Computer Science

CSC380: Principles of Data Science

Nonlinear Models 3

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Outline

- Basis Functions
- Support Vector Machine
- Neural Networks

Neural Networks

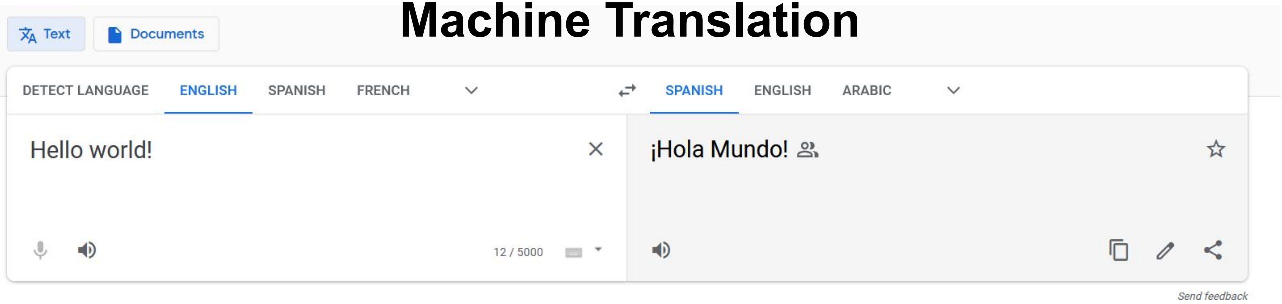
Forms of NNs are used all over the place nowadays…

FB Auto Tagging

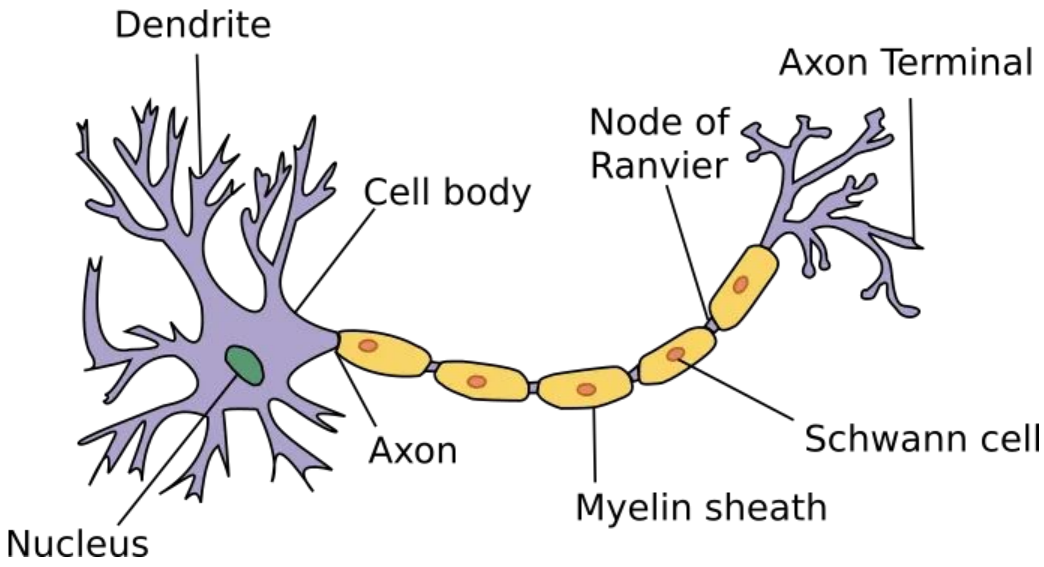
Self-Driving Cars

Creepy Robots

Machine Translation



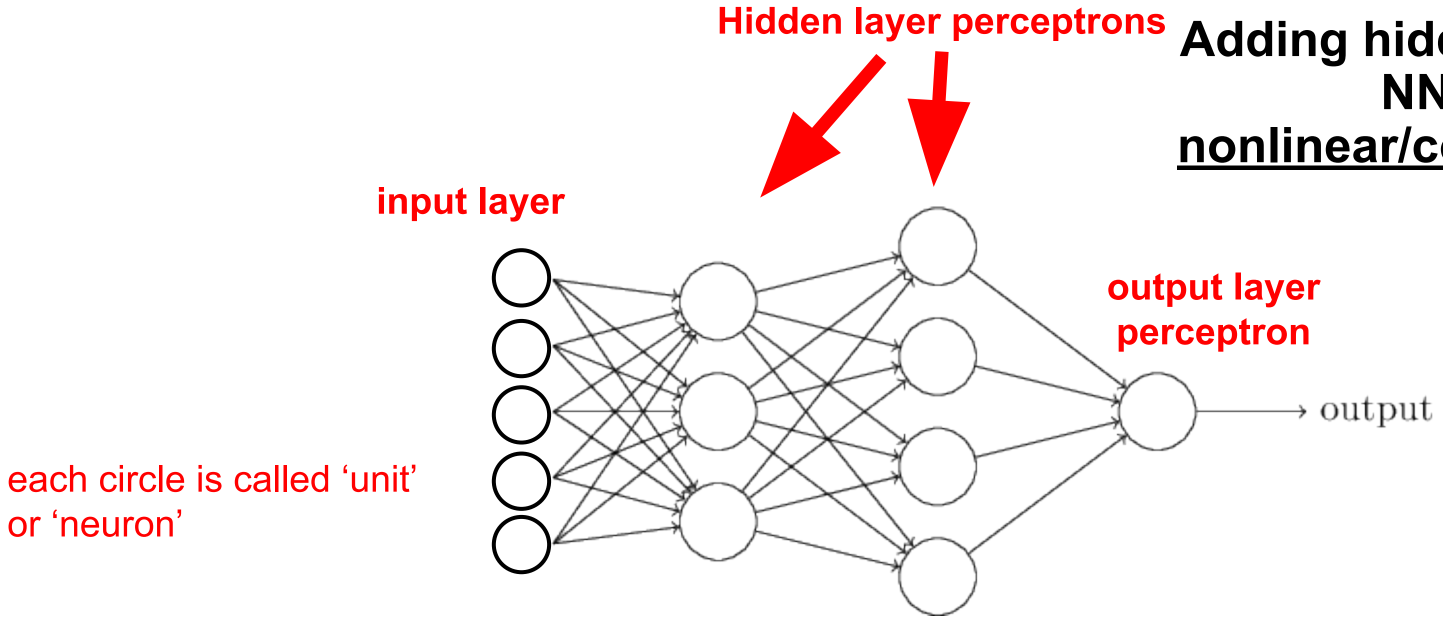
Biological Neuron



1. It takes inputs from its dendrites;
2. A weighted sum of inputs is passed on to the axon hillock;
3. If weighted sum is larger than threshold limit, the neuron will fire. Otherwise, it stays at rest.
4. The state of our neuron (on or off) then propagates through its axon and is passed on to the other connected neurons via its synapses.

Multilayer Perceptron

Adding hidden layers allows NN to learn <u>nonlinear/complex</u> functions



This is the quintessential *(Artificial) Neural Network…*

… the image above is a special case called *Feed Forward Neural Net*

feed forward: no backward connection

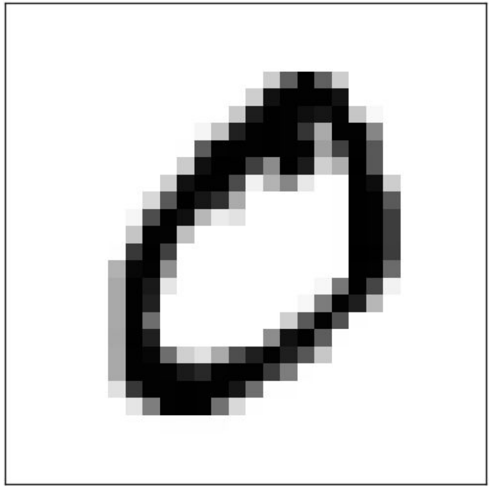
[Source: http://neuralnetworksanddeeplearning.com]

Handwritten Digit Classification

Classifying handwritten digits is the “Hello World” of NNs

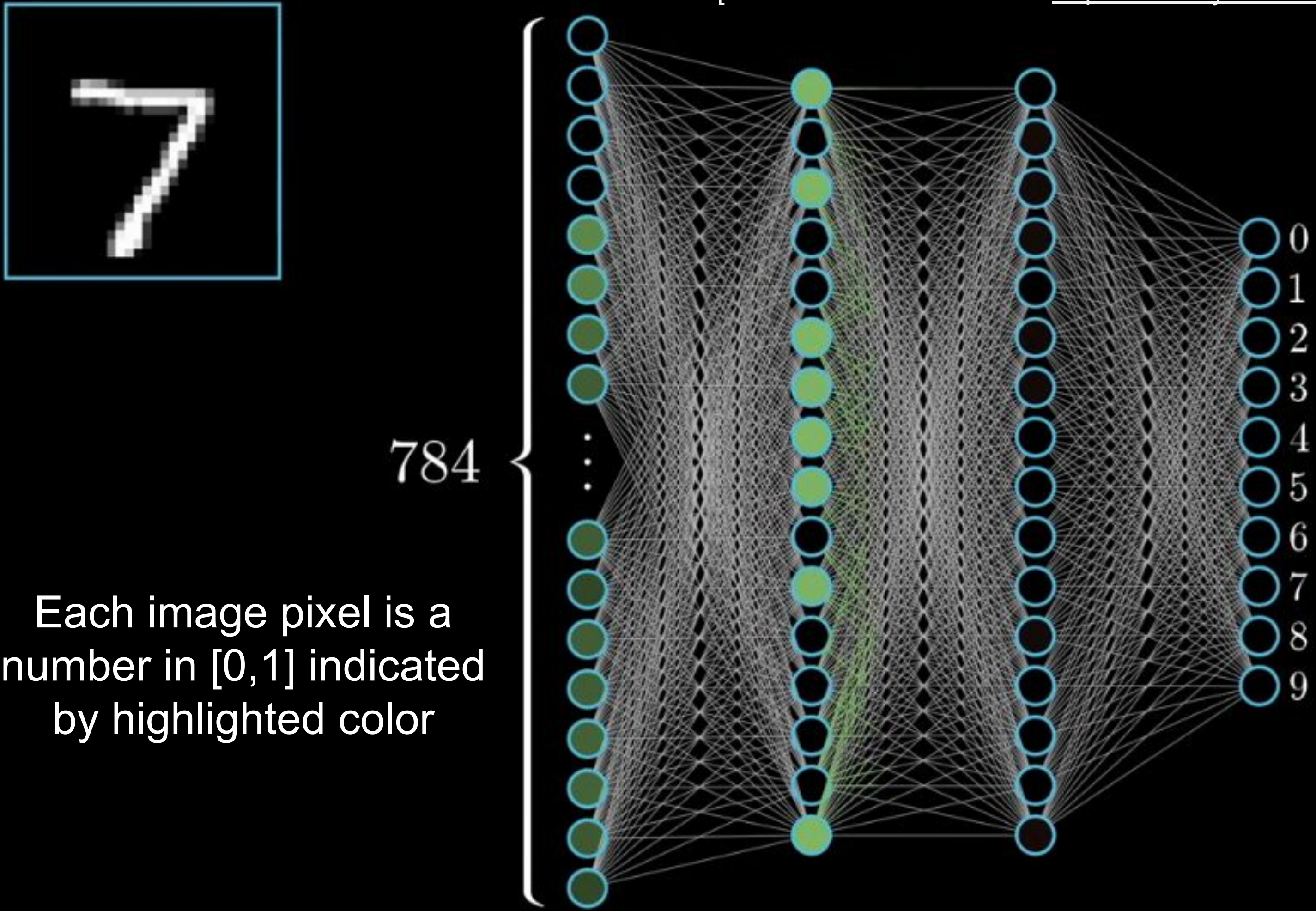
Modified National Institute of Standards and Technology (MNIST) database contains 60k training and 10k test images

Each character is centered in a 28x28=784 pixel grayscale image



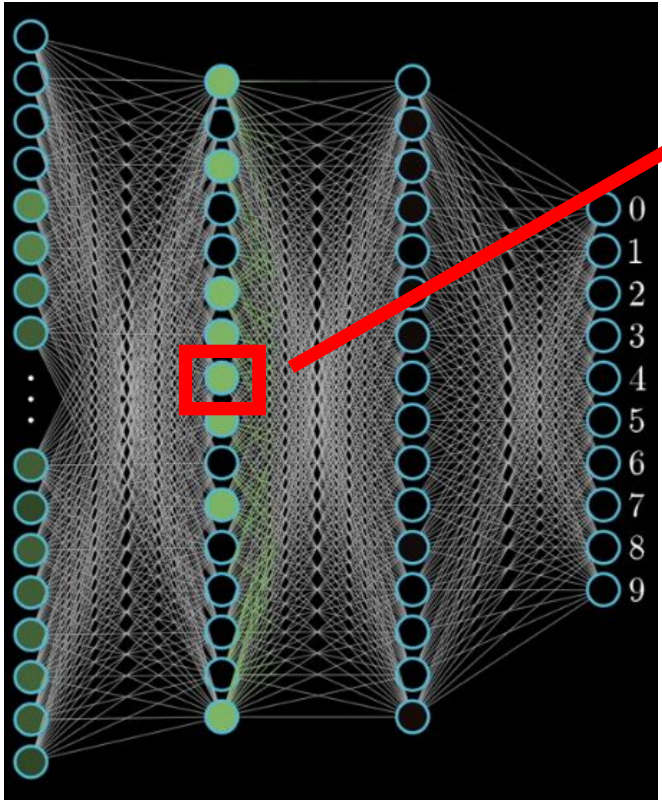
Fun fact: Kernel Ridge Regression with RBF kernel with no regularization gives 1.2% test error rate.

[Source : 3Blue1Brown : https://www.youtube.com/watch?v=aircAruvnKk]



Each image pixel is a number in [0,1] indicated by highlighted color

Feedforward Procedure



Each node computes a *weighted combination* of nodes at the previous layer…

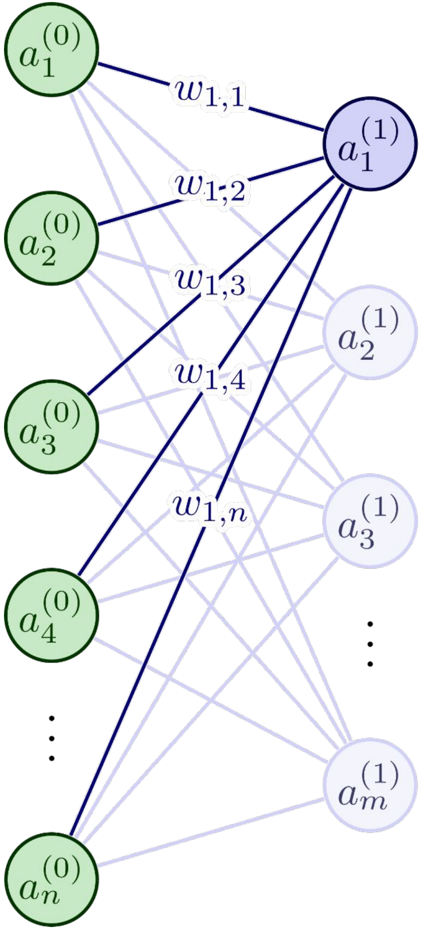
$$w_1 x_1 + w_2 x_2 + \ldots + w_n x_n$$

Then applies a *nonlinear function* to the result

$$\sigma(w_1 x_1 + w_2 x_2 + \ldots + w_n x_n + b)$$

Usually, we also introduce a constant *bias* parameter (usually hidden when we visualize the network)

Feedforward Procedure



$$= \sigma\left(w_{1,0}a_0^{(0)} + w_{1,1}a_1^{(0)} + \ldots + w_{1,n}a_n^{(0)} + b_1^{(0)}\right)$$

$$= \sigma\left(\sum_{i=1}^{n} w_{1,i}a_i^{(0)} + b_1^{(0)}\right)$$

$$\begin{pmatrix} a_1^{(1)} \\ a_2^{(1)} \\ \vdots \\ a_m^{(1)} \end{pmatrix} = \sigma\left[\begin{pmatrix} w_{1,0} & w_{1,1} & \ldots & w_{1,n} \\ w_{2,0} & w_{2,1} & \ldots & w_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{m,0} & w_{m,1} & \ldots & w_{m,n} \end{pmatrix} \begin{pmatrix} a_1^{(0)} \\ a_2^{(0)} \\ \vdots \\ a_n^{(0)} \end{pmatrix} + \begin{pmatrix} b_1^{(0)} \\ b_2^{(0)} \\ \vdots \\ b_m^{(0)} \end{pmatrix}\right]$$

$$a^{(1)} = \sigma\left(\mathbf{W}^{(0)}a^{(0)} + \mathbf{b}^{(0)}\right)$$

Number of parameters in this example: $m \times n + m$

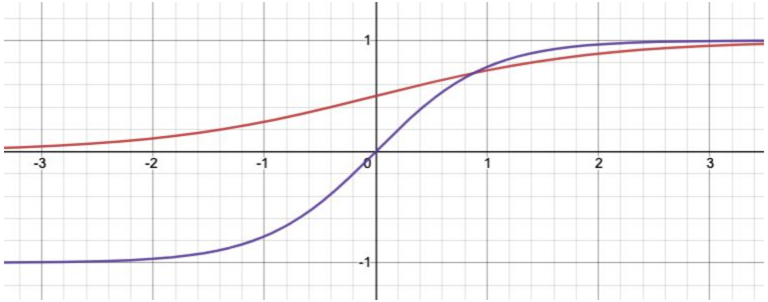
Activation functions

We call this an *activation function* and typically write it in vector form,

$$\sigma(w_1x_1 + w_2x_2 + \ldots + w_nx_n + b) = \sigma(w^Tx + b)$$

An early choice was the *logistic function*,

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$



Later, people found that a scaled version called **<u>tanh</u>** trains faster (=converges faster)

$$\tanh(z) = 2\sigma(2z) - 1$$

1

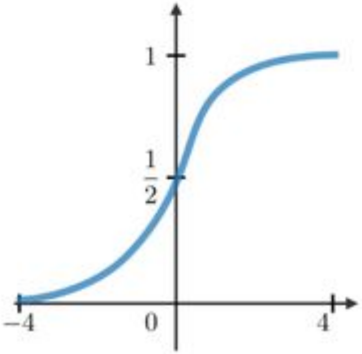
$$\frac{1}{(1 + e^{-x})} = \sigma(z)$$

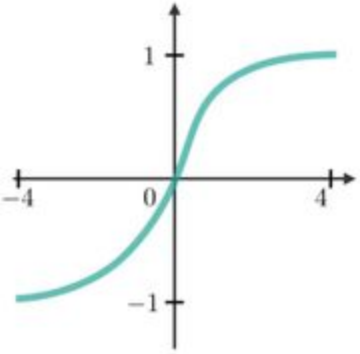
2

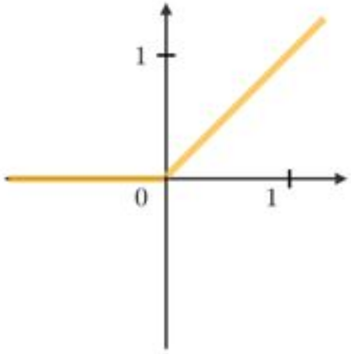
$$\frac{(e^z - e^{-z})}{e^z + e^{-z}} = \tanh(z)$$

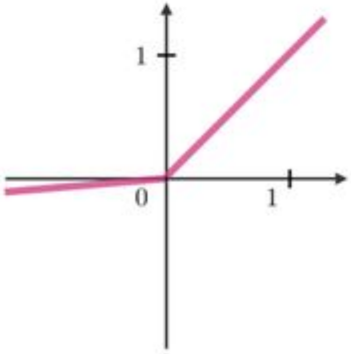
Activation functions

Sigmoid	Tanh	ReLU	Leaky ReLU
$g(z) = \dfrac{1}{1+e^{-z}}$	$g(z) = \dfrac{e^{z}-e^{-z}}{e^{z}+e^{-z}}$	$g(z) = \max(0, z)$	$g(z) = \max(\epsilon z, z)$ with $\epsilon \ll 1$

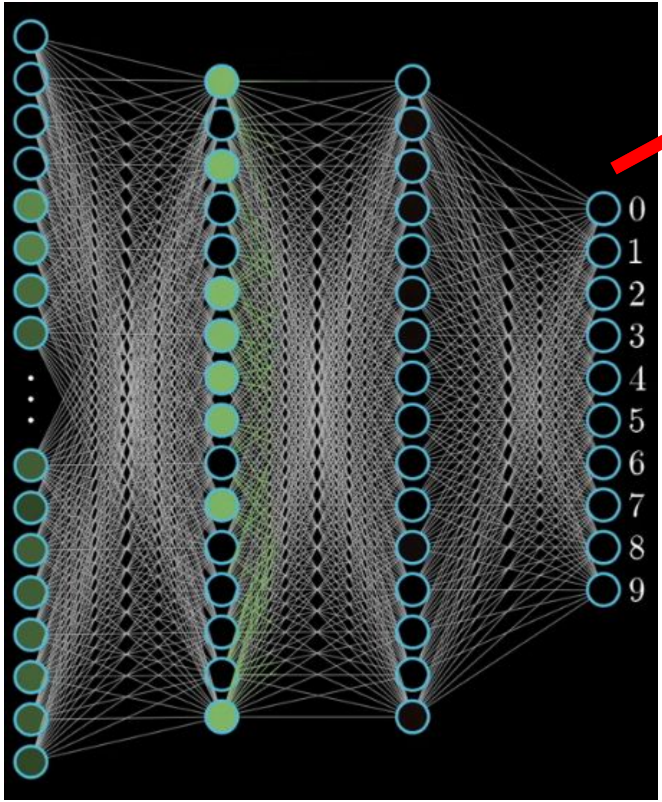








Multilayer Perceptron



Final layer is a linear model…

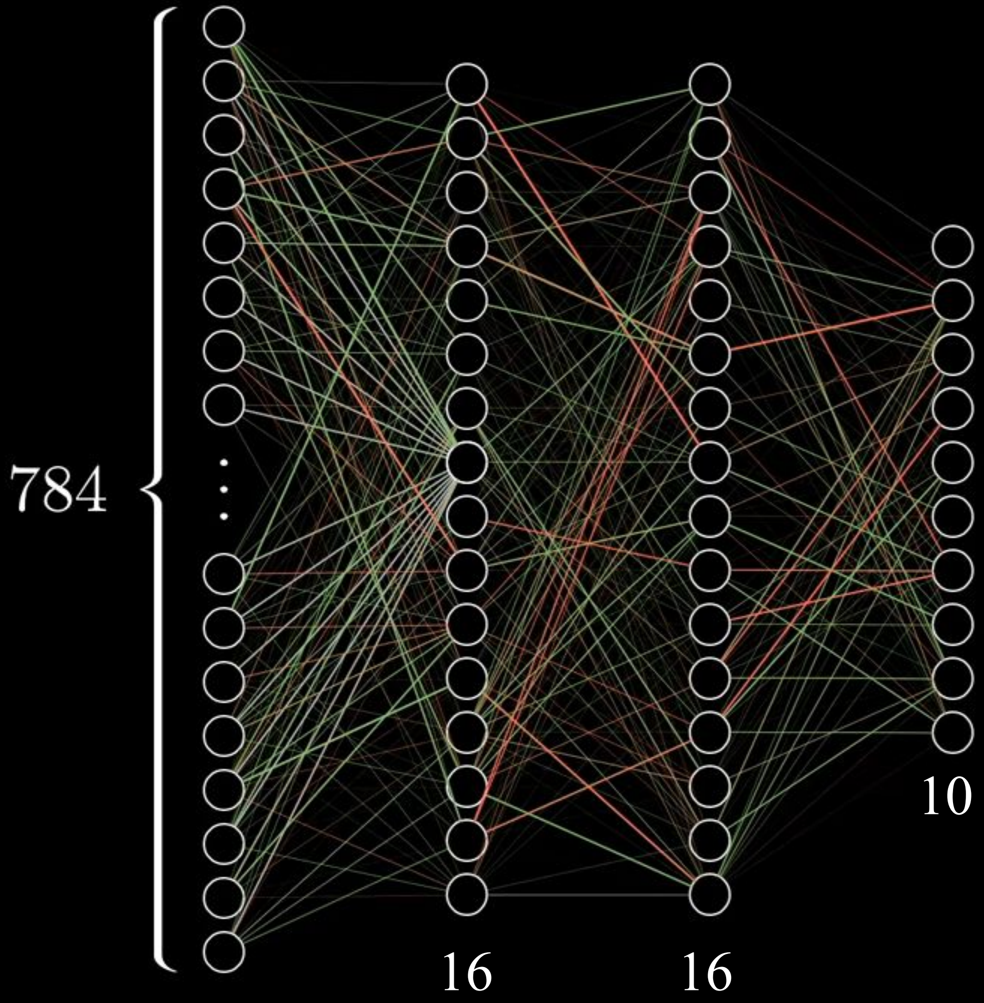
for classification this is a logistic regression

$$\sigma(w^T x + b) = \frac{1}{1 + e^{-(w^T x + b)}}$$

Vector of activations from previous layer

Note: we don't use ReLU for the last layer

[Source : 3Blue1Brown : https://www.youtube.com/watch?v=aircAruvnKk]



$$784\times16+16\times16+16\times10$$

weights

$$16\ +16+10$$

biases

13,002

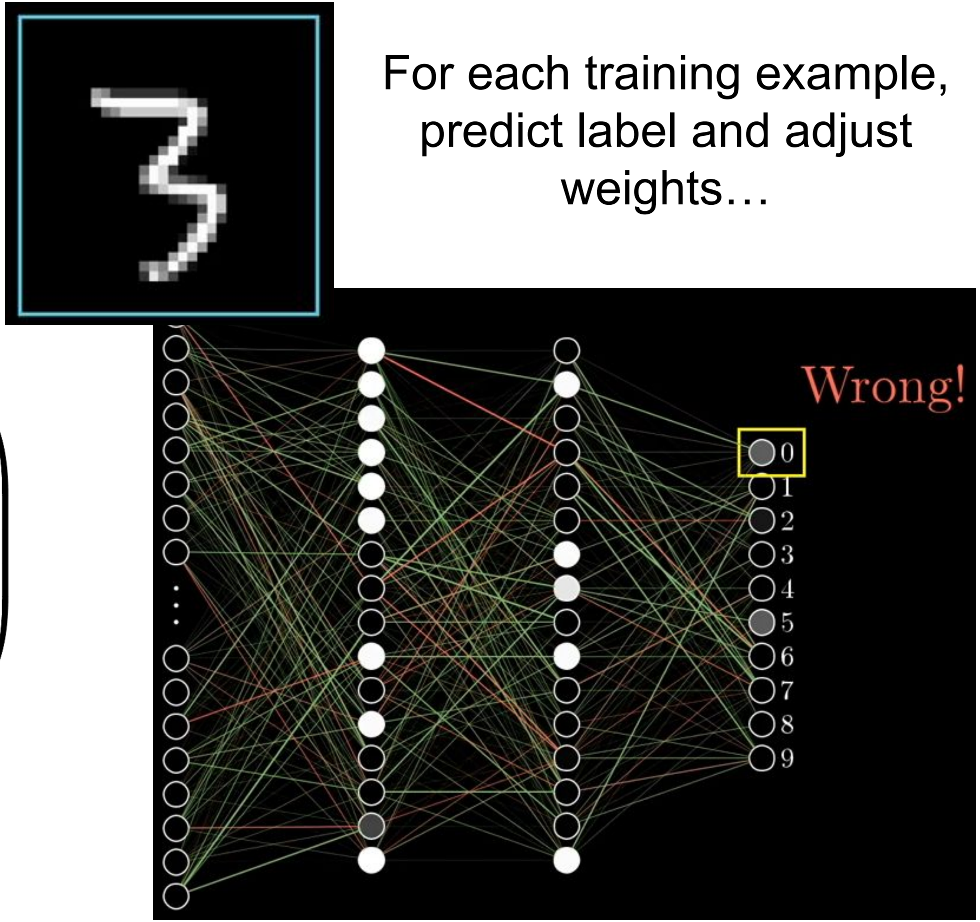
Each parameter has some impact on the output…need to train all these parameters simultaneously to have a good prediction accuracy

Training Multilayer Perceptron

$$X^{\text{Train}} =$$

$$Y^{\text{Train}} = \begin{pmatrix} 0 & 4 & 1 & \dots & 3 \\ 5 & 3 & 6 & \dots & 4 \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 7 & 4 & 6 & \dots & 5 \end{pmatrix}$$

For each training example, predict label and adjust weights…

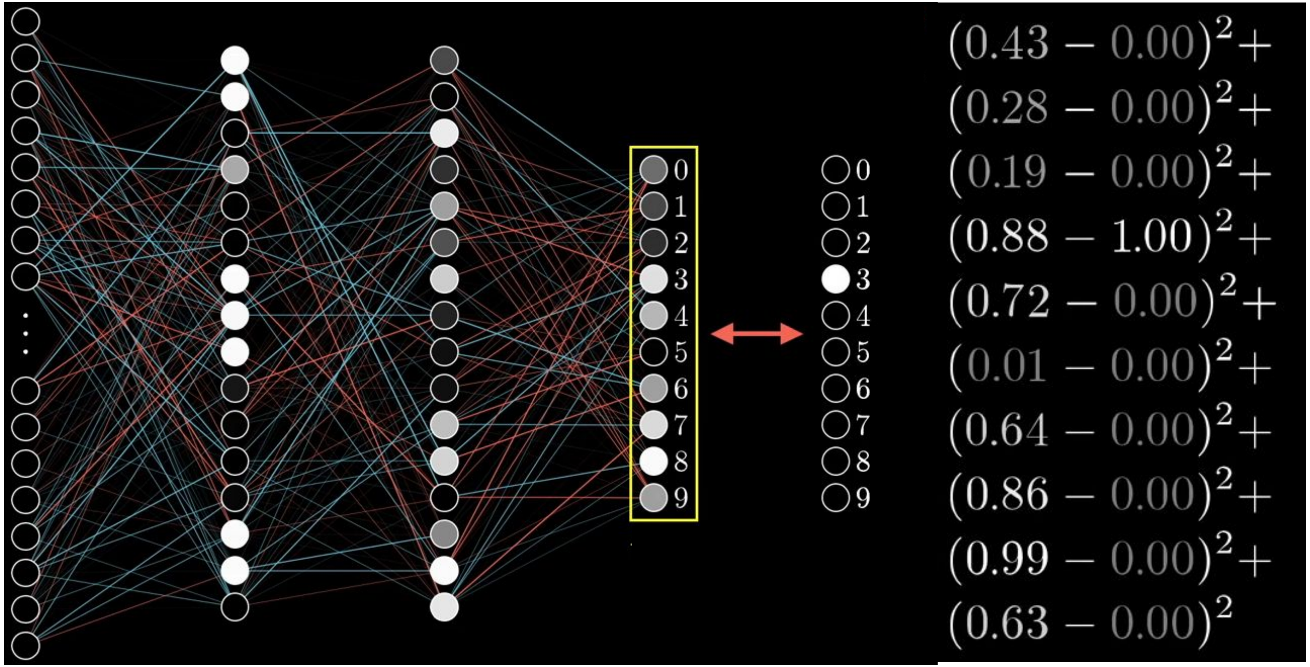


- How to score final layer output?
- How to adjust weights?

Training Multilayer Perceptron

Score based on difference between final layer and one-hot vector of true class…

Input



Training Multilayer Perceptron

Our cost function for i[th] input is error in terms of weights / biases…

$$\underbrace{\text{Cost}_i(w_1, \ldots, w_n, b_1, \ldots, b_n)}_{\text{13,002 Parameters in this network}}$$

…minimize cost over all training data…

$$\min_{w,b} \mathcal{L}(w, b) = \sum_i \text{Cost}_i(w_1, \ldots, w_n, b_1, \ldots, b_n)$$

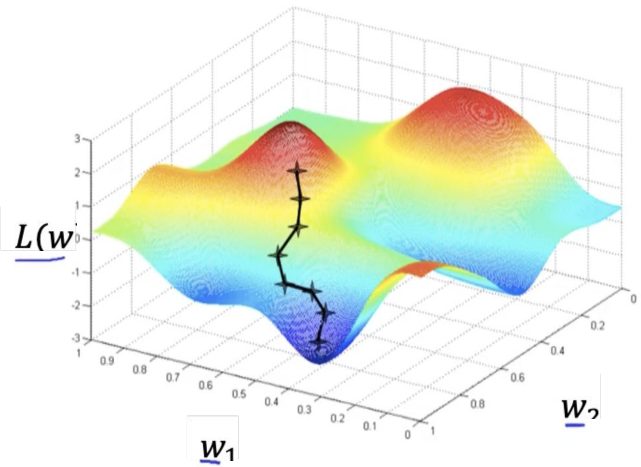
This is a super high-dimensional optimization (13,002 dimensions in this example)…how do we solve it?

Gradient descent!

Gradient Descent

How to minimize a function?

$$\arg\min_w L(w)$$



Randomly start from some $w^{(1)} \in \mathbb{R}^d$

For $t = 1,2,\ldots$

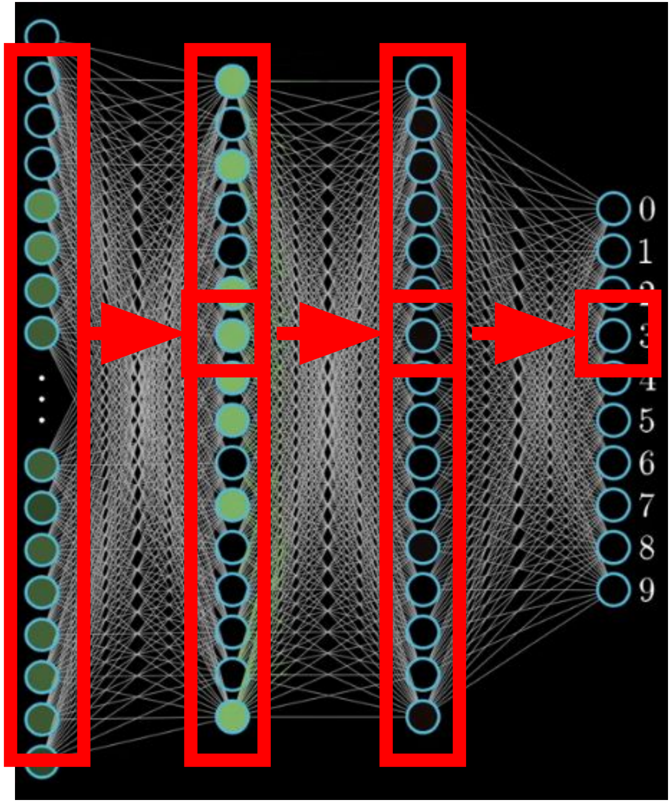
- Compute the gradient $g_t \in \mathbb{R}^d$ at the location $w^{(t)}$
- Move to that direction:
$$w^{(t+1)} = w^{(t)} - \eta_t \cdot g^{(t)}$$
where $\eta_t > 0$ is a stepsize parameter.
- If $L\left(w^{(t+1)}\right) \approx L\left(w^{(t)}\right)$, stop.

The choice of η_t matters! (default: $\eta_t = 0.01$)

https://zitaoshen.rbind.io/project/optimization/1-min-of-machine-learning-gradient-decent/

Backpropagation

[Source : 3Blue1Brown : https://www.youtube.com/watch?v=aircAruvnKk]



Randomly initialize $\{w^{(u)}\}_{u \in \text{units in neural net}}$

For $i \in \{1, \ldots, \text{n\_epochs}\}$

- For (x,y) in train set:
  - Forward pass:
    - evaluate the neural net output
    - measure the loss
  - Backward pass: compute the gradients.
  - Take the gradient step to update the weights $\{w^{(u)}\}$

Dependencies between layers.

No dependencies between units at the same layer.

$\Rightarrow$ Many GPU supported libraries available.

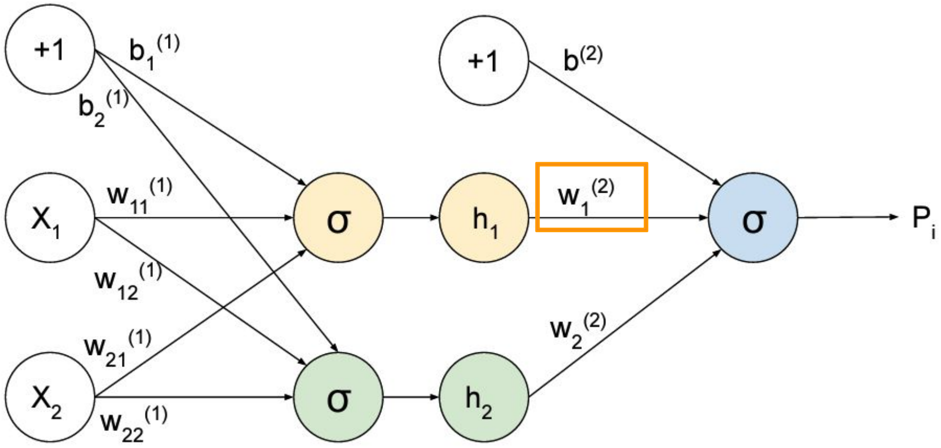
Backpropagation: an example

$$\begin{pmatrix} z_1^{(1)} = w_{11}^{(1)}x_1 + w_{21}^{(1)}x_2 + b_1^{(1)} \\ z_2^{(1)} = w_{12}^{(1)}x_1 + w_{22}^{(1)}x_2 + b_2^{(1)} \end{pmatrix}$$

$$\begin{pmatrix} h_1 = \sigma\left(z_1^{(1)}\right) \\ h_2 = \sigma\left(z_2^{(1)}\right) \end{pmatrix}$$

$$\left(z^{(2)} = w_1^{(2)}h_1 + w_2^{(2)}h_2 + b^{(2)} \right)$$

$$\left(p_i = \sigma\left(z^{(2)}\right) \right)$$



$$Error:\ L = \frac{1}{2}\|p - y\|^2 = \sum_i \frac{1}{2}(p_i - y_i)^2$$

$$Compute:\ \frac{\partial L}{\partial w_1^{(2)}}$$

Useful to know:

$$If\ p = \sigma(x) = \frac{1}{1+e^{-x}}$$

$$Then\ \frac{dp}{dx} = \left(1+e^{-x}\right)^{-2} e^{-x} = \frac{1}{1+e^{-x}} \times \frac{e^{-x}}{1+e^{-x}} = p(1-p)$$

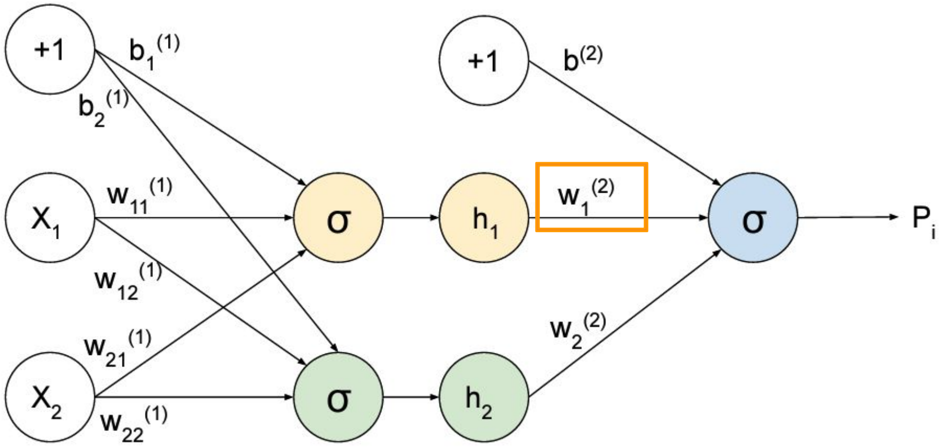
Backpropagation: an example

$$\begin{pmatrix} z_1^{(1)} = w_{11}^{(1)}x_1 + w_{21}^{(1)}x_2 + b_1^{(1)} \\ z_2^{(1)} = w_{12}^{(1)}x_1 + w_{22}^{(1)}x_2 + b_2^{(1)} \end{pmatrix}$$

$$\begin{pmatrix} h_1 = \sigma\left(z_1^{(1)}\right) \\ h_2 = \sigma\left(z_2^{(1)}\right) \end{pmatrix}$$

$$\left(z^{(2)} = w_1^{(2)}h_1 + w_2^{(2)}h_2 + b^{(2)} \right)$$

$$\left(p_i = \sigma\left(z^{(2)}\right) \right)$$



$$\frac{\partial L}{\partial w_1^{(2)}} = \sum_i \frac{\partial L_i}{\partial w_1^{(2)}}$$

$$Error: L = \frac{1}{2}\|p - y\|^2 = \sum_i \frac{1}{2}(p_i - y_i)^2$$

$$\frac{\partial L_i}{\partial w_1^{(2)}} = \frac{\partial z^{(2)}}{\partial w_1^{(2)}} \times \frac{\partial p_i}{\partial z^{(2)}} \times \frac{\partial L_i}{\partial p_i} = h_1 \times p_i(1 - p_i) \times (p_i - y)$$

$$Compute: \frac{\partial L}{\partial w_1^{(2)}}$$

Chain rule

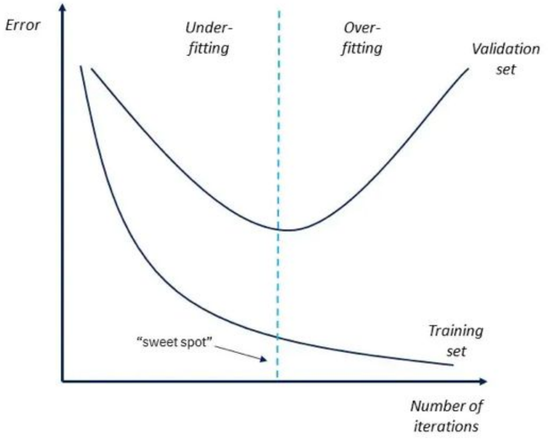
With four parameters I can fit an elephant. With five I can make him wiggle his trunk. - John von Neumann

$$w = \arg\min_{w} \mathrm{Cost}(w) + \alpha \cdot \mathrm{Regularizer}(\mathrm{Model})$$

Our example model has 13,002 parameters…that's a lot of elephants! Regularization is critical to avoid overfitting…

…numerous regularization schemes are used in training neural networks.

but the standard is of course, $\sum_i w_i^2$



sklearn.neural_network.MLPClassifier

hidden_layer_sizes : *tuple, length = n_layers - 2, default=(100,)*

The ith element represents the number of neurons in the ith hidden layer.

activation : *{'identity', 'logistic', 'tanh', 'relu'}, default='relu'*

Activation function for the hidden layer.

solver : *{'lbfgs', 'sgd', 'adam'}, default='adam'*

The solver for weight optimization.

alpha : *float, default=0.0001*

L2 penalty (regularization term) parameter.

learning_rate : *{'constant', 'invscaling', 'adaptive'}, default='constant'*

Learning rate schedule for weight updates.

early_stopping : *bool, default=False*

Whether to use early stopping to terminate training when validation score is not improving. If set to true,

Scikit-Learn : Multilayer Perceptron

Fetch MNIST data from www.openml.org :

```
X, y = fetch_openml("mnist_784", version=1, return_X_y=True)
X = X / 255.0
```

Train test split (60k / 10k),

```
X_train, X_test = X[:60000], X[60000:]
y_train, y_test = y[:60000], y[60000:]
```

Create MLP classifier instance,

- Single hidden layer (50 nodes)
- Use stochastic gradient descent
- Maximum of 10 learning iterations
- Small L2 regularization alpha=1e-4

```
mlp = MLPClassifier(
    hidden_layer_sizes=(50,),
    max_iter=10,
    alpha=1e-4,
    solver="sgd",
    verbose=10,
    random_state=1,
    learning_rate_init=0.1,
)
```

Scikit-Learn : Multilayer Perceptron

Fit the MLP and print stuff…

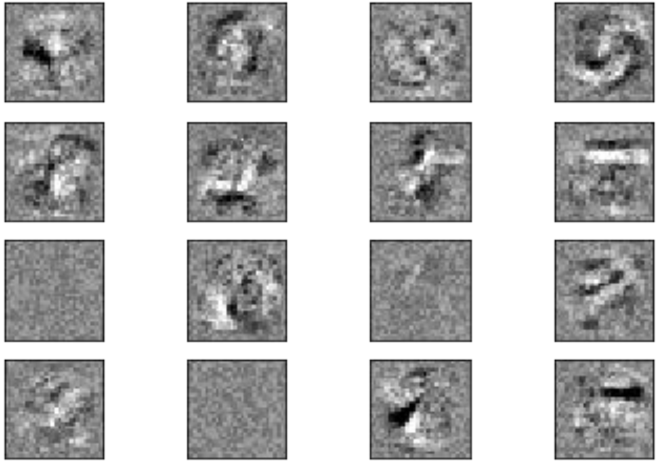
```
mlp.fit(X_train, y_train)

print("Training set score: %f" % mlp.score(X_train, y_train))
print("Test set score: %f" % mlp.score(X_test, y_test))
```

```
Iteration 1, loss = 0.32009978
Iteration 2, loss = 0.15347534
Iteration 3, loss = 0.11544755
Iteration 4, loss = 0.09279764
Iteration 5, loss = 0.07889367
Iteration 6, loss = 0.07170497
Iteration 7, loss = 0.06282111
Iteration 8, loss = 0.05530788
Iteration 9, loss = 0.04960484
Iteration 10, loss = 0.04645355
Training set score: 0.986800
Test set score: 0.970000
```

Visualize the weights for each node…

coefs_[i]: n_input x n_output matrix of weights for layer i

```
vmin, vmax = mlp.coefs_[0].min(), mlp.coefs_[0].max()
for coef, ax in zip(mlp.coefs_[0].T, axes.ravel()):
    ax.matshow(coef.reshape(28, 28), cmap=plt.cm.gray,
               vmin=0.5 * vmin, vmax=0.5 * vmax)
    ax.set_xticks(())
    ax.set_yticks(())
```



…magnitude of weights indicates which input features are important in prediction

More Advanced Topics

Many other NN architectures exist beyond MLP

- **Convolutional NN (CNN)** For image processing / computer viz.
- **Recurrent NN (RNN)** For sequence data (e.g. acoustic signals, video, etc.) , long short-term memory (LSTM) is popular
- **Generative Adversarial Nets (GANs)** For generating creepy deepfakes
- **Restricted Boltzmann Machine (RBM)** Another generative model

Many open areas being researched

- More reliable uncertainty estimates
- Robustness to exploits
- Interpretability
- Better scalability

Example

Play with a small multilayer perceptron on a binary classification task…

https://playground.tensorflow.org/