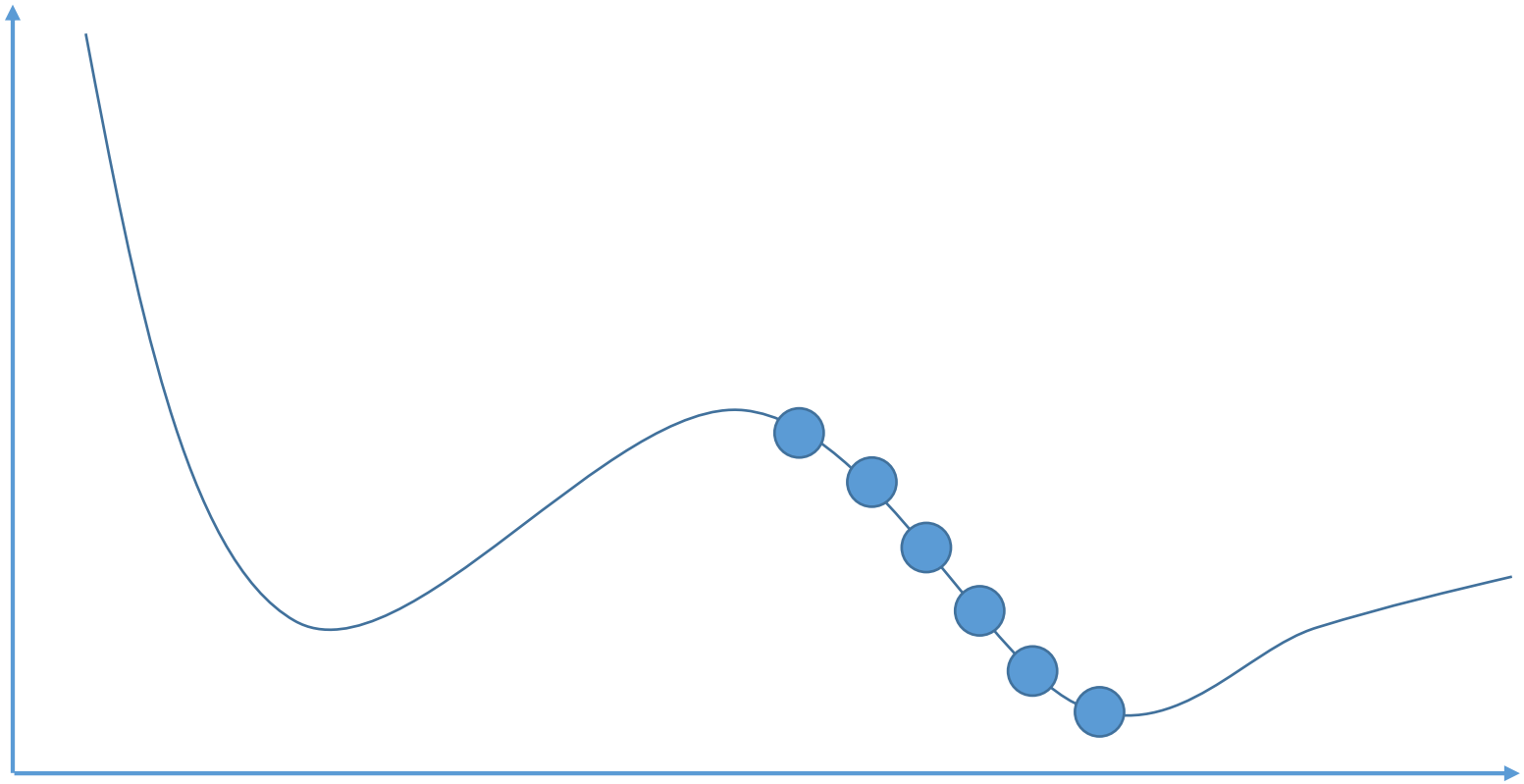
Deep Learning: Pre-Requisites

Understanding gradient descent, autodiff, and softmax

Gradient Descent



autodiff

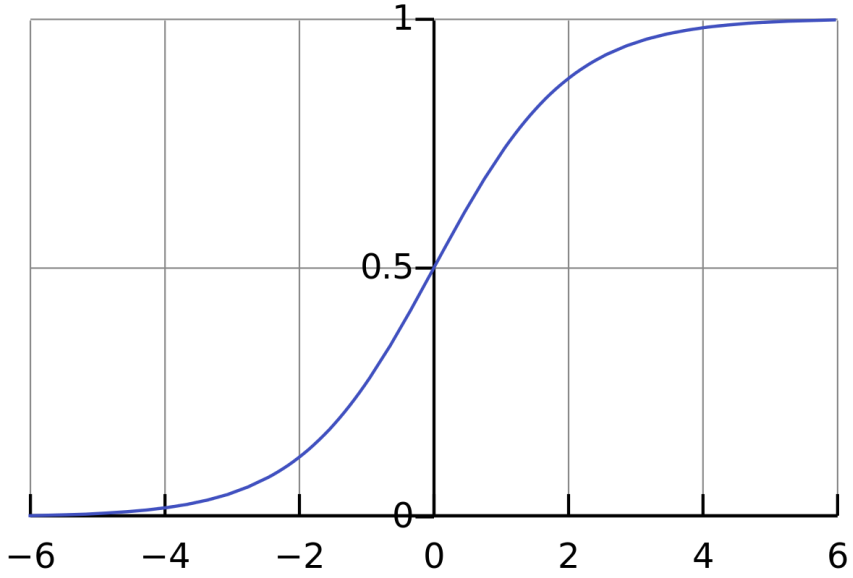
- Gradient descent requires knowledge of, well, the gradient from your cost function (MSE)
- Mathematically we need the first partial derivatives of all the inputs
  - This is hard and inefficient if you just throw calculus at the problem
- Reverse-mode autodiff to the rescue!
  - Optimized for many inputs + few outputs (like a neuron)
  - Computes all partial derivatives in # of outputs + 1 graph traversals
  - Still fundamentally a calculus trick – it’s complicated but it works
  - This is what Tensorflow uses

softmax

- Used for classification
  - Given a score for each class
  - It produces a probability of each class
  - The class with the highest probability is the “answer” you get

$$h_\theta(x) = \frac{1}{1 + \exp(-\theta^T x)},$$

x is a vector of input values
theta is a vector of weights



In review:

- Gradient descent is an algorithm for minimizing error over multiple steps
- Autodiff is a calculus trick for finding the gradients in gradient descent
- Softmax is a function for choosing the most probable classification given several input values

Introducing Artificial Neural Networks

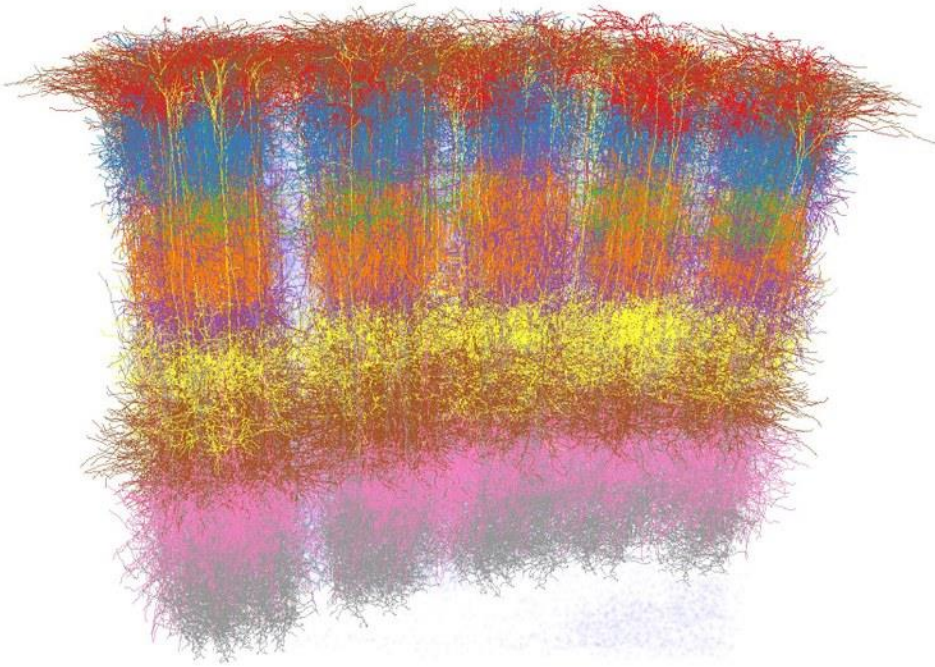
Evolving beyond nature

The biological inspiration

- Neurons in your cerebral cortex are connected via axons
- A neuron “fires” to the neurons it’s connected to, when enough of its input signals are activated.
- Very simple at the individual neuron level – but layers of neurons connected in this way can yield learning behavior.
- Billions of neurons, each with thousands of connections, yields a mind

Cortical columns

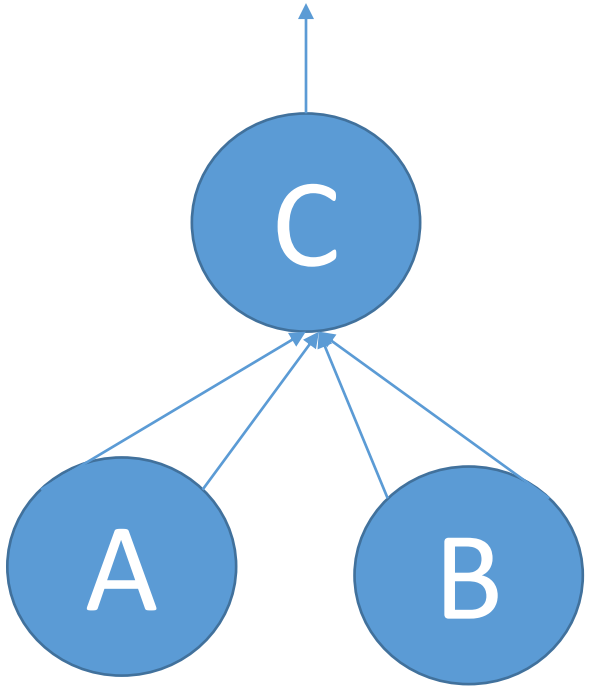
- Neurons in your cortex seem to be arranged into many stacks, or “columns” that process information in parallel
- “mini-columns” of around 100 neurons are organized into larger “hyper-columns”. There are 100 million mini-columns in your cortex
- This is coincidentally similar to how GPU’s work…



(credit: Marcel Oberlaender et al.)

The first artificial neurons

- 1943!!



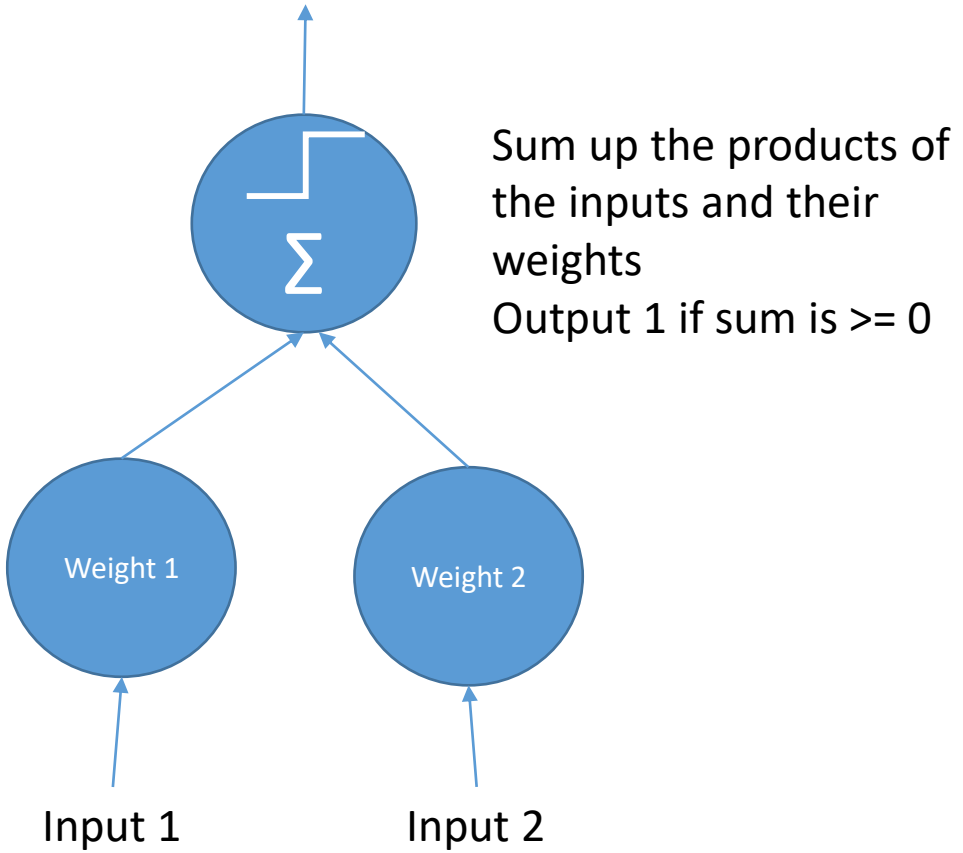
An artificial neuron “fires” if more than N input connections are active.

Depending on the number of connections from each input neuron, and whether a connection activates or suppresses a neuron, you can construct AND, OR, and NOT logical constructs this way.

This example would implement C = A OR B if the threshold is 2 inputs being active.

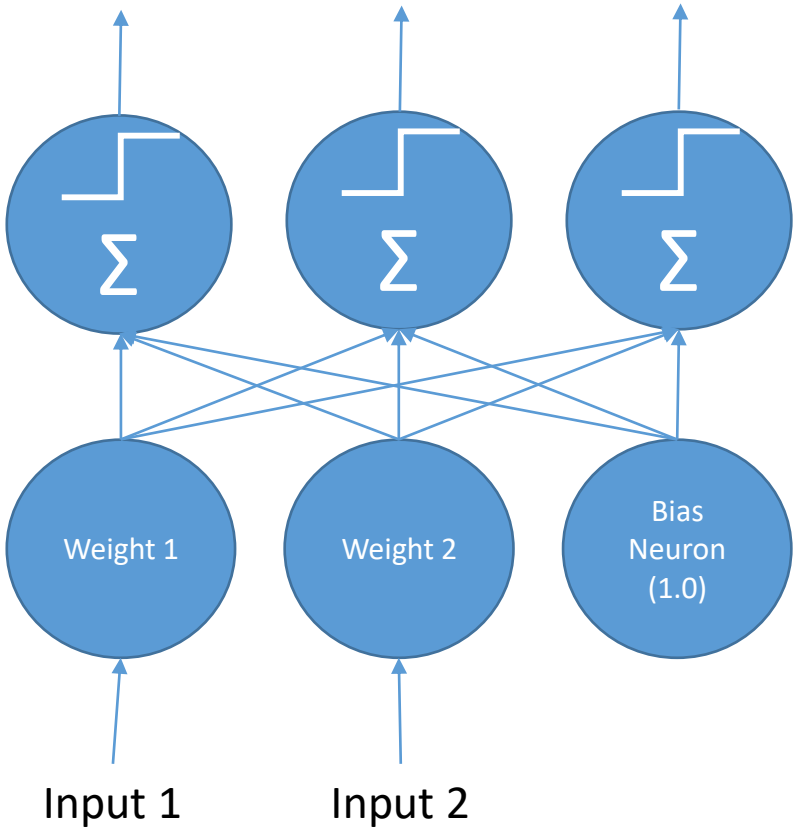
The Linear Threshold Unit (LTU)

- 1957!
- Adds weights to the inputs; output is given by a step function



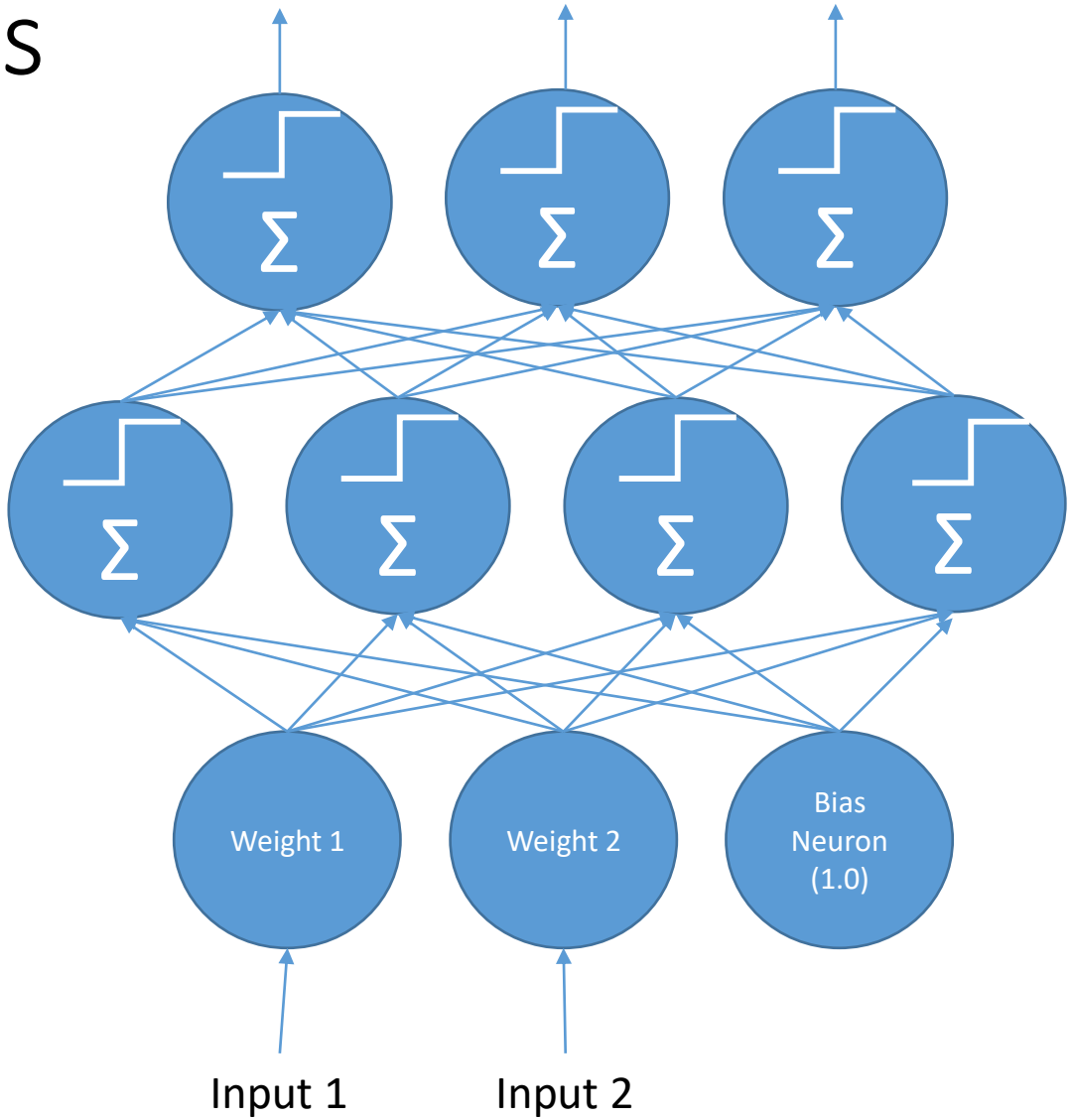
The Perceptron

- A layer of LTU's
- A perceptron can learn by reinforcing weights that lead to correct behavior during training
- This too has a biological basis ("cells that fire together, wire together")



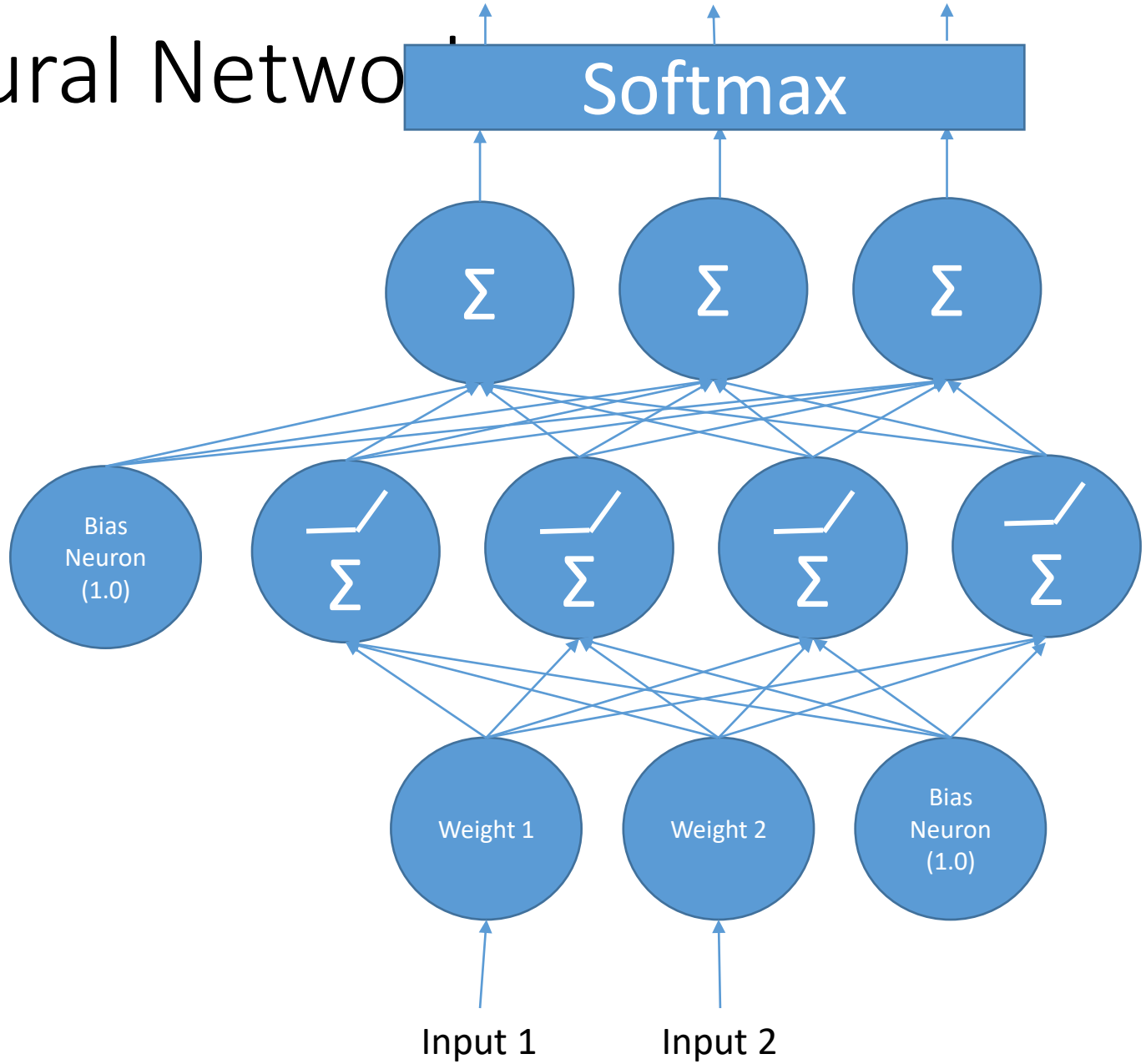
Multi-Layer Perceptrons

- Addition of “hidden layers”
- This is a Deep Neural Network
- Training them is trickier – but we’ll talk about that.



A Modern Deep Neural Netwo

- Replace step activation function with something better
- Apply softmax to the output
- Training using gradient descent



Let’s play

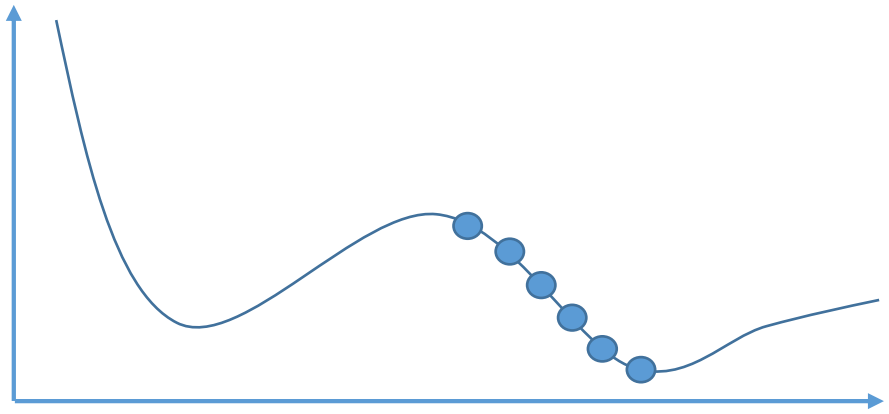
playground.tensorflow.org

Deep Learning

Constructing, training, and tuning multi-layer perceptrons

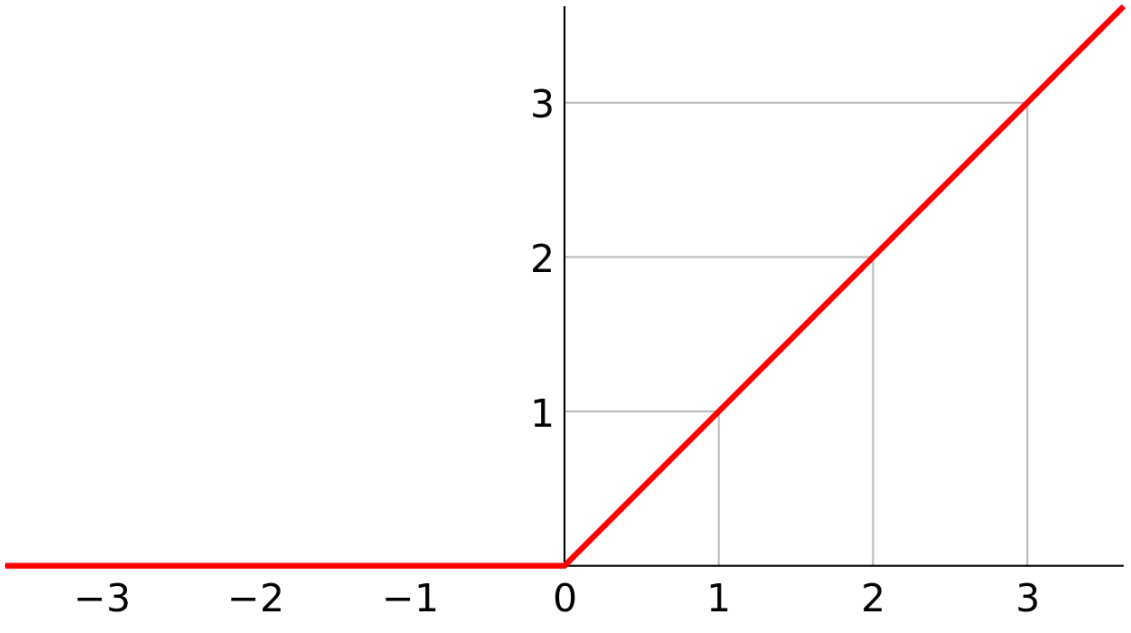
Backpropagation

- How do you train a MLP's weights? How does it **learn**?
- Backpropagation… or more specifically: Gradient Descent using reverse-mode autodiff!
- For each training step:
  - Compute the output error
  - Compute how much each neuron in the previous hidden layer contributed
  - Back-propagate that error in a reverse pass
  - Tweak weights to reduce the error using gradient descent



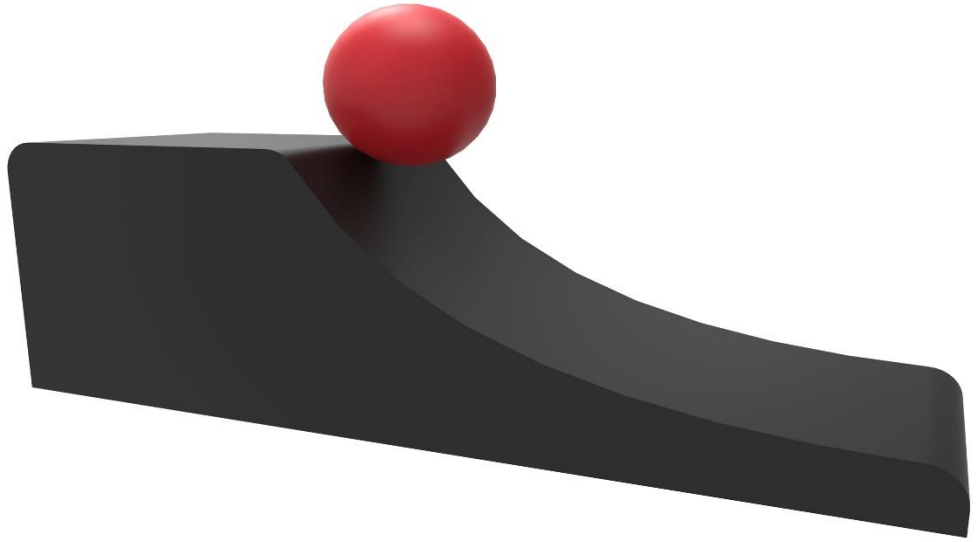
Activation functions (aka rectifier)

- Step functions don't work with gradient descent – there is no gradient!
  - Mathematically, they have no useful derivative.
- Alternatives:
  - Logistic function
  - Hyperbolic tangent function
  - Exponential linear unit (ELU)
  - ReLU function (Rectified Linear Unit)
- ReLU is common. Fast to compute and works well.
  - Also: "Leaky ReLU", "Noisy ReLU"
  - ELU can sometimes lead to faster learning though.



ReLU function

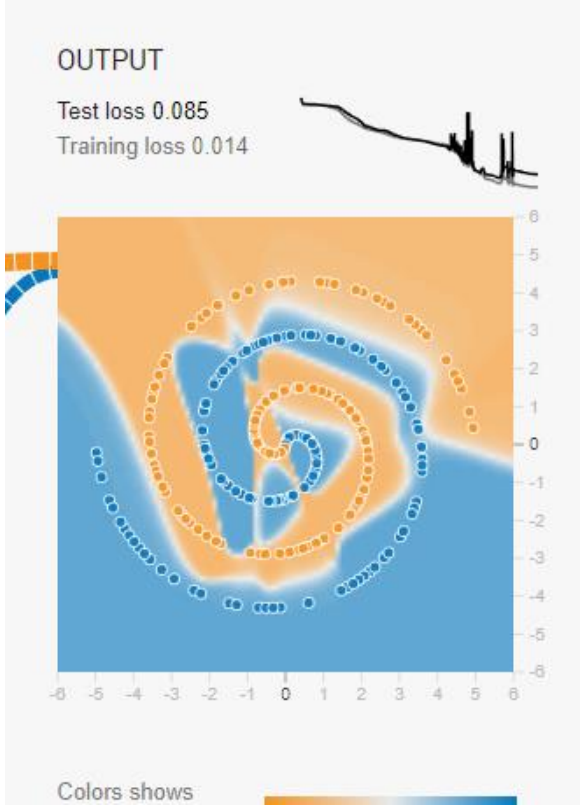
Optimization functions



- There are faster (as in faster learning) optimizers than gradient descent
  - Momentum Optimization
    - Introduces a momentum term to the descent, so it slows down as things start to flatten and speeds up as the slope is steep
  - Nesterov Accelerated Gradient
    - A small tweak on momentum optimization – computes momentum based on the gradient slightly ahead of you, not where you are
  - RMSProp
    - Adaptive learning rate to help point toward the minimum
  - Adam
    - Adaptive moment estimation – momentum + RMSProp combined
    - Popular choice today, easy to use

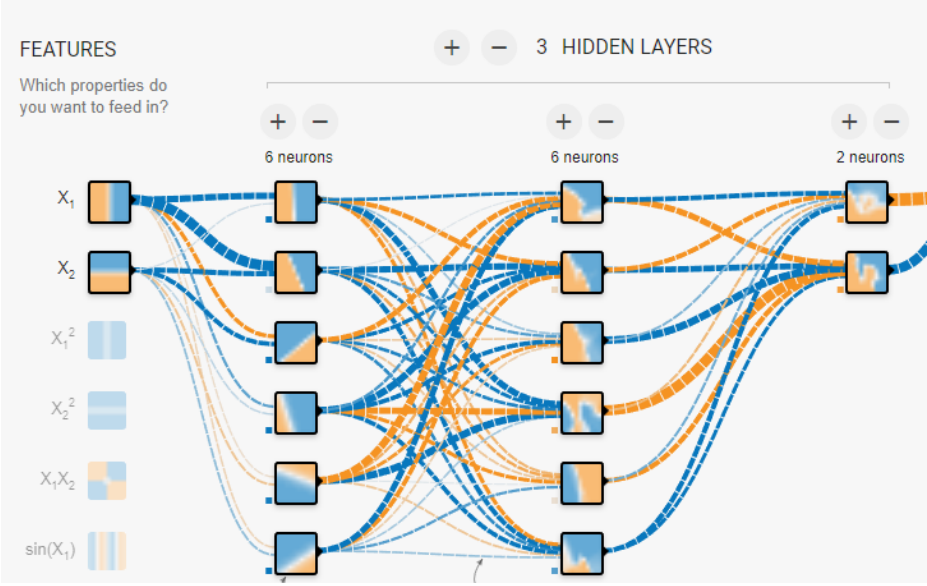
Avoiding Overfitting

- With thousands of weights to tune, overfitting is a problem
- Early stopping (when performance starts dropping)
- Regularization terms added to cost function during training
- Dropout – ignore say 50% of all neurons randomly at each training step
  - Works surprisingly well!
  - Forces your model to spread out its learning



Tuning your topology

- Trial & error is one way
  - Evaluate a smaller network with less neurons in the hidden layers
  - Evaluate a larger network with more layers
    - Try reducing the size of each layer as you progress – form a funnel
- More layers can yield faster learning
- Or just use more layers and neurons than you need, and don't care because you use early stopping.
- Use "model zoos"



Tensorflow

Why Tensorflow?

- It’s not specifically for neural networks– it’s more generally an architecture for executing a graph of numerical operations
- Tensorflow can optimize the processing of that graph, and distribute its processing across a network
  - Sounds a lot like Apache Spark, eh?
- It can also distribute work across GPU’s!
  - Can handle massive scale – it was made by Google
- Runs on about anything
- Highly efficient C++ code with easy to use Python API’s

Tensorflow basics

- Install with pip install tensorflow or pip install tensorflow-gpu
- A tensor is just a fancy name for an array or matrix of values
- To use Tensorflow, you:
  - Construct a graph to compute your tensors
  - Initialize your variables
  - Execute that graph – nothing actually happens until then

World's simplest Tensorflow app:

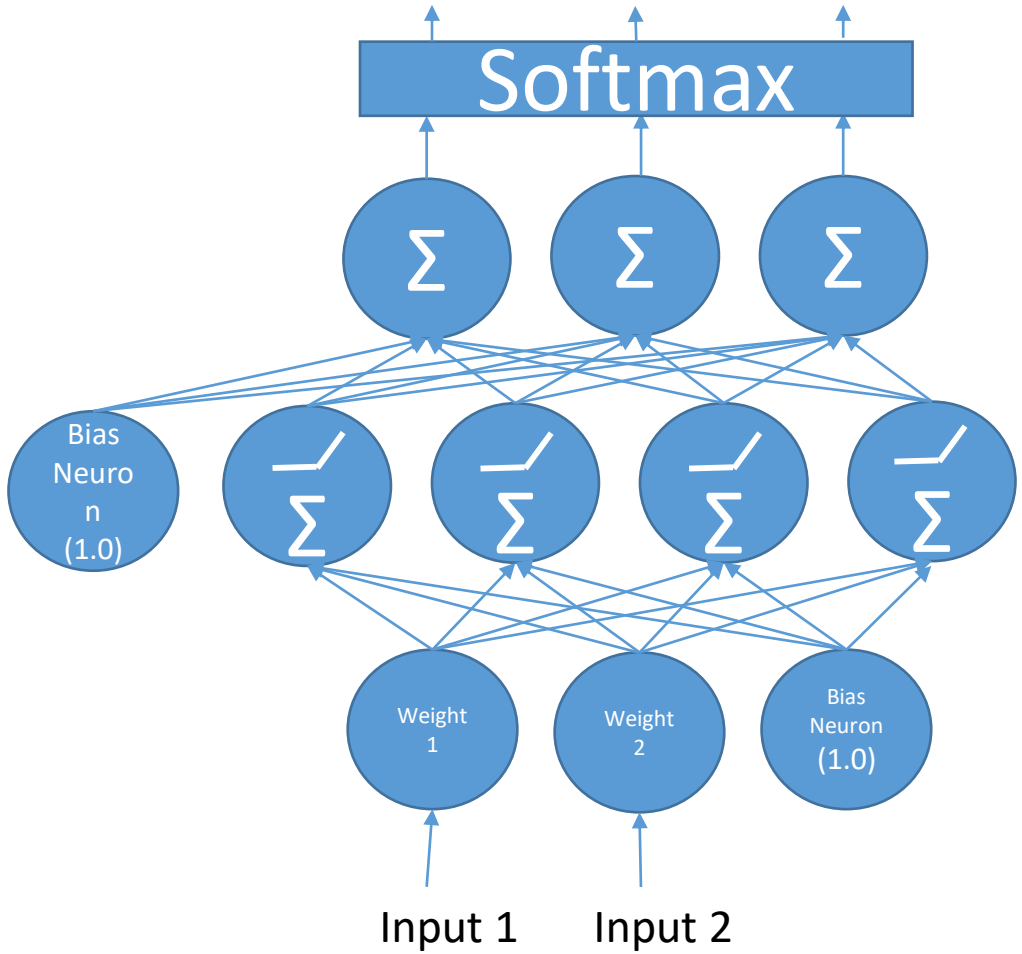
```
import tensorflow as tf

a = tf.Variable(1, name="a")
b = tf.Variable(2, name="b")
f = a + b

init = tf.global_variables_initializer()
with tf.Session() as s:
    init.run()
    print( f.eval() )
```

Creating a neural network with Tensorflow

- Mathematical insights:
  - All those interconnected arrows multiplying weights can be thought of as a big matrix multiplication
  - The bias term can just be added onto the result of that matrix multiplication
- So in Tensorflow, we can define a layer of a neural network as:

```
output = tf.matmul(previous_layer, layer_weights) + layer_biases
```

- By using Tensorflow directly we're kinda doing this the "hard way."



Creating a neural network with Tensorflow

- Load up our training and testing data
- Construct a graph describing our neural network
  - Use **placeholders** for the input data and target labels
    - This way we can use the same graph for training and testing!
  - Use **variables** for the learned weights for each connection and learned biases for each neuron
    - Variables are preserved across runs within a Tensorflow session
- Associate an optimizer (ie gradient descent) to the network
- Run the optimizer with your training data
- Evaluate your trained network with your testing data

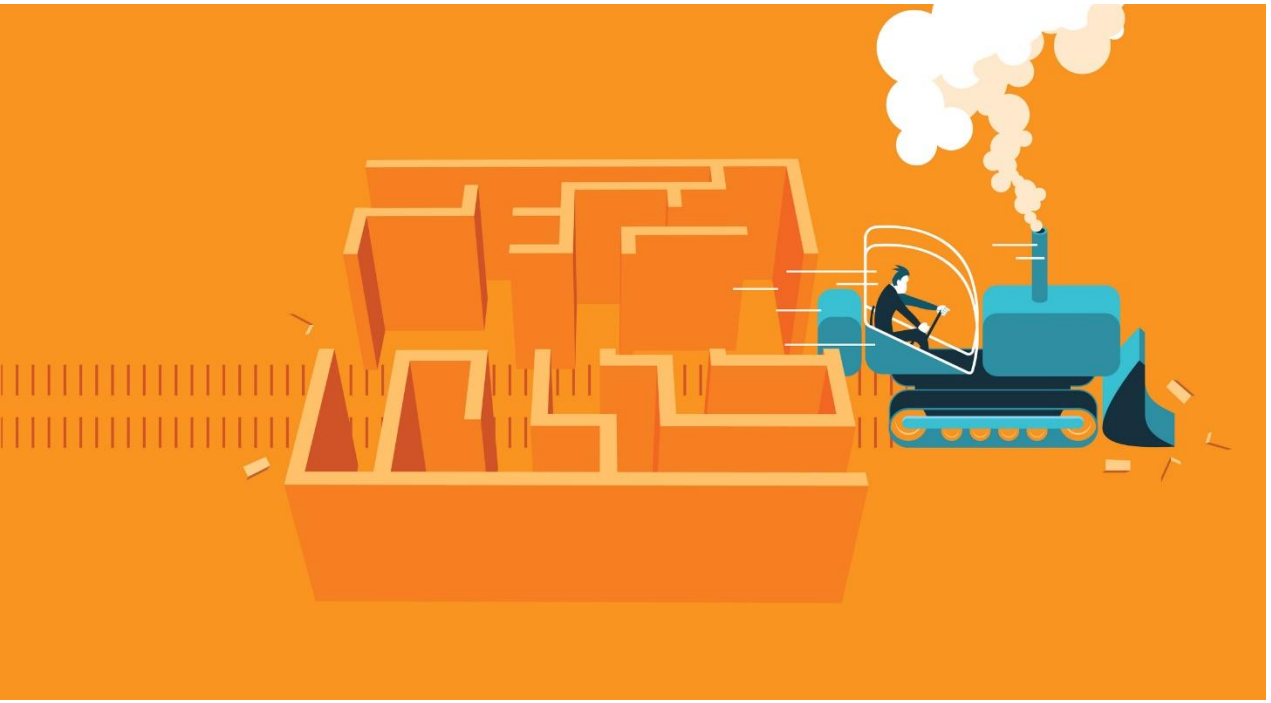
Make sure your features are normalized

- Neural networks usually work best if your input data is normalized.
  - That is, 0 mean and unit variance
  - The real goal is that every input feature is comparable in terms of magnitude
- scikit_learn's StandardScaler can do this for you
- Many data sets are normalized to begin with – such as the one we're about to use.

Let’s try it out

Keras

Why Keras?



- Easy and fast prototyping
  - Runs on top of TensorFlow (or CNTK, or Theano)
  - scikit_learn integration
  - Less to think about – which often yields better results without even trying
  - This is really important! The faster you can experiment, the better your results.

Let’s dive in: MNIST with Keras

Example: multi-class classification

- MNIST is an example of multi-class classification.

```
model = Sequential()

model.add(Dense(64, activation='relu', input_dim=20))
model.add(Dropout(0.5))
model.add(Dense(64, activation='relu'))
model.add(Dropout(0.5))
model.add(Dense(10, activation='softmax'))
sgd = SGD(lr=0.01, decay=1e-6, momentum=0.9,
        nesterov=True)
model.compile(loss='categorical_crossentropy',
        optimizer=sgd, metrics=['accuracy'])
```

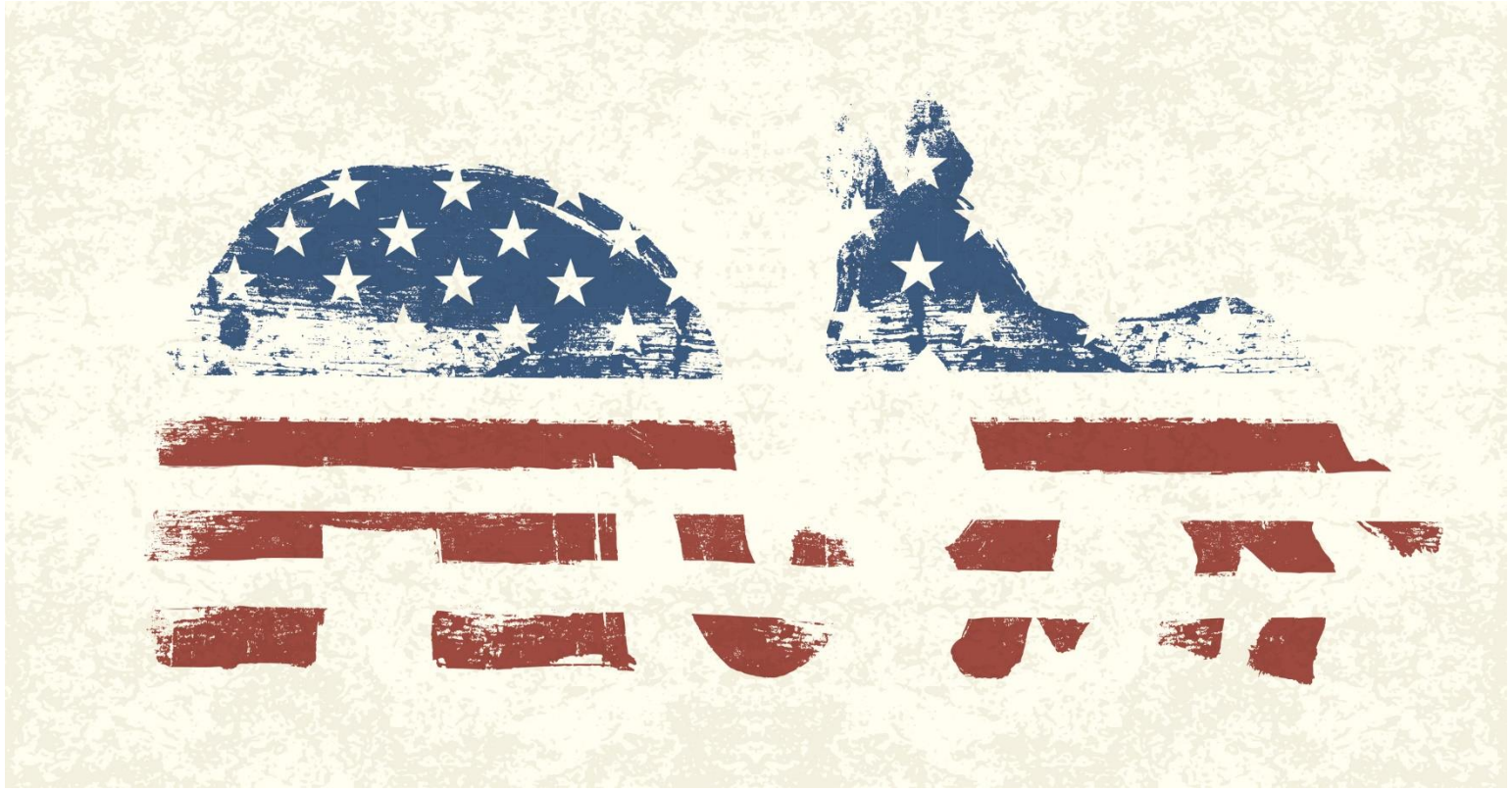
Example: binary classification

```
model = Sequential()
model.add(Dense(64, input_dim=20, activation='relu'))
model.add(Dropout(0.5))
model.add(Dense(64, activation='relu'))
model.add(Dropout(0.5))
model.add(Dense(1, activation='sigmoid'))
model.compile(loss='binary_crossentropy', optimizer='rmsprop',
        metrics=['accuracy'])
```

Integrating Keras with scikit_learn

```
from keras.wrappers.scikit_learn import KerasClassifier

def create_model():
    model = Sequential()
    model.add(Dense(6, input_dim=4, kernel_initializer='normal', activation='relu'))
    model.add(Dense(4, kernel_initializer='normal', activation='relu'))
    model.add(Dense(1, kernel_initializer='normal', activation='sigmoid'))
    model.compile(loss='binary_crossentropy', optimizer='rmsprop', metrics=['accuracy'])
    return model

estimator = KerasClassifier(build_fn=create_model, nb_epoch=100, verbose=0)

cv_scores = cross_val_score(estimator, features, labels, cv=10)
print(cv_scores.mean())
```

Let’s try it out: predict political parties with Keras

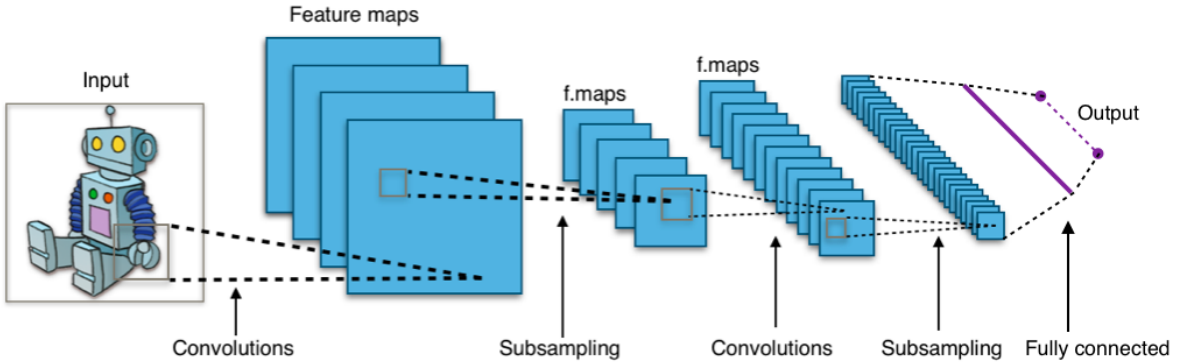


Convolutional Neural Networks

CNN's: what are they for?

- When you have data that doesn't neatly align into columns
  - Images that you want to find features within
  - Machine translation
  - Sentence classification
  - Sentiment analysis
- They can find features that aren't in a specific spot
  - Like a stop sign in a picture
  - Or words within a sentence
- They are "feature-location invariant"

CNN's: how do they wor



- Inspired by the biology of the visual cortex
  - Local receptive fields are groups of neurons that only respond to a part of what your eyes see (subsampling)
  - They overlap each other to cover the entire visual field (convolutions)
  - They feed into higher layers that identify increasingly complex images
    - Some receptive fields identify horizontal lines, lines at different angles, etc. (filters)
    - These would feed into a layer that identifies shapes
    - Which might feed into a layer that identifies objects
  - For color images, extra layers for red, green, and blue

How do we “know” that’s a stop sign?

- Individual local receptive fields scan the image looking for edges, and pick up the edges of the stop sign in a layer
- Those edges in turn get picked up by a higher level convolution that identifies the stop sign’s shape (and letters, too)
- This shape then gets matched against your pattern of what a stop sign looks like, also using the strong red signal coming from your red layers
- That information keeps getting processed upward until your foot hits the brake!
- A CNN works the same way

CNN's with Keras

- Source data must be of appropriate dimensions
  - ie width x length x color channels
- Conv2D layer type does the actual convolution on a 2D image
  - Conv1D and Conv3D also available – doesn't have to be image data
- MaxPooling2D layers can be used to reduce a 2D layer down by taking the maximum value in a given block
- Flatten layers will convert the 2D layer to a 1D layer for passing into a flat hidden layer of neurons
- Typical usage:
  - Conv2D -> MaxPooling2D -> Dropout -> Flatten -> Dense -> Dropout -> Softmax

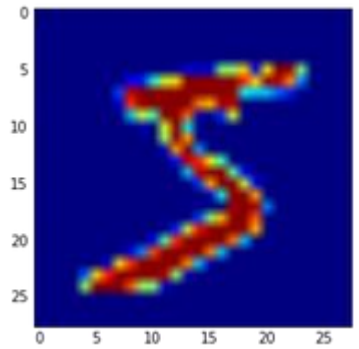
CNN’s are hard

- Very resource-intensive (CPU, GPU, and RAM)
- Lots of hyperparameters
  - Kernel sizes, many layers with different numbers of units, amount of pooling… in addition to the usual stuff like number of layers, choice of optimizer
- Getting the training data is often the hardest part! (As well as storing and accessing it)

Specialized CNN architectures

- Defines specific arrangement of layers, padding, and hyperparameters
- LeNet-5
  - Good for handwriting recognition
- AlexNet
  - Image classification, deeper than LeNet
- GoogLeNet
  - Even deeper, but with better performance
  - Introduces *inception modules* (groups of convolution layers)
- ResNet (Residual Network)
  - Even deeper – maintains performance via *skip connections*.

Let’s try it out

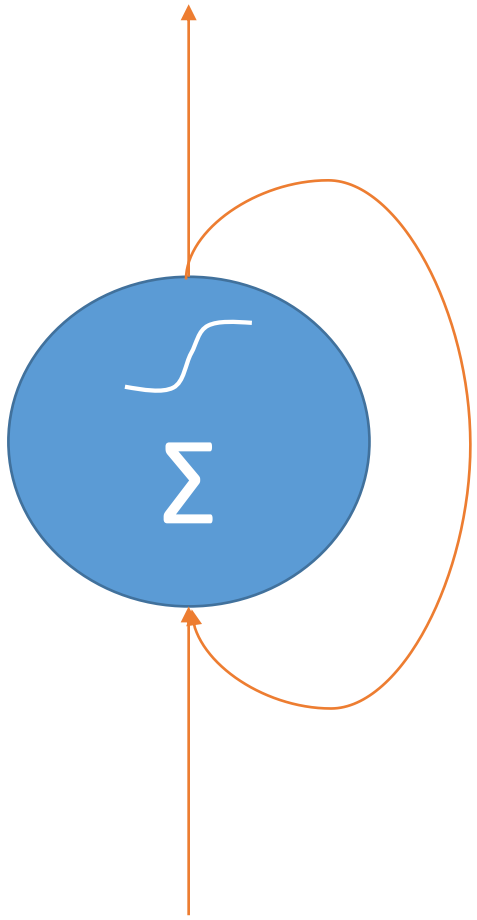


Recurrent Neural Networks

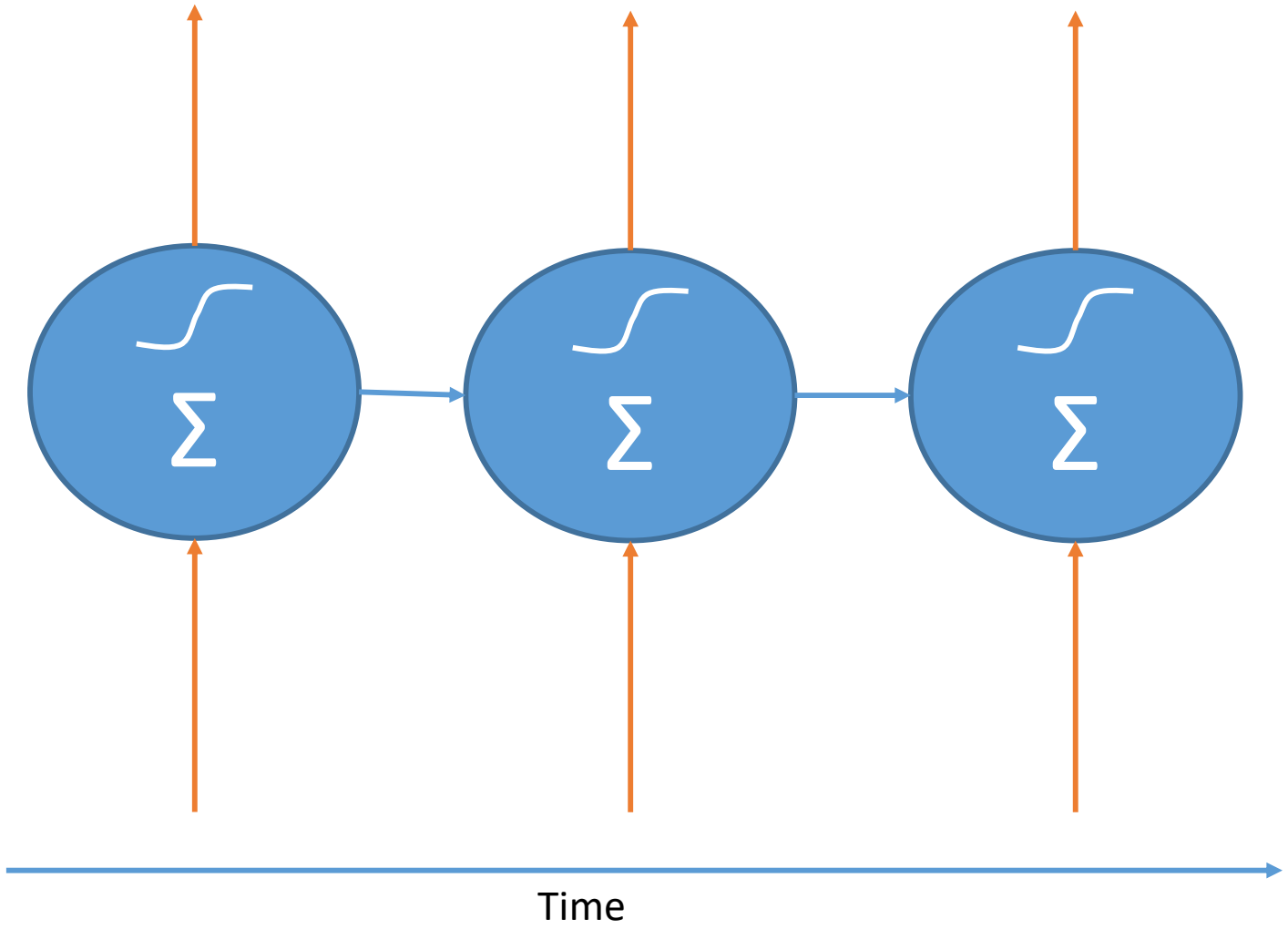
RNN's: what are they for?

- Time-series data
  - When you want to predict future behavior based on past behavior
  - Web logs, sensor logs, stock trades
  - Where to drive your self-driving car based on past trajectories
- Data that consists of sequences of arbitrary length
  - Machine translation
  - Image captions
  - Machine-generated music

A Recurrent Neuron

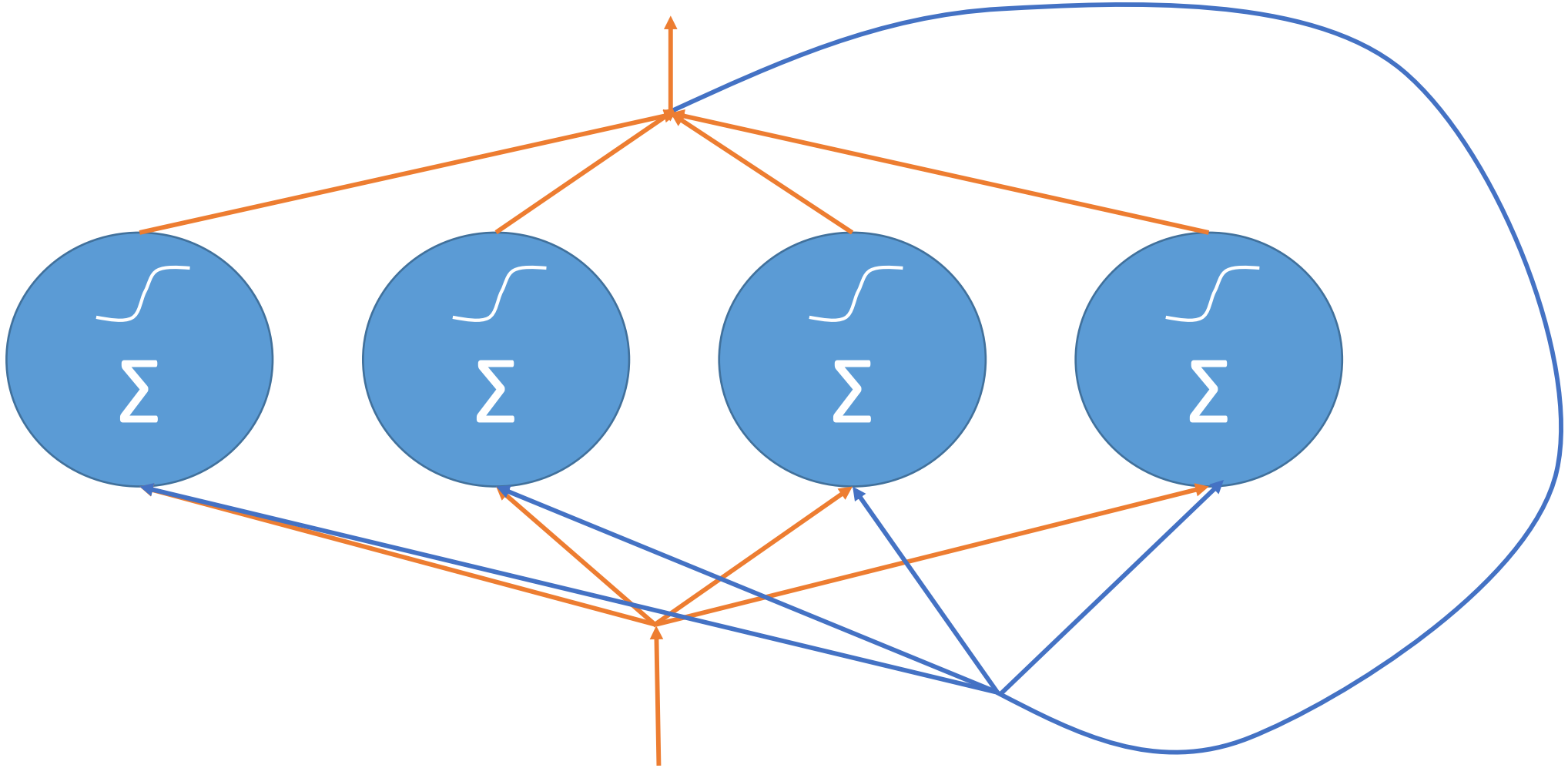


Another Way to Look At It



A “Memory Cell”

A Layer of Recurrent Neurons



RNN Topologies

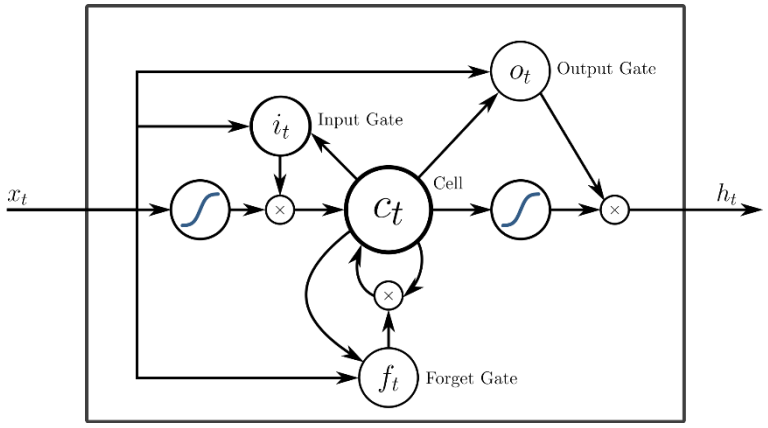
- Sequence to sequence
  - i.e., predict stock prices based on series of historical data
- Sequence to vector
  - i.e., words in a sentence to sentiment
- Vector to sequence
  - i.e., create captions from an image
- Encoder -> Decoder
  - Sequence -> vector -> sequence
  - i.e., machine translation

Training RNN's

- Backpropagation through time
  - Just like backpropagation on MLP's, but applied to each time step.
- All those time steps add up fast
  - Ends up looking like a really, really deep neural network.
  - Can limit backpropagation to a limited number of time steps (truncated backpropagation through time)

Training RNN's

- State from earlier time steps get diluted over time
  - This can be a problem, for example when learning sentence structures
- LSTM Cell
  - Long Short-Term Memory Cell
  - Maintains separate short-term and long-term states
- GRU Cell
  - Gated Recurrent Unit
  - Simplified LSTM Cell that performs about as well



Training RNN's

- It's really hard
  - Very sensitive to topologies, choice of hyperparameters
  - Very resource intensive
  - A wrong choice can lead to a RNN that doesn't converge at all.

Let’s run an example.

The Ethics of Deep Learning

Types of errors

- Accuracy doesn’t tell the whole story
- Type 1: False positive
  - Unnecessary surgery
  - Slam on the brakes for no reason
- Type 2: False negative
  - Untreated conditions
  - You crash into the car in front of you

- Think about the ramifications of different types of errors from your model, tune it accordingly

Hidden biases

- Just because your model isn't human doesn't mean it's inherently fair
- Example: train a model on what sort of job applicants get hired, use it to screen resumes
  - Past biases toward gender / age / race will be reflected in your model, because it was reflected in the data you trained the model with.

Is it really better than a human?

- Don’t oversell the capabilities of an algorithm in your excitement
- Example: medical diagnostics that are almost, but not quite, as good as a human doctor
- Another example: self-driving cars that can kill people

Unintended applications of your research

- Gather ‘round the fire while Uncle Frank tells you a story.

Learning More about Deep Learning