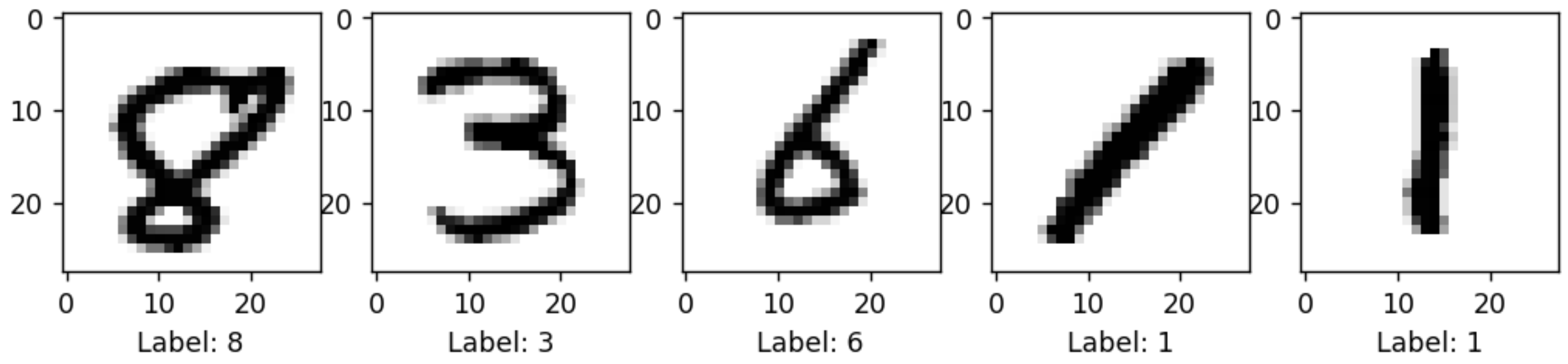
# Neural Networks

## Mathematical Foundations

- A first example
- Tensors and tensor operations
- Backpropagation and gradient descent

## A first example: classifying digits

- This example is meant to introduce the main concepts. We'll cover them in more detail later.
- MNIST dataset contains 28x28 pixel images of handwritten digits (0-9)
- The goal is to classify each image as one of the possible digits
- We **reshape** the data to a 70000x28x28 **tensor** (n-dimensional matrix)
  `X = X.reshape(70000, 28, 28)`
- Traditional holdout uses the last 10,000 images for testing



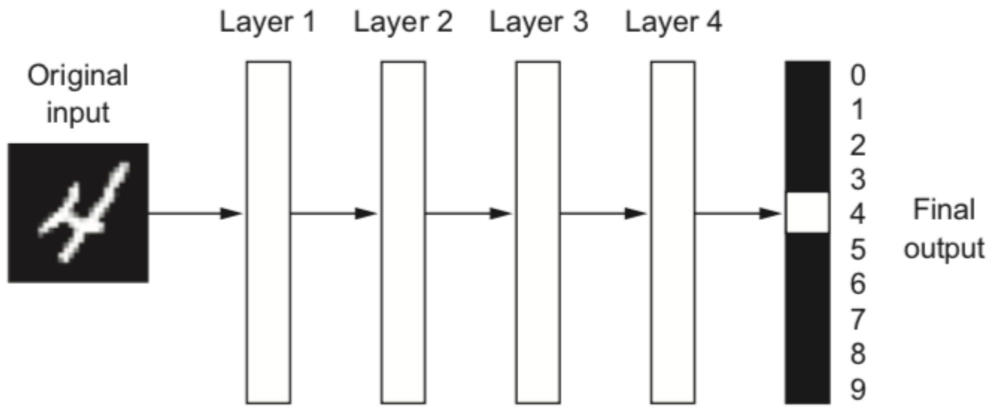
```
Training set:  (60000, 28, 28)
Test set:  (10000, 28, 28)
```

Note: this is also one of the datasets that comes included with Keras:

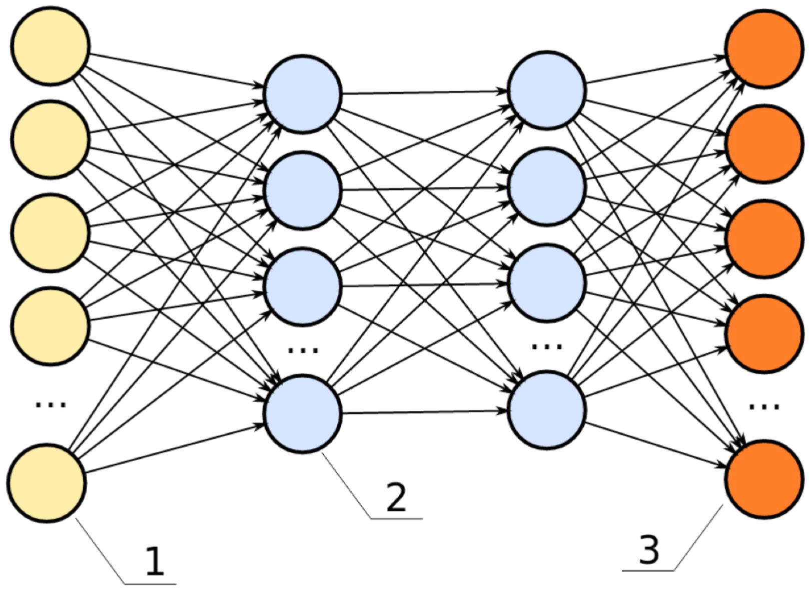
```
from keras.datasets import mnist
(train_images, train_labels), (test_images, test_labels) = mnist.load_da
ta()
```

## 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

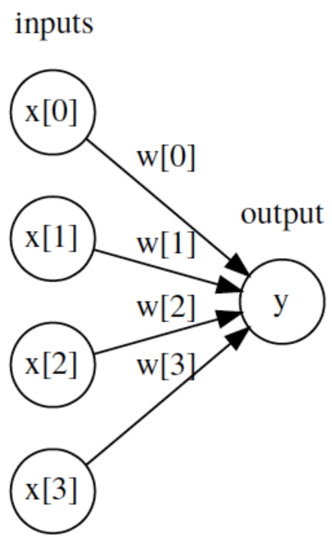


- The pixel values are fed to individual *nodes* of the *input layer* (yellow)
- The data then passes through one or more *hidden layers* (blue)
    - One type of layer is the *dense* or *fully connected* layer
    - Every node is connected to all nodes in the previous and subsequent layers
- The *output layer* has a node for every possible outcome (digits 0-9) (red)
    - I.e. The first node returns the probability that the input image represents a '0'



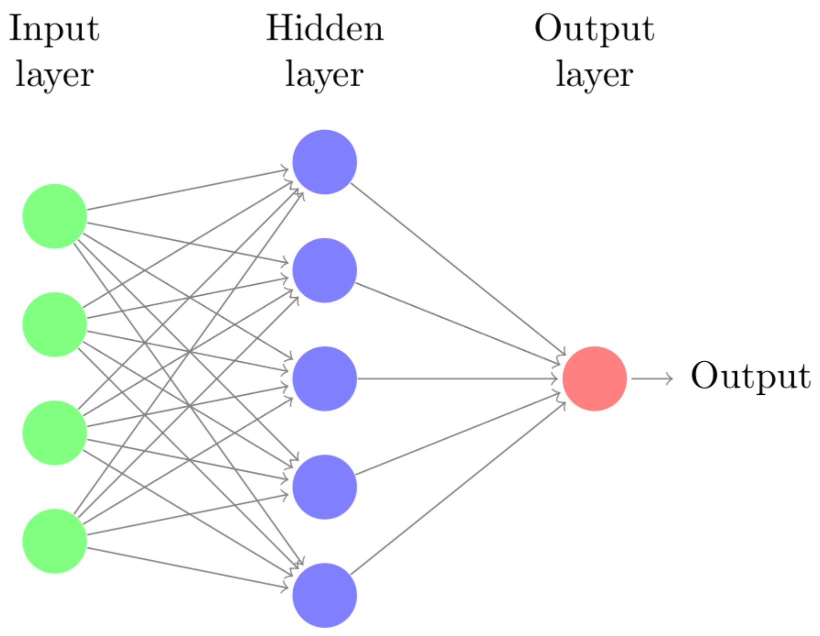
## The perceptron

- In its simplest form, each node outputs a weighted sum of the inputs: $y = \sum_i x_i w_i + b$
- It needs to learn the optimal set of weights to produce the right output
  - *Bias $b$*: modelled as the weight of an extra input that's always '1'
- This is the same as a linear model, can only learn linear decision boundaries.
  - Even a deep neural net of perceptrons can only learn a linear model



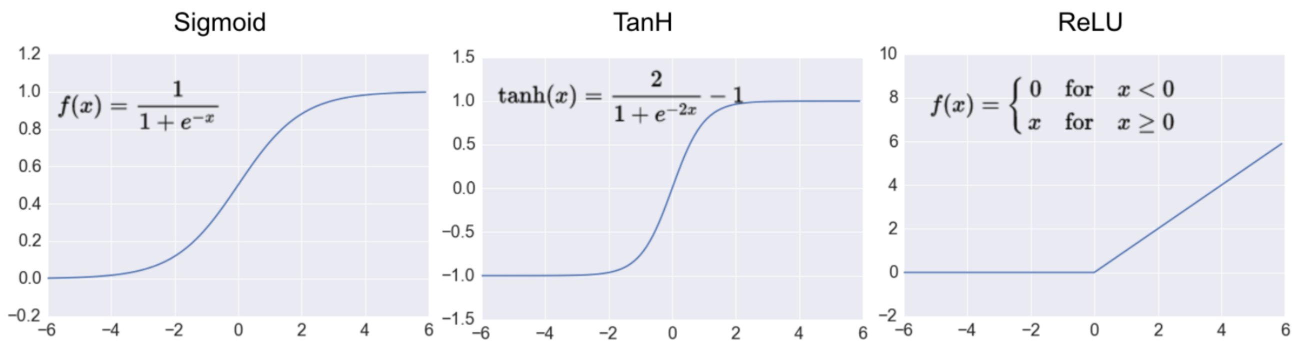
## Activation functions

- To learn a non-linear model, each hidden node has to output a non-linear *activation function* $f$ on the weighted sum of the inputs: $h(x) = f(W_1 x + b_1)$
- Likewise, the output nodes use an activation function $g$ on the weighted outputs of the previous layer: $o(x) = g(W_2 h(x) + b_2)$



## 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 outcome)
    - This is exactly what we used for logistic regression!



We can now build a simple neural network for MNIST:

- One dense hidden ReLU layer with 512 nodes
    - Input from a 28x28 matrix
- Output softmax layer with 10 nodes

```
from keras import models
from keras import layers

network = models.Sequential()
network.add(layers.Dense(512, activation='relu', input_shape=(28 * 28
,)))
network.add(layers.Dense(10, activation='softmax'))
```

'Visualize' the model using `summary()`

- Also shows the number of model parameters (weights) that need to be learned

```
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_3 (Dense)              (None, 512)               401920
_________________________________________________________________
dense_4 (Dense)              (None, 10)                5130
=================================================================
Total params: 407,050
Trainable params: 407,050
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)
- **Metrics** to monitor performance during training and testing.
    - e.g. accuracy

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

## Preprocessing

- Neural networks are sensitive to scaling, so always scale the inputs
- The network expects the data in shape (n, 28 * 28), so we also need to reshape
- We also need to categorically encode the labels
    - e.g. '4' becomes [0,0,0,0,1,0,0,0,0,0]

```
from keras.utils import to_categorical
y_train = to_categorical(y_train)
y_test = to_categorical(y_test)
```

## Training

Training (fitting) is done by **stochastic gradient descent** (SGD).

- Optimizes the model parameters (weights)
- We'll come back to this soon

```
Epoch 1/5
60000/60000 [==============================] - 4s 74us/step - loss: 0.0281
- acc: 0.9916
Epoch 2/5
60000/60000 [==============================] - 4s 63us/step - loss: 0.0208
- acc: 0.9939
Epoch 3/5
60000/60000 [==============================] - 4s 63us/step - loss: 0.0156
- acc: 0.9955
Epoch 4/5
60000/60000 [==============================] - 4s 63us/step - loss: 0.0121
- acc: 0.9965
Epoch 5/5
60000/60000 [==============================] - 4s 63us/step - loss: 0.0098
- acc: 0.9972
```

## Prediction

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

```
np.set_printoptions(precision=7)
print("Prediction: ",network.predict(X_test)[0])
```

```
Prediction:  [0.        0.0000002 0.        0.000001  0.9863701 0.000019
0.
 0.0000008 0.0005651 0.0130437]
Label:  [0. 0. 0. 0. 1. 0. 0. 0. 0. 0.]
```

## Evaluation

Evaluate the trained model on the entire test set

```python
test_loss, test_acc = network.evaluate(X_test, y_test)
print('Test accuracy:', test_acc)
```

```
10000/10000 [==============================] - 1s 57us/step
Test accuracy: 0.9793
```

## Overfitting

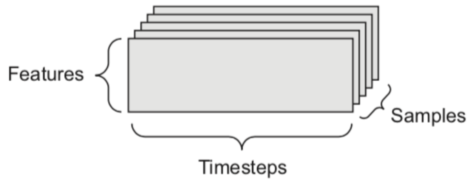
- Our test set accuracy is quite a bit lower than our training set accuracy
- We've already seen many choices (moving pieces) that can still be optimized:
    - Number of layers
    - Number of nodes per layer
    - Activation functions
    - Loss function (and hyperparameters)
    - SGD optimizer (and hyperparameters)
    - Batch size
    - Number of epochs

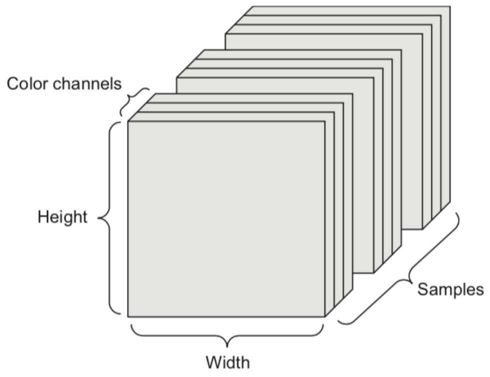
## Tensors and tensor operations

Representing data and learning better representations

## Tensors

- A *tensor* is simply an 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)





## Tensor operations

The operations that neural network layers perform on the data can be reduced to a handful of tensor operations.

```
keras.layers.Dense(512, activation='relu')
```

can be interpreted as a function

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

- takes a 2D tensor $x$ and returns a new 2D tensor $y$
- uses a 2D weight tensor $W$ and a bias vector $b$
- 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]])
```

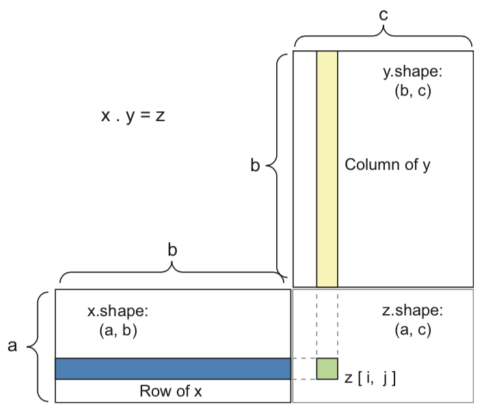
## Tensor dot

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

```
z = np.dot(x, y)
```

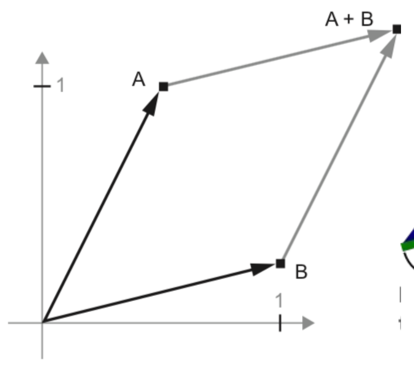
where

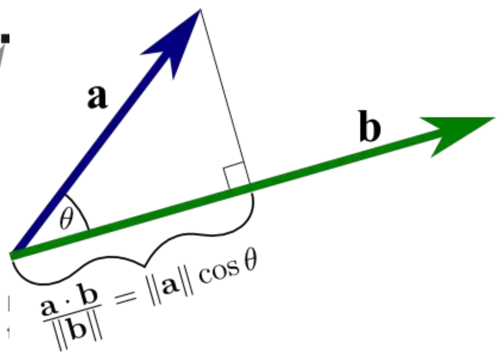
```
z[i,j] = x[i,:] * y[:,j]
```



## Geometric interpretation

- Dot products and additions change how data points relate to each other
- We aim to find a transformation of the data points so that it becomes easy to:
    - separate the classes (classification)
    - learn a simple function (regression)





## Gradient-based optimization

- We saw that a layer performs an operation like:

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

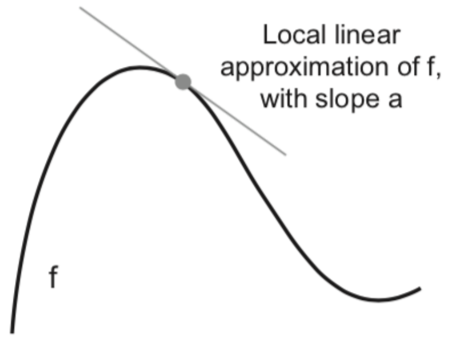
- How to find good values for $W$ and $b$ so that the data is transformed to a useful representation?
- Start with a random initialization, then loop:
    1. Draw a batch of training data $x$
    2. *Forward pass*: run the network on $x$ to yield $y_{pred}$ (tensor operations)
    3. Compute the loss (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 given current batch x
- Keep the one that reduces the loss most, then repeat

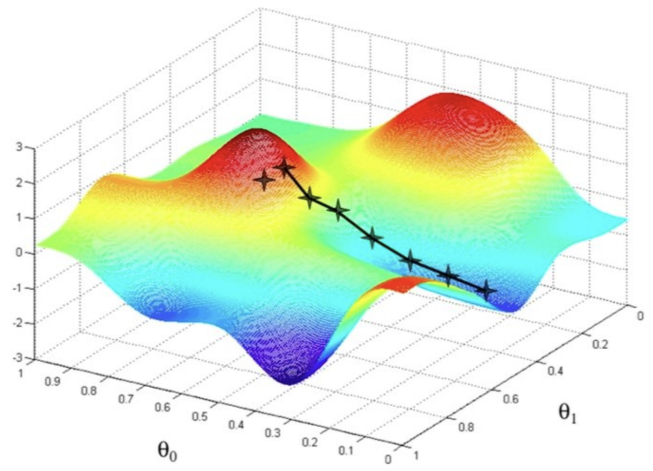
Better:



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

## Gradients

- A *gradient* is the generalization of a derivate to n-dimensional inputs
  - Approximates the *curvature* of the loss function $f(x, W)$ around a given point $W$
- Update: if $f$ is differentiable, then $W_1 = W_0 - \frac{\partial f(W_0)}{\partial W} * step$
  - step is a small scaling factor
  - Go against the curvature to a lower place on the curve
- Now repeat with a new batch of data $x$



## Stochastic gradient descent (SGD)

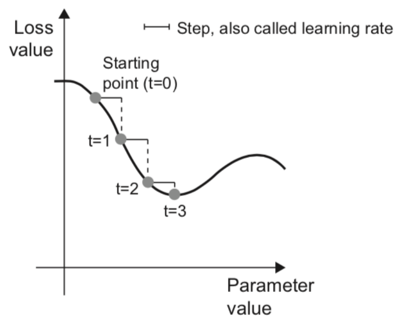
Mini-batch SGD:

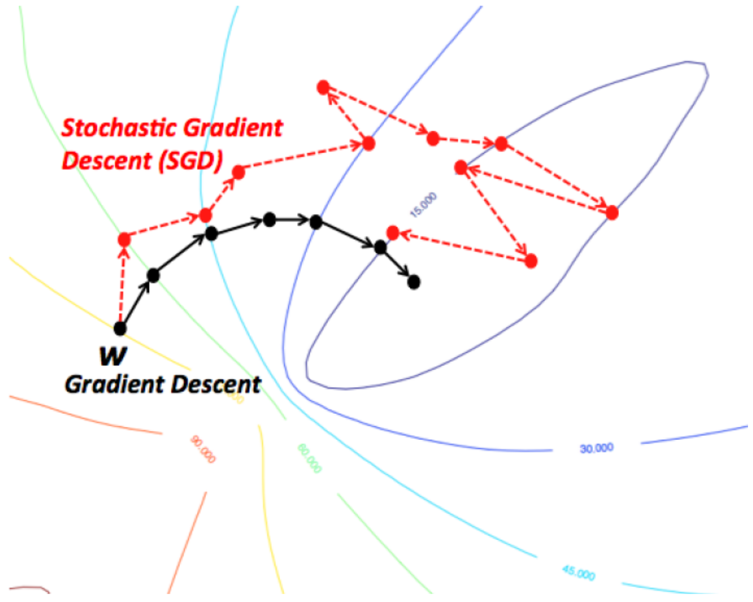
1. Draw a batch of *batch_size* training data $x$ and $y$
2. *Forward pass*: run the network on $x$ to yield $y_{pred}$ (tensor operations)
3. Compute the loss L (mismatch between $y_{pred}$ and $y$)
4. *Backward pass*: Compute the gradient of the loss with regard to $W$
5. Update W: $W_{i+1} = W_i -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

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

SGD Variants:

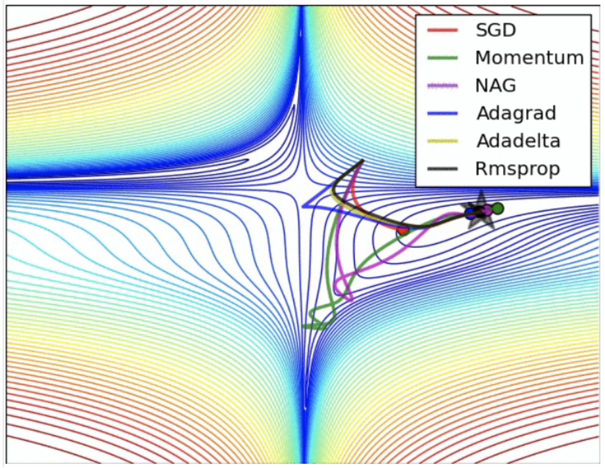
- Batch Gradient Descent: compute gradient on entire training set
    - More accurate gradients, but more expensive
- True Stochastic Gradient Descent: repeat for each individual data points (noisy)
- Minibatch SGD strikes a balance between the two (given the right batch size)





## 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. $f(W1, W2, W3) = a(W1, b(W2, c(W3)))$
- As long as each tensor operation is differentiable, we can still compute the gradient thanks to the chain rule:

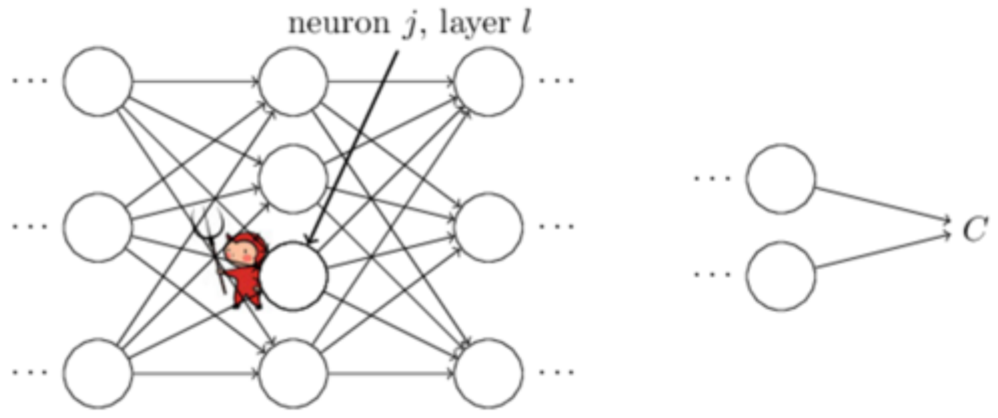
$$f(g(x)) = f'(g(x)) * g'(x)$$

- 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 $o(x) = g(W_2 h(x) + b_2)$

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

## Understanding $\frac{\partial h(\boldsymbol{x})}{\partial \boldsymbol{net}(\boldsymbol{x})}$

- Imagine a demon that adds a little change $\Delta u_k$ to the input of neuron $k$
    - The neuron now outputs $\sigma(u_k + \Delta u_k)$ instead of $\sigma(u_k)$
    - Propagates through network, ultimately causing an error $\frac{\delta E}{\delta u_k}\Delta u_k$
- A good demon helps you improve the error by trying to find a $\Delta u_k$ that reduces the error
    - If $\frac{\delta E}{\delta u_k}$ is large, choose $\Delta u_k$ to reduce it



## 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 (https://youtu.be/Ilg3gGewQ5U?list=PLZHQObOWTQDNU6R1_67000Dx_ZCJB-3pi)

## Symbolic and automatic differentiation

Symbolic differentiation: given a chain of operations with a known derivative, we can compute a *gradient function* for the chain

- Decomposes functions into simpler functions via the chain rule
- We can call the gradient function to get the gradient value for every model parameter

Automatic differentiation: evaluate the derivate of a function numerically for faster calculation

Modern tools such as TensorFlow do this for you so you don't have to implement backpropagation

## Further reading

https://www.tensorflow.org/versions/r0.10/tutorials/ (https://www.tensorflow.org/versions/r0.10/tutorials/)

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

https://www.tensorflow.org/versions/r0.10/get_started/basic_usage (https://www.tensorflow.org/versions/r0.10/get_started/basic_usage)

https://www.tensorflow.org/versions/r0.10/tutorials/mnist/beginners/ (https://www.tensorflow.org/versions/r0.10/tutorials/mnist/beginners/)

https://keras.io/ (https://keras.io/)

Tensorboard web interface