Lecture 12: Neural networks

STATS 202: Data Mining and Analysis

Linh Tran

tranlm@stanford.edu

Department of Statistics
Stanford University

August 4, 2021

Announcements

- Homework 3 is due this Friday.
  - Homework 4 will be released Friday.
- Confirmed for research panel on August 16.
- Final project review session this Friday.
  - Will be conducted like casual lab / office hours.

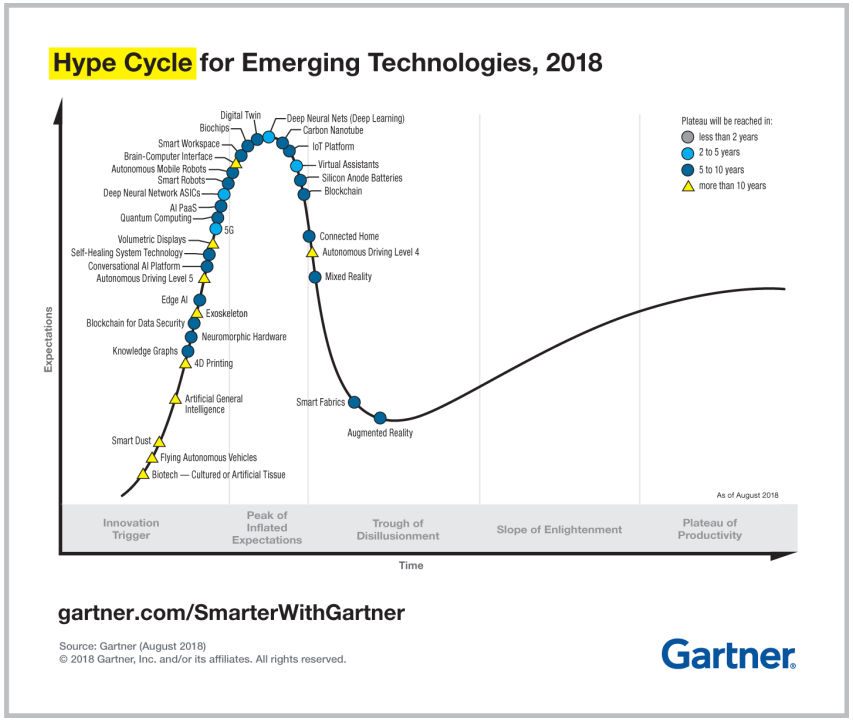
Outline

- Introduction
- Logistic regression
- Back propagation
- Function approximation
- Feature extraction
- Model generalization
- Advanced topics

Neural networks

Currently, the most popular algorithm amongst ML practitioners.

- Many times, used within the context of Artificial Intelligence.
- Simply a general function estimation algorithm.
- Though is often hyped up the media.



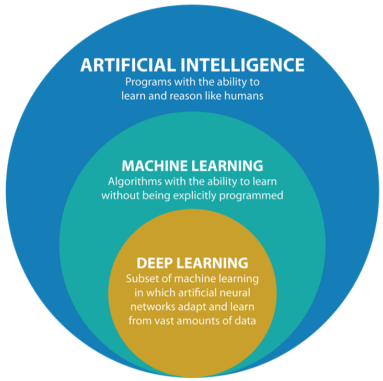
Gartner's hype cycle for 2018.

Neural networks

Lots of buzz words, but what do they mean?

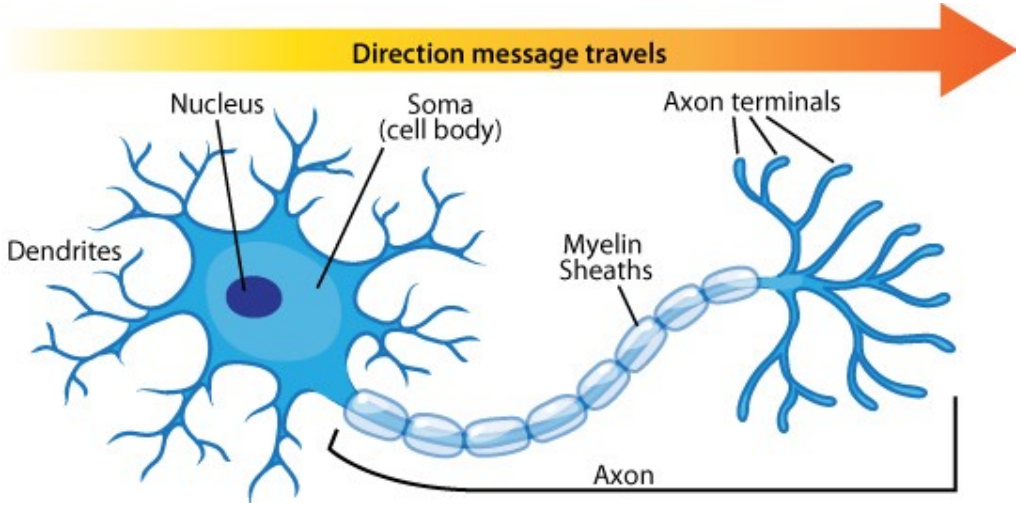
Definitions:

- *AI*: human-like machines or programs.
- *ML*: Algorithms that learn from data.
- *DL*: A type of ML algorithm, using neural networks (typically with many layers).



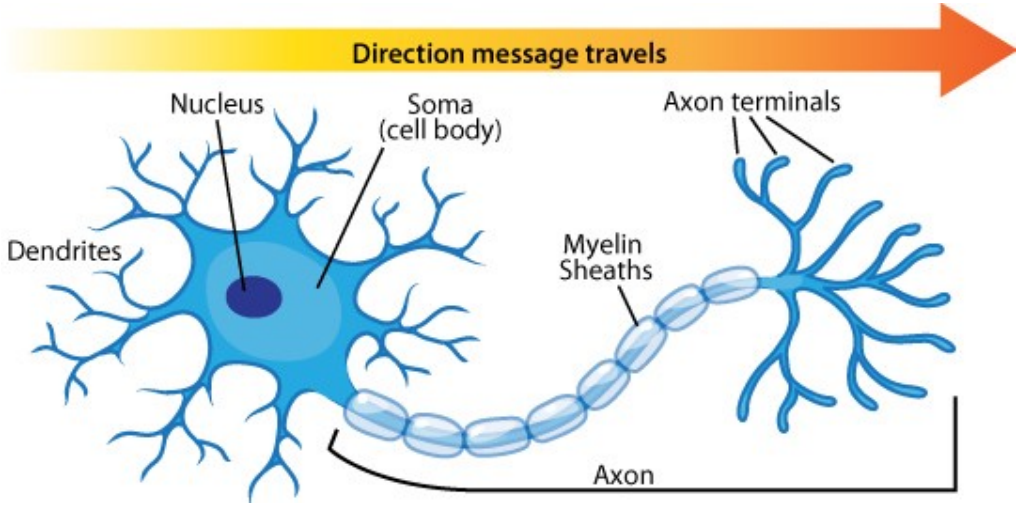
Neural networks

But: what exactly are neural networks?



Neural networks

But: what exactly are neural networks?

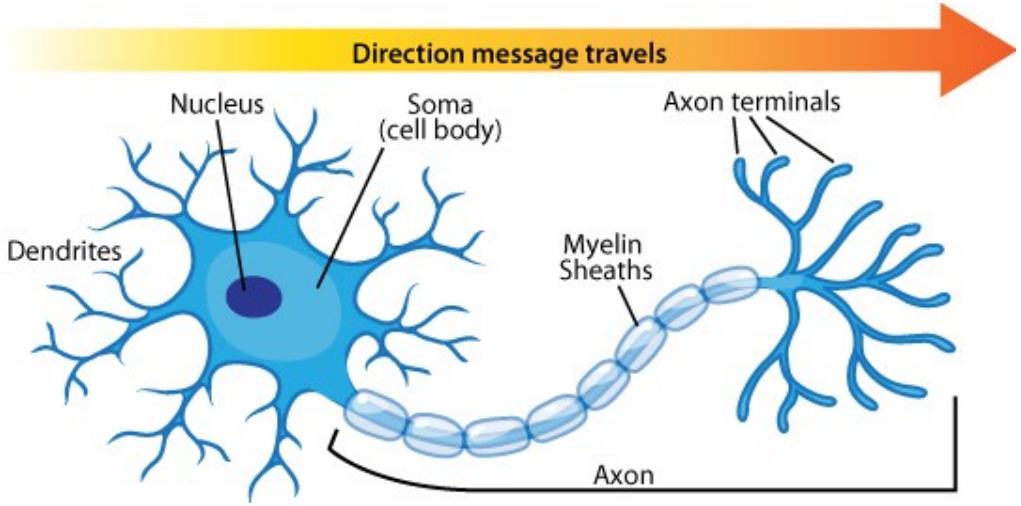


Some potential answers

- A *universal function approximator*.

Neural networks

But: what exactly are neural networks?

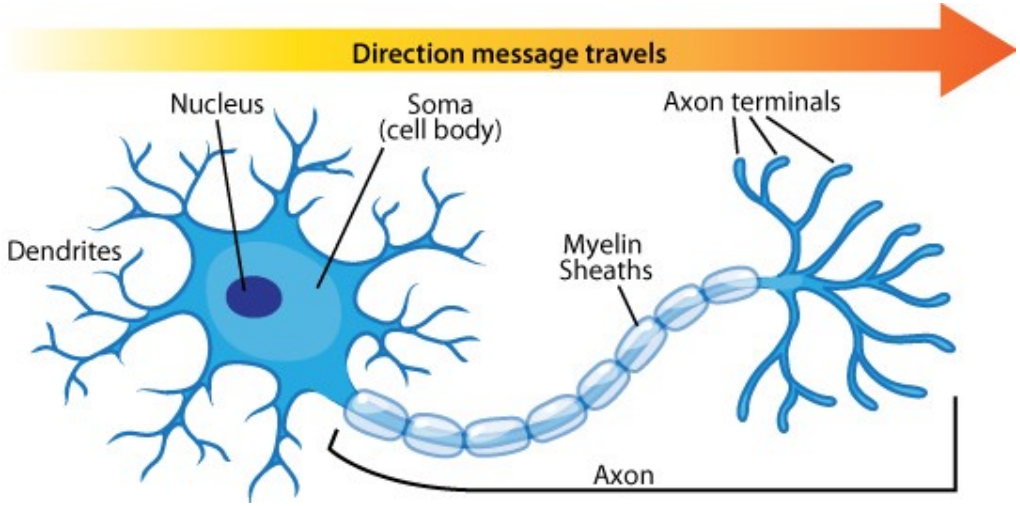


Some potential answers

- A *universal function approximator*.
- A *feature extractor*.

Neural networks

But: what exactly are neural networks?



Some potential answers

- A *universal function approximator*.
- A *feature extractor*.
- A *model generalizer*.

Logistic regression

Recall: logistic regression is a linear model with a logit link function, i.e.

$$\mathbb{P}(Y = 1|\mathbf{X}) = \sigma(\beta_0 + \beta_1 X_1 + ... + \beta_p X_p) : \sigma(z) = \frac{1}{1 + exp(-z)} \tag{1}$$

Let's rephrase this by:

1. Using b to denote β_0 (aka the bias)
2. Using $\mathbf{W}$ to denote $(\beta_1, ..., \beta_p)$ (aka the weights)
3. Using matrix notation

$$\mathbb{P}(Y = 1|\mathbf{X}) = \underbrace{\sigma}_{non-linearity}(\mathbf{X}\boldsymbol{W} + b) \tag{2}$$

Logistic regression

When the function is non-linear, our prior option was to do feature transformations, e.g.

- Expand predictor set (e.g. non-linear transformations, interactions, etc.).
- Define a kernel (e.g. find a function $f(\cdot, \cdot)$ that is positive definite).

Logistic regression

When the function is non-linear, our prior option was to do feature transformations, e.g.

- Expand predictor set (e.g. non-linear transformations, interactions, etc.).
- Define a kernel (e.g. find a function $f(\cdot, \cdot)$ that is positive definite).

Another option: build the non-linearity into the model specification, e.g.

$$\mathbb{P}(Y = 1|\mathbf{X}) = \sigma(\sigma(\mathbf{X}\boldsymbol{W}_1 + b_1)\boldsymbol{W}_2 + b_2) \tag{3}$$

Logistic regression

When the function is non-linear, our prior option was to do feature transformations, e.g.

- Expand predictor set (e.g. non-linear transformations, interactions, etc.).
- Define a kernel (e.g. find a function $f(\cdot, \cdot)$ that is positive definite).

Another option: build the non-linearity into the model specification, e.g.

$$\mathbb{P}(Y = 1|\mathbf{X}) = \sigma(\sigma(\mathbf{X}\boldsymbol{W}_1 + b_1)\boldsymbol{W}_2 + b_2) \tag{3}$$

This is a neural network (with 1 hidden layer)!

Hidden nodes

For logistic regression:

$$\mathbb{P}(Y = 1|\mathbf{X}) = \sigma(\mathbf{X} \underbrace{\boldsymbol{W}}_{p\times 1} + \underbrace{b}_{1\times 1}) \tag{4}$$

Hidden nodes

For logistic regression:

$$\mathbb{P}(Y = 1|\mathbf{X}) = \sigma(\mathbf{X} \underbrace{\boldsymbol{W}}_{p\times 1} + \underbrace{b}_{1\times 1}) \tag{4}$$

For neural networks:

$$\mathbb{P}(Y = 1|\mathbf{X}) = \sigma(\sigma(\mathbf{X} \underbrace{\boldsymbol{W}_1}_{p\times M} + \underbrace{b_1}_{1\times M}) \underbrace{\boldsymbol{W}_2}_{M\times 1} + \underbrace{b_2}_{1\times 1}) \tag{5}$$

M specifies how many hidden nodes we have

- Called '*hidden*' since it's not directly observed by us.
- Also referred to as '*embeddings*'.

Hidden nodes

$$\mathbb{P}(Y = 1|\mathbf{X}) = \sigma(\sigma(\mathbf{X} \underbrace{\boldsymbol{W}_1}_{p\times M} + \underbrace{b_1}_{1\times M}) \underbrace{\boldsymbol{W}_2}_{M\times 1} + \underbrace{b_2}_{1\times 1}) \quad (6)$$

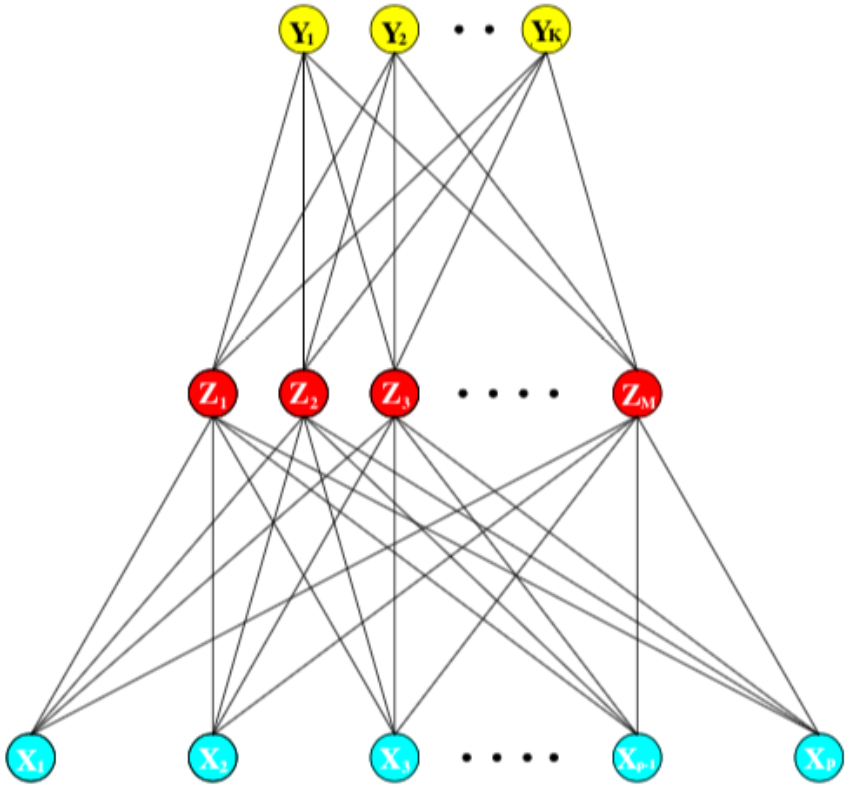


FIGURE 11.2. *Schematic of a single hidden layer, feed-forward neural network.*

Hidden layers

We can iteratively apply our non-linear operations, e.g.

$$\mathbb{P}(Y = 1|\mathbf{X}) = \sigma(\cdots\sigma(\sigma(\mathbf{X}\boldsymbol{W}_1 + b_1)\boldsymbol{W}_2 + b_2)\cdots\boldsymbol{W}_B + b_B) \quad (7)$$

Where B is the number of iterations (i.e. *hidden layers*).

Hidden layers

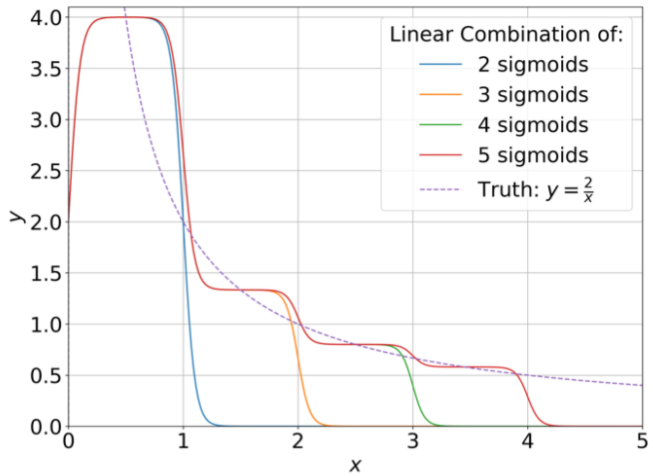
We can iteratively apply our non-linear operations, e.g.

$$\mathbb{P}(Y = 1|\mathbf{X}) = \sigma(\cdots\sigma(\sigma(\mathbf{X}\boldsymbol{W}_1 + b_1)\boldsymbol{W}_2 + b_2)\cdots\boldsymbol{W}_B + b_B) \quad (7)$$

Where B is the number of iterations (i.e. *hidden layers*).

Each activation (e.g. sigmoid) can approximate a local change

- B sigmoids $\implies$ approximate at $\approx B$ points



n.b. Each layer needs the number of hidden nodes specified.

Multinomial logistic regression

Our examples have been for binary outcomes so far.
Question: What about multinomial outcomes

- e.g. Which of digits 0 through 9 is this photo?

Multinomial logistic regression

Our examples have been for binary outcomes so far.
Question: What about multinomial outcomes

- e.g. Which of digits 0 through 9 is this photo?

Recall: for logistic regression, we're modeling

$$\log\left[\frac{\mathbb{P}(Y=1|\mathbf{X})}{1-\mathbb{P}(Y=1|\mathbf{X})}\right] = \beta_0+\beta_1X_1+\ldots+\beta_pX_p \quad (8)$$

$$= \mathbf{XW} \quad (9)$$

where $\mathbf{X}$ is our $n \times p$ design matrix and $\mathbf{W}$ is our $p \times 1$ parameter vector.

Multinomial logistic regression

For multinomial regression, let $Y \in \{1, \ldots, K\}$. We can model

$$\log\left[\frac{\mathbb{P}(Y=1|\mathbf{X})}{\mathbb{P}(Y=K|\mathbf{X})}\right] = \mathbf{X}\mathbf{W_1} \quad (10)$$

$$\log\left[\frac{\mathbb{P}(Y=2|\mathbf{X})}{\mathbb{P}(Y=K|\mathbf{X})}\right] = \mathbf{X}\mathbf{W_2} \quad (11)$$

$$\cdots = \cdots \quad (12)$$

$$\log\left[\frac{\mathbb{P}(Y=K-1|\mathbf{X})}{\mathbb{P}(Y=K|\mathbf{X})}\right] = \mathbf{X}\mathbf{W_{K-1}} \quad (13)$$

where each $\mathbf{W_k}$ is a $p \times 1$ parameter vector.

Exponentiating both sides and solving for $\mathbb{P}(Y=K|\mathbf{X})$ (using the fact that the probabilities have to sum to 1) gives us

$$\mathbb{P}(Y=K|\mathbf{X}) = \frac{1}{1+\sum_{k=1}^{K-1} e^{\mathbf{X}\mathbf{W_k}}} \quad (14)$$

Multinomial logistic regression

Equivalently, can represent the multinomial logistic model as

$$\begin{aligned}
\log \mathbb{P}(Y = 1|\mathbf{X}) &= \mathbf{X}\mathbf{W_1} - \log(Z) && (15)\\
\log \mathbb{P}(Y = 2|\mathbf{X}) &= \mathbf{X}\mathbf{W_2} - \log(Z) && (16)\\
\cdots &= \cdots && (17)\\
\log \mathbb{P}(Y = K|\mathbf{X}) &= \mathbf{X}\mathbf{W_K} - \log(Z) && (18)
\end{aligned}$$

resulting in the following probabilities

$$\begin{aligned}
\mathbb{P}(Y = 1|\mathbf{X}) &= \frac{\exp(\mathbf{X}\mathbf{W_1})}{\sum_{k=1}^{K} \exp(\mathbf{X}\mathbf{W_k})} && (19)\\
\mathbb{P}(Y = 2|\mathbf{X}) &= \frac{\exp(\mathbf{X}\mathbf{W_2})}{\sum_{k=1}^{K} \exp(\mathbf{X}\mathbf{W_k})} && (20)\\
\cdots &= \cdots && (21)\\
\mathbb{P}(Y = K|\mathbf{X}) &= \frac{\exp(\mathbf{X}\mathbf{W_K})}{\sum_{k=1}^{K} \exp(\mathbf{X}\mathbf{W_k})} && (22)
\end{aligned}$$

Multinomial logistic regression

This leads us to the softmax function, i.e.

$$\text{softmax}(\mathbf{XW_1}, \ldots, \mathbf{XW_K})_k = \frac{e^{\mathbf{XW_k}}}{\sum_{l=1}^{K} e^{\mathbf{XW_l}}} \tag{23}$$

Or, more succintly, we have

$$\text{softmax}(\mathbf{XW^K})_k = \frac{\exp((\mathbf{XW^K})_{k\cdot})}{\sum_{k=1}^{K} \exp((\mathbf{XW^K})_{k\cdot})} \tag{24}$$

where the $p \times K$ matrix $\mathbf{W^K}$ is simply the (concatenated) matrix of $\mathbf{W_1}, \ldots, \mathbf{W_K}$.

This is what multiclass neural networks are modeling!

The chain rule

Recall: In logistic regression we try to maximize the likelihood

- Equivalent to minimizing the cross-entropy

$$
\begin{aligned}
L(y_i, f(\mathbf{X}_i)) &= -y_i \log(p_i) - (1 - y_i) \log(1 - p_i), \text{ where} && (25) \\
p_i &= \frac{1}{1 + exp(-Z_i)} && (26) \\
Z_i &= \mathbf{X}_i \boldsymbol{W} && (27)
\end{aligned}
$$

The chain rule

Recall: In logistic regression we try to maximize the likelihood

- Equivalent to minimizing the cross-entropy

$$
\begin{aligned}
L(y_i, f(\mathbf{X}_i)) &= -y_i \log(p_i) - (1 - y_i) \log(1 - p_i), \text{ where} && (25)\\
p_i &= \frac{1}{1 + exp(-Z_i)} && (26)\\
Z_i &= \mathbf{X}_i \boldsymbol{W} && (27)
\end{aligned}
$$

Can apply *the derivative chain rule* to get our gradient, i.e.

$$
\frac{\partial L(y_i, f(\mathbf{X}_i))}{\partial \boldsymbol{W}} = \frac{\partial L(y_i, f(\mathbf{X}_i))}{\partial p_i} \times \frac{\partial p_i}{\partial Z_i} \times \frac{\partial Z_i}{\partial \boldsymbol{W}} \quad (28)
$$

The chain rule

Recall: In logistic regression we try to maximize the likelihood

- Equivalent to minimizing the cross-entropy

$$
\begin{aligned}
L(y_i, f(\mathbf{X}_i)) &= -y_i \log(p_i) - (1 - y_i) \log(1 - p_i), \text{ where} && (25)\\
p_i &= \frac{1}{1 + exp(-Z_i)} && (26)\\
Z_i &= \mathbf{X}_i \boldsymbol{W} && (27)
\end{aligned}
$$

Can apply *the derivative chain rule* to get our gradient, i.e.

$$\frac{\partial L(y_i, f(\mathbf{X}_i))}{\partial \boldsymbol{W}} = \frac{\partial L(y_i, f(\mathbf{X}_i))}{\partial p_i} \times \frac{\partial p_i}{\partial Z_i} \times \frac{\partial Z_i}{\partial \boldsymbol{W}} \quad (28)$$

Which gives us

$$\frac{\partial L(y_i, f(\mathbf{X}_i))}{\partial \boldsymbol{W}} = \mathbf{X}_i (y_i - p_i) \quad (29)$$

Backpropagation

Neural networks are simply a generalization of the logistic regression case, e.g. for

$$\mathbb{P}(Y = 1|\mathbf{X}) = \sigma(\sigma(\mathbf{X}\boldsymbol{W}_1)\boldsymbol{W}_2) \tag{30}$$

Backpropagation

Neural networks are simply a generalization of the logistic regression case, e.g. for

$$\mathbb{P}(Y = 1|\mathbf{X}) = \sigma(\sigma(\mathbf{X}\boldsymbol{W}_1)\boldsymbol{W}_2) \tag{30}$$

Our loss is

$$\begin{aligned}
L(y_i, f(\mathbf{X}_i)) &= -y_i \log(p_i) - (1 - y_i) \log(1 - p_i), \text{ where} && (31)\\
p_i &= \frac{1}{1 + exp(-Z_{2,i})} && (32)\\
Z_{2,i} &= h_i \boldsymbol{W}_2 && (33)\\
h_i &= \frac{1}{1 + exp(-Z_{1,i})} && (34)\\
Z_{1,i} &= \mathbf{X}\boldsymbol{W}_1 && (35)
\end{aligned}$$

Backpropagation

Our loss is

$$
\begin{aligned}
L(y_i, f(\mathbf{X}_i)) &= -y_i \log(p_i) - (1 - y_i) \log(1 - p_i), \text{ where} && (36)\\
p_i &= \frac{1}{1 + exp(-Z_{2,i})} && (37)\\
Z_{2,i} &= h_i \boldsymbol{W}_2 && (38)\\
h_i &= \frac{1}{1 + exp(-Z_{1,i})} && (39)\\
Z_{1,i} &= \mathbf{X} \boldsymbol{W}_1 && (40)
\end{aligned}
$$

Applying *the derivative chain rule*:

$$
\begin{aligned}
\frac{\partial L(y_i, f(\mathbf{X}_i))}{\partial \boldsymbol{W}_2} &= \frac{\partial L(y_i, f(\mathbf{X}_i))}{\partial p_i} \times \frac{\partial p_i}{\partial Z_{2,i}} \times \frac{\partial Z_{2,i}}{\partial \boldsymbol{W}_2}\\
\frac{\partial L(y_i, f(\mathbf{X}))}{\partial \boldsymbol{W}_1} &= \frac{\partial L(y_i, f(\mathbf{X}))}{\partial p_i} \times \frac{\partial p_i}{\partial Z_{2,i}} \times \frac{\partial Z_{2,i}}{\partial h_i} \times \frac{\partial h_i}{\partial Z_{1,i}} \times \frac{\partial Z_{1,i}}{\partial \boldsymbol{W}_1}
\end{aligned}
$$

Gradient descent

Our gradient is estimated using our data, i.e. $(y_i, \mathbf{X}_i) : i = 1, 2, \ldots, n$.

Gradient descent

Our gradient is estimated using our data, i.e. $(y_i, \mathbf{X}_i) : i = 1, 2, \ldots, n$.

We can estimate it using, e.g.

- **Stochastic gradient descent**: estimating our (full) gradient using just one observation.
- **Gradient descent**: estimating our (full) gradient using all observations.
- **Mini-batch gradient descent**: using a (random) subsample of our observations.

Each will trade off between variance for the gradient and memory size.

Gradient descent

Our gradient is estimated using our data, i.e. $(y_i, \mathbf{X}_i) : i = 1, 2, \ldots, n$.

We can estimate it using, e.g.

- **Stochastic gradient descent**: estimating our (full) gradient using just one observation.
- **Gradient descent**: estimating our (full) gradient using all observations.
- **Mini-batch gradient descent**: using a (random) subsample of our observations.

Each will trade off between variance for the gradient and memory size.

When done iteratively, we'll typically specify a stopping point (e.g. by using a dev set).

Gradient descent

The use of non-linearities results in multiple minima, tendency to overfit, and can be unstable.
Some considerations to make:

- Set initial weight values near zero.
- Over parameterize and regularize heavily.
- Standardize input features.
- Use a dev set and stop training earlier.
- Try out different weight randomizations and take the one with the lowest (validated) error.
    - Or average the predictions (or apply bagging).

Estimation summary

Estimating neural network parameters simply requires '*propagating back*' errors.

- We're just applying (matrix) multiplications
  - GPU's can be very good for this
- Matrix multiplications can get pretty big (for large networks)
  - Commonly not worth it to use the Hessian
- Should be careful with large values going into sigmoid activations
  - Results in saturated gradients

Universal approximation theorem

Hornik's theorem

Whenever the activation function is continuous, bounded, and non-constant, then, for arbitrary compact subsets $X \subseteq R^k$, standard multilayer feedforward networks can approximate any continuous function on X arbitrarily well with respect to uniform distance, provided that sufficiently many hidden units are avaiable.

Universal approximation theorem

Hornik's theorem

Whenever the activation function is continuous, bounded, and non-constant, then, for arbitrary compact subsets $X \subseteq R^k$, standard multilayer feedforward networks can approximate any continuous function on X arbitrarily well with respect to uniform distance, provided that sufficiently many hidden units are avaiable.

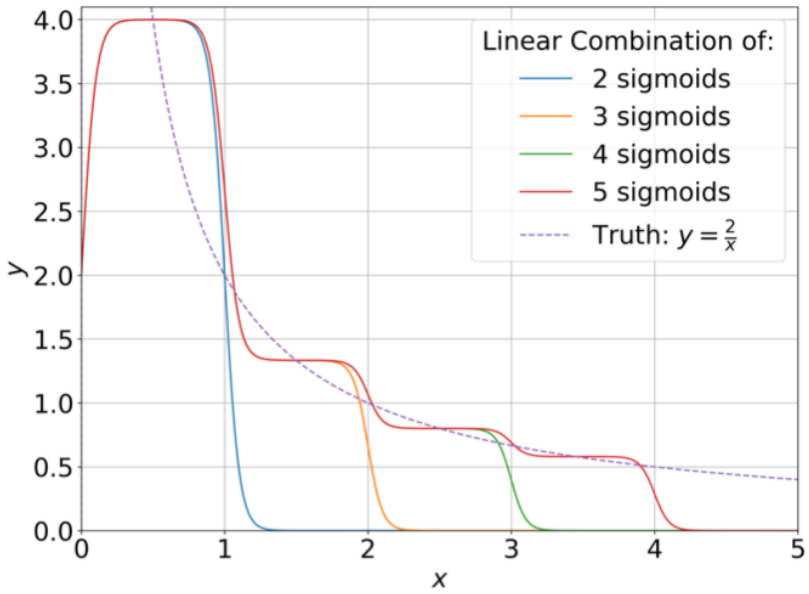
In words: A 2-layer neural network with enough hidden nodes can closely approximate any continuous function $f(x)$.

References:

Cybenko (1989) "Approximations by superpostions of sigmoidal function"
Hornik (1991) "Approximation Capabilities of Multilayer Feedforward Networks"
Leshno and Schocken (1993) "Multilayer Feedforward Networks with Non-Polynomial Activation Functions Can Approximate Any Function"

Universal approximation theorem

Given enough hidden nodes, we can approximate any function.



Check out this *visual example* of this.

Universal approximation theorem

Some caveats to the theorem

- We're approximating the function within some bound, i.e. $|\hat{f}_n(x) - f(x)| < \epsilon$.
- Result is meant for *continuous* functions on *compact* subsets of $\mathbb{R}$.
- Nothing is guaranteed on the how quickly we can learn the function's parameters.
- Other function estimators also do a good job approximating!

Features

For non-linear functions,

Logistic regression: expand our feature set via transformations

Neural network: define the model non-linearly

Features

For non-linear functions,

Logistic regression: expand our feature set via transformations

- We have to specify the feature transformations

Neural network: define the model non-linearly

- The model learns the feature transformations

Features

For non-linear functions,

Logistic regression: expand our feature set via transformations

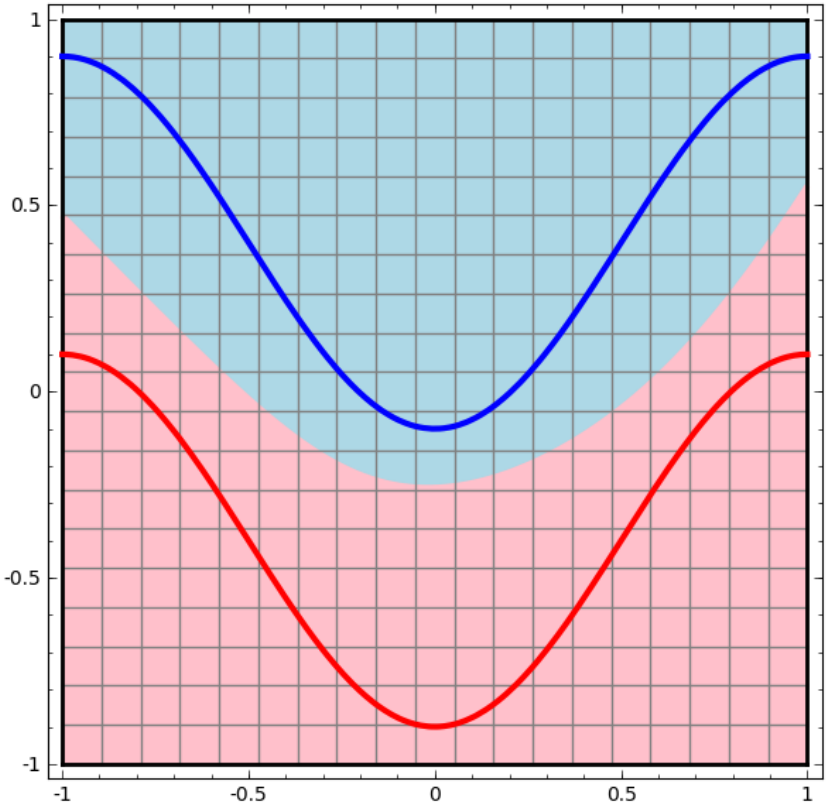
- We have to specify the feature transformations

Neural network: define the model non-linearly

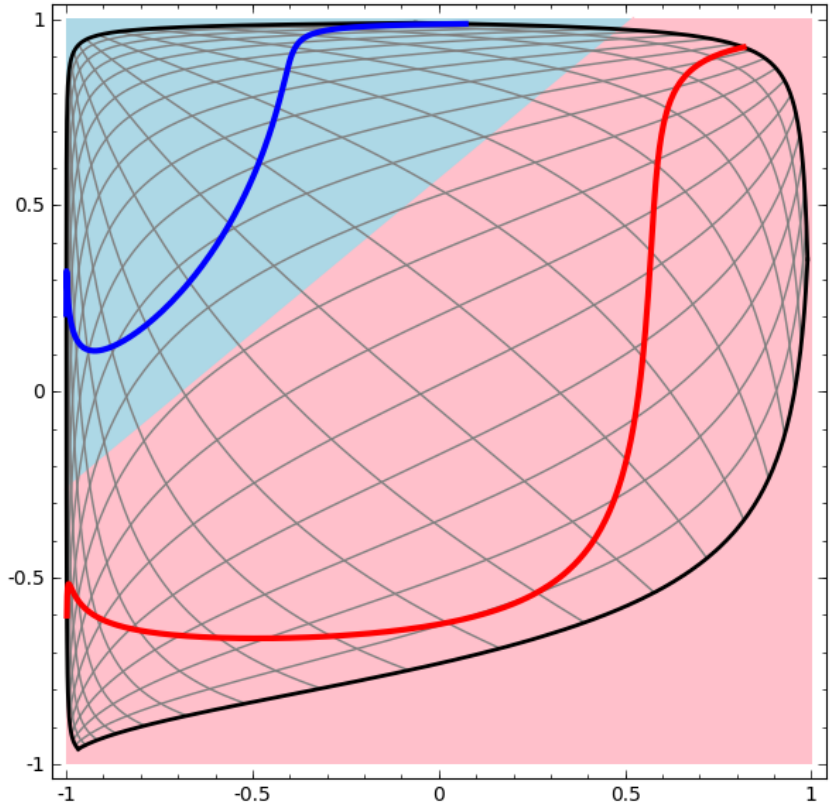
- The model learns the feature transformations
- *This helps us greatly when dealing with abstract or high dimensional problems (e.g. images & text)!*

Feature representation

How do the feature transformations get learned?



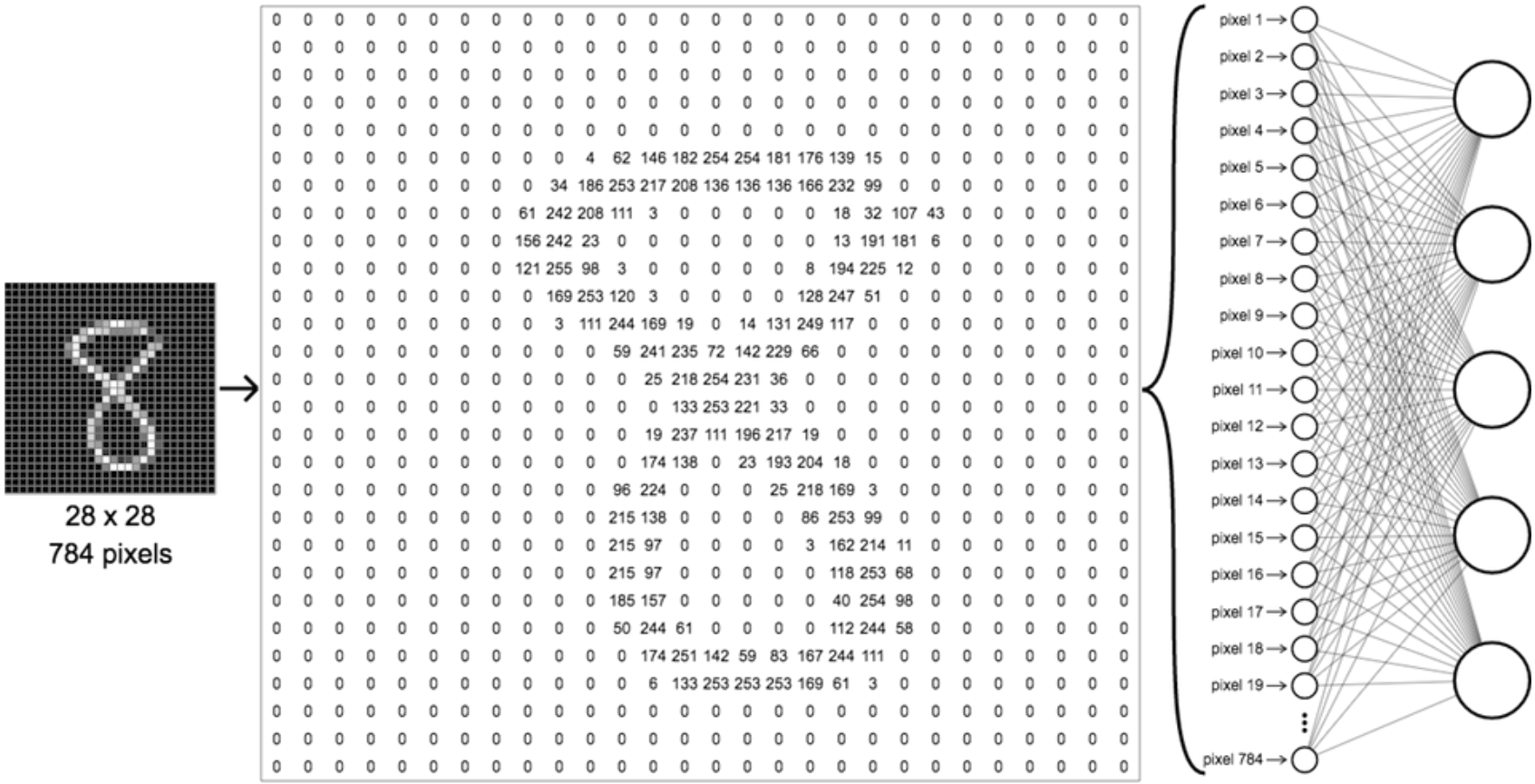
Original representation of curves



Hidden layer representation of curves

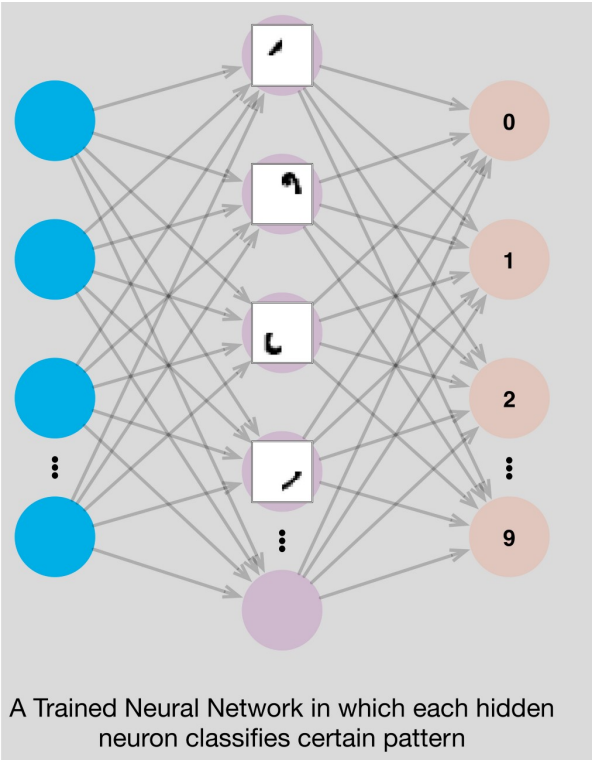
Well demonstrated by *Chris Olah's blog*.

Example: The MNIST data

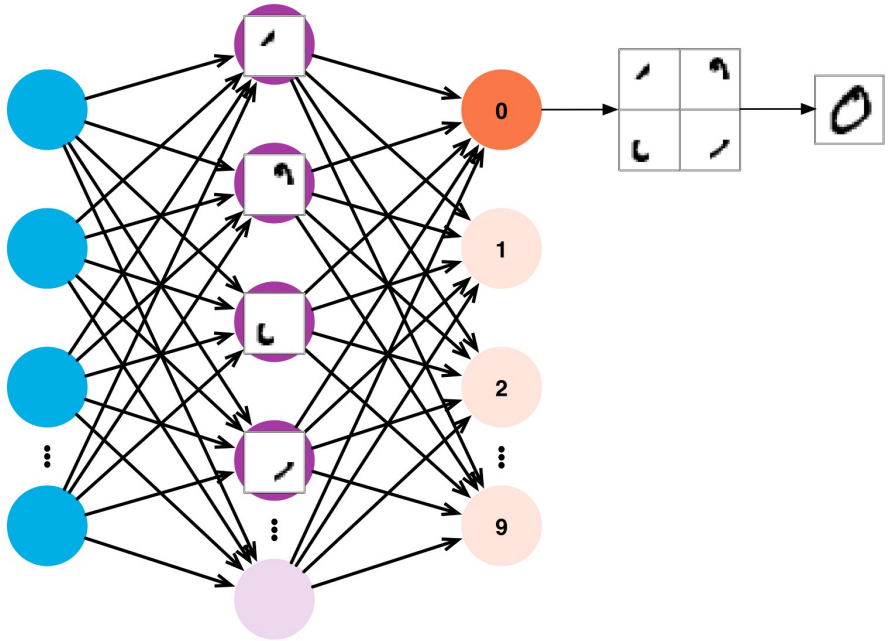


A linear model (e.g. for multinomial logistic regression)

Example: The MNIST data



A Trained Neural Network in which each hidden neuron classifies certain pattern

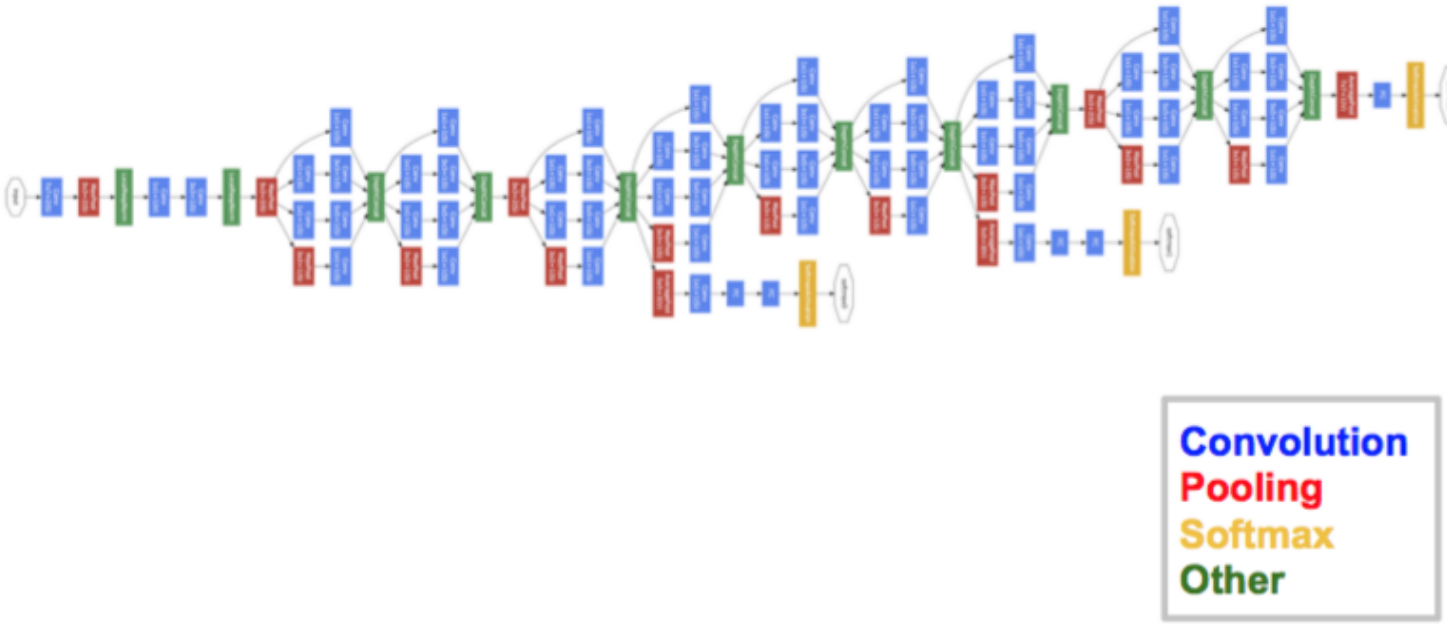


Feeding a handwritten digit of 0 should trigger the 4 hidden layer neurons, and then the first output neuron

Neural network's learned (kernel) features.

Model generalizations

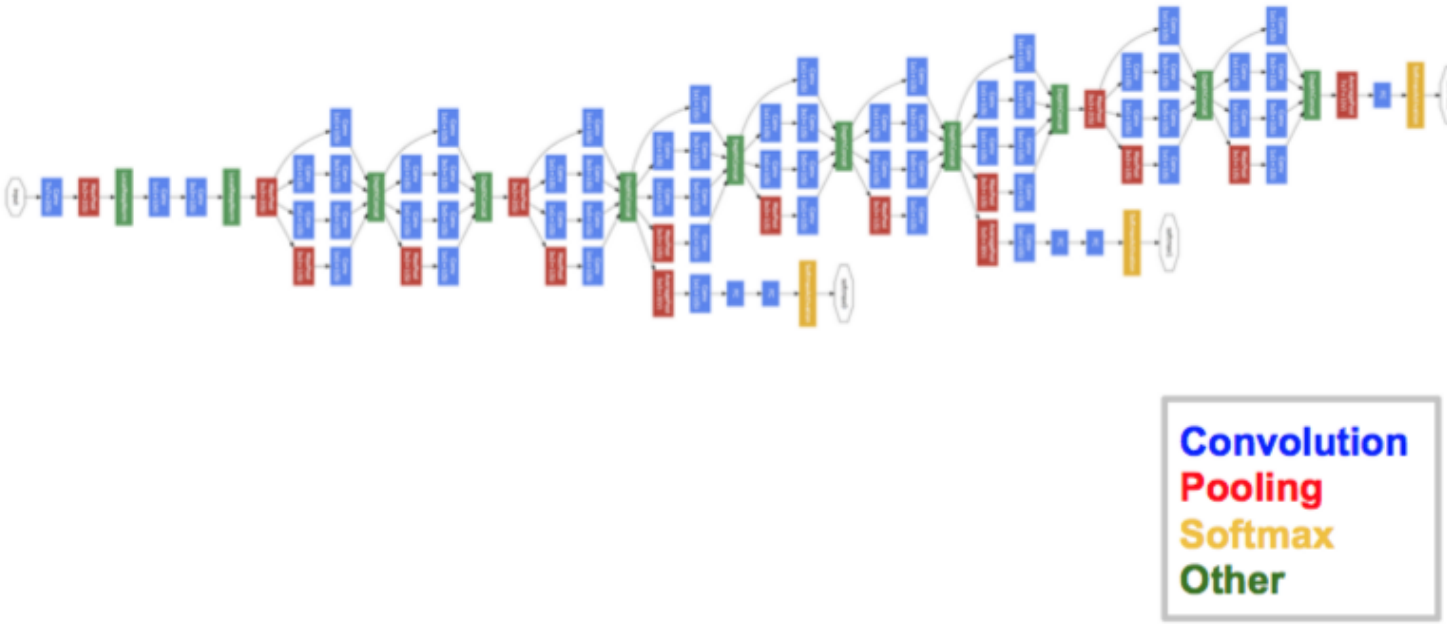
Knowing that we can simply back propagate errors via multiplication opens many doors for us, e.g.



Google's InceptionNet architecture

Model generalizations

Knowing that we can simply back propagate errors via multiplication opens many doors for us, e.g.



Google's InceptionNet architecture

Problem: *large networks are vulnerable to vanishing/exploding gradients.*

The vanishing gradient problem

Recall: Our gradient is simply a product of partial derivatives.

$$\frac{\partial C}{\partial b_1} = \sigma'(z_1) \times w_2 \times \sigma'(z_2) \times w_3 \times \sigma'(z_3) \times w_4 \times \sigma'(z_4) \times \frac{\partial C}{\partial a_4}$$

Neural Network

Example neural network and gradient.

The vanishing gradient problem

Recall: Our gradient is simply a product of partial derivatives.

$$\frac{\partial C}{\partial b_1} = \sigma'(z_1) \times w_2 \times \sigma'(z_2) \times w_3 \times \sigma'(z_3) \times w_4 \times \sigma'(z_4) \times \frac{\partial C}{\partial a_4}$$

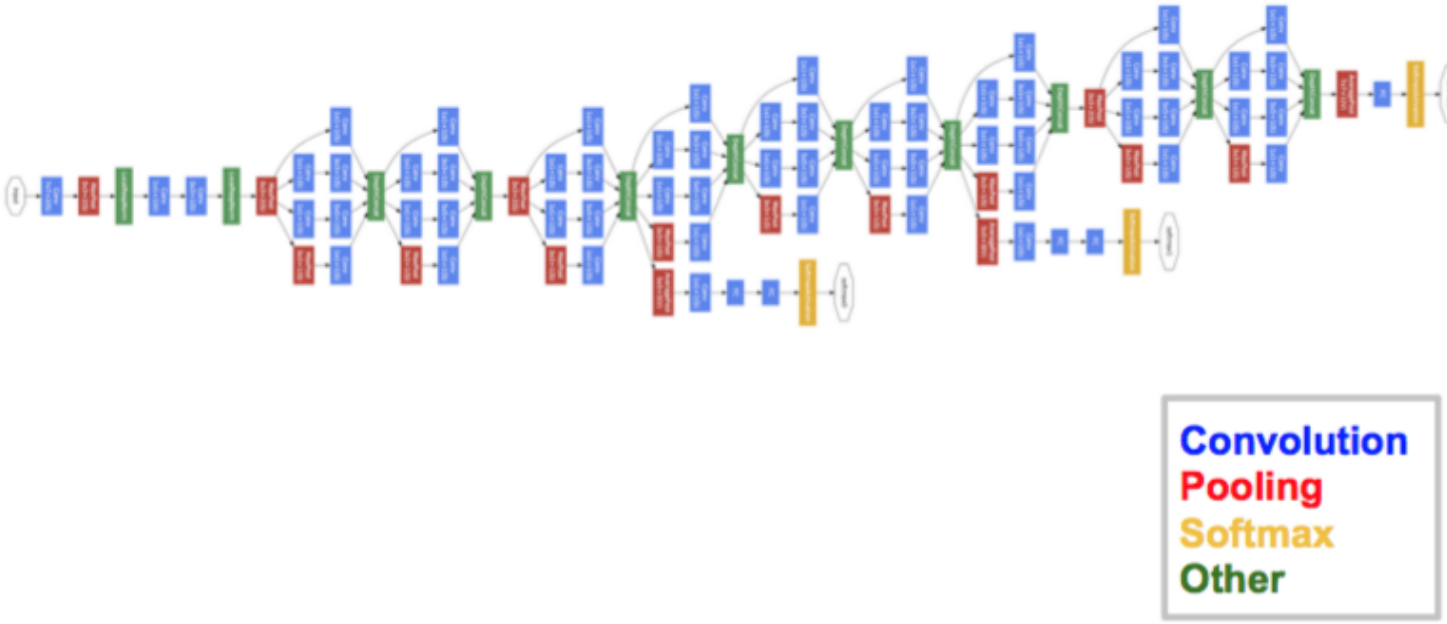
Neural Network

Example neural network and gradient.

Question: What is the derivative of the sigmoid function?

The vanishing gradient problem

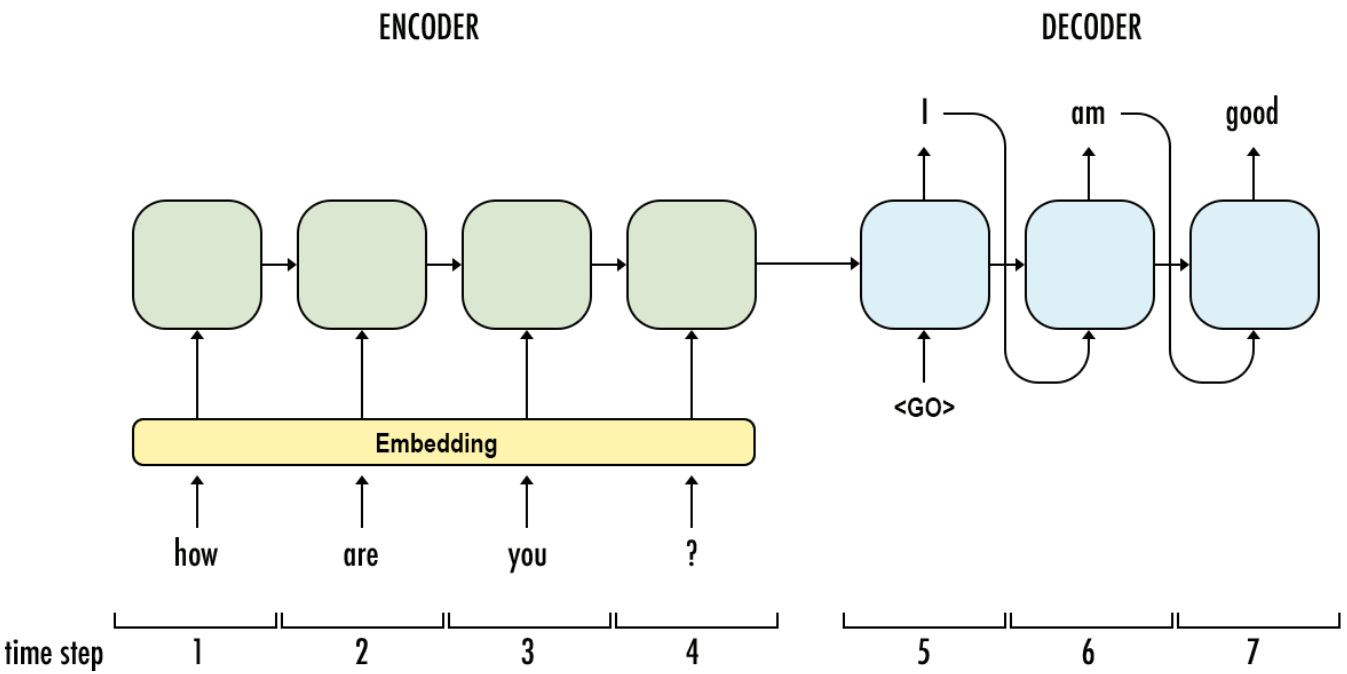
Google's InceptionNet address this via strategically placed loss functions.



Google's InceptionNet architecture

Model generalizations

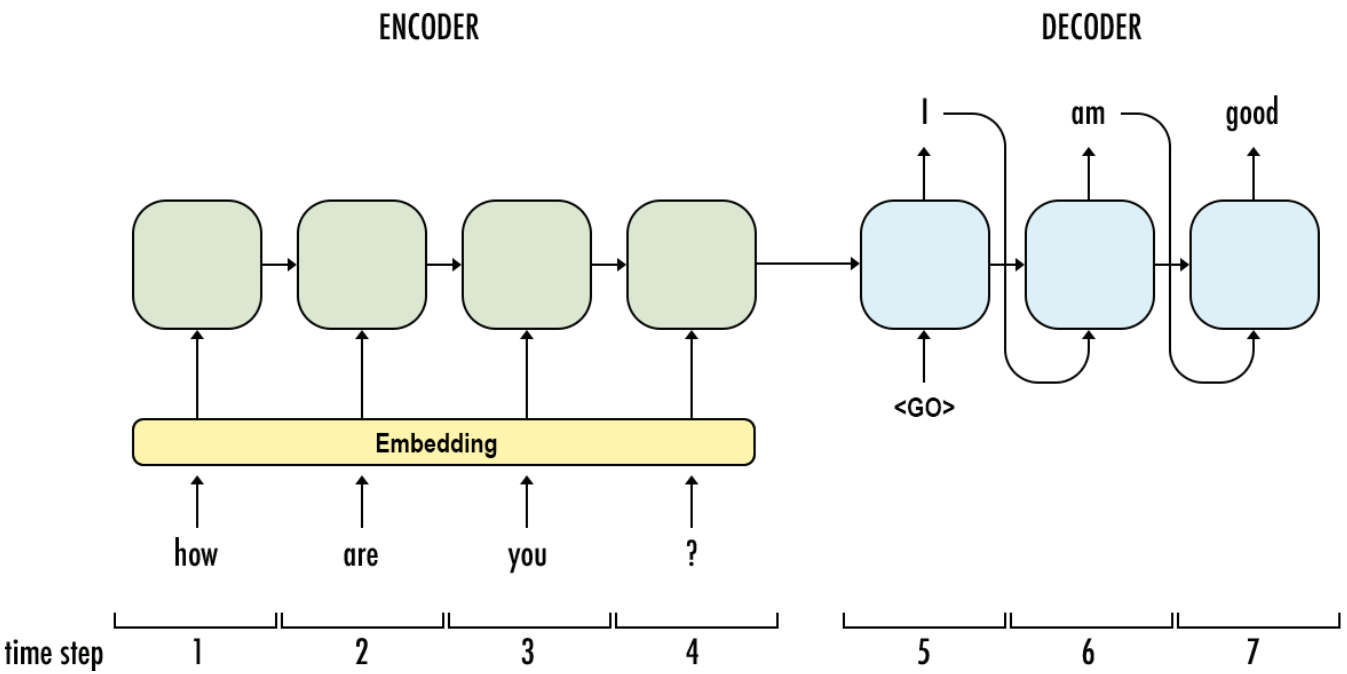
We can also train models end to end, e.g.



Encoder-decoder architecture

Model generalizations

We can also train models end to end, e.g.

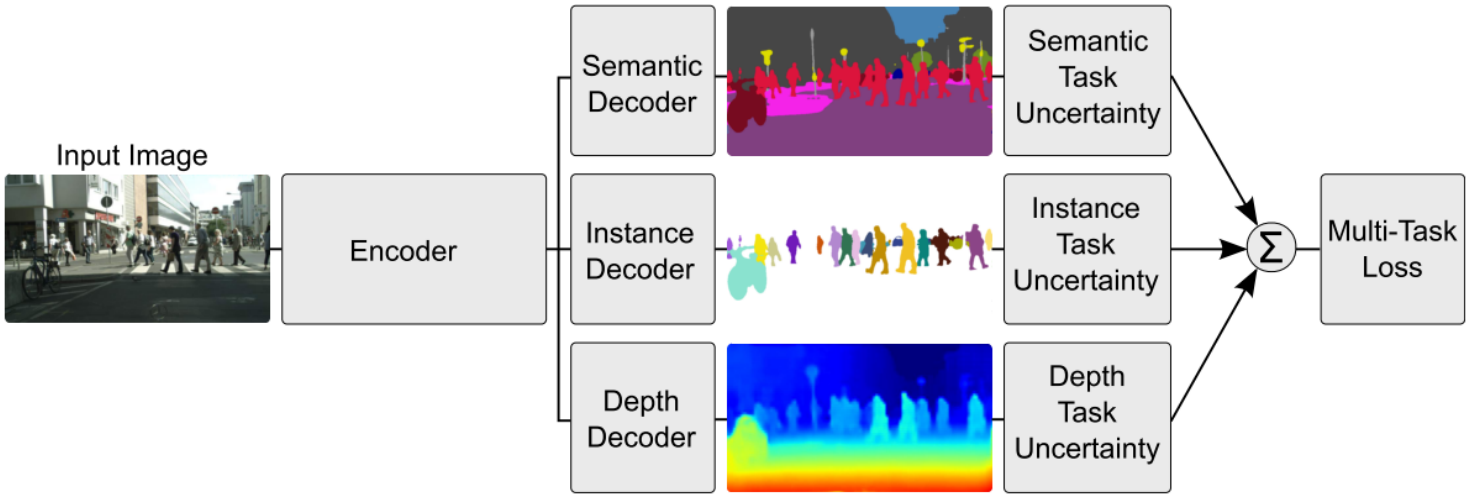


Encoder-decoder architecture

Or: in a modular fashion, e.g. pre-training.

Model generalizations

Or over multiple tasks (i.e. multi-task learning), e.g.



Kendall et al. 2017's multi-task model

Model generalizations

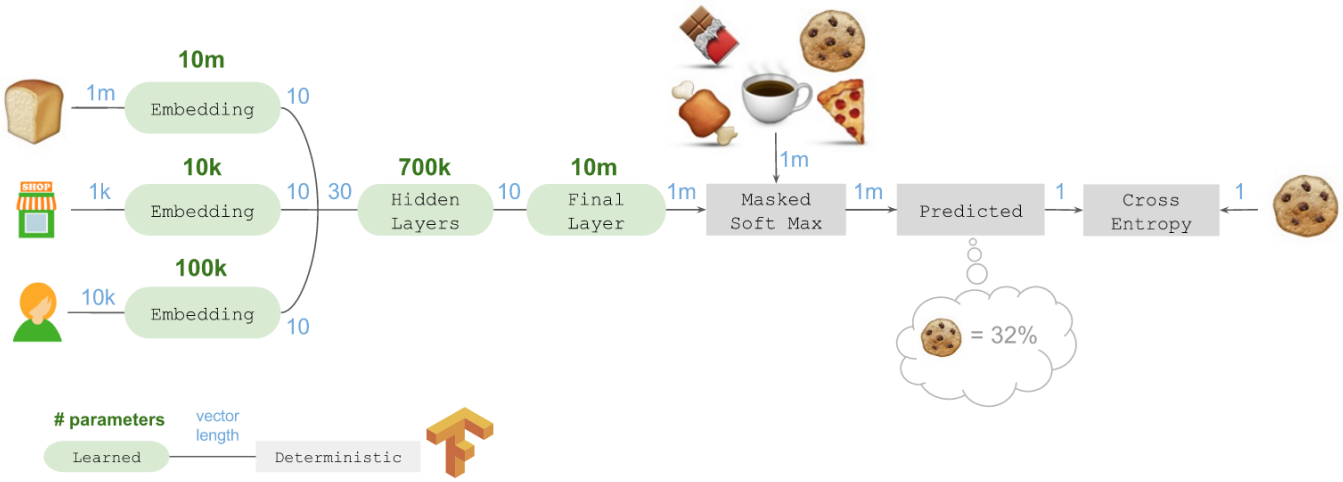
Many researchers will create unique architectures for specific problems, e.g. *Instacart*

The prediction problem

Model generalizations

Many researchers will create unique architectures for specific problems, e.g. *Instacart*

The prediction problem



The intial solution

Model generalizations

Another example using the Netflix data.

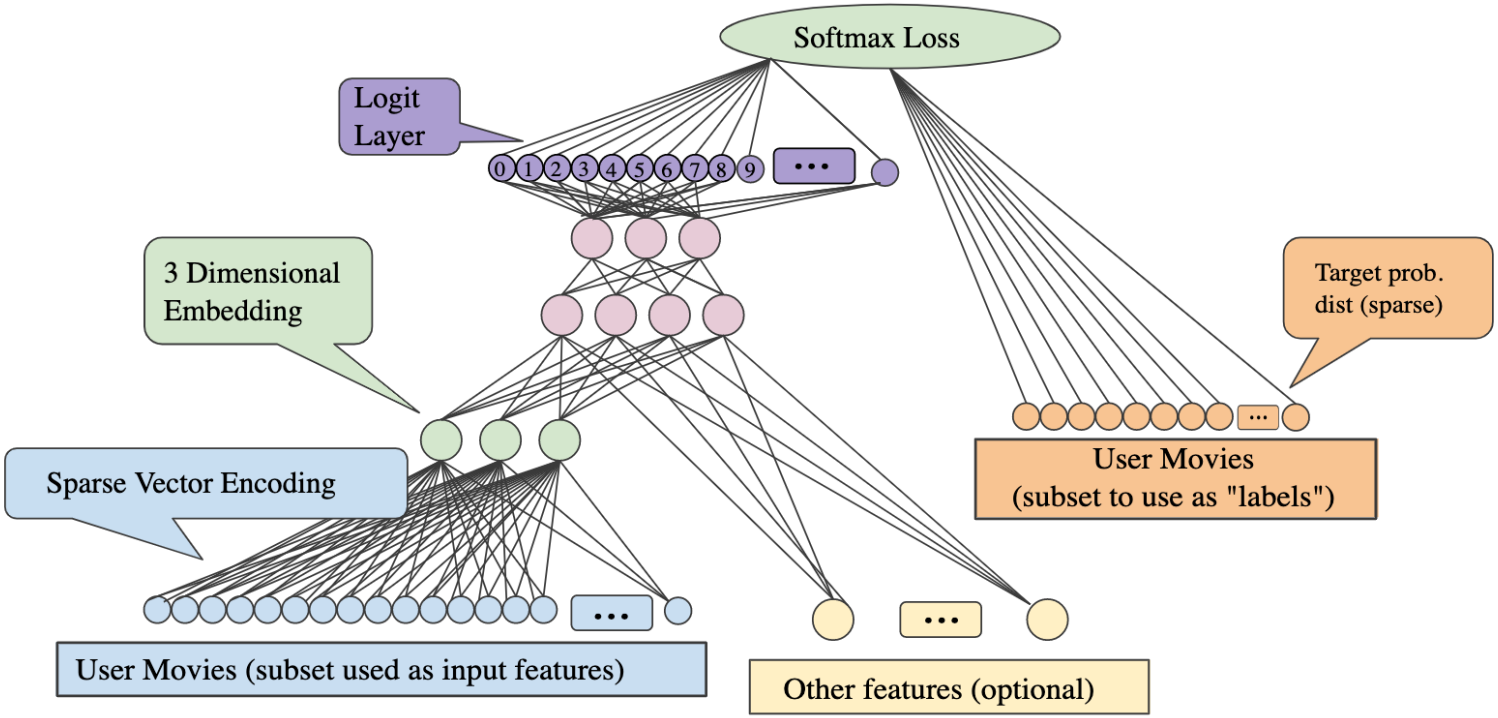
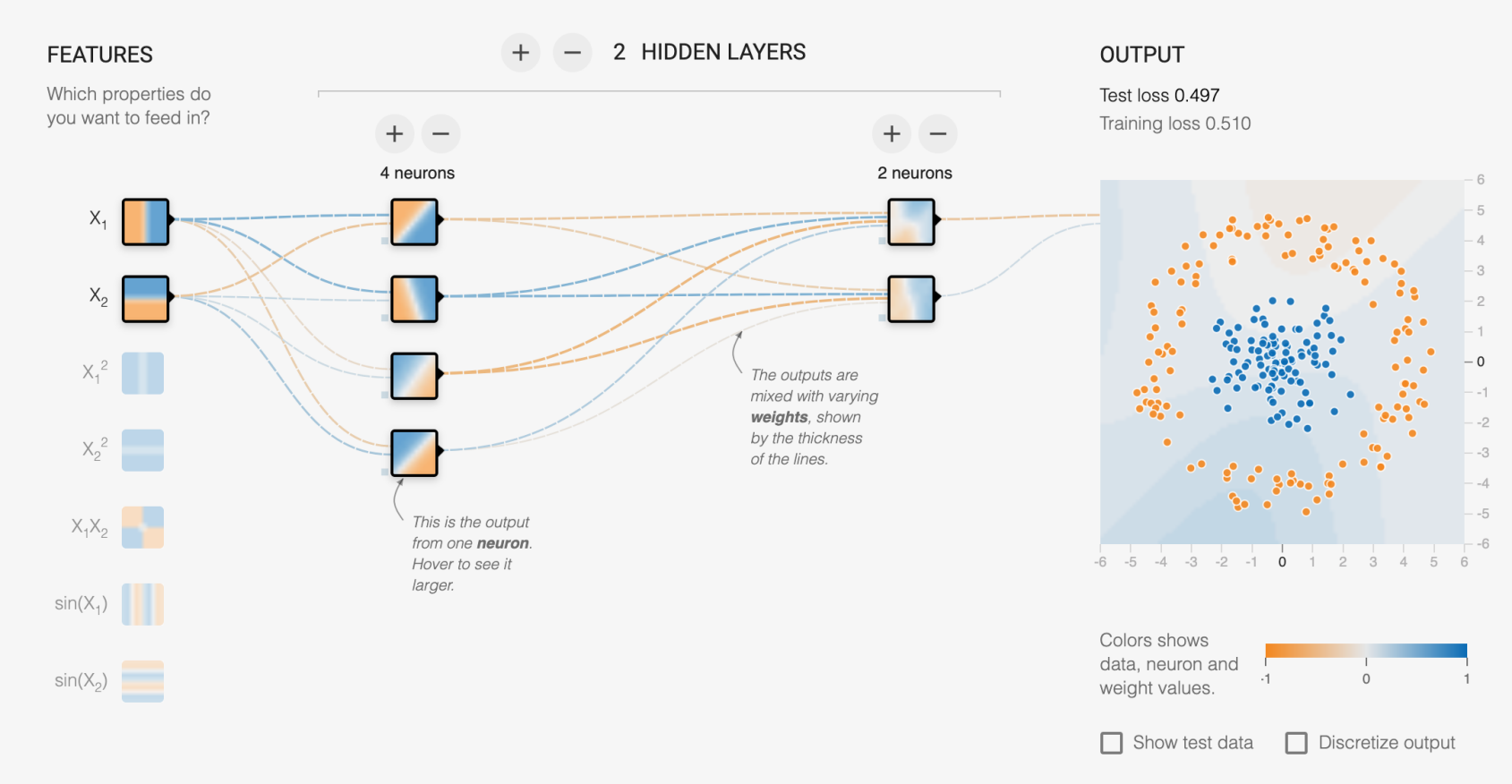


Figure 5. A sample DNN architecture for learning movie embeddings from collaborative filtering data.

The tensorflow playground

An *interactive demo* that allows you to play with a neural network.



Additional topics

Neural net related core topics:

- Weight initializations
- Activation functions
- Optimization functions
- Loss functions
- Normalization
- Regularization / dropout
- Model architectures
- Hyperparameter optimization
- Bayesian neural networks
- Computation graphs
- Software / platforms
- Encoding / adding outside knowledge
- Hardware accelerators

Additional topics

Neural net applied topics:

- Computer vision
- Natural language processing
- Signal processing
- Generative models
- Unsupervised learning
- Reinforcement learning
- One/Zero shot learning
- Transfer learning
- Auto-ML
- Memory Augmented Neural Networks

References

[1] ESL. Chapter 11