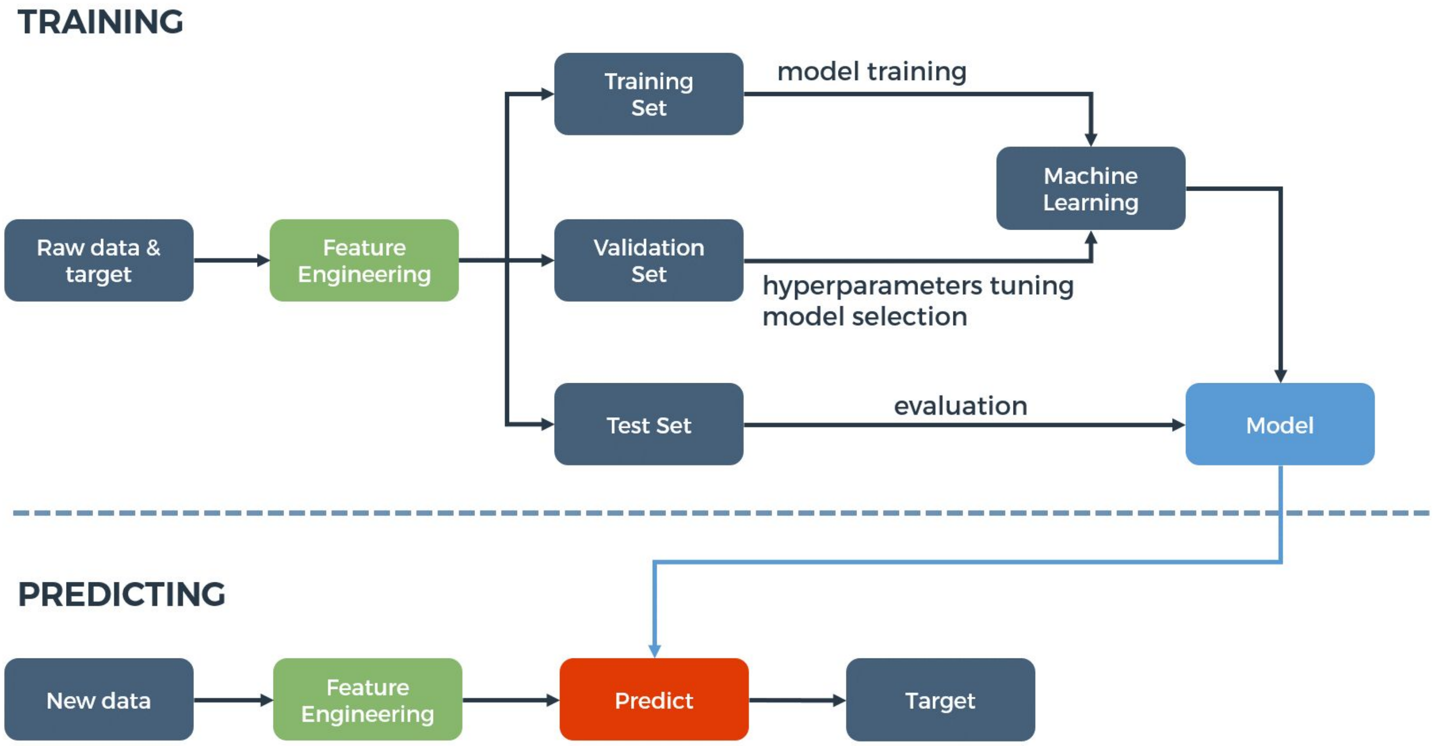






Choose an appropriate metric for your own problem
Always sanity check your model, is it better than a baseline?
An almost perfect classification score is always sketchy
Keep questioning the model, never trust it

Workflow



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04. DL Frameworks

Do not compute your own gradients

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

SURF

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

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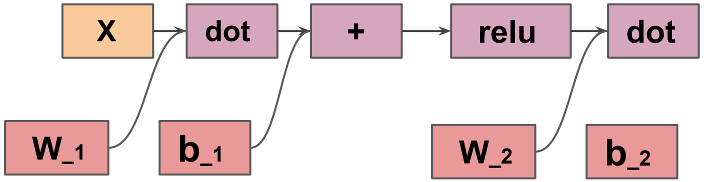

SURF

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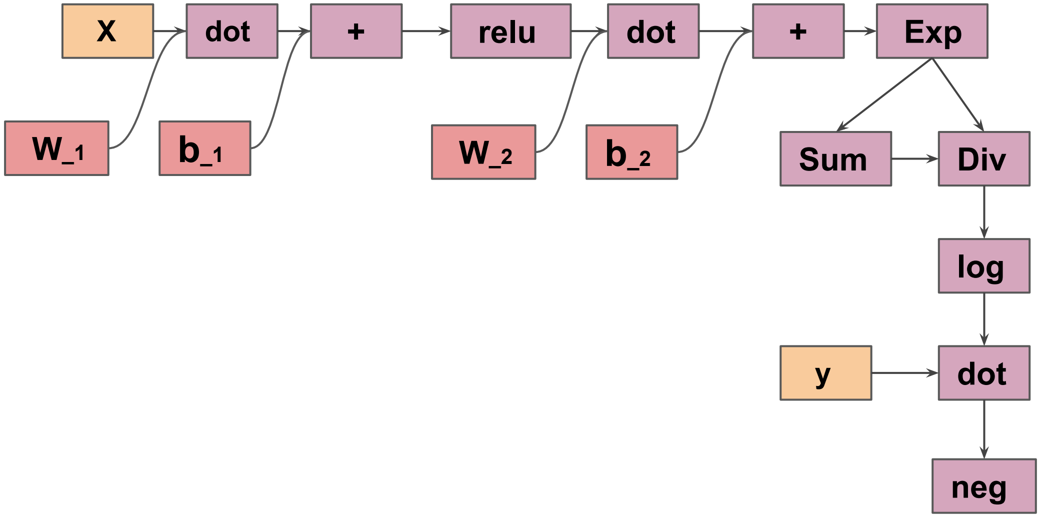

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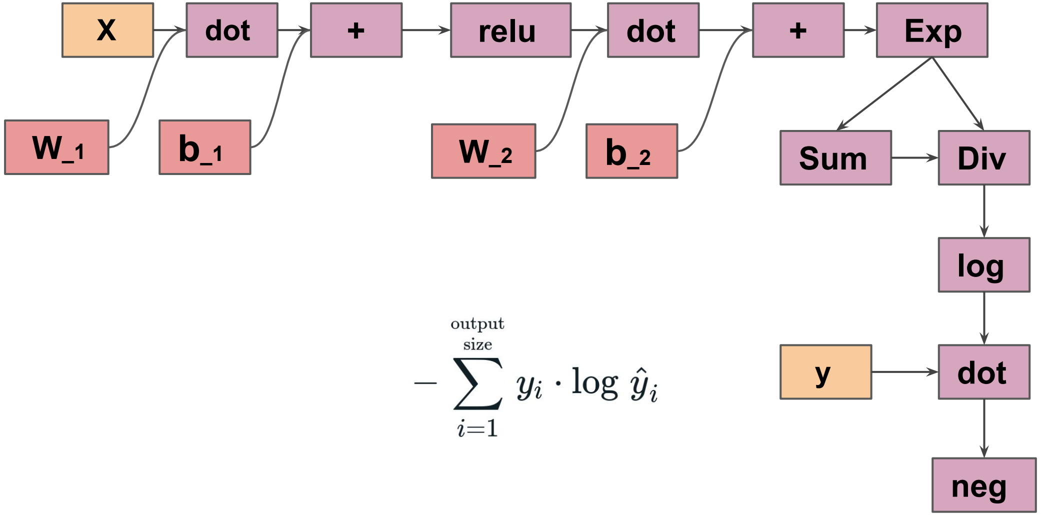

$$-\sum_{i=1}^{\text{output size}} y_i \cdot \log \hat{y}_i$$

SURF

PyTorch

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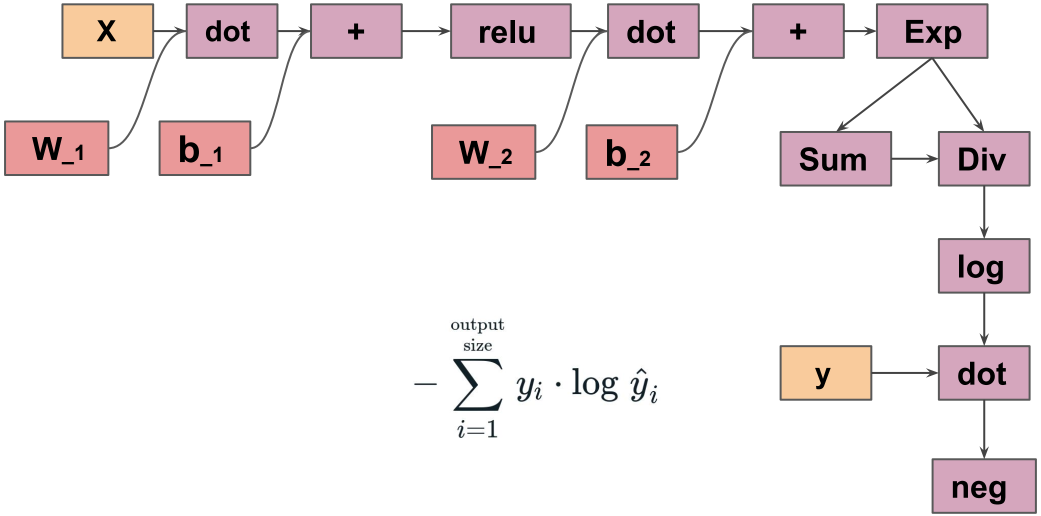

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SURF

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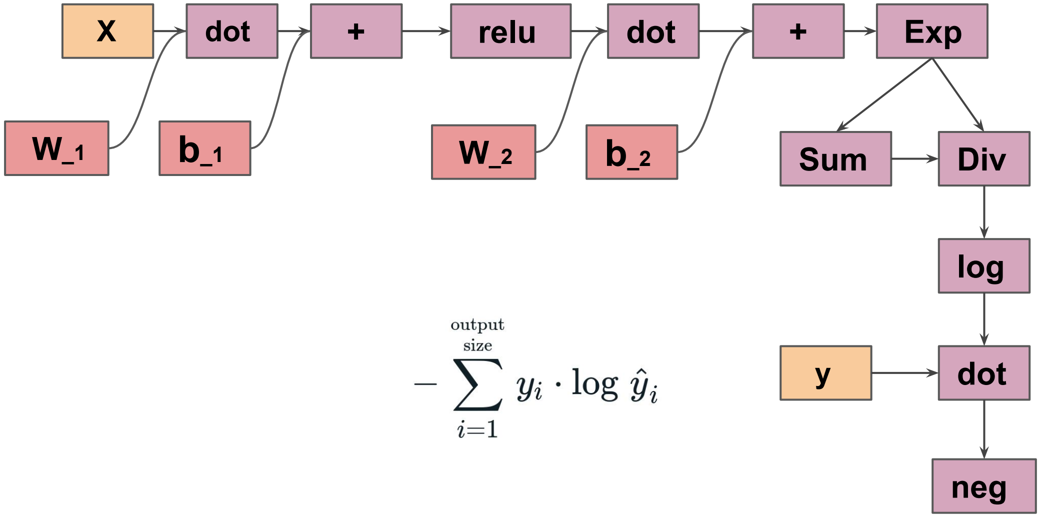
$$\hat{y} = g(\mathbf{W}_0 f(\mathbf{W}_1 \mathbf{x}))$$



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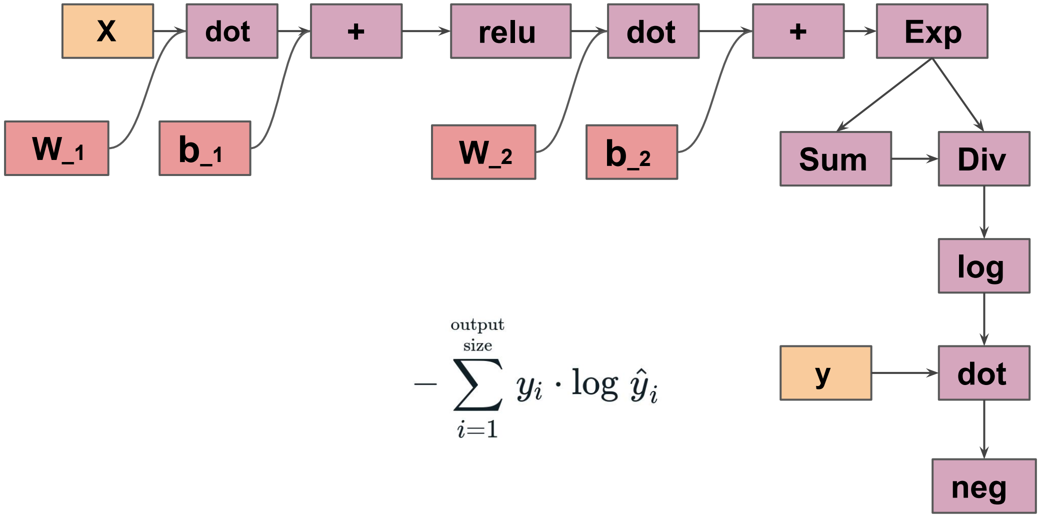

$$-\sum_{i=1}^{\text{output size}} y_i \cdot \log \hat{y}_i$$

Pytorch will helps us with

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

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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()

SURF

PyTorch

General Training Structure

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

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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()
```

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()
```

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

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()

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

```
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()
```

SURF

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

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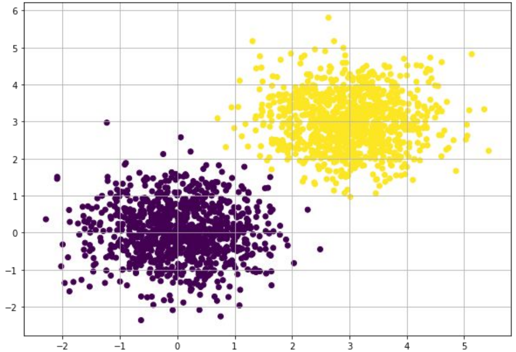

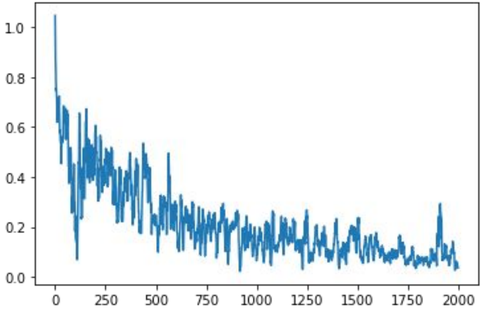

Thank You