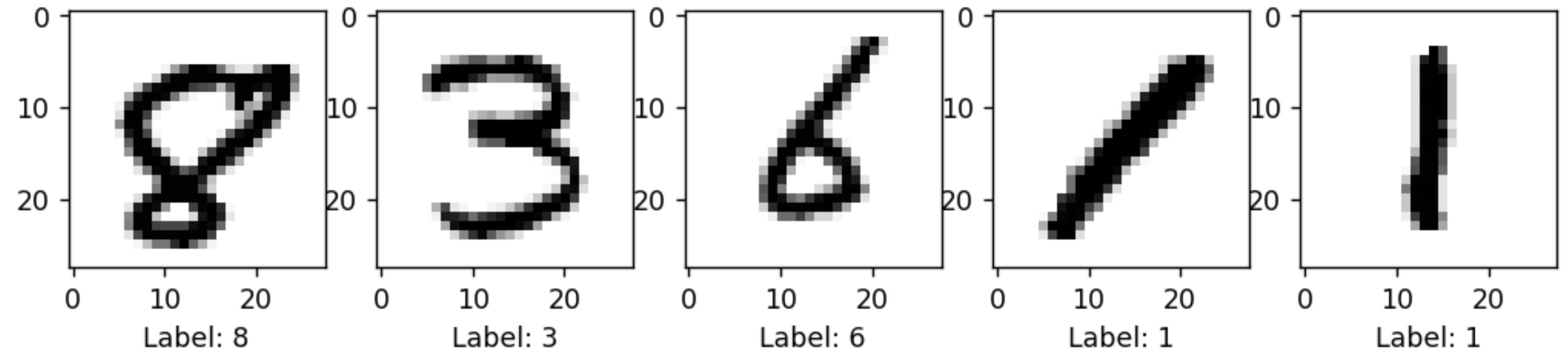
Neural Networks

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



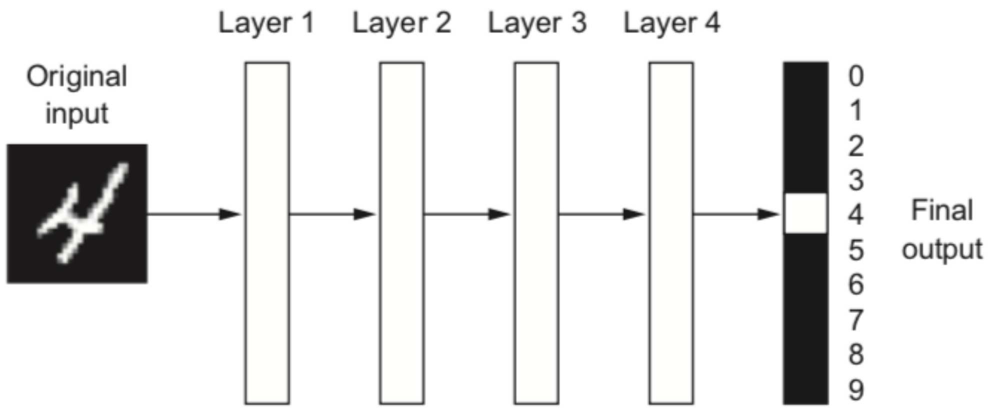
```
Training set:  (60000, 28, 28)
Test set:  (10000, 28, 28)
```

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

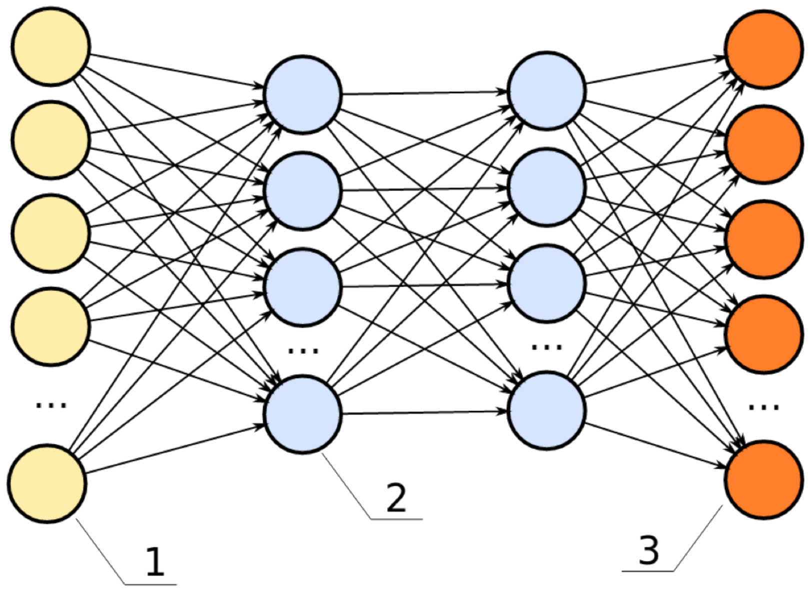
```
from keras.datasets import mnist
(train_images, train_labels), (test_images, test_labels) = mnist.load_da
ta()
```

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

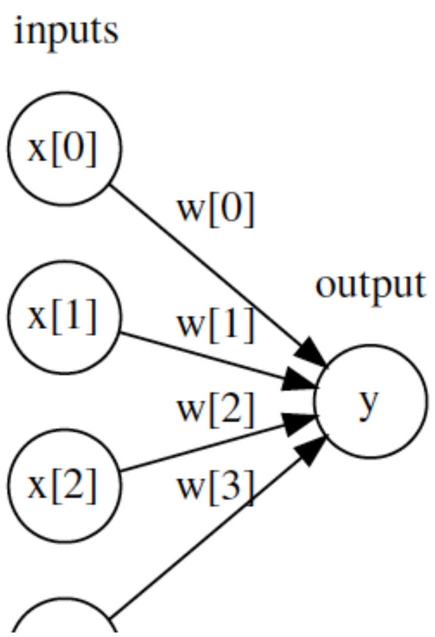


- The pixel values are fed to individual *nodes* of the *input layer* (yellow)
- The data then passes through one or more *hidden layers* (blue)
  - One type of layer is the *dense* or *fully connected* layer
  - Every node is connected to all nodes in the previous and subsequent layers
- The *output 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'



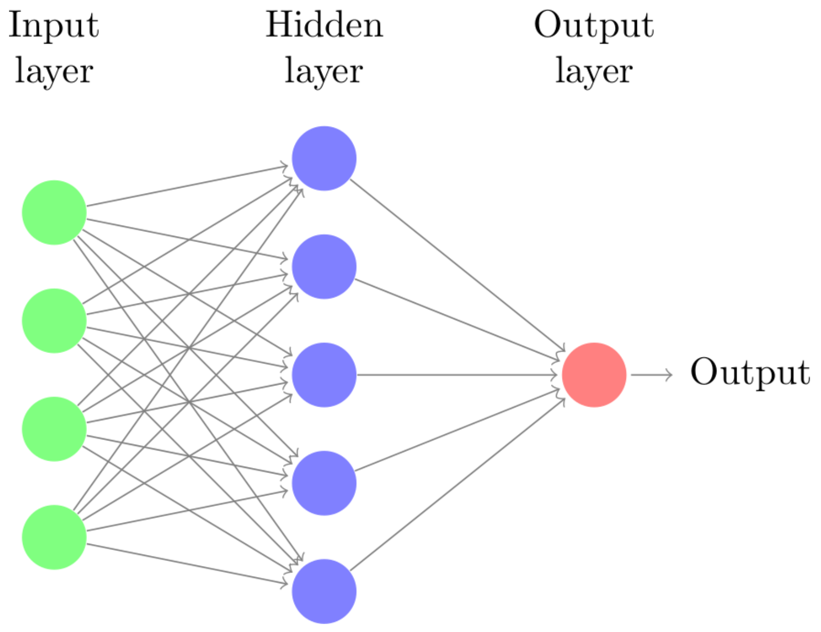
The perceptron

- 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
    - The *bias* b is modelled as the weight of an extra input that is always '1' (see later)
- This is exactly the same as a linear model. It can only learn linear decision boundaries.
    - Even a deep neural net of perceptrons can only learn a linear model



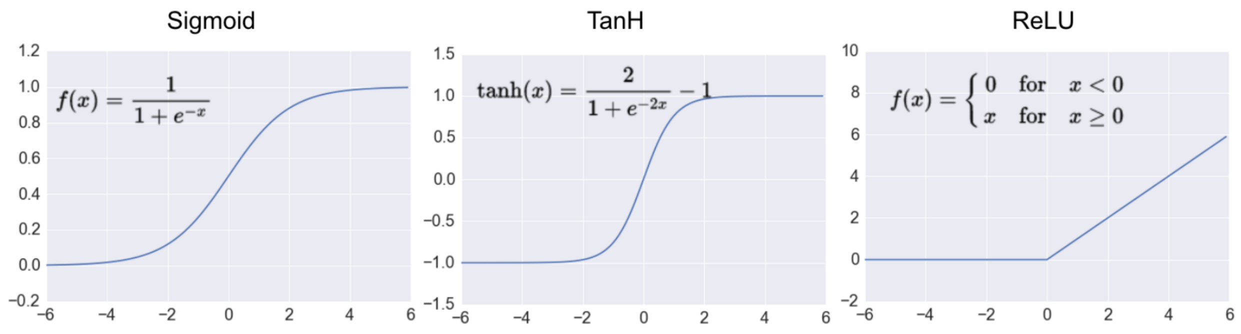
Activation functions

- 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 [==============================] - 5s 79us/step - loss: 0.2536
- acc: 0.9265
Epoch 2/5
60000/60000 [==============================] - 4s 75us/step - loss: 0.1032
- acc: 0.9699
Epoch 3/5
60000/60000 [==============================] - 5s 79us/step - loss: 0.0671
- acc: 0.9795
Epoch 4/5
60000/60000 [==============================] - 4s 74us/step - loss: 0.0491
- acc: 0.9854
Epoch 5/5
60000/60000 [==============================] - 4s 72us/step - loss: 0.0362
- acc: 0.9889
```

Prediction

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

```
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

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

Overfitting

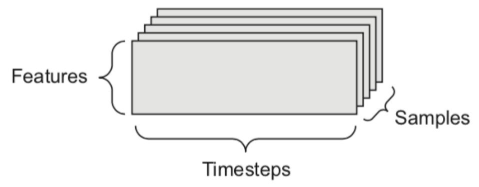
- Our test set accuracy is quite a bit lower than our training set accuracy
- We've already seen many choices (moving pieces) that can still be optimized:
    - Number of layers
    - Number of nodes per layer
    - Activation functions
    - Loss function (and hyperparameters)
    - SGD optimizer (and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

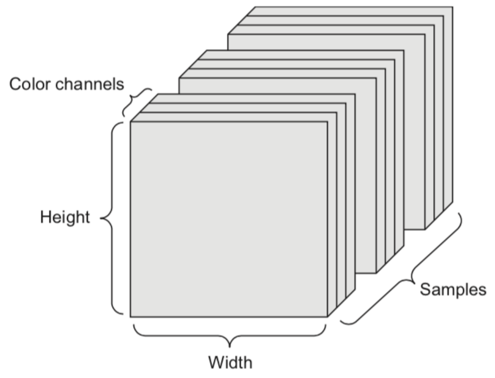
Tensors and tensor operations

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]])
```

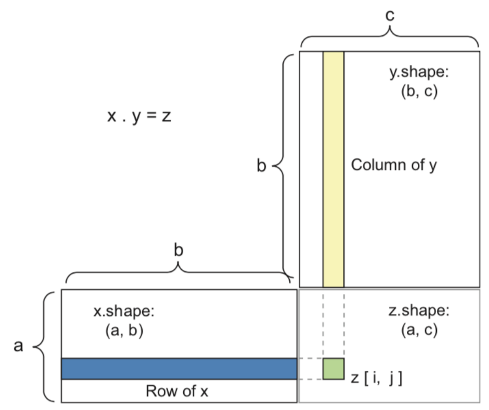
Tensor dot

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

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

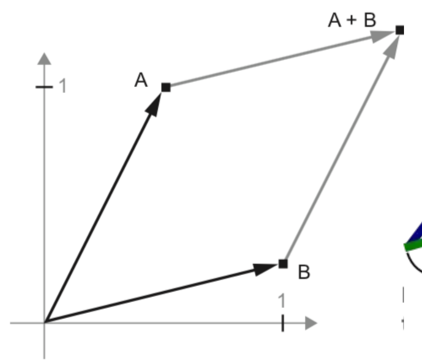
where

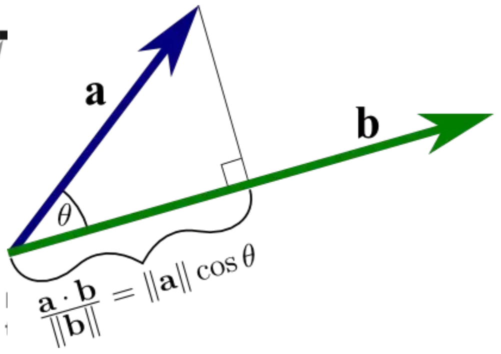
```
z[i,j] = x[i,:] * y[:,j]
```



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)




a
b
θ
$\frac{\mathbf{a}\cdot\mathbf{b}}{\|\mathbf{b}\|} = \|\mathbf{a}\|\cos\theta$

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?

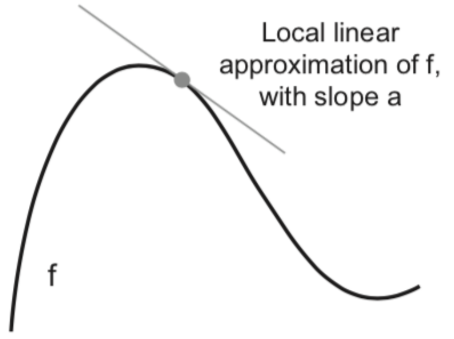
- Start with a random initialization, then loop:
  1. Draw a batch of training data x
  2. *Forward pass*: run the network on x to yield y_{pred} (tensor operations)
  3. Compute the loss (mismatch between y_{pred} and y)
  4. Update W, b in a way that slightly reduces the loss (OK, but how?)

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

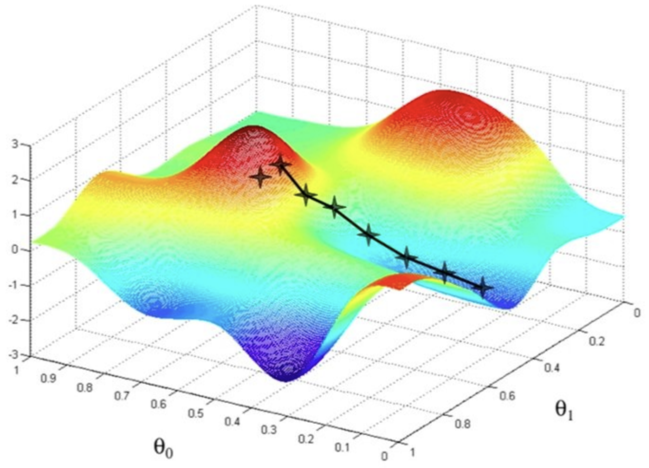
Better:



- 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)

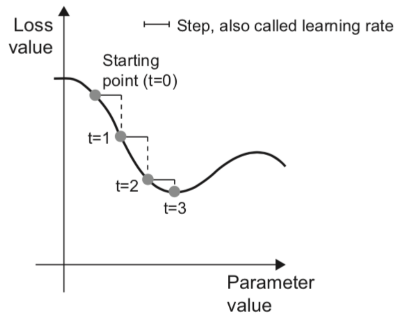
Mini-batch SGD:

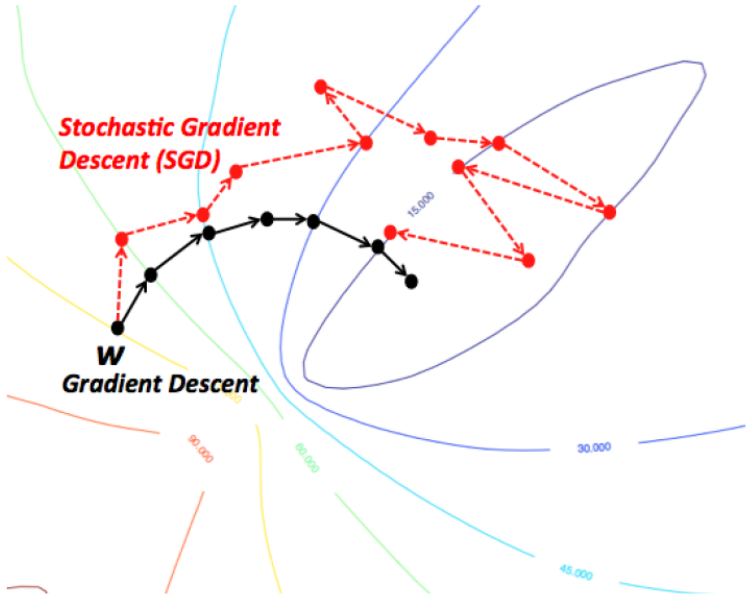
1. Draw a batch of *batch_size* training data x and y
2. *Forward pass*: run the network on x to yield y_{pred} (tensor operations)
3. Compute the loss L (mismatch between y_{pred} and y)
4. *Backward pass*: Compute the gradient of the loss with regard to W
5. Update W: $W_{i+1} = W_i - \frac{\partial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

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

SGD Variants:

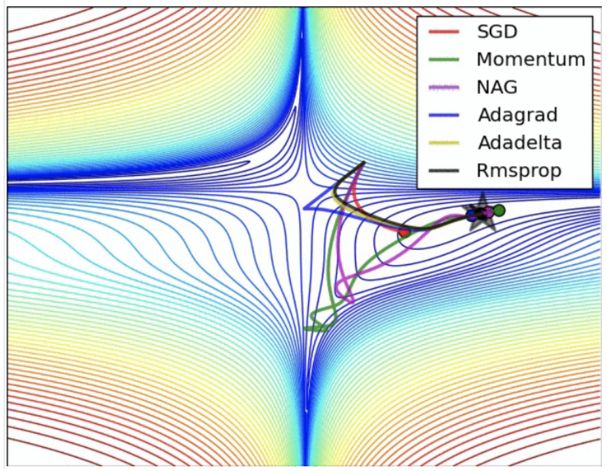
- Batch Gradient Descent: compute gradient on entire training set
    - More accurate gradients, but more expensive
- True Stochastic Gradient Descent: repeat for each individual data points (noisy)
- Minibatch SGD strikes a balance between the two (given the right batch size)





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 $h(x) = f(W_1x + b_1)$, $net(x) = W_1x + b_1$, and output node $o(x) = g(W_2h(x) + b_2)$

$$\frac{\partial o(\mathbf{x})}{\partial W_1} = \underbrace{\frac{\partial o(\mathbf{x})}{\partial h(\mathbf{x})}}_{\text{backpropagation of gradient of layer above.}} \underbrace{\frac{\partial h(\mathbf{x})}{\partial \mathrm{net}(\mathbf{x})}}_{\text{Gradient of Non-linearity f}} \underbrace{\frac{\partial \mathrm{net}(\mathbf{x})}{\partial W_1}}_{\text{Input to 1st layer x}}$$

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