Neural Networks

Deep Learning

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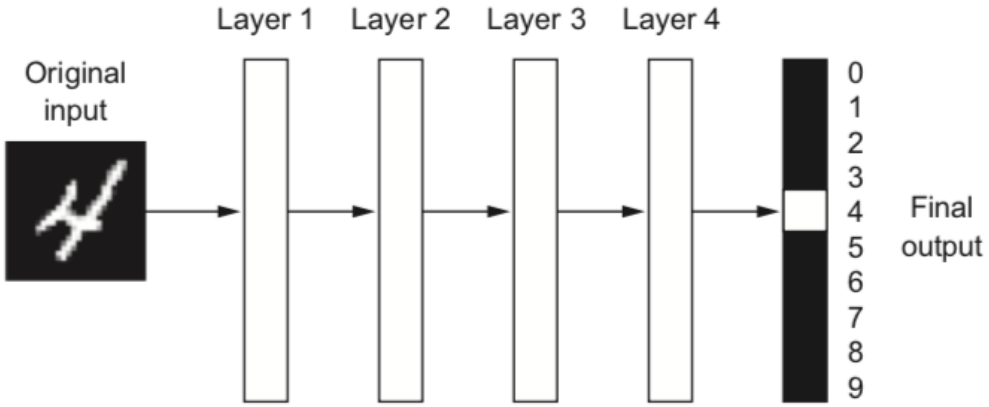
Overview

- Mathematical foundations
    - Tensors and tensor operations
    - Backpropagation and gradient descent
- Evaluation and Regularization
- Text Representations

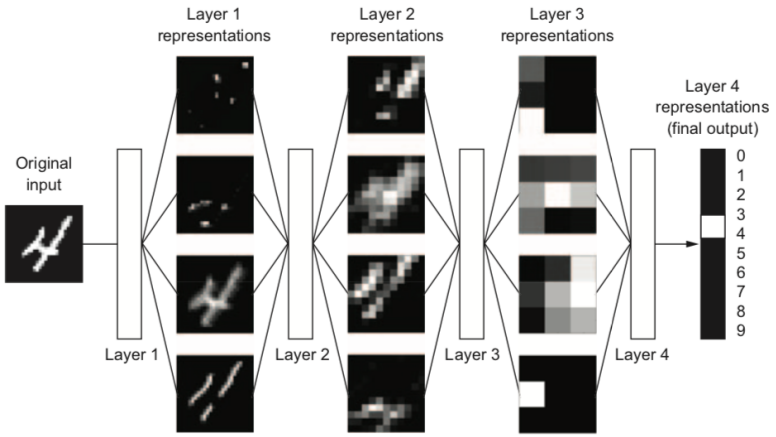
Neural networks

- The core building block of a neural network is the *layer*
- You can think of it as a *filter* for the data
    - Data goes in, and comes out in a more useful form
- Layers extract new *representations* of the data
- *Deep learning* models contain many such layers
    - They progressively *distill* (refine) the data



Feature maps

- Each layer transforms (maps) an input to possibly multiple outputs
- Each layer needs to *learn* how to do the mapping so that the final output is correct
- There are different *types* of layers that are constrained to certain mappings
    - Allows us to introduce mappings which we think are useful: *flexible!*

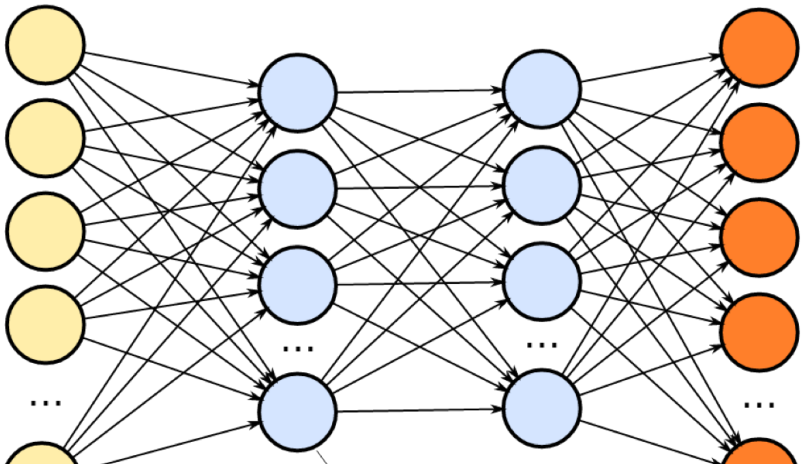


Terminology

1. Numerical(!) input features are fed to individual *nodes* of the *input layer* (yellow)
2. Each input is passed to a set of nodes in the *hidden layers* (blue)

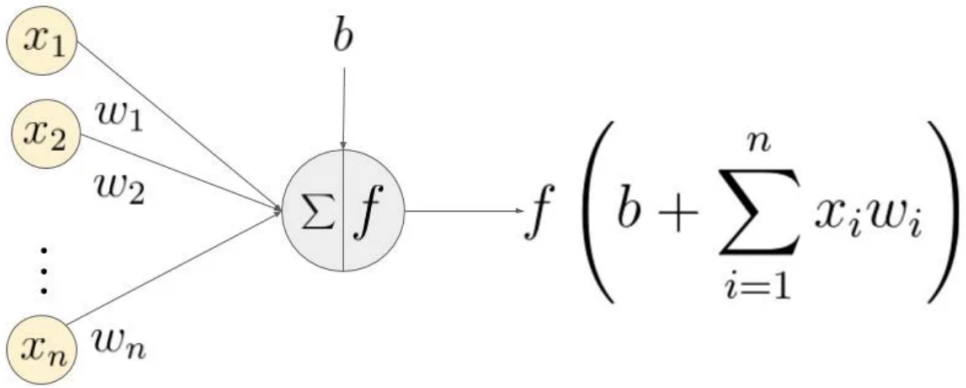
    - In *dense* layers, every previous layer node is connected to all nodes
    - Every node produces an output that is some function of all its inputs
3. The *output layer* has a node for every possible outcome (red)

    - A single regression value, multiple possible classes, or entire output images/signals/...



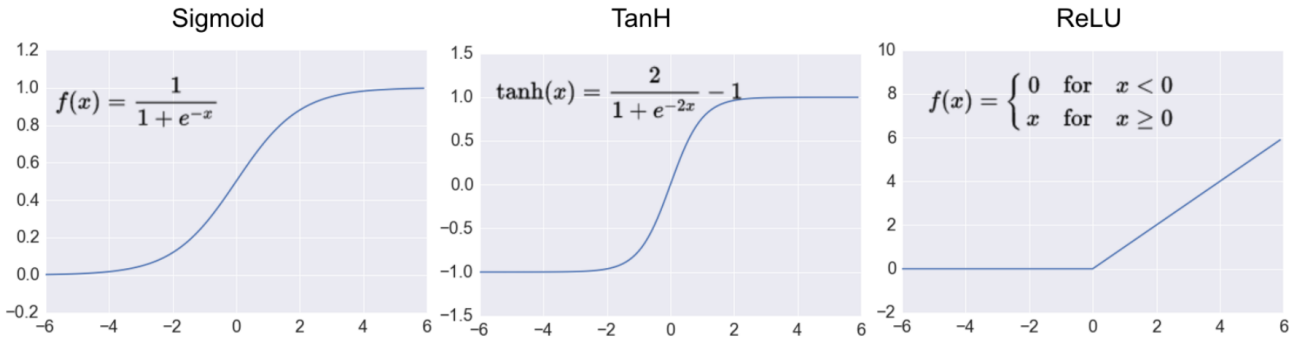
Nodes

- Each node gives each of its inputs a weight w_i
- Each node also has a bias b
    - Sometimes 'drawn' as an extra input with value '1'
- In its simplest form (a.k.a. the perceptron), each node outputs a weighted sum of the inputs: $y = \sum_i x_i w_i + b$
    - This is indeed equivalent to a linear model
- Even a deep neural net of perceptrons can only learn a linear model
    - To learn a non-linear model we need to transform y with an *activation function* f



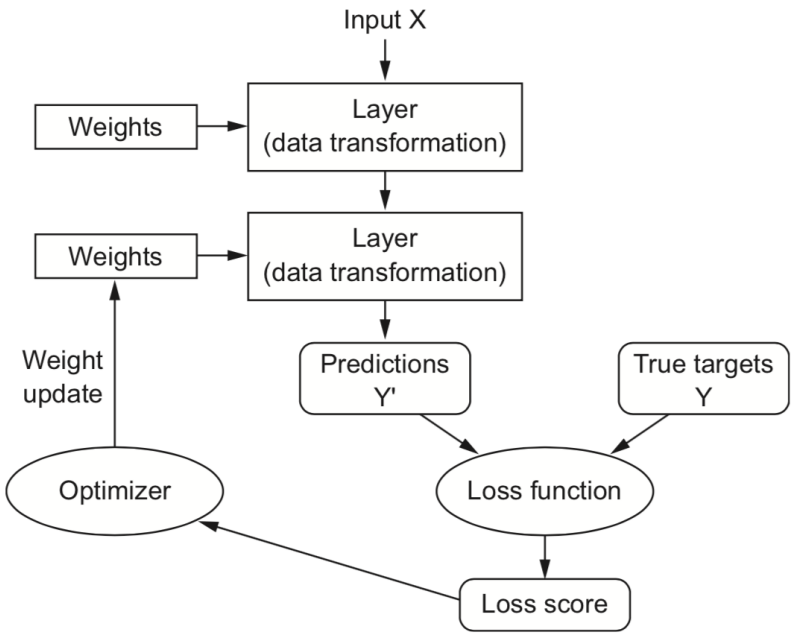
Activation functions

- For hidden nodes, popular choices are the *rectified linear unit* (ReLU) and *tanh*
    - There are many others. We'll come back to this soon!
    - ReLU is very cheap to compute, speeds up training
- For classification, we use *softmax* (or sigmoid)
    - Transforms the input into a probability for each specific class
    - This is exactly what we used for logistic regression!



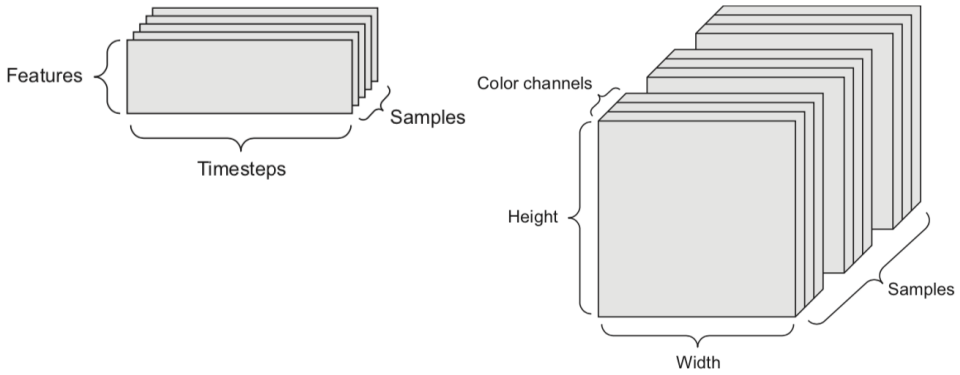
Training Neural Nets

- Each layer starts with random (small) weights
    - Or weights could be *transferred* from previously trained models (transfer learning or meta-learning)
- *Loss function*: Measures how well the model fits the training data
- *Optimizer*: Defines how to update the weights, e.g. gradient descent



Representing data

- We can represent all layer inputs (and outputs) as *tensors*
    - These are numerical n-dimensional array (with n axes)
    - 2D tensor: matrix (samples, features)
    - 3D tensor: grayscale images (samples, height, width)
        - or time series (samples, timesteps, features)
    - 4D tensor: color images (samples, height, width, channels)
    - 5D tensor: video (amples, frames, height, width, channels)



Implementing layers (from scratch)

- The operations that neural network layers perform on the data can be reduced to a *series of tensor operations*
- Imagine that we have a 2D input tensor **x**
- A dense layer with ReLU activation could be implemented as:

```
y = relu(dot(W, x) + b)
```

- Uses a 2D weight tensor **W**
    - One weight for every combination of input x_i and node n_j
- and a bias vector **b** (one value per node n_j)
- Performs a dot product, addition, and $relu(x) = max(x, 0)$

Element-wise operations

ReLU and addition are element-wise operations. Since numpy arrays support element-wise operations natively, these are simply:

```
def relu(x):
  return np.maximum(x, 0.)

def add(x, y):
  return x + y
```

Note: if y has a lower dimension than x, it will be *broadcasted*: axes are added to match the dimensionality, and y is repeated along the new axes

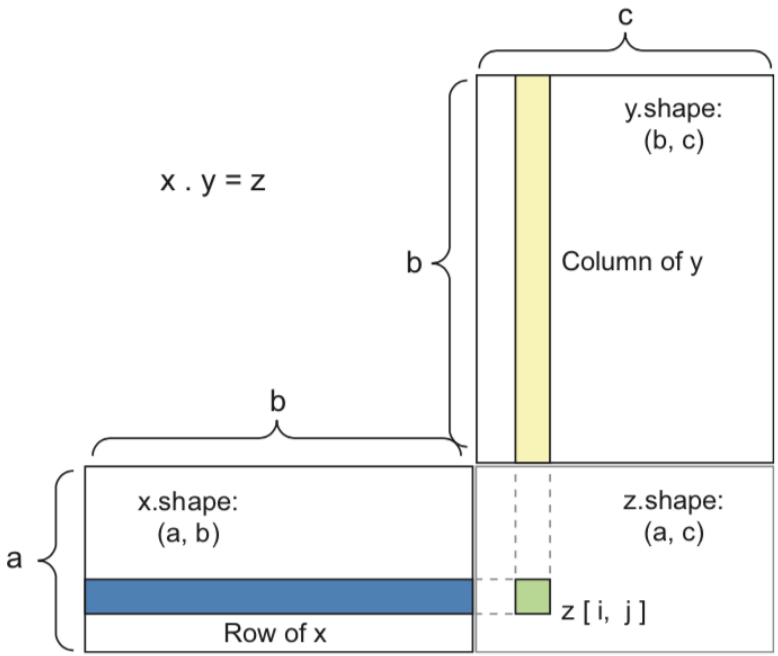
```
>>> np.array([[1,2],[3,4]]) + np.array([10,20])
array([[11, 22],
       [13, 24]])
```

Tensor dot

The dot product $x.\ y$ of two tensors can also be done easily with numpy:

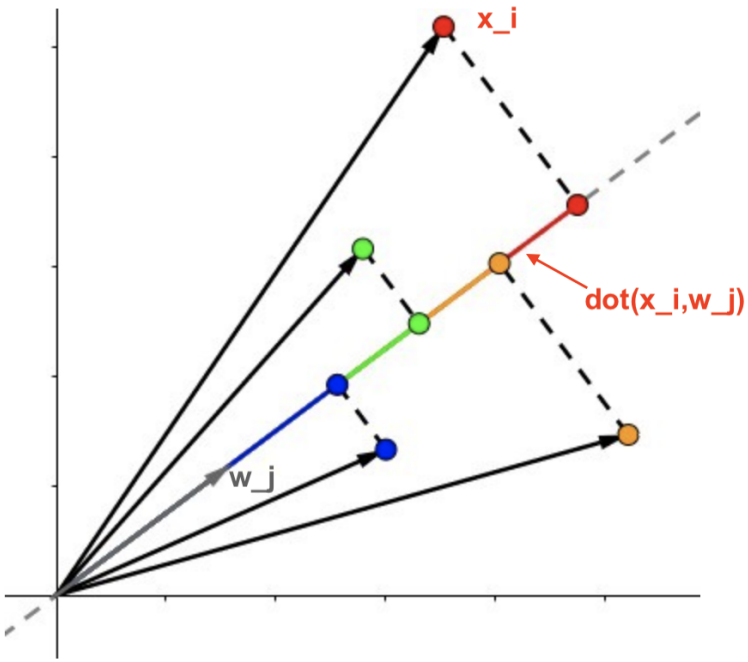
```
z = np.dot(x, y)
# z[i,j] = x[i,:] * y[:,j]
```

E.g. input **x** has *a* samples of *b* features, and **y** is the weight tensor for a dense layer with *c* nodes, then *z* is the layer output (with *c* features)



Geometric interpretation

- Dot product $z_{i,j} = x_i . w_j$ projects every vector x_i (colored) onto weight vector w_j (gray)
- $z_{i,j}$ is the projection length (colored line segment, until origin)
- In short, the dot product changes how the (colored) points relate to each other
- We aim to find a transformation $\mathbf{W}$ of x so that it becomes easy to:
    - separate the classes (classification)
    - learn a simple function (regression)



Gradient-based optimization

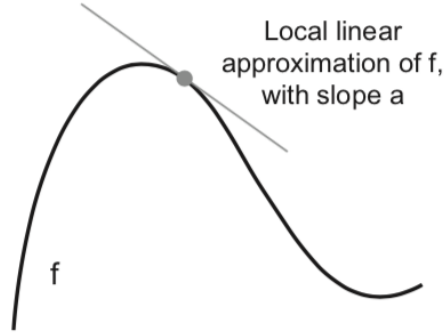
- How to find good values for W and b so that the data is transformed to a useful representation?
- Start with a random initialization, then loop:
    1. Draw a batch of training data x
    2. *Forward pass*: run the network on x to yield y_{pred} (tensor operations)
    3. Compute the loss (mismatch between y_{pred} and y)
    4. Update W, b in a way that slightly reduces the loss (OK, but how?)

Update rule

Naive approach (expensive):

- Choose one weight $w_{i,j}$ to optimize, freeze the others
- Run the network (twice) with $w_{i,j} - \epsilon$ and $w_{i,j} + \epsilon$
- Compute the losses $L(x, w_{i,j} - \epsilon)$ and $L(x, w_{i,j} + \epsilon)$ given current batch x
- Keep the one that reduces the loss most, then repeat

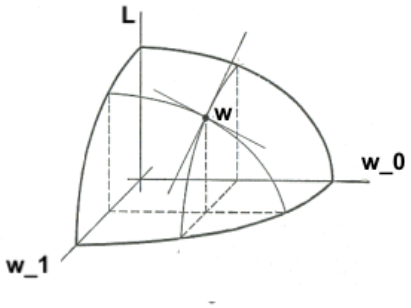
Better:

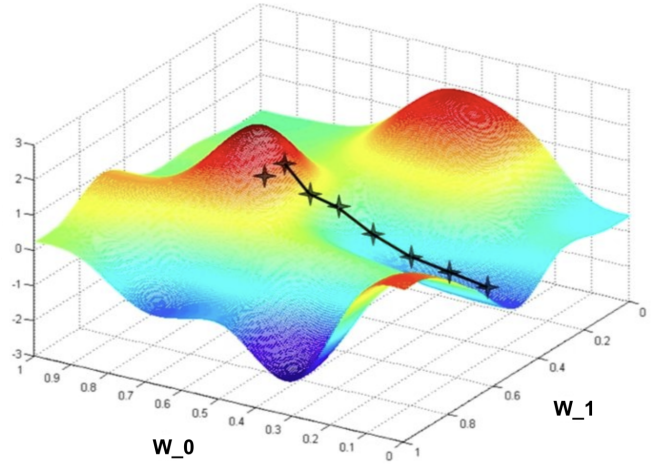


- Choose a loss function L that is *differentiable*
  - Also all underlying tensor operations need to be differentiable
- Then we can compute the derivative $\frac{\partial L(x,w_{i,j})}{\partial w_{i,j}} = a$
- So that $L(x, w_{i,j} + \epsilon) \approx y + a * \epsilon$
- We can now estimate weights without recomputing L

Gradients

- A *gradient* ∇L is the generalization of a derivate to n-dimensional inputs
  - Approximates the *curvature* of the loss function $L(x, W)$ around a given point W
  - Vector of partial derivatives $\nabla L = \left[\frac{\partial L}{\partial w_{0,0}}, \frac{\partial L}{\partial w_{0,1}}, \ldots \right]$
- Update: if L is differentiable, then *new* weight tensor $W_{i+1} = W_i - \frac{\partial L(W_i)}{\partial W} * step$
  - *step* is a small scaling factor (learning rate)
  - Go against the curvature to a lower place on the curve
- Now repeat with a new batch of data x





Stochastic gradient descent (SGD)

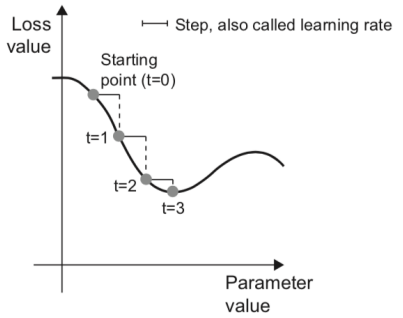
Mini-batch SGD:

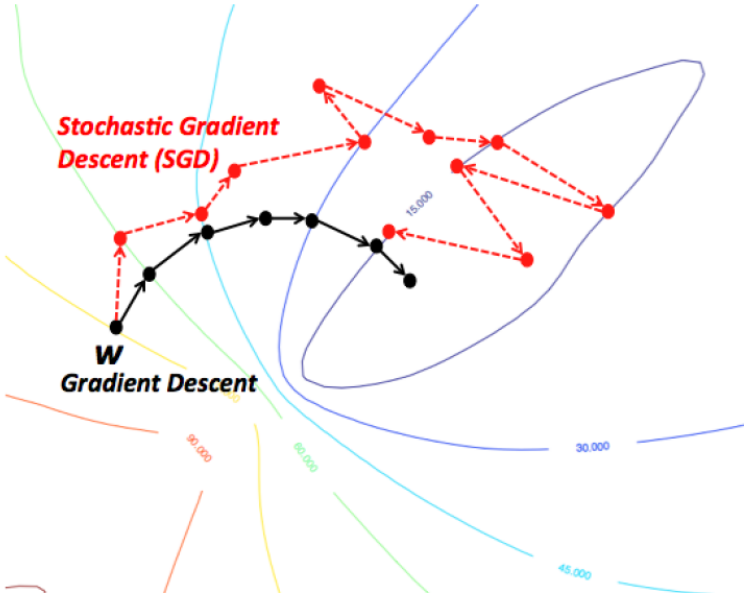
1. Draw a batch of *batch_size* training data x and y
2. *Forward pass*: run the network on x to yield y_{pred} (tensor operations)
3. Compute the loss L (mismatch between y_{pred} and y)
4. *Backward pass*: Compute the gradient of the loss with regard to W
5. Update W: $W_{i+1} = W_i - \frac{\partial L(x, W_i)}{\partial W} * step$

Repeat until n passes (epochs) are made through through the entire training set.

SGD Variants:

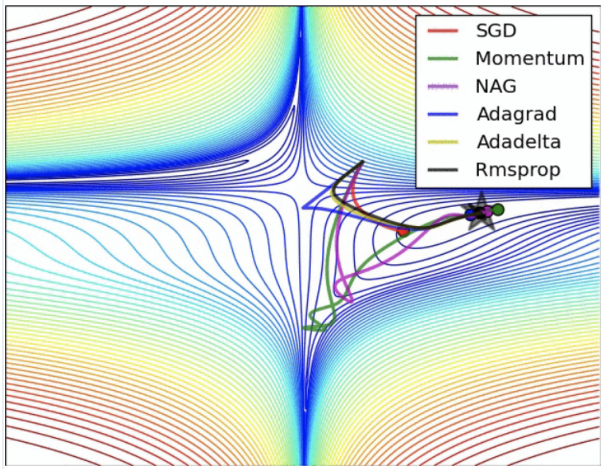
- Batch Gradient Descent: compute gradient on entire training set
    - More accurate gradients, but more expensive
- True Stochastic Gradient Descent: repeat for each individual data points (noisy)
- Minibatch SGD strikes a balance between the two (given the right batch size)





SGD: many more variants

- With SGD, it is quite easy to get stuck in a local minimum
- Learning rate decay: start with a big step size and then decrease
- Momentum: do a larger update if previous update has large loss improvement
    - Like a ball that gains speed if it goes down steeply
- Adaptive step size for each W_i: adam, Adagrad,...
    - See http://ruder.io/optimizing-gradient-descent/index.html (http://ruder.io/optimizing-gradient-descent/index.html)
- Some intuitions say that in high-dimensional spaces, most local minima are near the global minimum



Backpropagation

- In practice, a neural network function consist of many tensor operations chained together
  - e.g. $f(W1, W2, W3) = a(W1, b(W2, c(W3)))$
- How can we still compute $\frac{\partial L(x,W)}{\partial W}$?
- As long as each tensor operation is differentiable, we can still compute the gradient thanks to the chain rule:

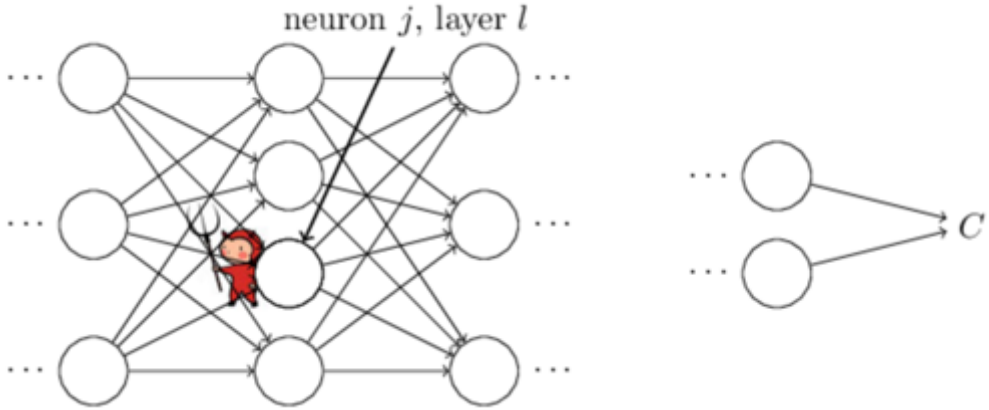
$$f(g(x)) = f'(g(x)) * g'(x)$$

- We can let the gradient *backpropagate* through the layers
- So, if we have a hidden node $h(x) = f(W_1 x + b_1)$, $net(x) = W_1 x + b_1$, and output node $o(x) = g(W_2 h(x) + b_2)$

$$\frac{\partial o(\mathbf{x})}{\partial W_1} = \underbrace{\frac{\partial o(\mathbf{x})}{\partial h(\mathbf{x})}}_{\text{Backpropagation of gradient of layer above}} \underbrace{\frac{\partial h(\mathbf{x})}{\partial \text{net}(\mathbf{x})}}_{\text{Gradient of Activation function f}} \underbrace{\frac{\partial \text{net}(\mathbf{x})}{\partial W_1}}_{\text{Input to 1st layer x}}$$

Intuition

- Imagine a demon that adds a change $\Delta x_j = x_{j,0}, x_{j,1}, \ldots$ to inputs of neuron j
  - The neuron now outputs $\sigma(x_j + \Delta x_j)$ instead of $\sigma(x_j)$
  - Propagates through network, ultimately causing an error $\frac{\delta E}{\delta x_j} \Delta x_j$
- A *good* demon tries to find a Δx_j that *reduces* the error
  - If it knows $\frac{\delta E}{\delta x_j}$ is large, it chooses Δx_j to reduce it
  - If gradient $\frac{\delta E}{\delta x_j} > 0$, increasing the output of x_j will increase the error
  - Decrease the output by increasing the weights of negative inputs, or decreasing the weights of positive inputs.

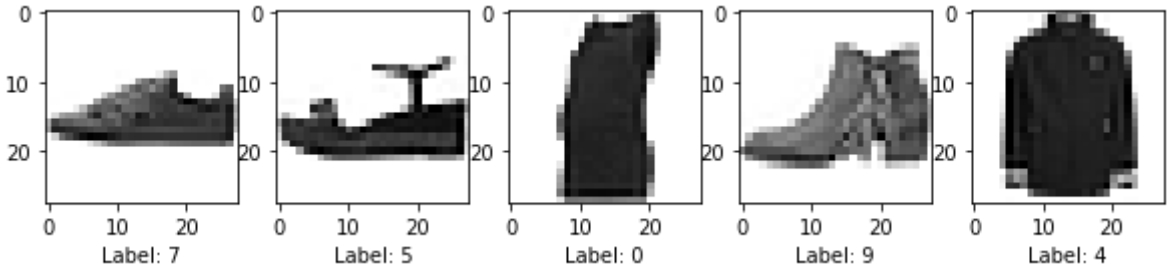


Backpropagation in action

To get an intuitive understanding of how backpropagation works, here is a nice animation of the entire process: https://youtu.be/Ilg3gGewQ5U?list=PLZHQObOWTQDNU6R1_67000Dx_ZCJB-3pi&t=403 (https://youtu.be/Ilg3gGewQ5U?list=PLZHQObOWTQDNU6R1_67000Dx_ZCJB-3pi&t=403)

Using neural networks

Example: Fashion-MNIST dataset contains 28x28 pixel images of 10 classes of fashion items



Building the network

- One dense hidden ReLU layer with 128 nodes
  - Input from a 28x28 matrix
- Output softmax layer with 10 nodes
- Example using Keras, a well-known API for building neural networks
  - Integrated in Tensorflow, but also in other backends

```
from tensorflow.keras import models
from tensorflow.keras import layers

network = models.Sequential()
network.add(layers.Dense(128, activation='relu', input_shape=(28 * 28
,)))
network.add(layers.Dense(10, activation='softmax'))
```

Model summary

- Lots of parameters (weights and biases) to learn!
  - hidden layer: (28 *28 + 1)* 128 = 100480
  - output layer: (128 + 1) * 10

```
Model: "sequential"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense (Dense)                (None, 128)               100480
_________________________________________________________________
dense_1 (Dense)              (None, 10)                1290
=================================================================
Total params: 101,770
Trainable params: 101,770
Non-trainable params: 0
_________________________________________________________________
```

Compilation

We still need to specify how we want the network to be trained:

- **Loss function**: The objective function used to measure how well the model is doing, and steer itself in the right direction
  - e.g. Cross Entropy (*negative log likelihood* or *log loss*) for classification
- **Optimizer**: How to optimize the model weights in every iteration.
  - usually a variant of stochastic gradient descent (http://ruder.io/optimizing-gradient-descent/index.html#momentum)
  - `RMSprop` uses different learning rates for every weight
- **Metrics** to monitor performance during training and testing.
  - e.g. accuracy

```
network.compile(optimizer='rmsprop',
                loss='categorical_crossentropy',
                metrics=['accuracy'])
```

Cross-entropy loss

- We've seen *cross-entropy loss* (or *log loss*) over C classes before
  - Measures how similar the actual and predicted probability distributions are
  - Compute cross-entropy $H(y, \hat{y})$ between true y and predicted $\hat{y}$

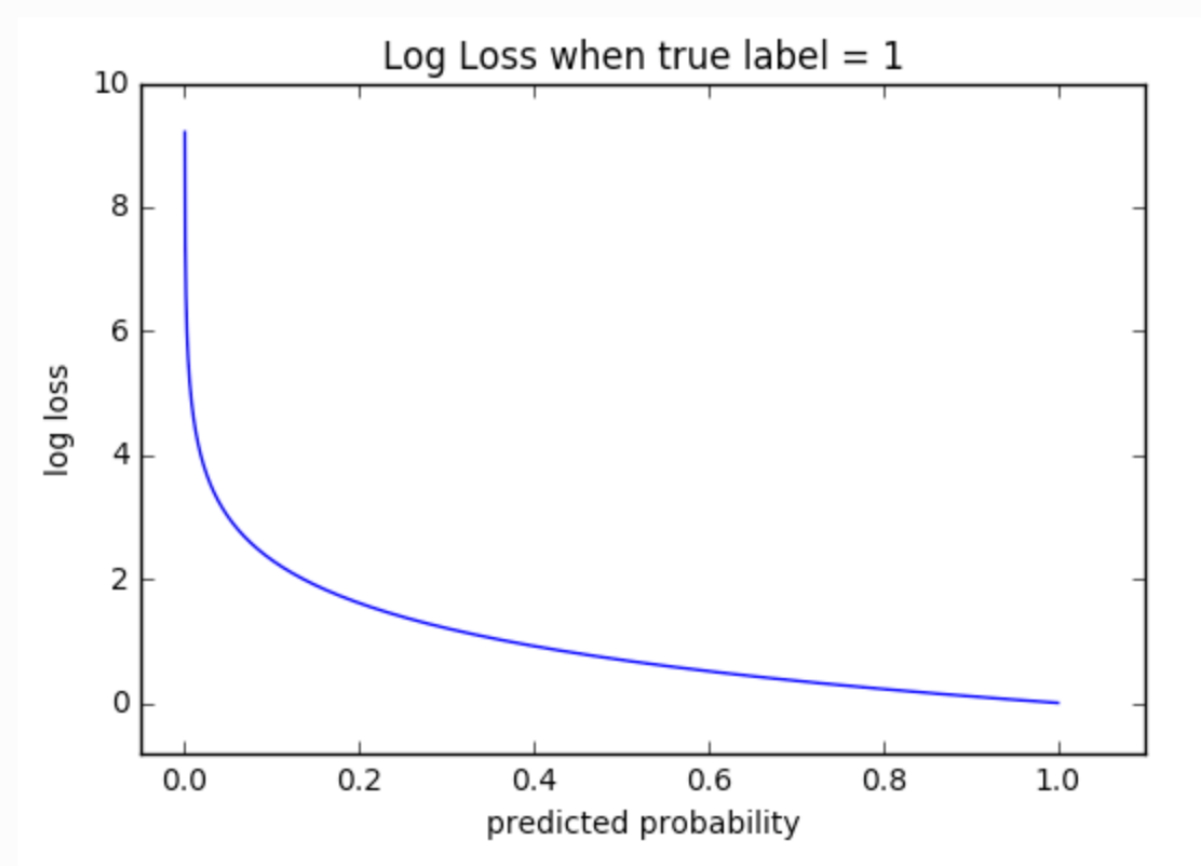
$$H(y, \hat{y}) = -\sum_{c=1}^{C} y_c \log(\hat{y}_c)$$

  - Sum up over all training samples
- *binary cross-entropy loss* is the case for 2 classes ($i = 0, 1$ $y_1 = y$, $y_0 = 1 - y$, $y_1 = \hat{y}$, $y_0 = 1 - \hat{y}$)

$$H(y, \hat{y}) = -ylog(\hat{y}) - (1 - y)log(1 - \hat{y})$$

Cross-entropy loss

- exponentially larger penalty as the predicted probability $\hat{y}$ is further away from the ground truth (here: $y = 1$)



Preprocessing

- Neural networks are sensitive to scaling, so always scale the inputs
- The network expects the data in a certain shape, e.g. (n, 28 * 28)
    - reshape the tensor to the correct input shape
- In classification, every class is an output node, so categorically encode the labels
    - e.g. class '4' becomes [0,0,0,0,1,0,0,0,0,0]

Training

- Optimizes the model parameters (weights) with mini-batch SGD
- We choose 5 epochs and a batch size of 128

```
Train on 60000 samples
Epoch 1/5
60000/60000 [==============================] - 6s 99us/sample - loss: 0.50
78 - accuracy: 0.8192
Epoch 2/5
60000/60000 [==============================] - 6s 96us/sample - loss: 0.38
29 - accuracy: 0.8632
Epoch 3/5
60000/60000 [==============================] - 5s 84us/sample - loss: 0.35
16 - accuracy: 0.8753
Epoch 4/5
60000/60000 [==============================] - 6s 102us/sample - loss: 0.3
341 - accuracy: 0.8824
Epoch 5/5
60000/60000 [==============================] - 6s 98us/sample - loss: 0.32
23 - accuracy: 0.8868
```

Prediction

We can now call `predict` or `predict_proba` to generate predictions

```
network.predict(X_test)
```

```
Prediction:  [0.994607  0.        0.0000003 0.0000022 0.        0.
0.0053905
 0.        0.        0.       ]
```

Evaluation

Evaluate the trained model on the entire test set

```
test_loss, test_acc = network.evaluate(X_test, y_test)
```

```
10000/10000 [==============================] - 1s 58us/sample - loss: 0.33
82 - accuracy: 0.8824
Test accuracy: 0.8824
```

Tuning the model

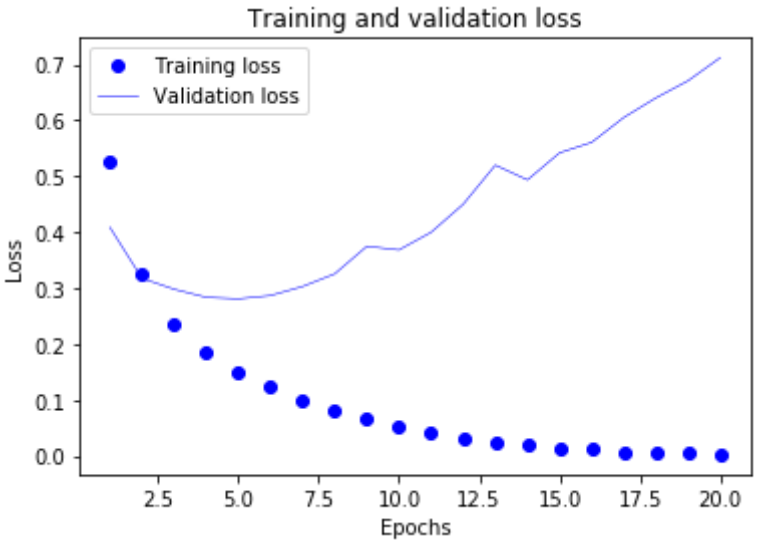
- There are a *lot* of choices that can (should) be optimized:
    - Number and types of layers
    - Layer hyperparameters
        - Number of nodes, shape
        - Activation functions
        - ...
    - Loss function (and hyperparameters)
    - SGD optimizer (and hyperparameters)
        - Learning rate
        - Batch size
        - Number of epochs
        - ...

Tuning the number of epochs

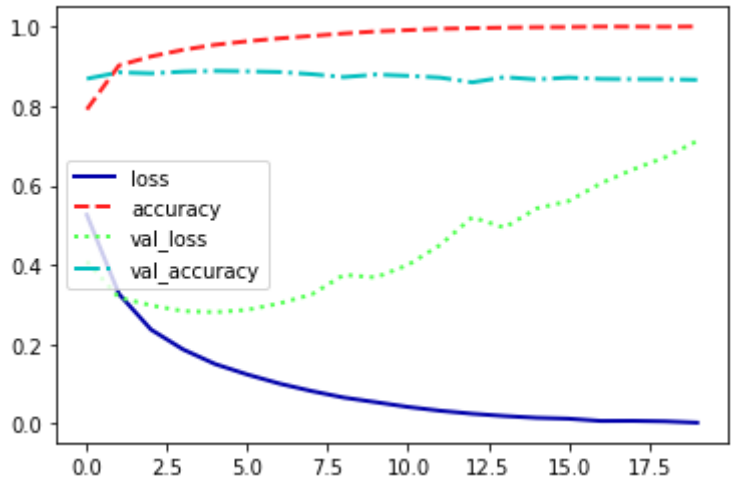
- How many epochs do we need for training?
- Train the neural net and track the loss after every iteration on a validation set
- We start with 20 epochs in minibatches of 512 samples

We can now retrieve visualize the loss on the validation data

- The training loss keeps decreasing, due to gradient descent
- The validation loss peaks after a few epochs, after which the model starts to overfit



Confirm that accuracy follows the same (although inverse) behavior as the loss



Early stopping

One simple technique to avoid overfitting is to use the validation set to 'tune' the optimal number of epochs

- In this case, we could stop after 4 epochs
- Note: validation loss can be bumpy, best use a moving average of inspect manually.

```
model.fit(x_train, y_train, epochs=4, batch_size=512, verbose=0)
result = model.evaluate(x_test, y_test)
```

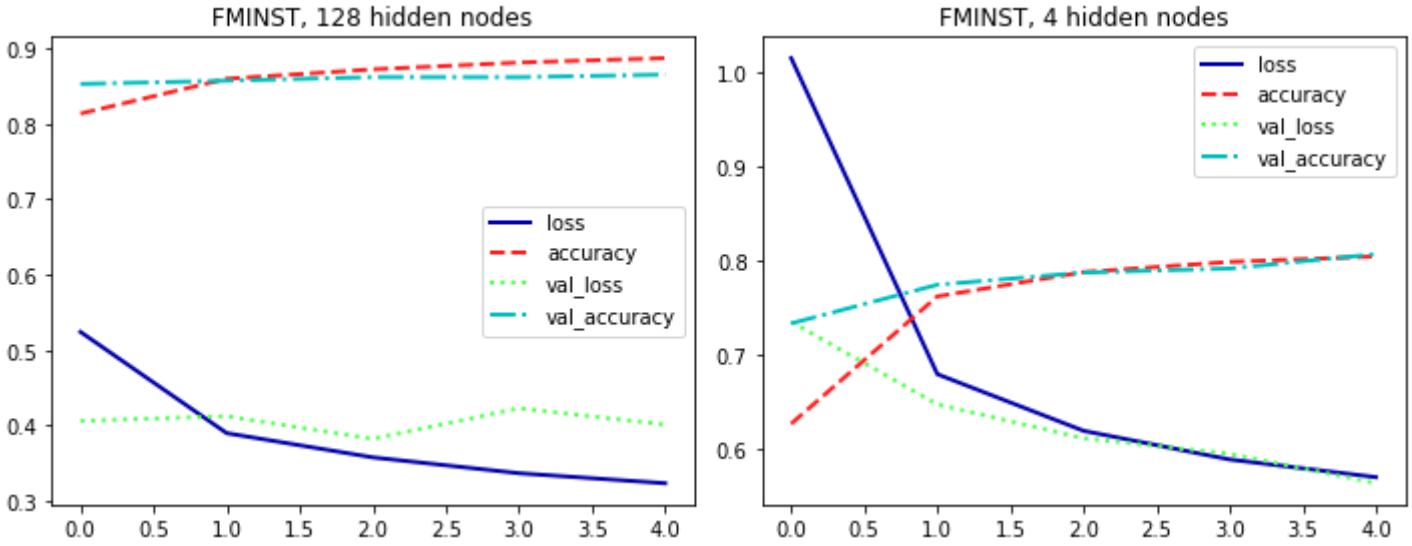
```
25000/25000 [==============================] - 4s 157us/sample - loss: 0.4
960 - accuracy: 0.8604
Loss: 0.4960, Accuracy:  0.8604
```

Regularization: build smaller networks

- The easiest way to avoid overfitting is to use a simpler model
- The number of learnable parameters is called the model *capacity*
- A model with more parameters has a higher *memorization capacity*
    - The entire training set can be `stored` in the weights
    - Learns the mapping from training examples to outputs
- Forcing the model to be small forces it to learn a compressed representation that generalizes better
    - Always a trade-off between too much and too little capacity
- Start with few layers and parameters, incease until you see diminisching returns

Tuning the number of nodes

- If a layer is too 'narrow', it will 'drop' some information, which can never be recovered by subsequent layers
    - *Information bottleneck*: information-theoretic framework to compute a bound on the `capacity` of the network
- Imagine that you need to learn 10 outputs (e.g. classes) and your hidden layer has 2 nodes
    - This is like trying to learn 10 separating hyperplanes from a 2-dimensional representation
- If your layers are too 'wide', the network will overfit, basically 'memorizing' the training data
    - Try to make the layers as small as possible (e.g. using the validation set), but not smaller


FMINST, 128 hidden nodes
loss
accuracy
val_loss
val_accuracy
FMINST, 4 hidden nodes
loss
accuracy
val_loss
val_accuracy

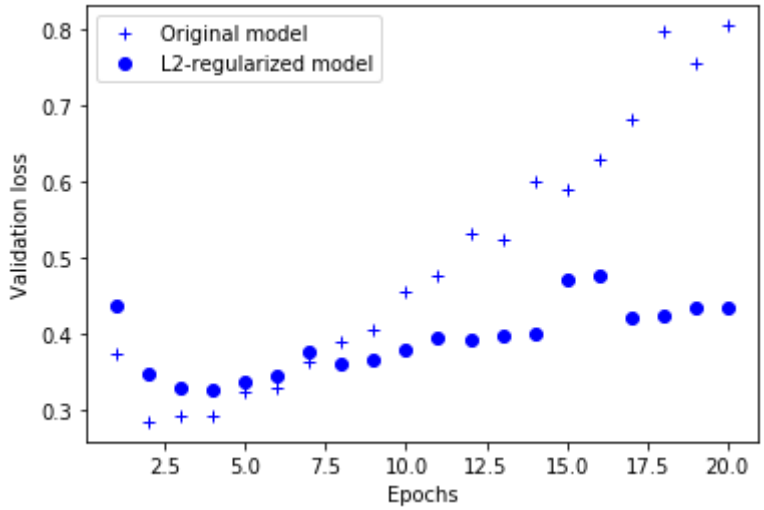
Weight regularization

- As we did many times before, we can also add weight regularization to our loss function
- L1 regularization: leads to *sparse networks* with many weights that are 0
- L2 regularization: leads to many very small weights
    - Also called *weight decay* in neural net literature
- In Keras, add `kernel_regularizer` to every layer

```
from keras import regularizers

l2_model = models.Sequential()
l2_model.add(layers.Dense(16, kernel_regularizer=regularizers.l2(0.001),
                          activation='relu', input_shape=(10000,)))
l2_model.add(layers.Dense(16, kernel_regularizer=regularizers.l2(0.001),
                          activation='relu'))
l2_model.add(layers.Dense(1, activation='sigmoid'))
```

L2 regularized model is much more resistant to overfitting, even though both have the same number of parameters



You can also try L1 loss or both at the same time

```
from keras import regularizers

# L1 regularization
regularizers.l1(0.001)

# L1 and L2 regularization at the same time
regularizers.l1_l2(l1=0.001, l2=0.001)
```

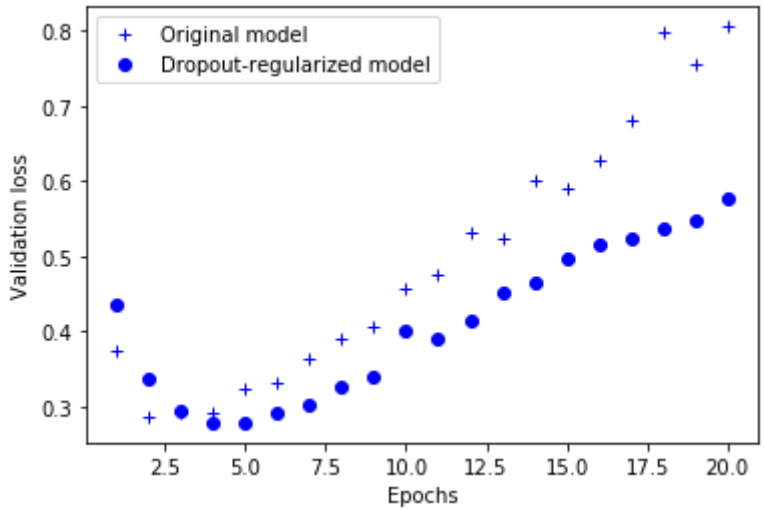
Dropout

- One of the most effective and commonly used regularization techniques
- Randomly set a number of outputs of the layer to 0 every iteration
- Idea: break up accidental non-significant learned patterns
- *Dropout rate*: fraction of the outputs that are zeroed-out
    - Usually between 0.2 and 0.5
- At test time, nothing is dropped out, but the output values are scaled down by the dropout rate
    - Balances out that more units are active than during training
- In Keras: add `Dropout` layers between the normal layers

```
dpt_model = models.Sequential()
dpt_model.add(layers.Dense(16, activation='relu', input_shape=(10000,)))
dpt_model.add(layers.Dropout(0.5))
dpt_model.add(layers.Dense(16, activation='relu'))
dpt_model.add(layers.Dropout(0.5))
dpt_model.add(layers.Dense(1, activation='sigmoid'))

dpt_model.compile(optimizer='rmsprop',
                  loss='binary_crossentropy',
                  metrics=['acc'])
```

Dropout finds a better model, and overfits more slowly as well



Batch Normalization

- Normalization (in general) aims to make different examples more similar to each other
    - Easier to learn and generalize
- Batch normalization layer adaptively normalizes data, even as the mean and variance change over time during training.
    - It works by internally maintaining an exponential moving average of the batch-wise mean and variance of training data
    - Helps with gradient propagation, allows for deeper networks.

```
dense_model.add(layers.Dense(32, activation='relu'))
dense_model.add(layers.BatchNormalization())
```

SGD Hyperparameter tuning

SGD has many important hyperparameters to tune:

- Learning rate
    - Too low: slow convergence, may get stuck in local minima
    - Too high: may lead to *divergence*: train loss *increases* with training
- Learning rate decay
    - It is often useful to start with a high learning rate and then decrease it during training
    - Many variants of this approach exist
- Batch size
    - Small batch size may be slower, more erratic
    - Medium batch sizes (24-32) often recommended
    - Large batch sizes can decrease performance ('generalization gap')
    - Intense research topic (https://openreview.net/pdf?id=B1Yy1BxCZ)
- ...

Tuning multiple hyperparameters

- You can wrap Keras models as scikit-learn and use any of its tuning techniques
- Keras also has built-in RandomSearch (and HyperBand - see later)

```
def build_model(hp){
    m.add(Dense(units=hp.Int('units', min_value=32, max_value=512, step=
32)))
    m.compile(optimizer=Adam(hp.Choice('learning rate', [1e-2, 1e-3, 1e-
4])))
    return model;}

from tensorflow.keras.wrappers.scikit_learn import KerasClassifier
clf = KerasClassifier(make_model)
grid = GridSearchCV(clf, param_grid=param_grid, cv=3)

from kerastuner.tuners import RandomSearch
tuner = keras.RandomSearch(build_model, max_trials=5)
```

Regularization recap

- Get more training data
- Reduce the capacity of the network
- Try weight regularization, dropout, batch normalization
- Start with a simple model and add capacity, or start with a complex model and then regularize

Handling textual data

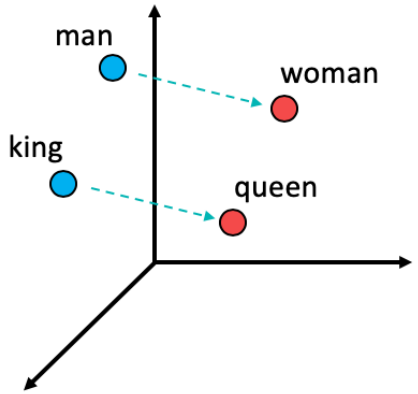
Textual data can be represented in different ways

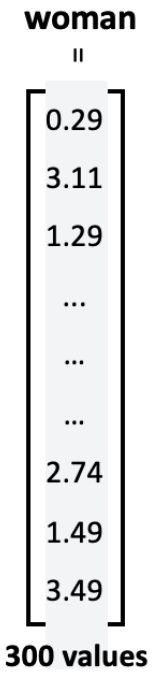
- Every 'document' (e.g. a review, tweet,...) is represented by a vector
- Bag-of-words representation
    - Build a dictionary of the most frequent words (e.g. 10000)
    - One-hot-encoding: 10000 features, '1.0' if the word occurs
    - TF-IDF: Term frequency over inverse document frequency
        - Count how many times each word occurs and normalize by the frequency across documents
- Word embeddings

Word Embeddings

- An embedding maps each word to a point in an n-dimensional space (e.g. 300 values), so that similar words are close to each other
    - Can usually be imported as an 'Embedding' layer
- There are different ways to learn word embeddings. Most common are:
    - Word2Vec: Learn encoding based on the words that are typically in a window around the word
        - Encoding is learned using a 1-layer neural net
    - GloVe (Global Vector): Count co-occurrences of words in a matrix
        - Use a low-rank approximation to get a condensed vector representation
    - FastText: learns embedding for n-grams rather than complete words
        - Can also produce embeddings for new words
    - BERT, ELMO,...: learn a context-dependent embedding: the some word has a different embedding depending on the sentence it appears in

Word embeddings: Word2Vec and GloVe





Word2Vec (prediction)

I	like	playing	**football**	with	my	friends

This is	the	tallest	**tree**	I	have	ever seen

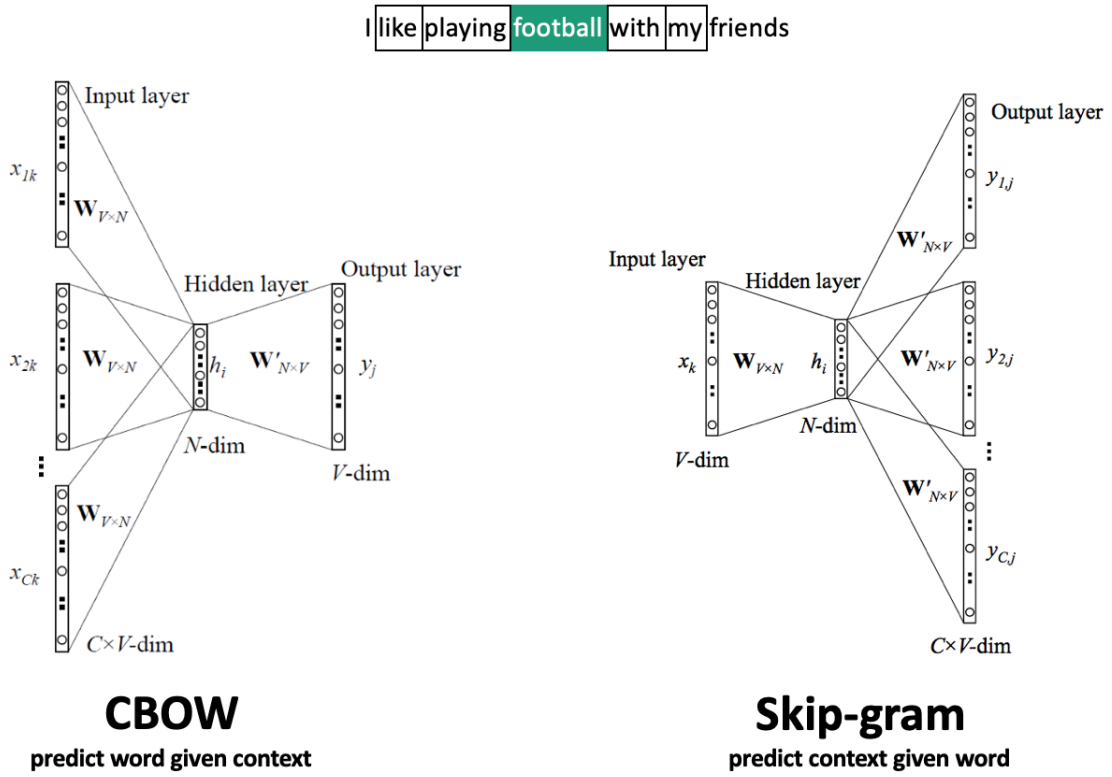
I have	trained	my	**dog**	well

GloVe (count)

	my	tallest	trained
football	1	0	0
tree	0	1	0
dog	1	0	1

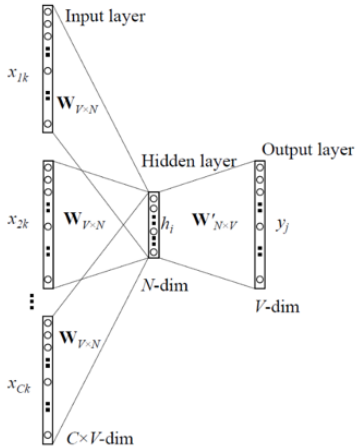
Word2Vec

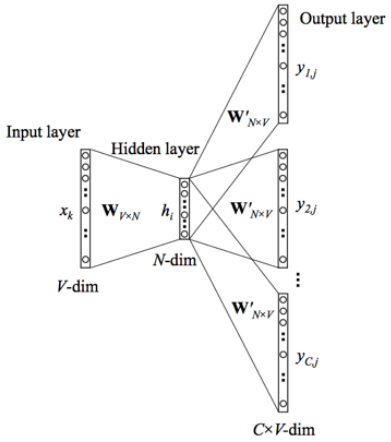
- Continuous bag of words (CBOW): train model to predict word given context, use weights of last layer as embedding
- Skip-Gram: train model to predict context given word, use weights of first layer as embedding (better for large corpora)



FastText

Like CBOW or SkipGram, but using n-grams instead of words





Character-level ngrams

- apple = “ ap” + “app” + “ppl” + “ple” + “ le”

Benefits

- Better embeddings for rare words
- Out-of-vocabulary words

BERT, ELMO, GPT,...

- Uses *transformer networks* to learn contextual embeddings
- Devlin et al. (2018) BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding

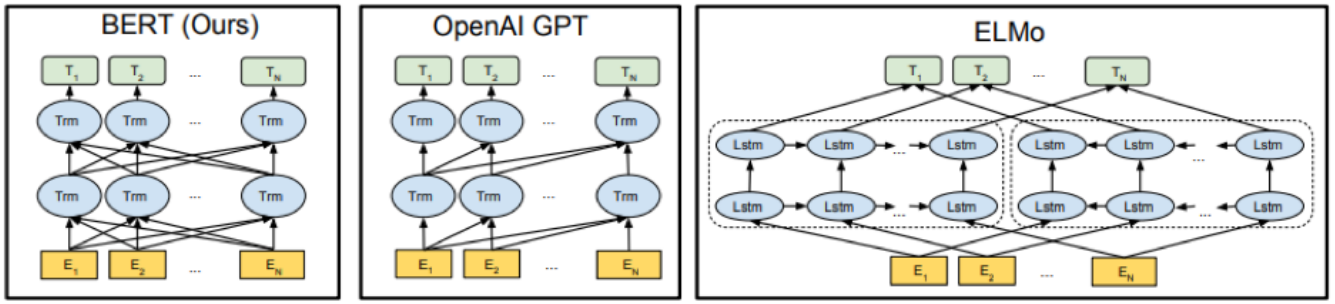


Figure 1: Differences in pre-training model architectures. BERT uses a bidirectional Transformer. OpenAI GPT uses a left-to-right Transformer. ELMo uses the concatenation of independently trained left-to-right and right-to-left LSTM to generate features for downstream tasks. Among three, only BERT representations are jointly conditioned on both left and right context in all layers.

Further reading

https://www.tensorflow.org/learn (https://www.tensorflow.org/learn)

http://playground.tensorflow.org (http://playground.tensorflow.org)

https://www.tensorflow.org/tensorboard
(https://www.tensorflow.org/tensorboard)