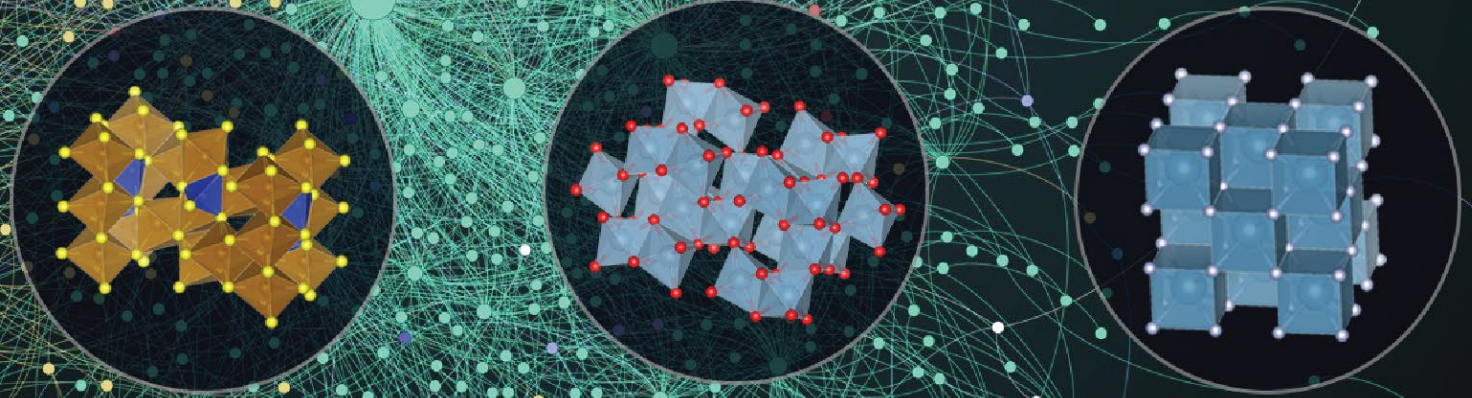
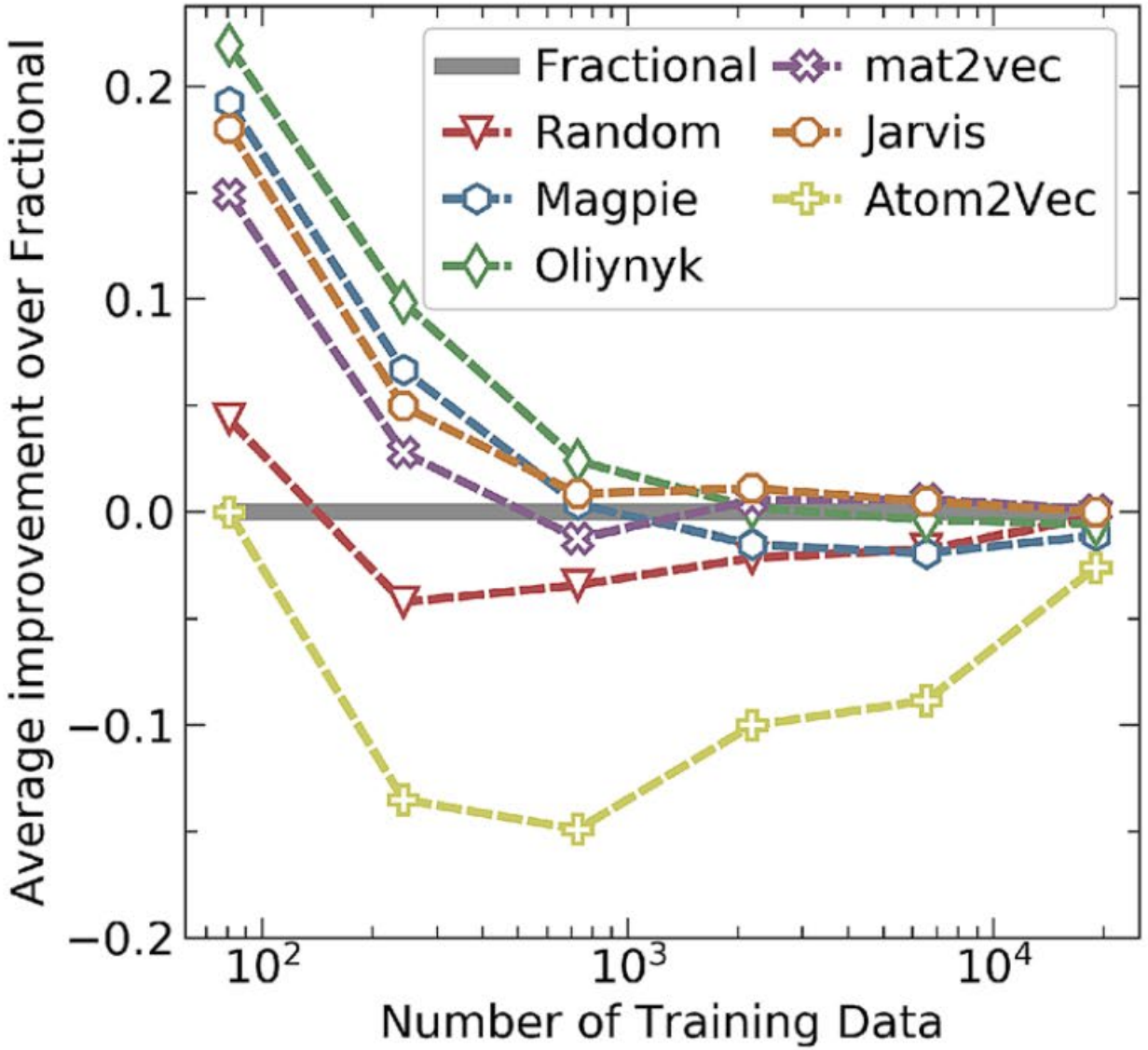
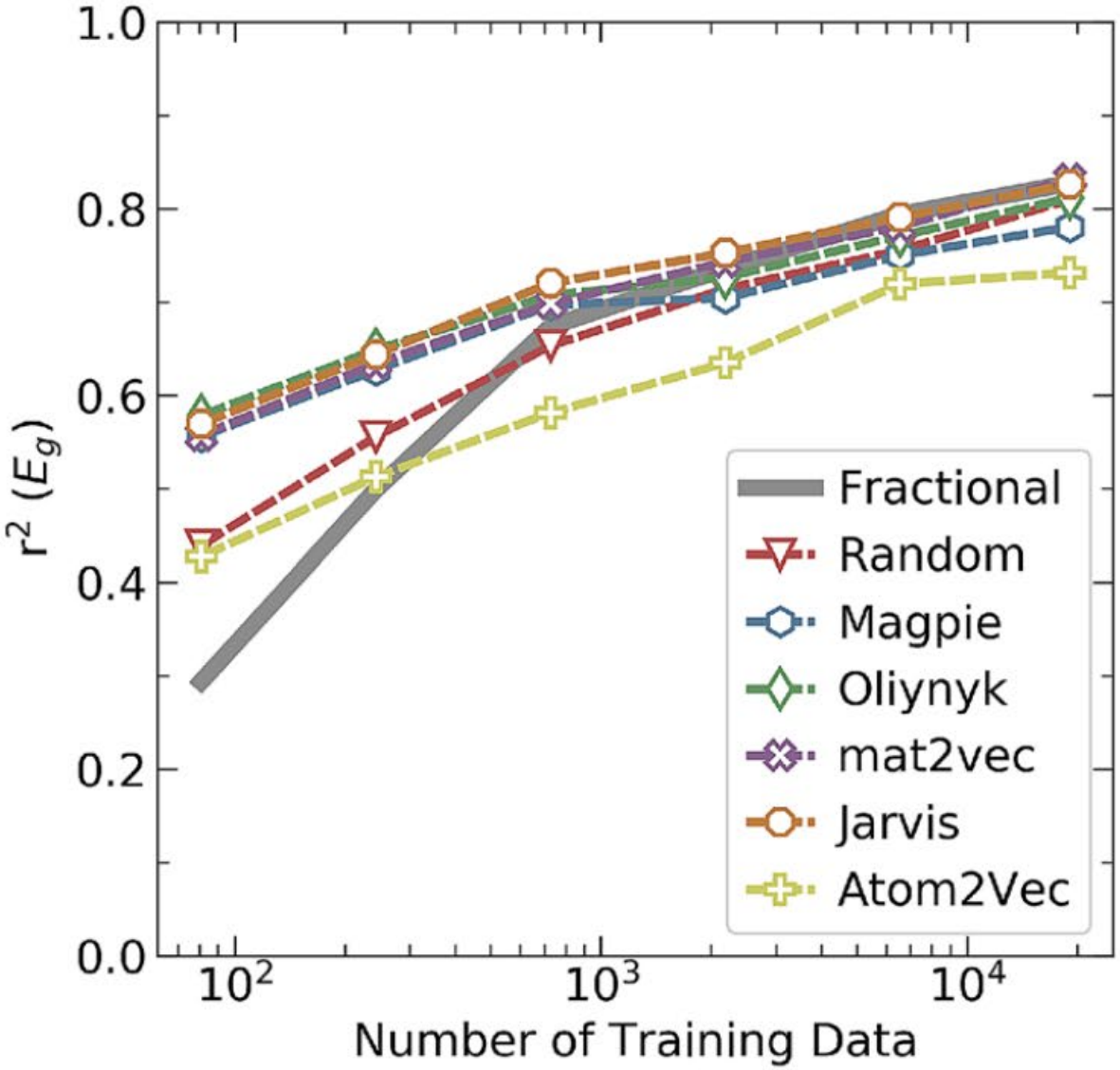
neural networks



Neural networks have emerged as one of the most powerful machine learning algorithms





Neural networks are meant to mimic how neurons in the brain pass information

Major differences:

Size (86 billions vs 10-1000)

Topology (neurons not really connected)

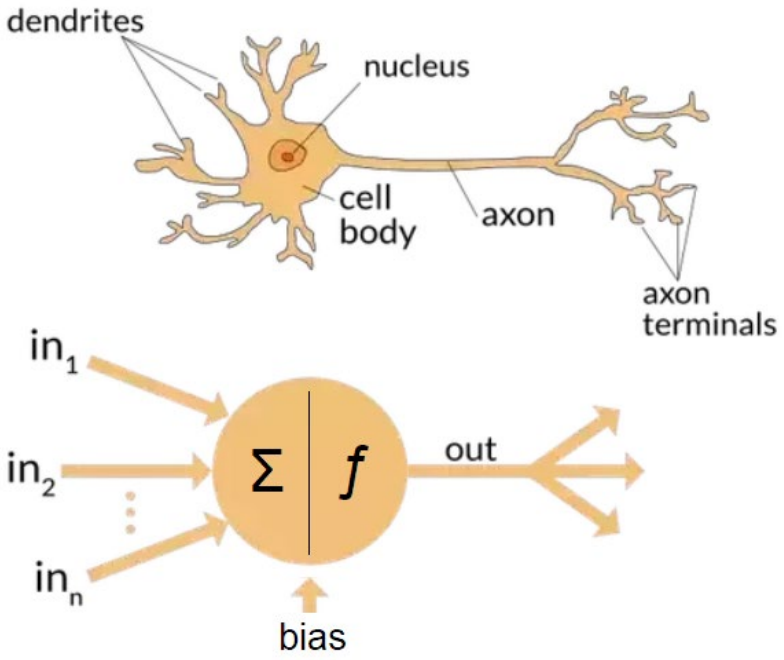
Speed (much faster in computer, and no rest periods)

Fault tolerance (artificial has no redundant info wired into system)

Power consumption (brain runs at 20W, Nvidia GeForce Titan X GPU is 250W)

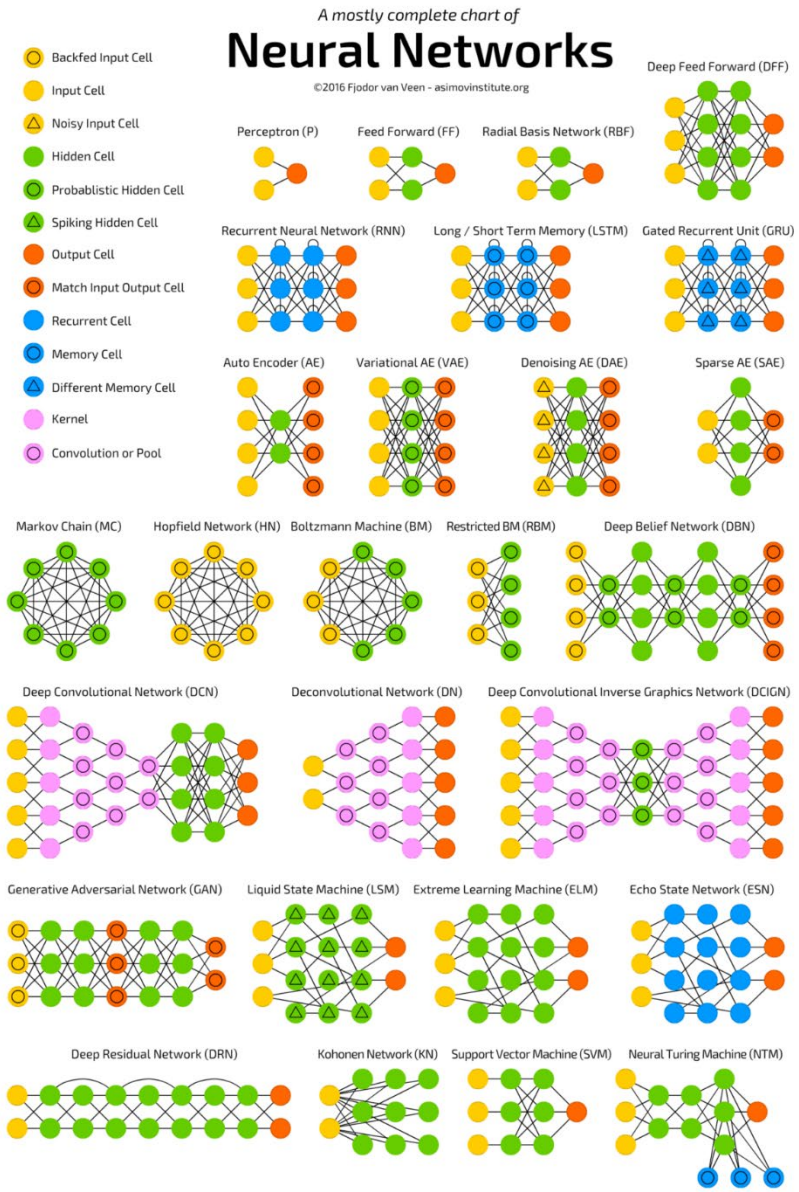
Signal (0 or 1 for brain, no intermediate)

Learning (all at once or reinforced over time, predefined model or one that evolves)



https://towardsdatascience.com/the-differences-between-artificial-and-biological-neural-networks-a8b46db828b7

Neural networks come in different flavors



https://towardsdatascience.com/the-mostly-complete-chart-of-neural-networks-explained-3fb6f2367464

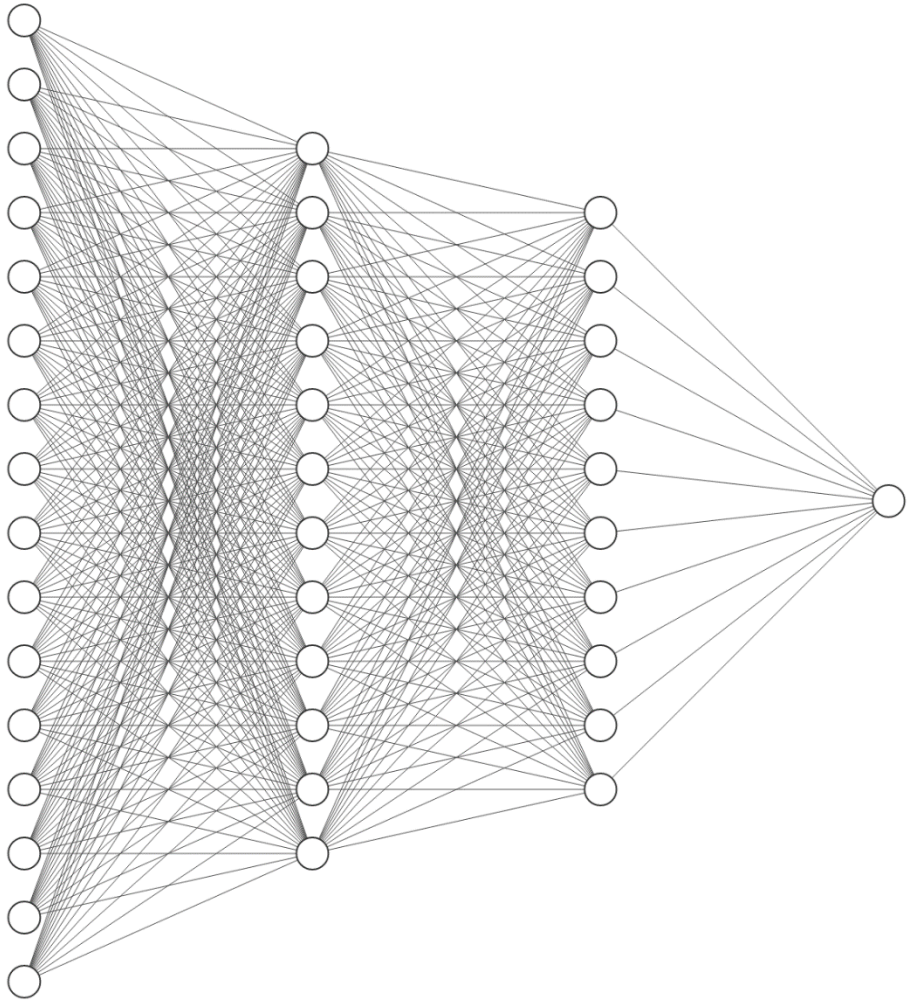
Neural networks are made up of layers of interconnected nodes

Nodes store numbers

- “activated” with a value between 0 and 1
- Functions that pass information

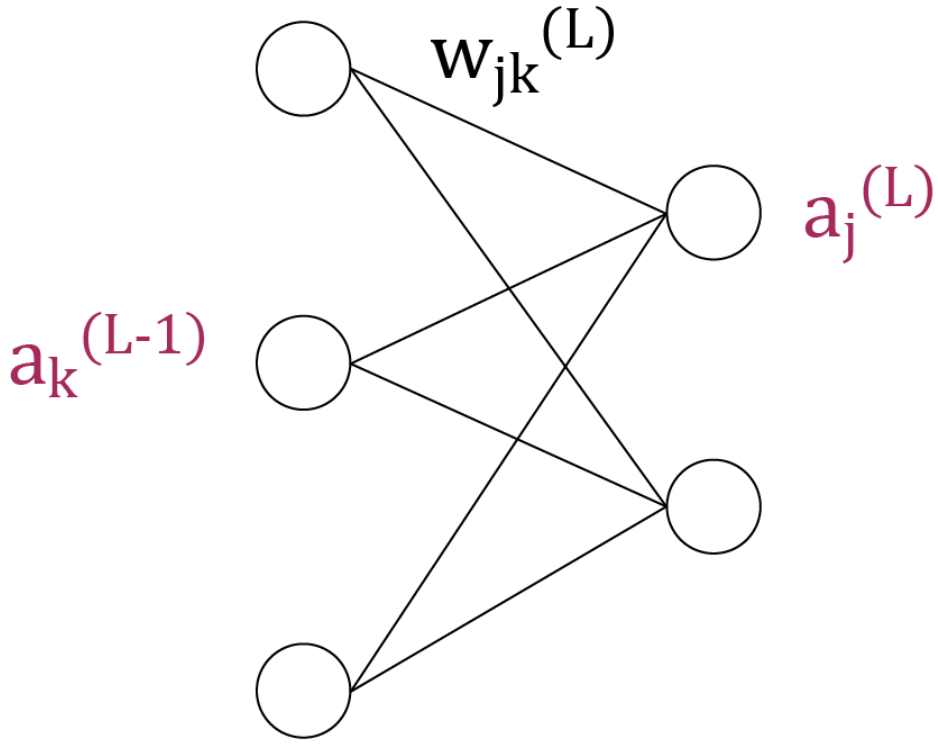
End result of network is a prediction (regression or classification)

Do intermediate layers build up in explainable way to the outcome you obtain?



Neural networks are made up of layers of interconnected nodes

- Each node is fully connected to previous layer
- Information is passed and summed to new node
- Node value is “squished” to between 0 and 1 via an activation function



$a_0^{(1)}$ means 0-th node of first layer

$$a_0^{(1)} = \sigma\left(w_{0,0}a_0^{(0)} + w_{0,1}a_1^{(0)} + \cdots + w_{0,n}a_n^{(0)} + b_0\right)$$

Tunable parameters are weights and biases!

Machine learning is just linear algebra

$$\sigma\left(\begin{bmatrix} w_{0,0} & w_{0,1} & \cdots & w_{0,n} \\ w_{1,0} & w_{1,1} & \cdots & w_{1,n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{k,0} & w_{k,1} & \cdots & w_{k,n} \end{bmatrix} \begin{bmatrix} a_0^{(0)} \\ a_1^{(0)} \\ \vdots \\ a_n^{(0)} \end{bmatrix} + \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_n \end{bmatrix}\right)$$

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

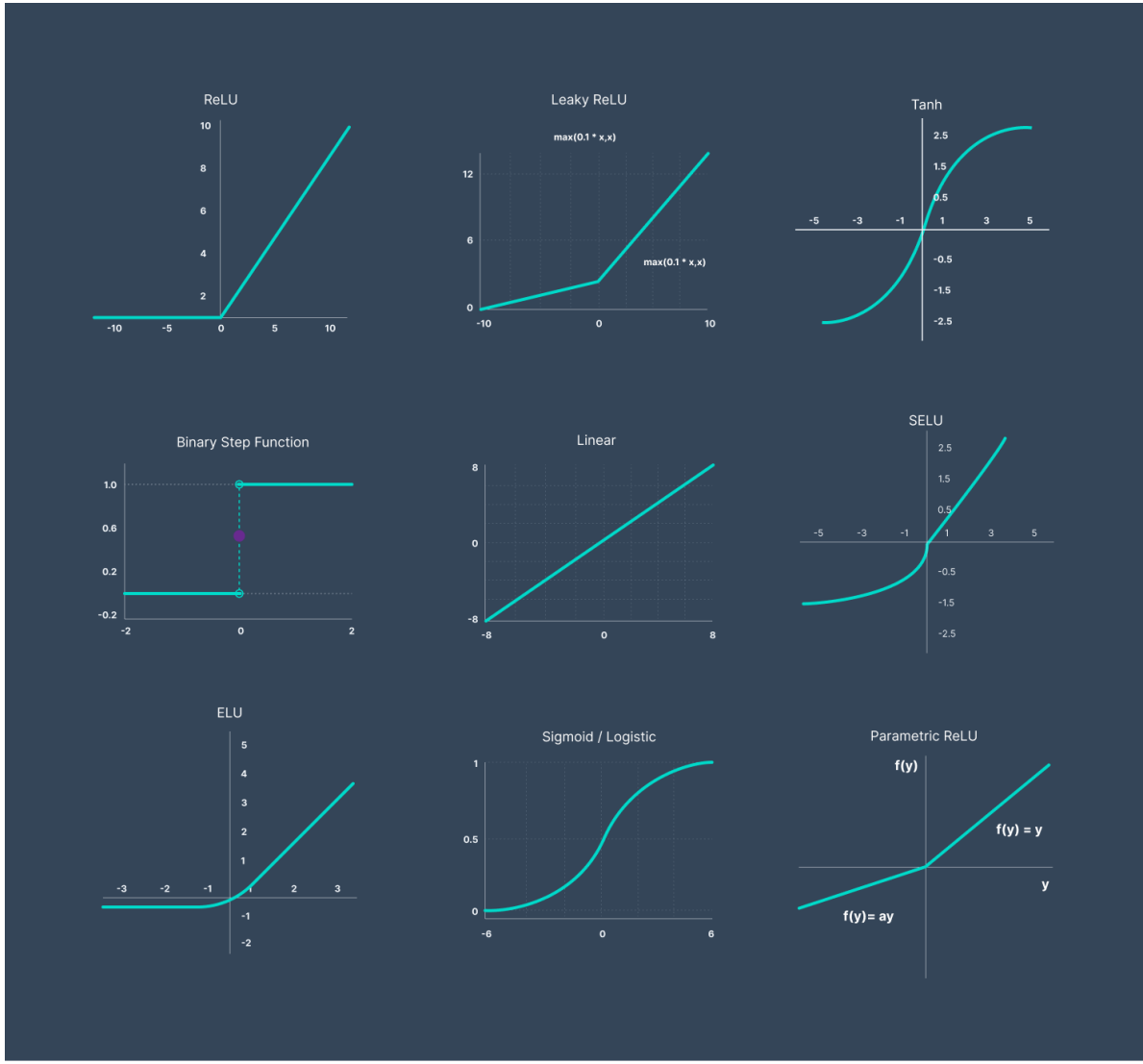
Many different activation functions are available

Sigmoid was a popular early choice, but is a slow learner

ReLU (Rectified linear unit) has become much more common

$$ReLU(a) = \max(0, a)$$

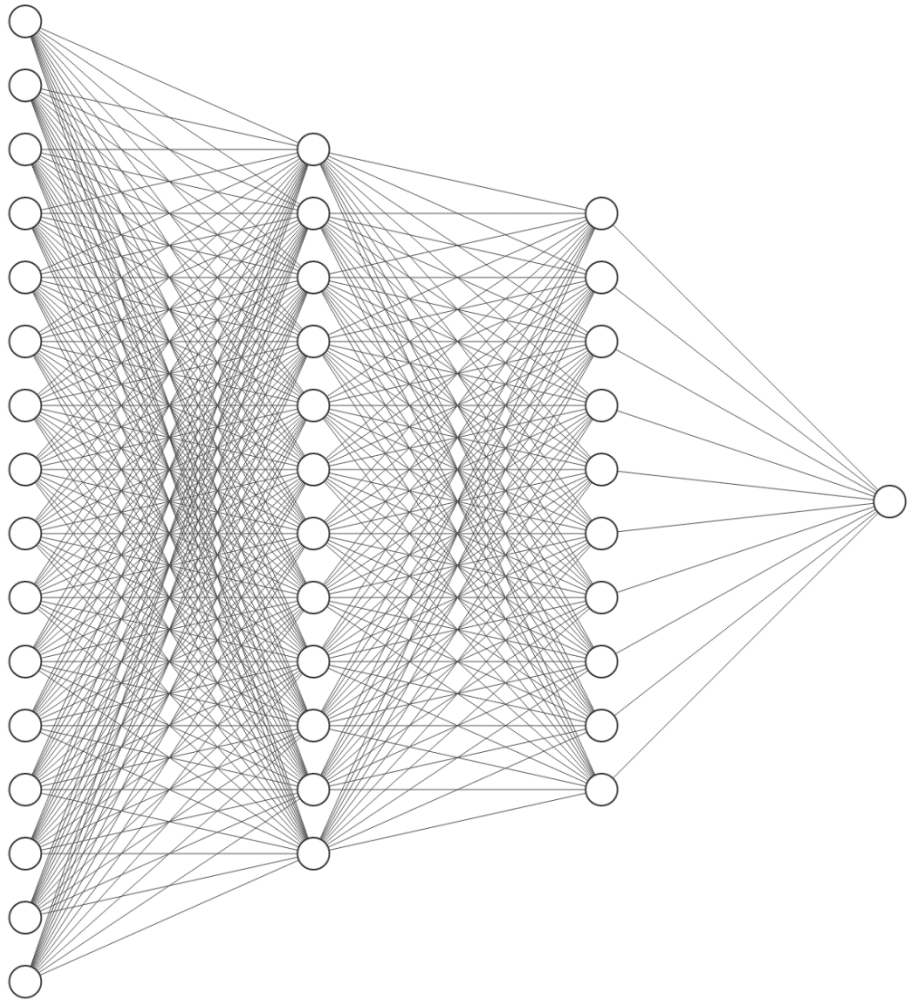
Inactive before some threshold, f(a)=a after threshold



How does a neural network learn then?

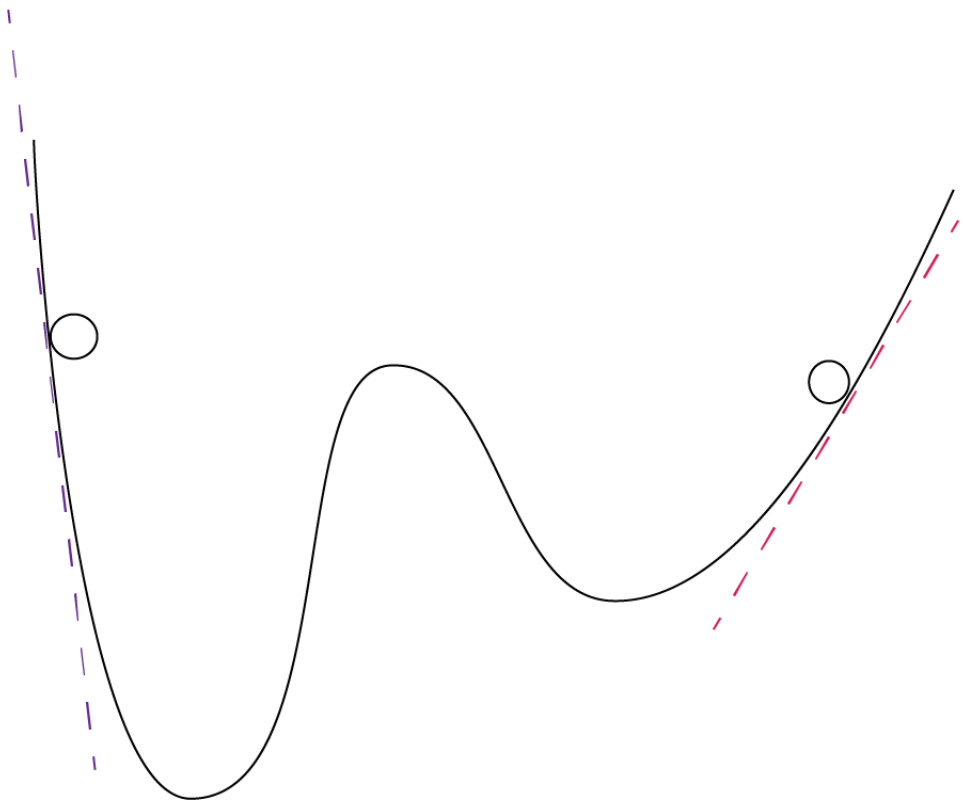
- Randomly initializing all weights and biases
- Introduce a cost function
  - Add up the square of the differences of each node in final layer
  - “the cost of a single training run”
  - Calculate the average cost over all of the data available to train from
- Adjust the free parameters in order to minimize our cost function

How???



A gradient allows us to find the most efficient minimization of our cost function

- Calculate the slope of our function to decide where to move next
- Beware of local vs global minimum
- Make step size proportional to the slope!



Learning steps:
Calculate gradient
Take step in negative gradient direction
Repeat

Gradient just gets multiplied by the parameters to nudge these all in the right direction

$$-\nabla C[\overrightarrow{W}]$$

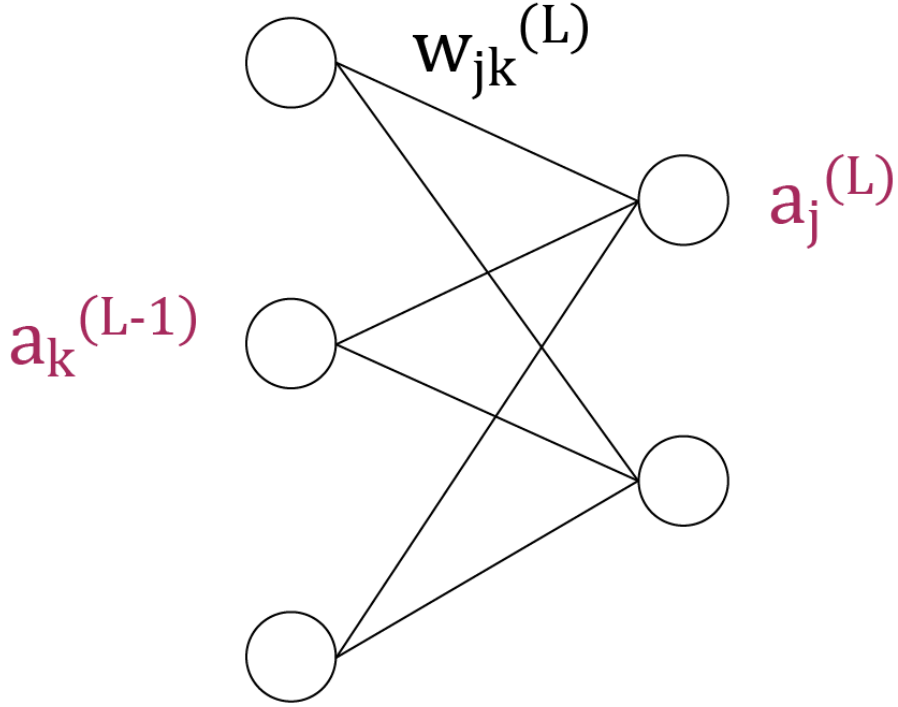
if we treat the weights as a vector, it just changes the direction!

Backpropagation is the process of applying gradients to update our free parameters

The magnitude of each element in your gradient tells you how sensitive that weight is for your cost function

Remember: $a^{(L)} = \sigma(Wa^{(L-1)} + b)$

To increase a final node we can…
1. increase bias
2. increase weights
3. ~~change~~ influence activations from previous layer



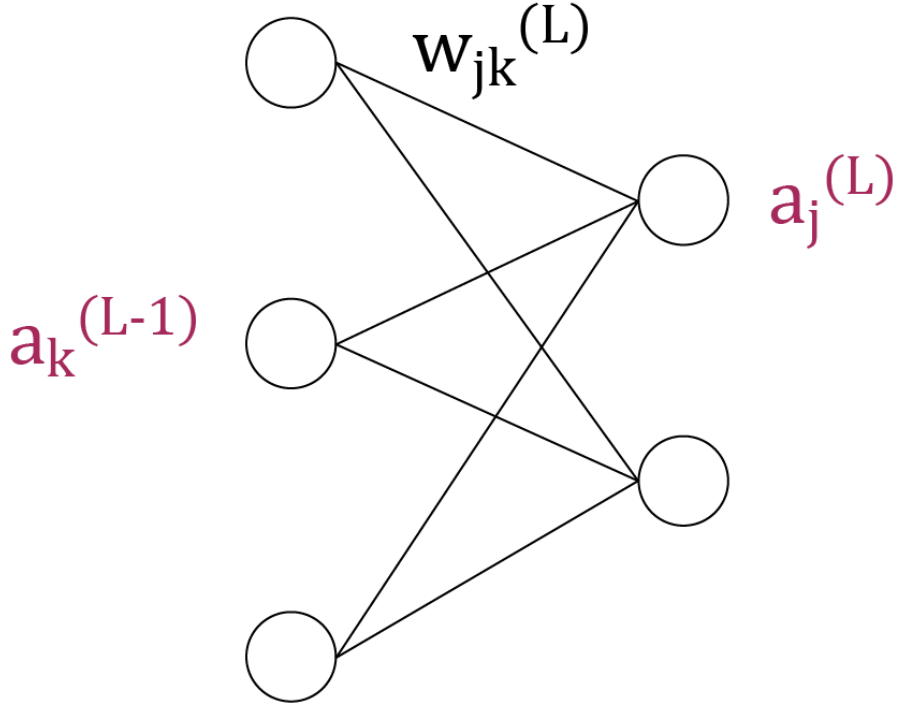
The corrections of each node in our final output get averaged

Backpropagation moves from final desired output backwards

For each step you are getting a list of nudges you want to happen to previous layer, so collect them for all weights and biases in whole network

Generate this list of nudges for each and every sample in training data and then average across all samples

This average is the negative gradient of the cost function!!! (or at least something proportional to it)



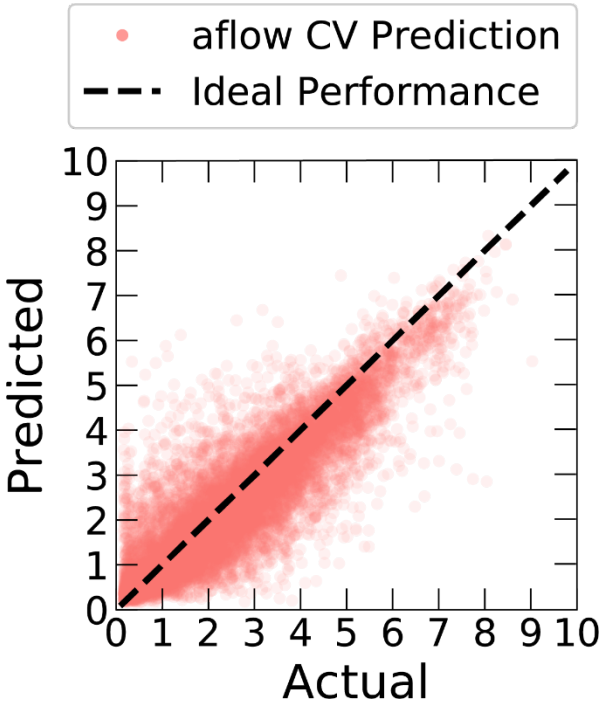
Backpropagation would be way too slow if we did every step on every sample

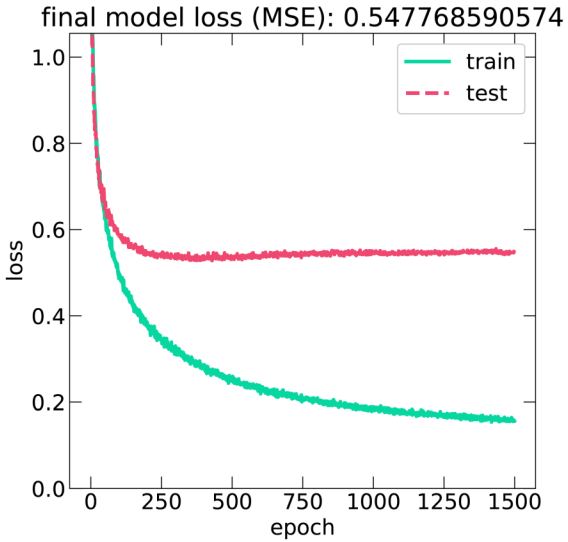
To speed training up, we perform calculations on mini-batches

- “stochastic gradient descent”
- Randomly shuffle data and then divide into mini-batches
- Compute a step (gradient calculation) according to mini batch
- Pretty good approximation, but not technically the steepest descent, but way faster

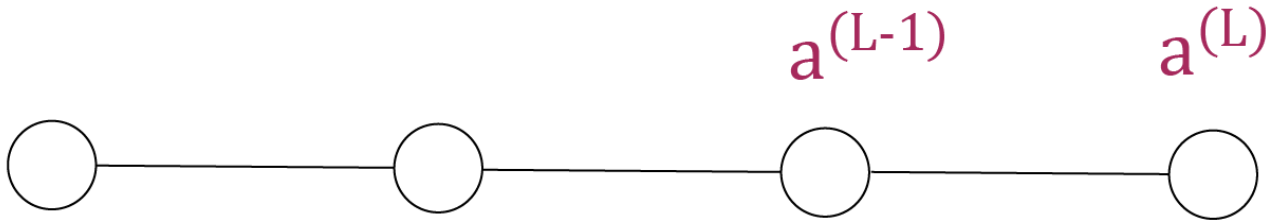
As you train you actually go through your whole dataset multiple times

- Epoch is when entire dataset is passed through one time





Let's look at the math of backpropagation in a really simple network



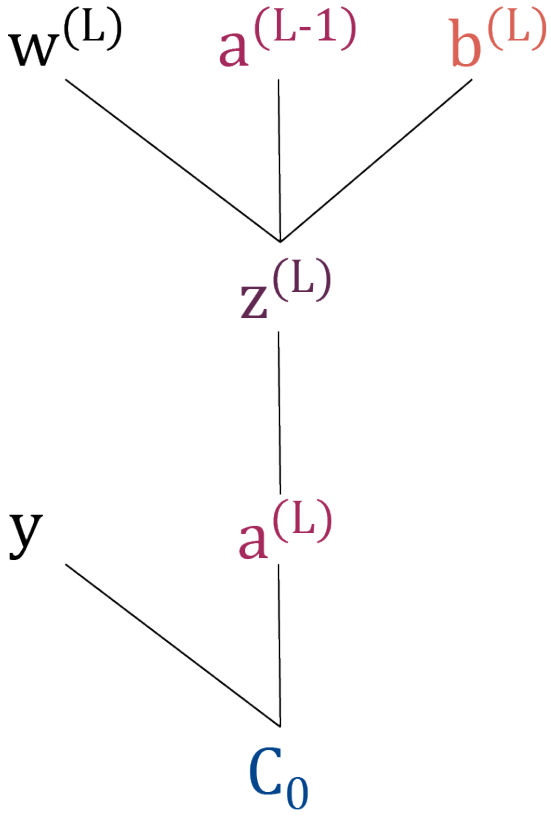
What free parameters do we have?

$$C(w_1, b_1, w_2, b_2, w_3, b_4)$$

How sensitive is our cost function to these variables?

$$C_0(\dots) =$$

$$a^{(L)} =$$



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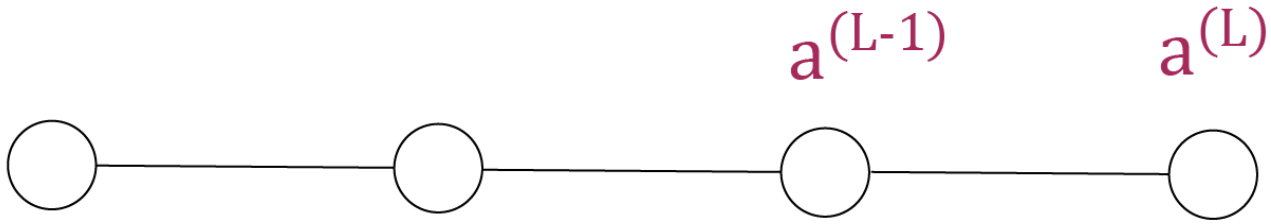


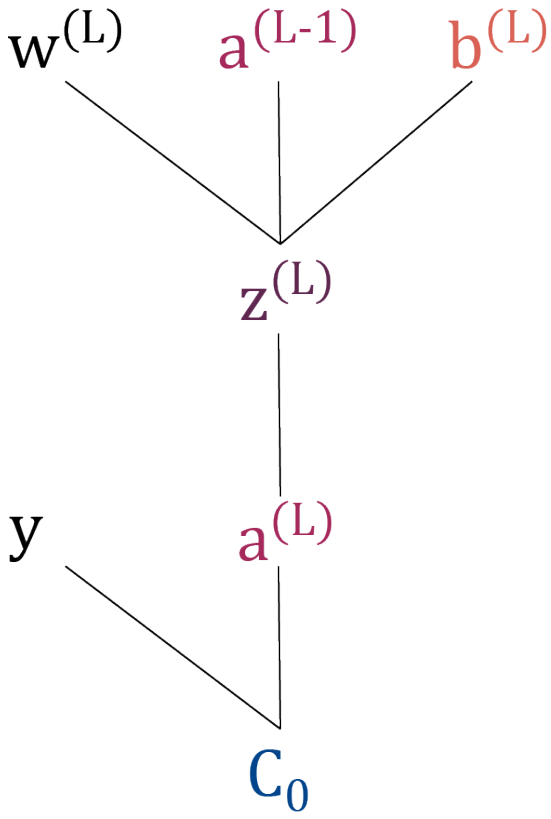
What free parameters do we have?

$$C(w_1, b_1, w_2, b_2, w_3, b_4)$$

How sensitive is our cost function to these variables?

$$C_0(\dots) = \left(a^{(L)} - y\right)^2$$

$$a^{(L)} = \sigma\left(w^{(L)} a^{(L-1)} + b^{(L)}\right) = \sigma\left(z^{(L)}\right)$$



Derivatives let us calculate how much to change our parameters to affect cost function

These happen sequentially

$$\frac{\partial C_0}{\partial w^{(L)}} =$$

Derivatives

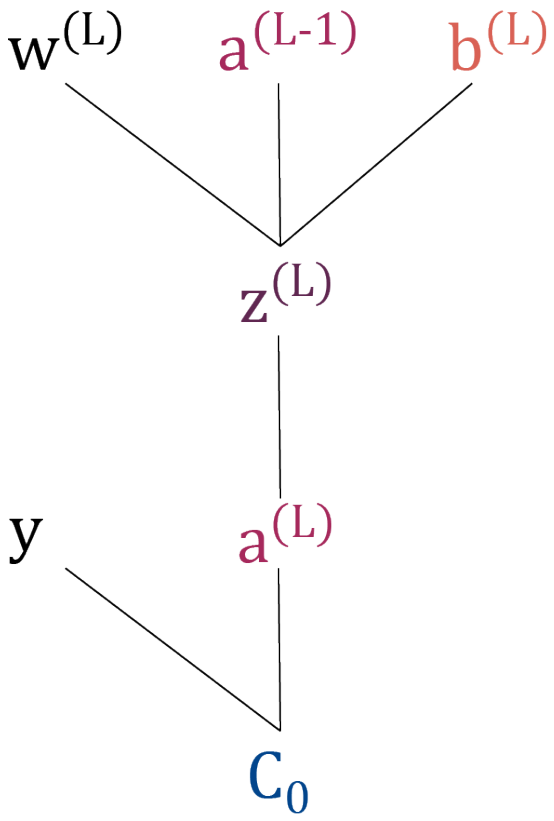
$$\frac{\partial C_0}{\partial a^{(L)}} =$$

$$\frac{\partial a^{(L)}}{\partial z^{(L)}} =$$

$$\frac{\partial z^{(L)}}{\partial w^{(L)}} =$$

Then average across all training examples

$$\frac{\partial C_0}{\partial w^{(L)}} =$$



Derivatives let us calculate how much to change our parameters to affect cost function

These happen sequentially

$$\frac{\partial C_0}{\partial w^{(L)}} = \frac{\partial z^{(L)}}{\partial w^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L)}} \frac{\partial C_0}{\partial a^{(L)}}$$

Derivatives

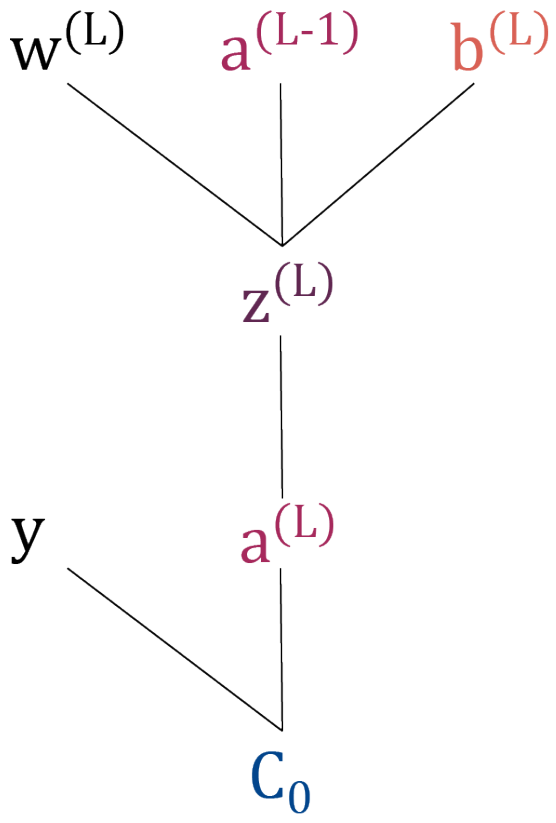
$$\frac{\partial C_0}{\partial a^{(L)}} = 2(a^{(L)} - y)$$

$$\frac{\partial a^{(L)}}{\partial z^{(L)}} = \sigma'\left(z^{(L)}\right)$$

$$\frac{\partial z^{(L)}}{\partial w^{(L)}} = a^{(L-1)}$$

Then average across all training examples

$$\frac{\partial C_0}{\partial w^{(L)}} = \frac{1}{n} \sum_{n} 2(a^{(L)} - y)\sigma'\left(z^{(L)}\right) a^{(L-1)}$$



Derivatives let us calculate how much to change our parameters to affect cost function

$\frac{\partial C_0}{\partial b^{(L)}}$ is nearly identical

These happen sequentially

$$\frac{\partial C_0}{\partial b^{(L)}} = \frac{\partial z^{(L)}}{\partial b^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L)}} \frac{\partial C_0}{\partial a^{(L)}}$$

Derivatives

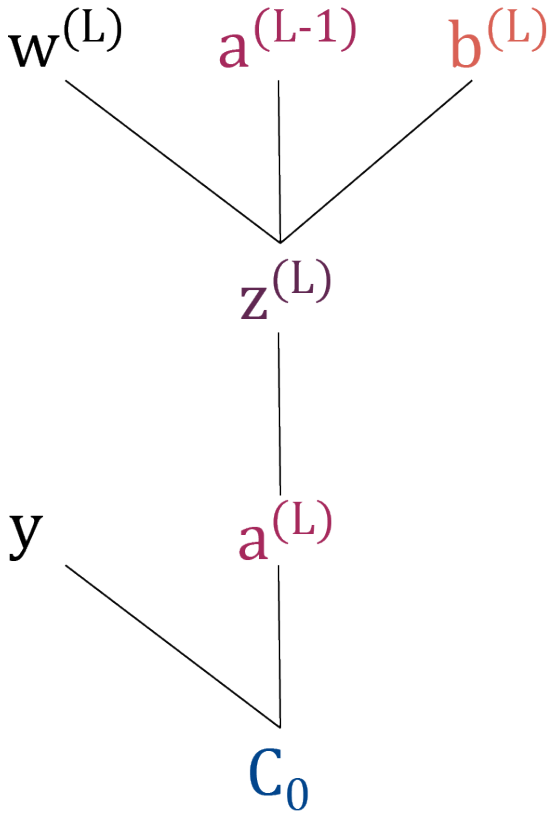
$$\frac{\partial C_0}{\partial a^{(L)}} = 2(a^{(L)} - y)$$

$$\frac{\partial a^{(L)}}{\partial z^{(L)}} = \sigma'(z^{(L)})$$

$$\frac{\partial z^{(L)}}{\partial b^{(L)}} = 1$$

Then average across all training examples

$$\frac{\partial C_0}{\partial b^{(L)}} = \frac{1}{n} \sum_{n} 2(a^{(L)} - y)\sigma'(z^{(L)})$$



Remember, gradient depends on all of our parameters, not just one

Gradient is over all tunable parameters

$$\nabla C = \begin{bmatrix} \frac{\partial C}{\partial w^{(1)}} \\ \frac{\partial C}{\partial b^{(1)}} \\ \vdots \\ \frac{\partial C}{\partial w^{(L)}} \\ \frac{\partial C}{\partial b^{(L)}} \end{bmatrix}$$

For more realistic networks (more than 1 node, it's not that much crazier…)

Backpropagation for arbitrary layer size

Cost function

$$C_0 = \sum_{j=0}^{n_L-1} \left(a_j^{(L)} - y_j\right)^2$$

Our z becomes

$$z_j^{(L)} = w_{j0}^{(L)} a_0^{(L-1)} + w_{j1}^{(L)} a_1^{(L-1)} + w_{j2}^{(L)} a_2^{(L-1)} + b_j^{(L)}$$

Activation of node in final layer is then just

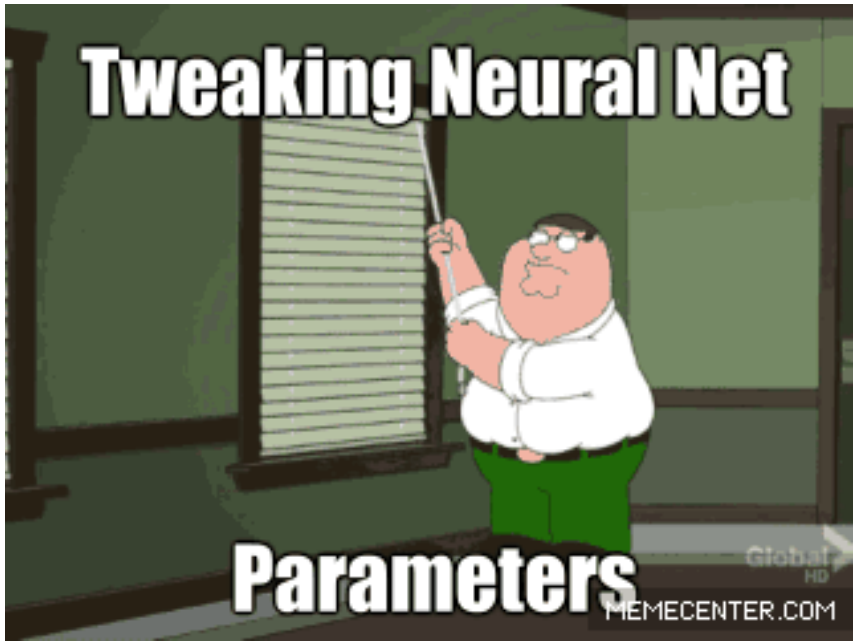
$$\sigma\left(z_j^{(L)}\right)$$

Chain rule cost sensitivity expression becomes

$$\frac{\partial C_0}{\partial w_{jk}^{(L)}} = \frac{\partial z_j^{(L)}}{\partial w_{jk}^{(L)}} \frac{\partial a_j^{(L)}}{\partial z_j^{(L)}} \frac{\partial C_0}{\partial a_j^{(L)}}$$

Tuning neural networks can be tricky

Parameters:
Architecture (number of nodes, number of layers)
Learning rates and weights (7 optimizers to choose from)
Activation function
Batch size (small is faster, higher variance; large is slow, less variance)
Epochs used for training
Regularization (dropout)



https://www.analyticsvidhya.com/blog/2021/05/tuning-the-hyperparameters-and-layers-of-neural-network-deep-learning/

Deep learning can get a little bit out of hand, it's helpful to do some sanity checks

Consider ElemNet

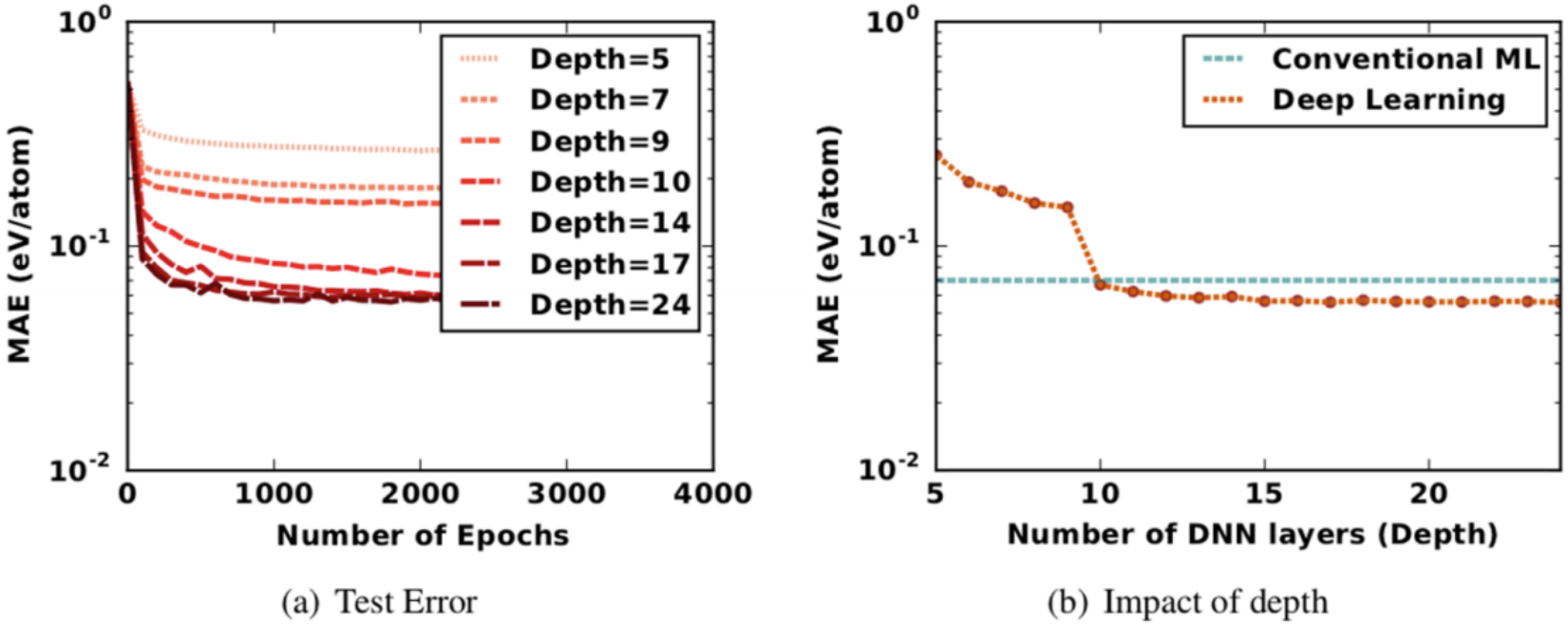
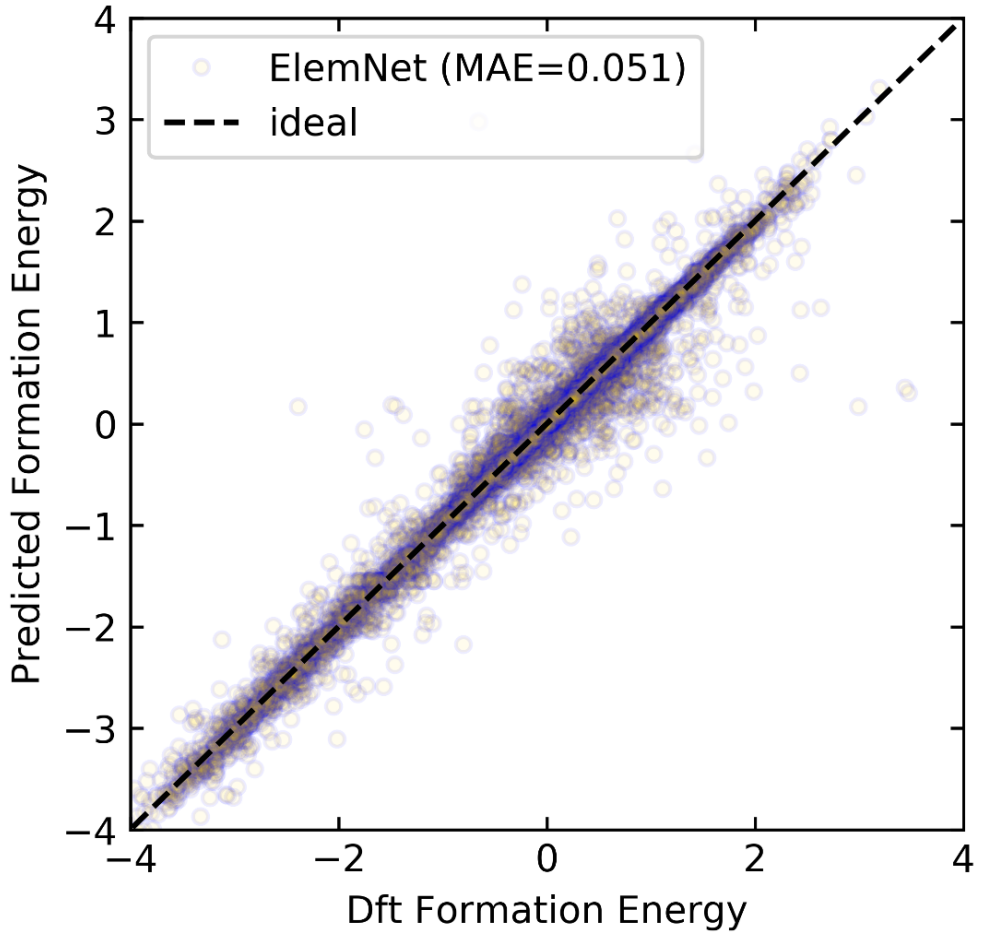
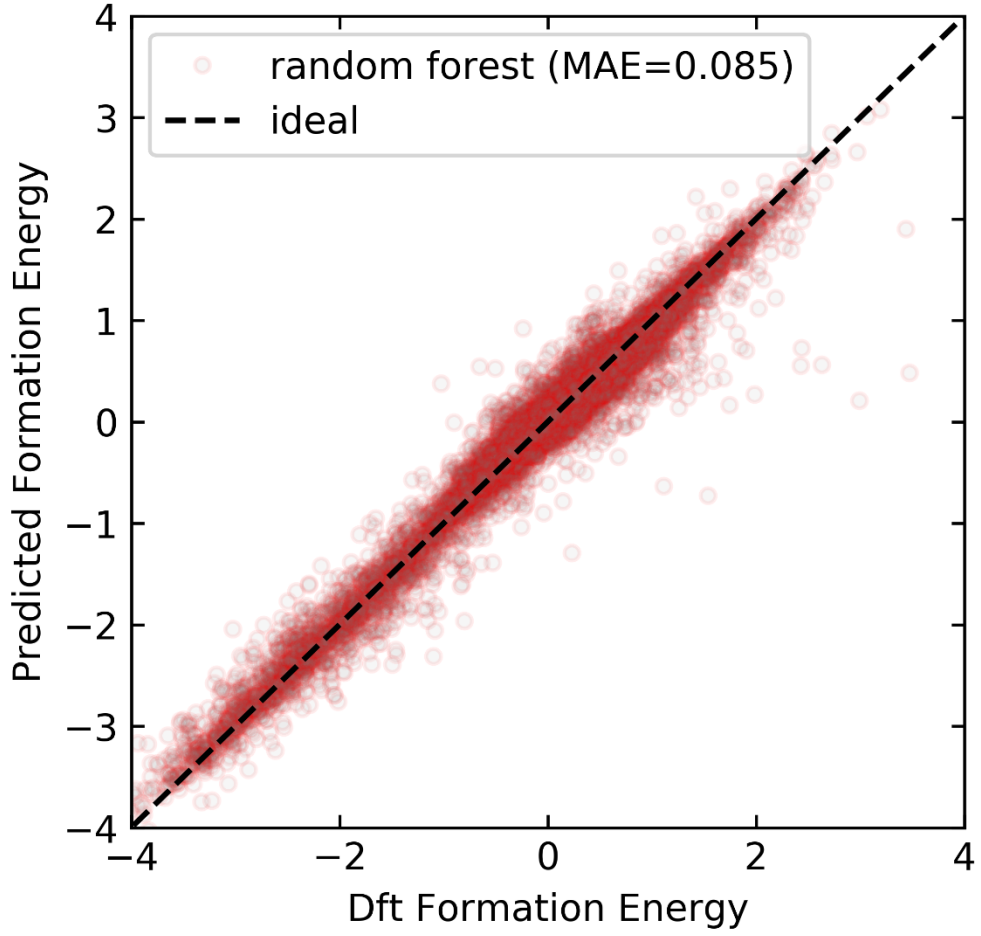


Figure 2. Performance of deep learning models of different depths in model architecture. The models are trained and tested on the lowest DFT-computed formation enthalpy of 256, 622 compounds. Here, we present the impact of depth of architecture for one sample split from our ten-fold cross validation. (**a**) Shows the mean absolute error (MAE) on the test dataset of 25, 662 compounds with unique compositions at different epochs for one split from the cross validation. The DNN models keep learning new features from the training dataset with the increase in the number of layers up to 17 layers, after which they begin to slowly overfit to the training data. (**b**) Shows the MAE for different depths of deep learning model architectures and also illustrates mean absolute error of the best performing conventional ML model trained using physical attributes computed on the same training and test sets. The deep learning model starts outperforming the best performing conventional ML model with an architecture depth of 10 layers, achieving the best performance at 17 layers, we refer to the best performing DNN model as *ElemNet*. The detailed architecture for *ElemNet* is available in the Method section.

Jha et al. ElemNet: Deep Learning the Chemistry of Materials From Only Elemental Composition, Sci Rep, 2018

How good is good enough? How much improvement will deep learning give us?



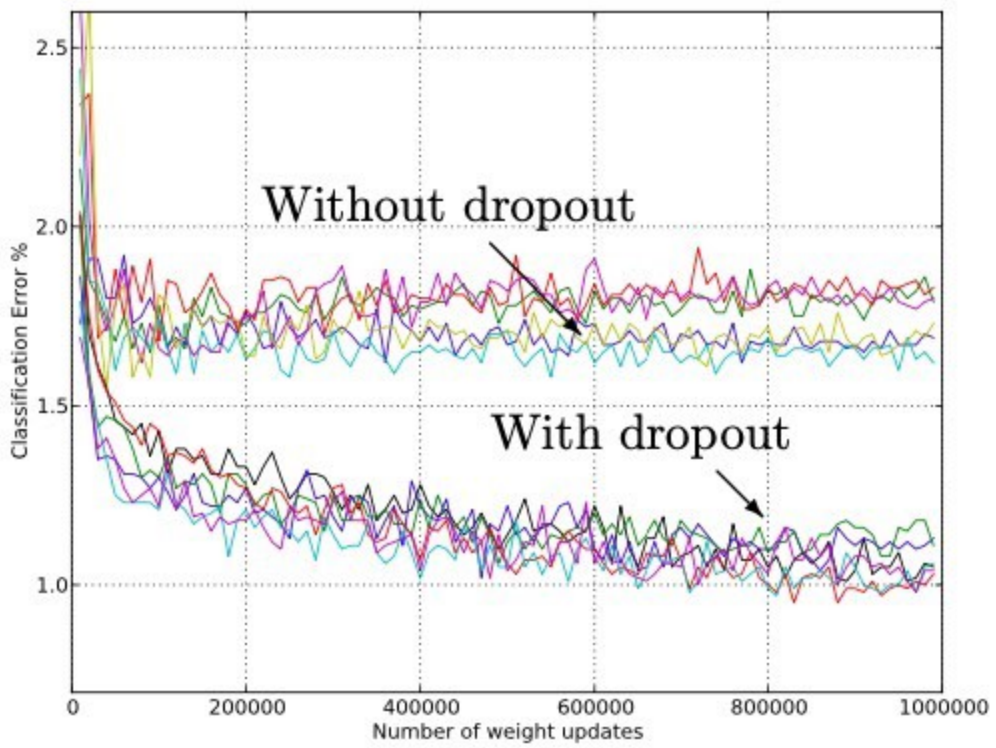


Classical models are absurdly easy to implement, in comparison

The random forest version of predicting formation energy is already absurdly easy to setup if we are willing to settle for the slightly worse performance

```
1import pandas as pd
2import matplotlib.pyplot as plt
3from utils.composition import generate_features as gf
4from sklearn.ensemble import RandomForestRegressor
5path = 'data/material_properties/elemnet_energy_atom/'
6df_train = pd.read_csv(path+'/train.csv')
7df_test = pd.read_csv(path+'test.csv')
8X_train, y_train, formulae_train = gf(df_train)
9X_test, y_test, formulae_test = gf(df_test, features_style='magpie')
10rf = RandomForestRegressor(n_estimators=100, max_features='auto')
11rf.fit(X_train, y_train)
12y_test_pred = rf.predict(X_test)
```

Dropout is a good way to prevent overfitting




```
#create model
model = Sequential()
#add model layers
model.add(Conv2D(64, kernel_size=3, activation='relu', input_shape=(28,28,1)))
model.add(Conv2D(32, kernel_size=3, activation='relu'))
model.add(Dropout(.5, noise_shape=None, seed=None)) #dropout layer
model.add(Conv2D(32, kernel_size=3, activation='relu'))

model.add(Flatten())
model.add(Dense(10, activation='softmax'))
```

Srivastava et al. Dropout: a simple way to prevent neural networks from overfitting, JMLR 2014

advanced deep learning