CSE/STAT 416

Deep Learning

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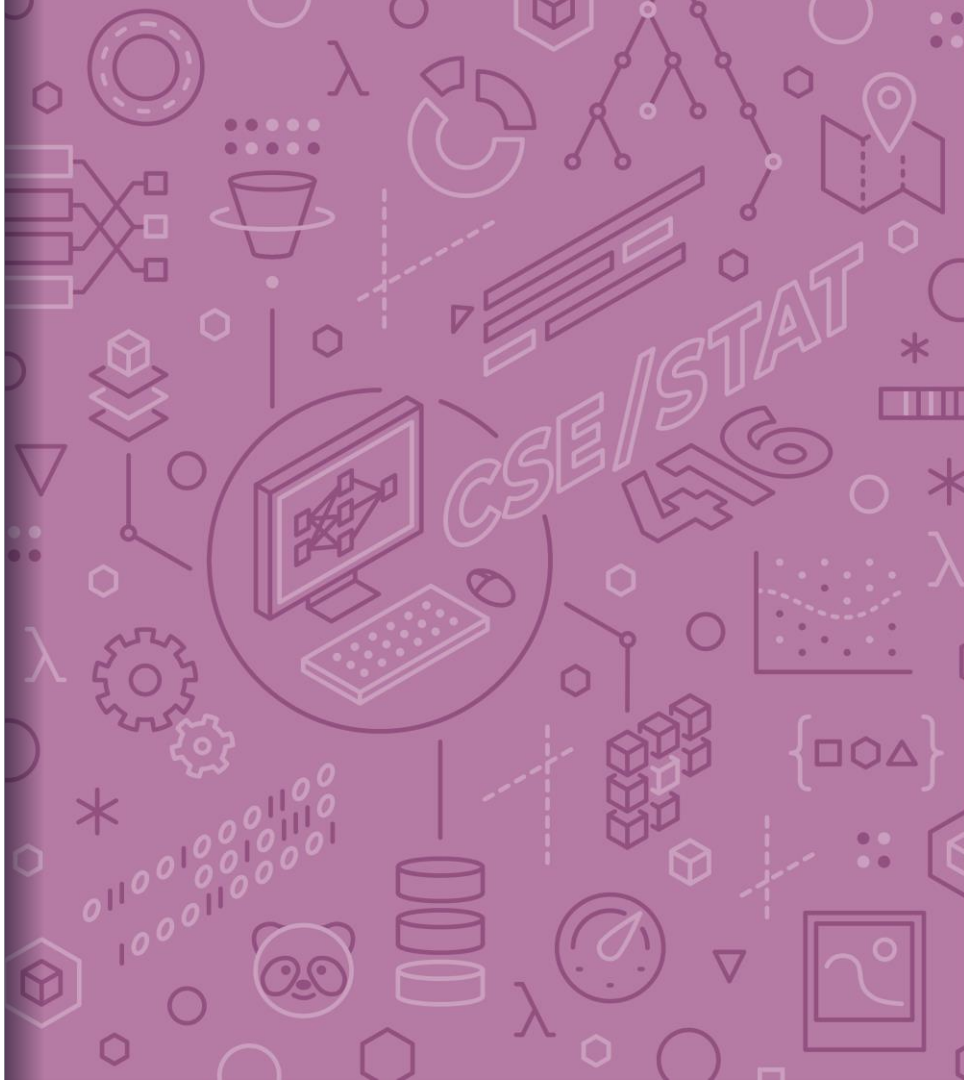
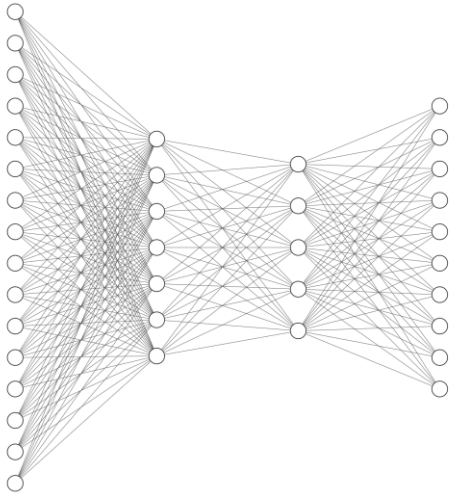
May 24, 2021



Deep Learning

A lot of the buzz about ML recently has come from recent advancements in **deep learning.**

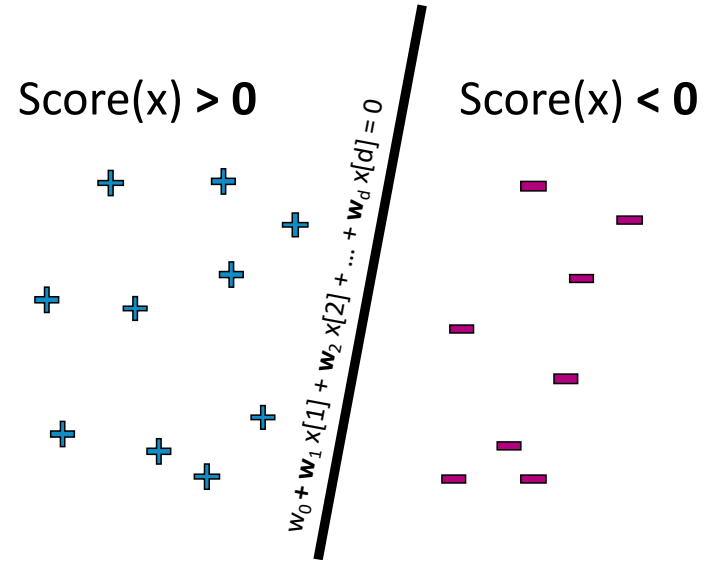
When people talk about “deep learning” they are generally talking about a class of models called **neural networks** that are a loose approximation of how our brains work.



Recall: Linear Classifier

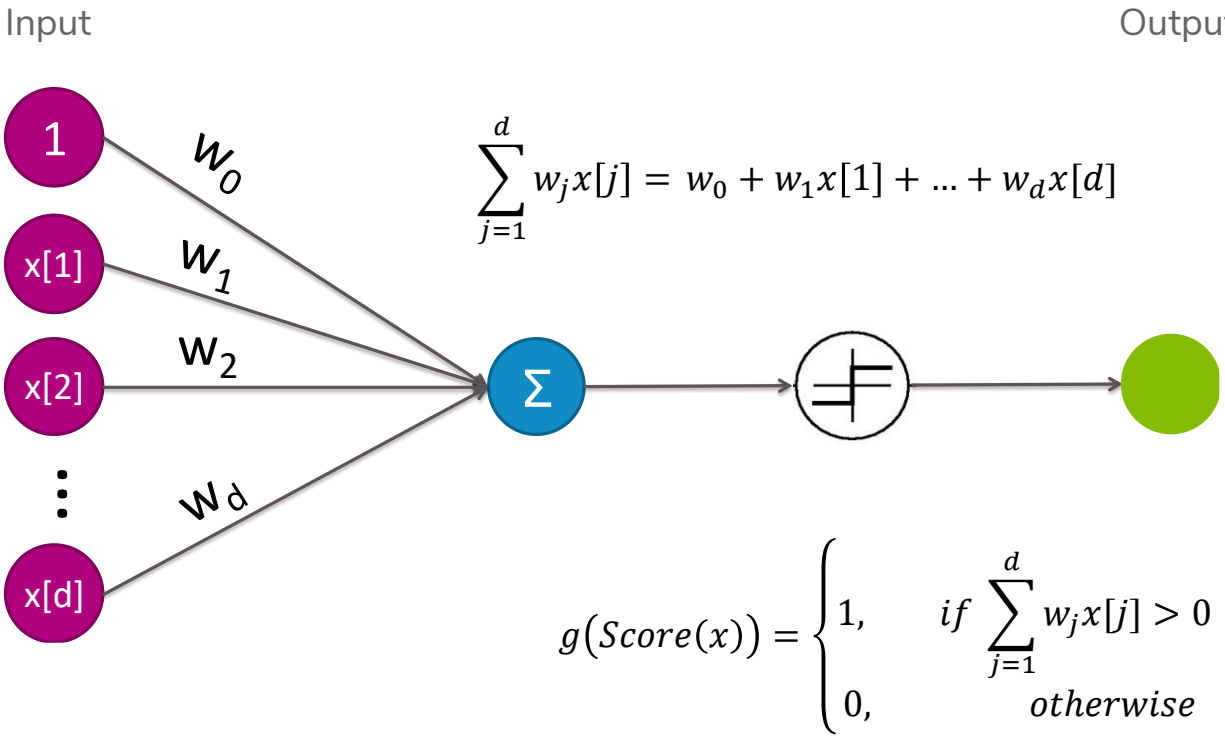
Remember the linear classifier based on score

$$\text{Score}(x) = w_0 + \mathbf{w}_1\, x[1] + \mathbf{w}_2\, x[2] + \ldots + \mathbf{w}_d\, x[d]$$



Perceptron

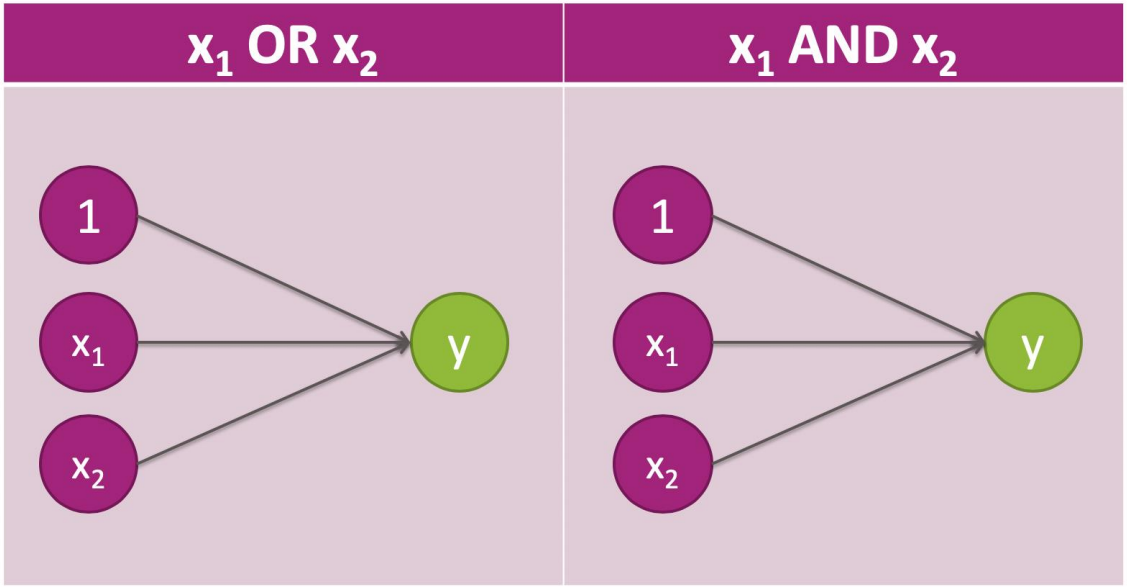
Graphical representation of this same classifier



This is called a **perceptron**

Learnable

What can a perceptrons represent?



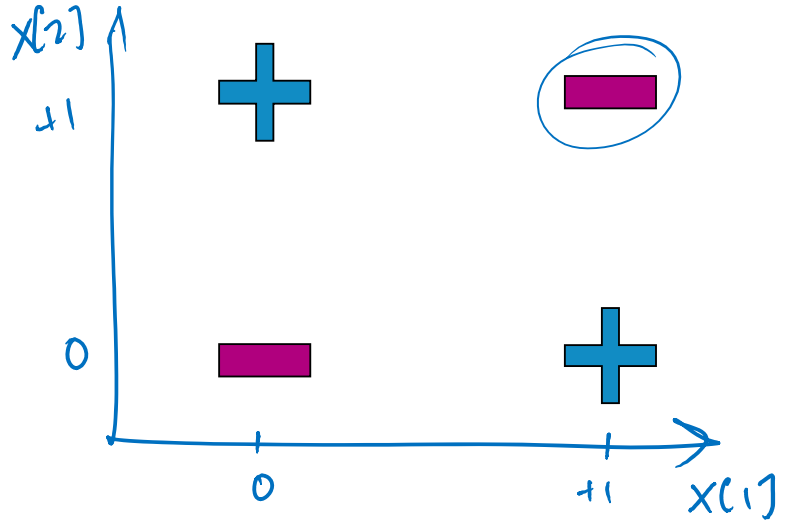
x_1	x_2	y
0	0	0
0	1	1
1	0	1
1	1	1

x_1	x_2	y
0	0	0
0	1	0
1	0	0
1	1	1

XOR

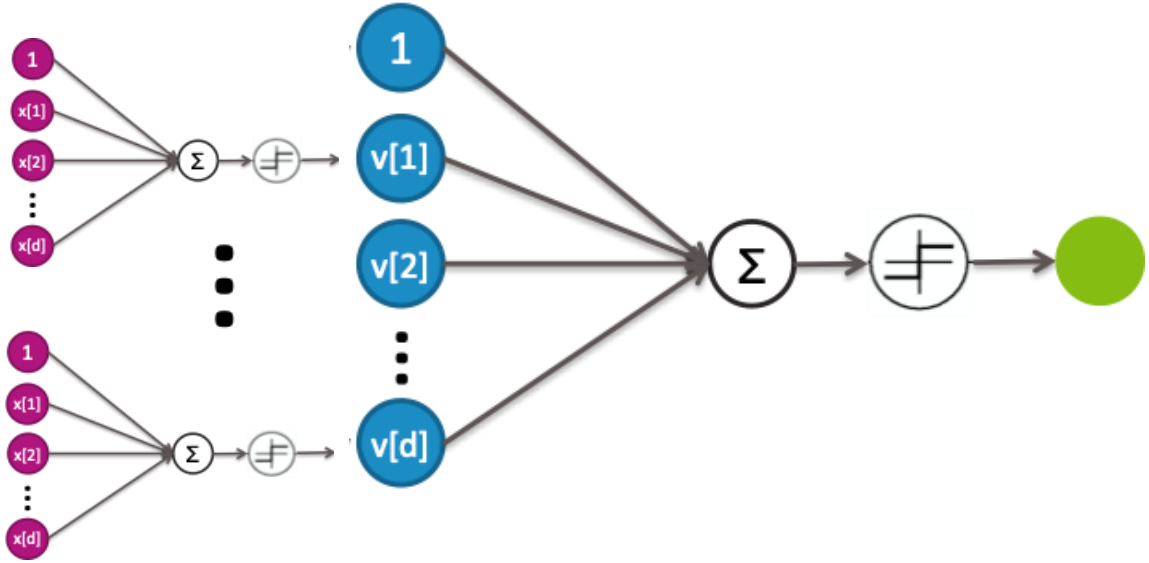
The perceptron can learn most boolean functions, but XOR always has to ruin the fun.

This data is not **linearly separable**, therefore can't be learned with the perceptron



Neural Network

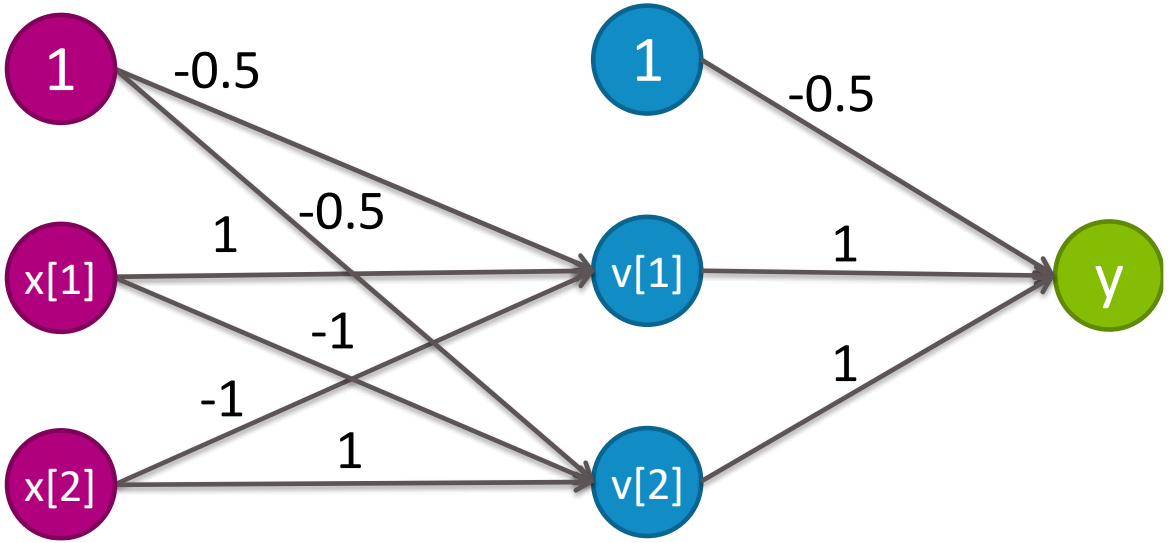
Idea: Combine these perceptrons in layers to learn more complex functions.



XOR

Notice that we can represent

$$x[1]\ XOR\ x[2] = (x[1]\ AND\ !\,x[2])\ OR\ (!\,x[1]\ AND\ x[2])$$



XOR

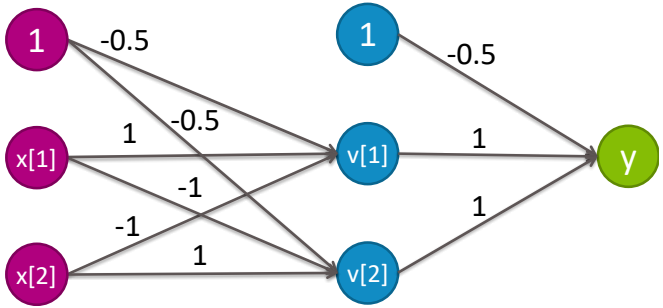
This is a 2-layer neural network

$$y = x[1]\ XOR\ x[2] = (x[1]\ AND\ !\,x[2])\ OR\ (!\,x[1]\ AND\ x[2])$$

$$v[1] = (x[1]\ AND\ !\,x[2])$$
$$= g(-0.5 + x[1] - x[2])$$

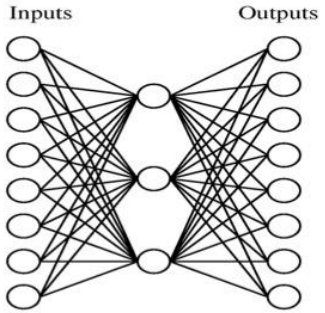
$$v[2] = (!\,x[1]\ AND\ x[2])$$
$$= g(-0.5 - x[1] + x[2])$$

$$y = v[1]\ OR\ v[2]$$
$$= g(-0.5 + v[1] + v[2])$$



Neural Network

Two layer neural network (alt. one hidden-layer neural network)



Single

$$out(x) = g\left(w_0 + \sum_j w_j x[j]\right)$$

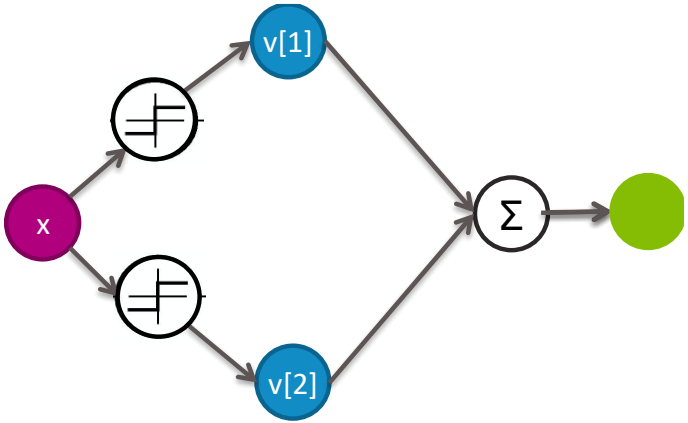
1-hidden layer

$$out(x) = g\left(w_0 + \sum_k w_k g\left(w_0^{(k)} + \sum_j w_j^{(k)} x[j]\right)\right)$$

Power of 2-layer NN

A surprising fact is that a 2-layer network can represent any function, if we allow enough nodes in hidden layer.

For this example, consider regression function with one input.



See more here:
http://neuralnetworksanddeeplearning.com/chap4.html

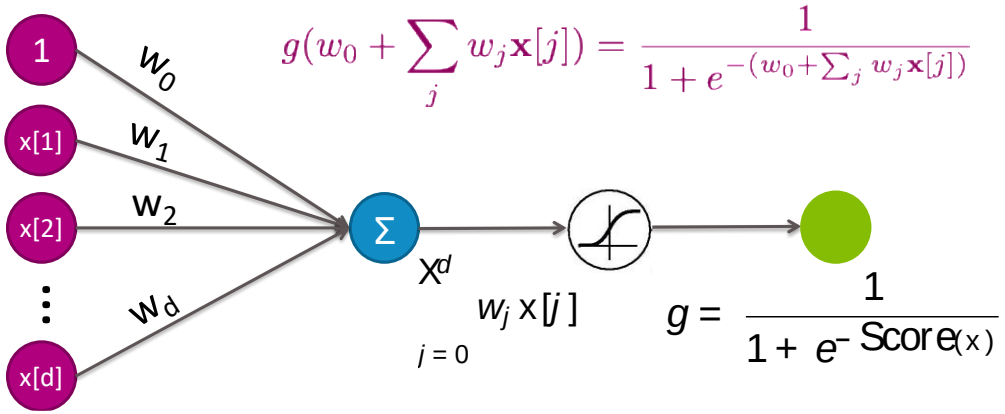
Class Session

Activation Function

Before, we were using the sign activation function.

- This is not generally used in practice.
  - Not differentiable
  - No notion of confidence

Generally, people use different sigmoid functions as activation functions. For example, the logistic function



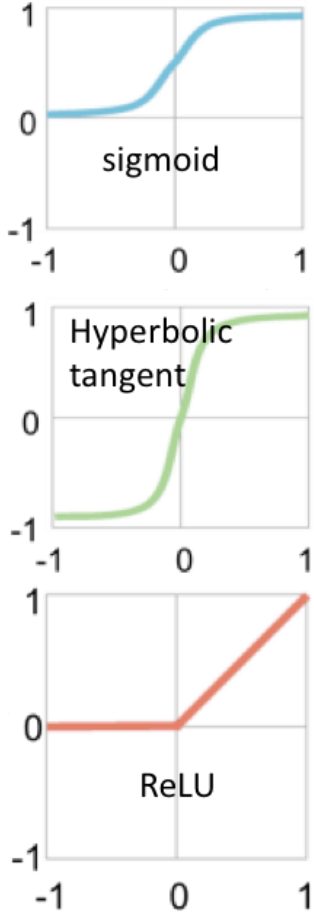
Sigmoid Functions

•Sigmoid
-Historically popular, but (mostly) fallen out of favor
•Neuron's activation saturates
(weights get very large -> gradients get small)
•Not zero-centered -> other issues in the gradient steps
-When put on the output layer, called "softmax" because interpreted as class probability (soft assignment)

•Hyperbolic tangent $g(x) = \tanh(x)$
-Saturates like sigmoid unit, but zero-centered

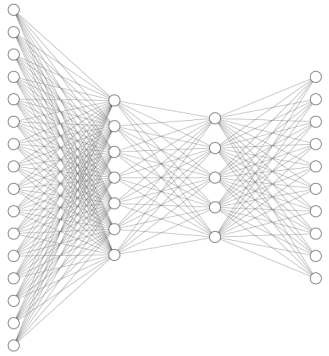
•Rectified linear unit (ReLU) $g(x) = x^+ = \max(0,x)$
-Most popular choice these days
-Fragile during training and neurons can "die off"… be careful about learning rates
-"Noisy" or "leaky" variants

•Softplus $g(x) = \log(1+\exp(x))$
-Smooth approximation to rectifier activation



Neural Networks

Generally layers and layers of linear models and non-linearities (activation functions).



Have been around for about 50 years

- Fell in “disfavor” in the 90s when simpler models were doing well

In the last few years, have had a huge resurgence

- Impressive accuracy on several benchmark problems
- Have risen in popularity due to huge datasets, GPUs, and improvements to

Overfitting NNs

Are NNs likely to overfit? **YES**.

- Consequence of being able to fit any function!

How to avoid overfitting?

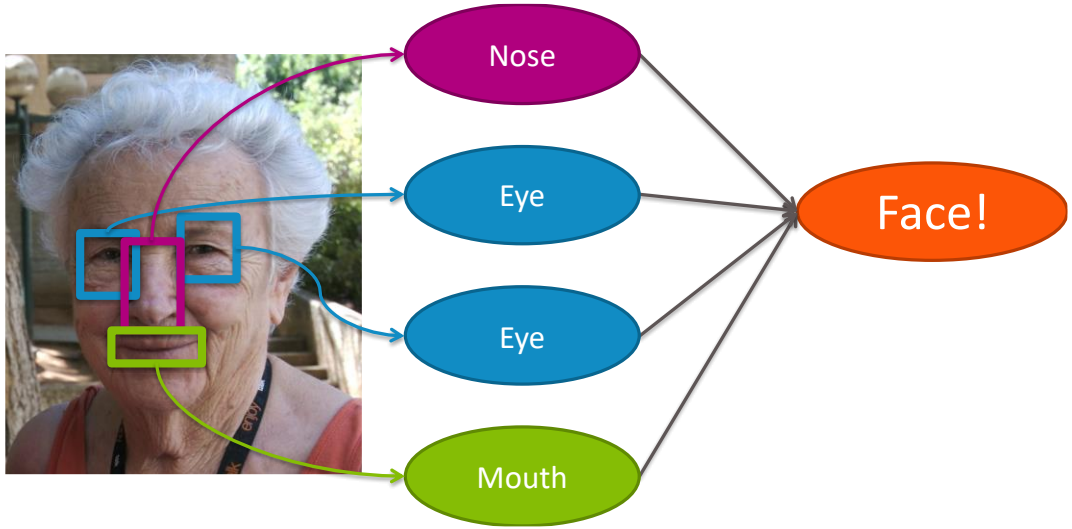
- Get more training data
- Few hidden nodes / better topology
  - **Rule of thumb:** 3-layer NNs outperform 2-layer NNs, but going deeper only helps if you are very careful (different story next time with convolutional neural networks)
- Regularization
  - Dropout
- Early stopping

Application to Computer Vision

Image Features

Features in computer vision are local detectors

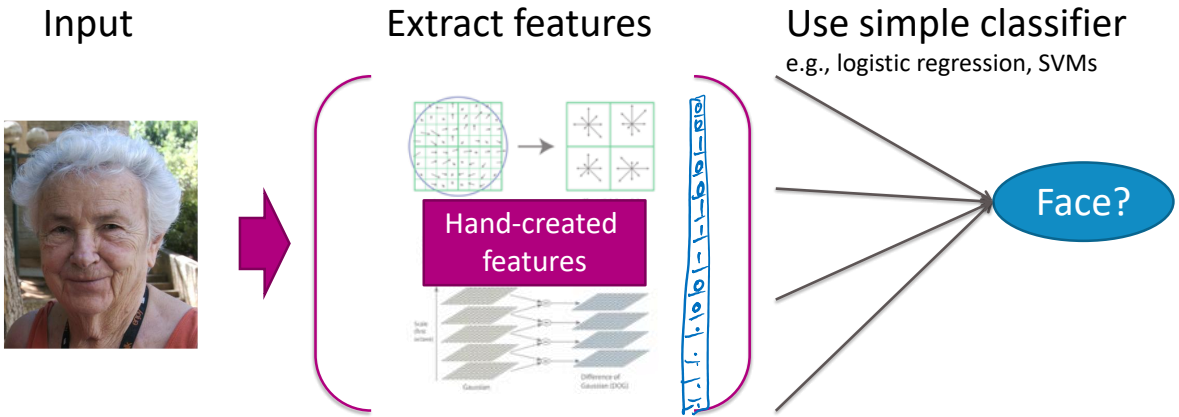
- Combine features to make prediction



In reality, these features are much more low level (e.g. Corner?)

The Past

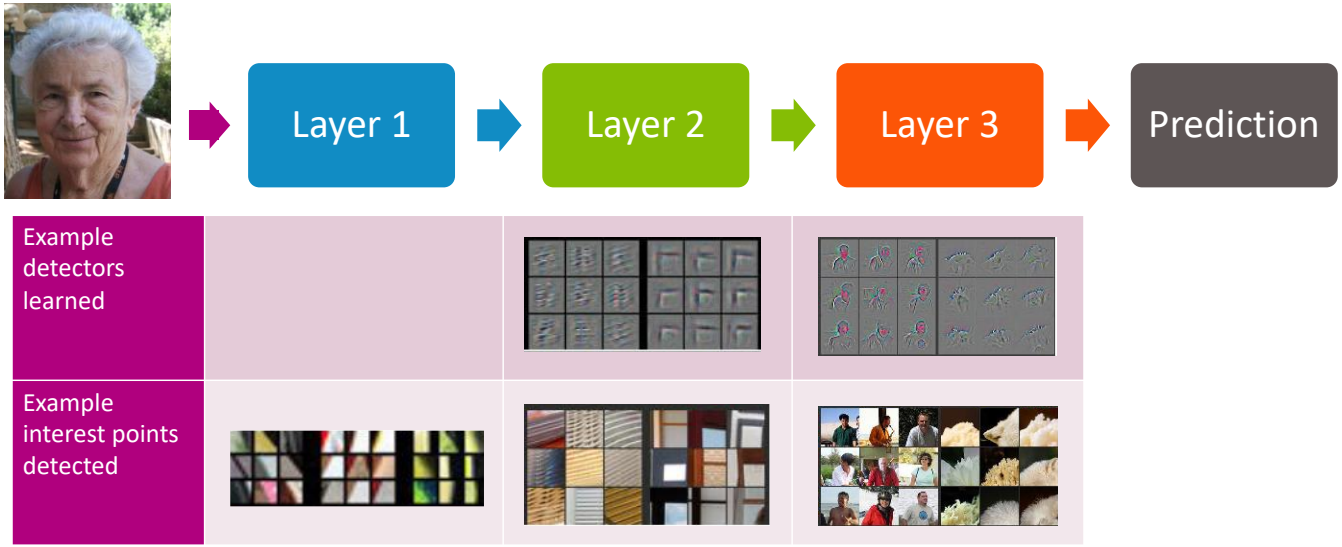
A popular approach to computer vision was to make hand-crafted features for object detection



Relies on coming up with these features by hand (yuck!)

NN to the Rescue

Neural Networks implicitly find these low level features for us!



[Zeiler & Fergus '13]

Each layer learns more and more complex features

Brain Break

Classification or Regression

You can use neural networks for classification and regression!

Regression

The output layer will generally have one node that is the output (outputs a single number)

Classification

The output layer will have one node per class. Usually take the node with the highest score as the prediction for an example. Can also use the logistic function to turn scores into probabilities!

Learning Coefficients

So the idea of neural networks might make sense, but how do we actually go about learning the coefficients in the layers?

First we need to define a quality metric or cost function

- For regression, generally use RSS or RMSE
- For classification, generally use something call the Cross Entropy loss.

Can we use gradient descent here? Actually yes!

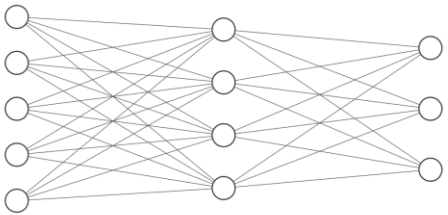
- How do we take the derivative of a network?
- Are there convergence guarantees?

Backpropagation

What does gradient descent do in general? Have the model make predictions and update the model in a special way such that the new weights have lower error.

To do gradient descent with neural networks, we generally use the **backpropagation algorithm.**

1. Do a forward pass of the data through the network to get predictions
2. Compare predictions to true values
3. Backpropagate errors so the weights make better predictions



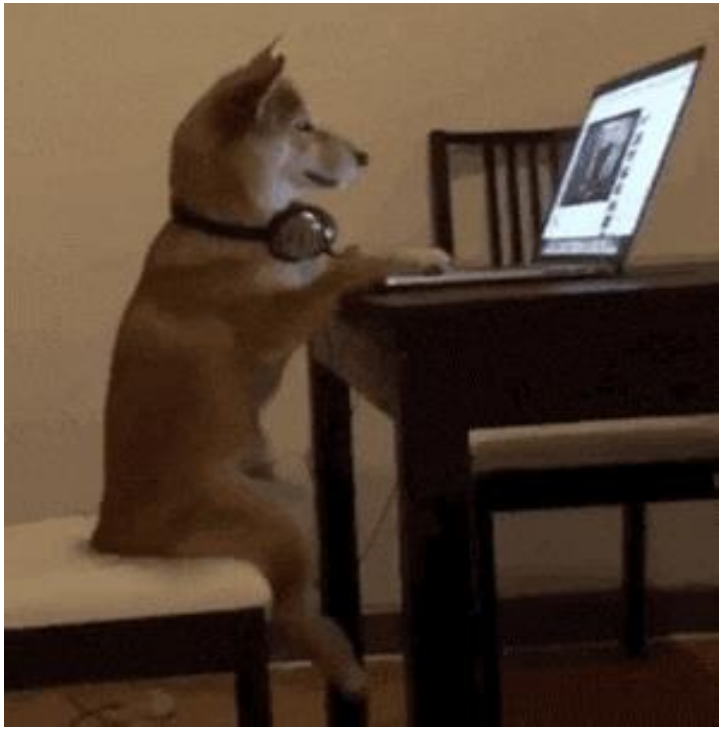
Training NN

It's pretty expensive to do this update for the entire dataset at once, so it's common to break it up into small batches to process individually.

However, processing each batch only once isn't enough. You generally have to repeatedly update the model parameters. We call an iteration that goes over every batch once an **epoch**.

```
for i in range(num_epochs):
  for batch in batches(training_data):
    preds = model.predict(batch.data) # Forward pass
    diffs = compare(preds, batch.labels)  # Compare
    model.backprop(diffs)          # Backpropagation
```

Brain Break



Training NN

Neural Networks have MANY hyperparameters

- How many hidden layers and hidden neurons?
- What activation function?
- What is the learning rate for gradient descent?
- What is the batch size?
- How many epochs to train?
- And much much more!

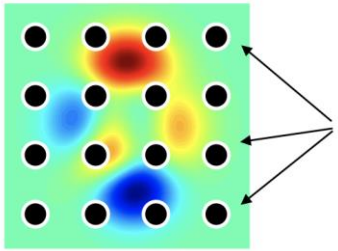
How do you decide these values should be? ¯_(ツ)_/¯

The most frustrating thing is that we don't have a great grasp on how these things impact performance, so you generally have to try them all.

Hyperparameter Optimization

How do we choose hyperparameters to train and evaluate?

Grid search:



Hyperparameters on 2d uniform grid

Hyperparameter Optimization

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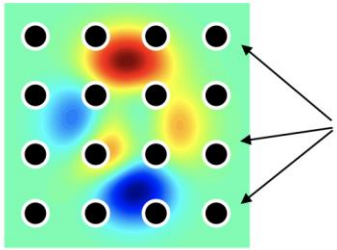
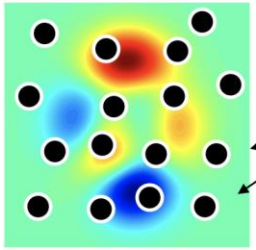


Hyperparameters on 2d uniform grid

Random search:



Hyperparameters randomly chosen

Hyperparameter Optimization

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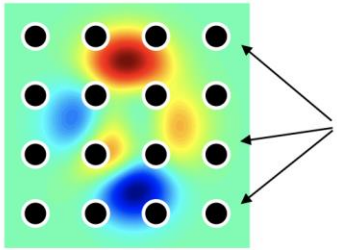
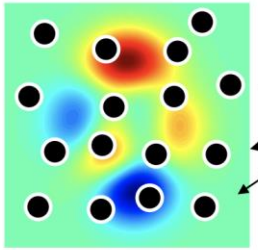


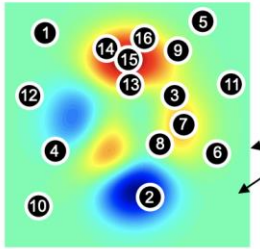
Hyperparameters on 2d uniform grid

Random search:



Hyperparameters randomly chosen

Bayesian Optimization:



Hyperparameters ***adaptively*** chosen

Hyperparameter Optimization

Recent work attempts to speed up hyperparameter evaluation by stopping poor performing settings before they are fully trained.

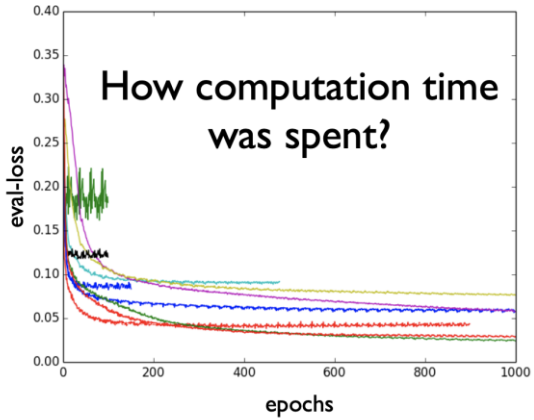
Kevin Swersky, Jasper Snoek, and Ryan Prescott Adams. Freeze-thaw bayesian optimization. arXiv:1406.3896, 2014.

Alekh Agarwal, Peter Bartlett, and John Duchi. Oracle inequalities for computationally adaptive model selection. COLT, 2012.

Domhan, T., Springenberg, J. T., and Hutter, F. Speeding up automatic hyperparameter optimization of deep neural networks by extrapolation of learning curves. In *IJCAI*, 2015.

András György and Levente Kocsis. Efficient multi-start strategies for local search algorithms. JAIR, 41, 2011.

Li, Jamieson, DeSalvo, Rostamizadeh, Talwalkar. Hyperband: A Novel Bandit-Based Approach to Hyperparameter Optimization. ICLR 2016.



Hyperparameter Optimization

In general, hyperparameter optimization is a non-convex optimization problem where we know very little about how the function behaves.

Your time is valuable and compute time is cheap. Write your code to be modular so you can use compute time to try a range of values.

Tools for different purposes

- Very few evaluations: use random search (and pray)
- Few evaluations and long-run computations: See last slide
- Moderate number of evaluations: Bayesian optimization
- Many evaluations possible: Use random search. Why overthink it?

NN Convergence

In general, loss functions with neural networks are **not** convex.

This means the backprop algorithm for gradient descent will only converge to a local optima.

Like with k-means, this means that how you initialize the weights is really important and can impact the final result.

How should you initialize weights? ¯_(ツ)_/¯

- Usually people do random initialization

All the same rules apply from gradient descent with a learning rate, you might miss the mark of the local optima if the step size is too large.