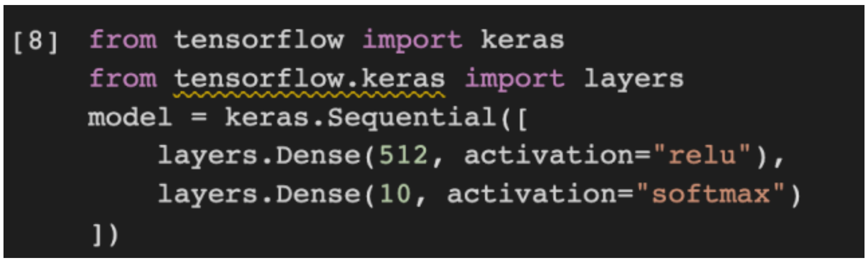
Lecture3 Engine Neural Network

1. How does learning happen?

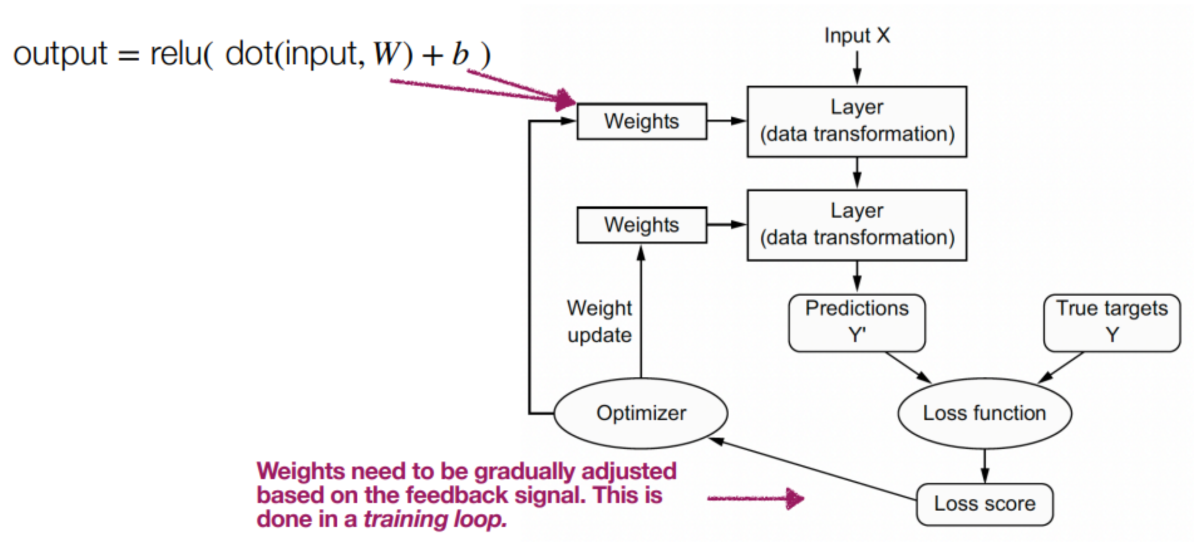
Kernel and Bias



```
[8] from tensorflow import keras
    from tensorflow.keras import layers
    model = keras.Sequential([
        layers.Dense(512, activation="relu"),
        layers.Dense(10, activation="softmax")
    ])
```

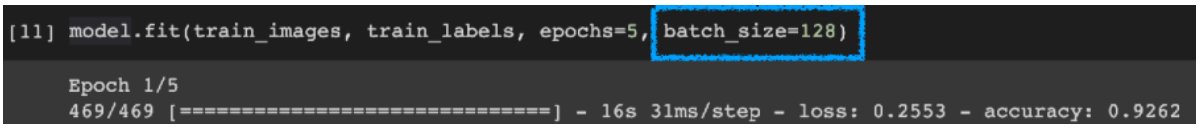
$$\text{output} = \text{relu}(\text{dot}(\text{input}, W) + b)$$

- We saw that dense layers are these combination of operations, where W and b are **parameters** of the layer
- Those two matrices are called the **kernel** and **bias** attributes of the dense layer
- Initially, they are **randomized**
  - i.e. assigned random values


output = relu(dot(input, W) + b)
Input X
Weights
Layer (data transformation)
Weights
Layer (data transformation)
Weight update
Predictions Y'
True targets Y
Optimizer
Loss function
Loss score
Weights need to be gradually adjusted based on the feedback signal. This is done in a training loop.

Training loop

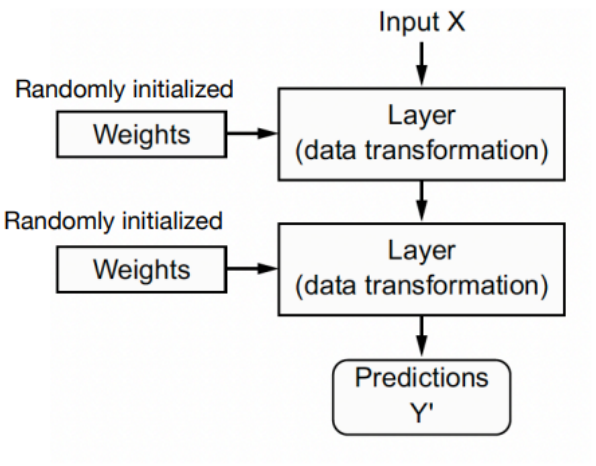
1. Draw a batch of training samples `x`, and corresponding labels `y_pred`.



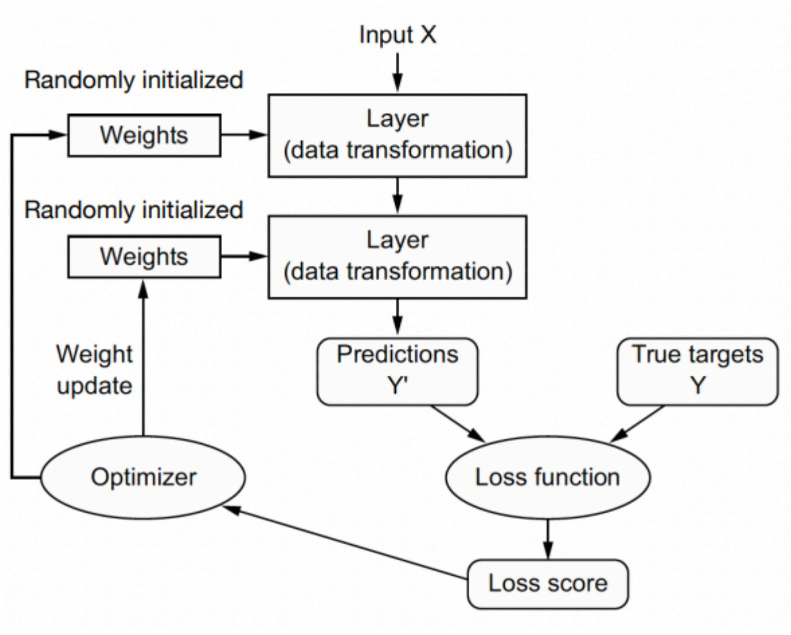
```
[11] model.fit(train_images, train_labels, epochs=5, batch_size=128)

     Epoch 1/5
     469/469 [==============================] - 16s 31ms/step - loss: 0.2553 - accuracy: 0.9262
```

```python
batch = train_images[:128]
batch = train_images[128:256]
n = 3
batch = train_images[128*n:128*(n+1)]
```

2. Run the model on `x` (**forward pass**) to obtain predictions `y_pred`



3. Compute the **loss** of the model on the batch, a measure of the mismatch between `y_pred` and `y_true`
4. Update all weights of the model in a way that slightly reduces the loss on this batch.



2. How to Update Weight?

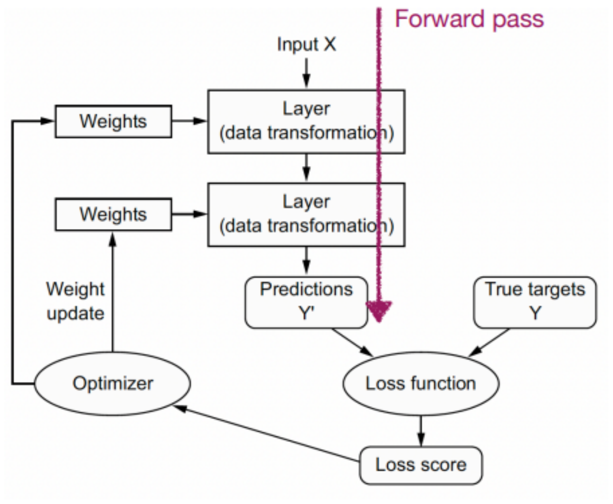
Weight initialization: Randomly

$$W = \begin{bmatrix} 0.30 & 0.45 & 0.10 \\ 0.70 & 0.56 & 0.32 \end{bmatrix} \qquad b = \begin{bmatrix} 0.50 \\ 0.21 \end{bmatrix}$$

- A linear layer with
  - 3 inputs
  - 2 outputs

    - its weight (w) is a (2 x 3) matrix (and a bias term (b))
- **This layer wouldn't do anything useful**.
    - (I.e., a randomly initialized model for MNIST classification would show about 10% accuracy)

Update the weights - A naive approach (X)



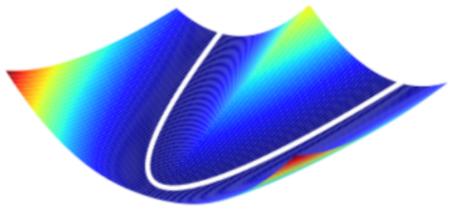
- Change one coefficient at a time,
    - e.g. increase its value by a little.
- Do the forward pass again, see if the loss improved.

Weight Adjustment	**Loss Computation**
Weight Initialization	$W = \begin{bmatrix} 0.30 & 0.45 & 0.10 \\ 0.70 & 0.56 & 0.32 \end{bmatrix} \longrightarrow \ell = 0.5$ $b = \begin{bmatrix} 0.50 \\ 0.21 \end{bmatrix}$
Increase the first element in W, loss increases	$W = \begin{bmatrix} \boxed{0.35}\uparrow & 0.45 & 0.10 \\ 0.70 & 0.56 & 0.32 \end{bmatrix} \longrightarrow \ell = 0.6$ $b = \begin{bmatrix} 0.50 \\ 0.21 \end{bmatrix}$
Decrease the first element in W, loss decreases	$W = \begin{bmatrix} \boxed{0.25}\downarrow & 0.45 & 0.10 \\ 0.70 & 0.56 & 0.32 \end{bmatrix} \longrightarrow \ell = 0.4$ $b = \begin{bmatrix} 0.50 \\ 0.21 \end{bmatrix}$

- This is terribly inefficient
- For a middle size network, e.g. 400k parameters, this is 800k forward passes
- In other words, we'd like a method that can **update all the weights** (slightly increase or decrease the value in a way that the model gets **better** (show a lower loss)

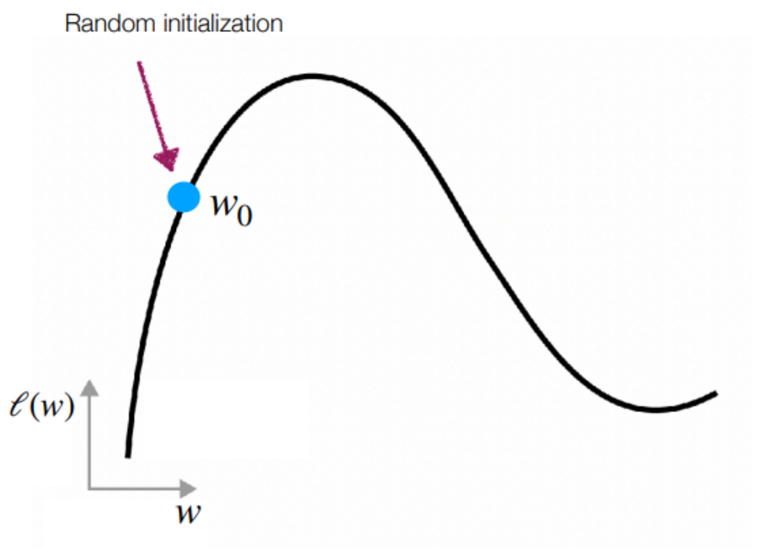
Gradient Descent

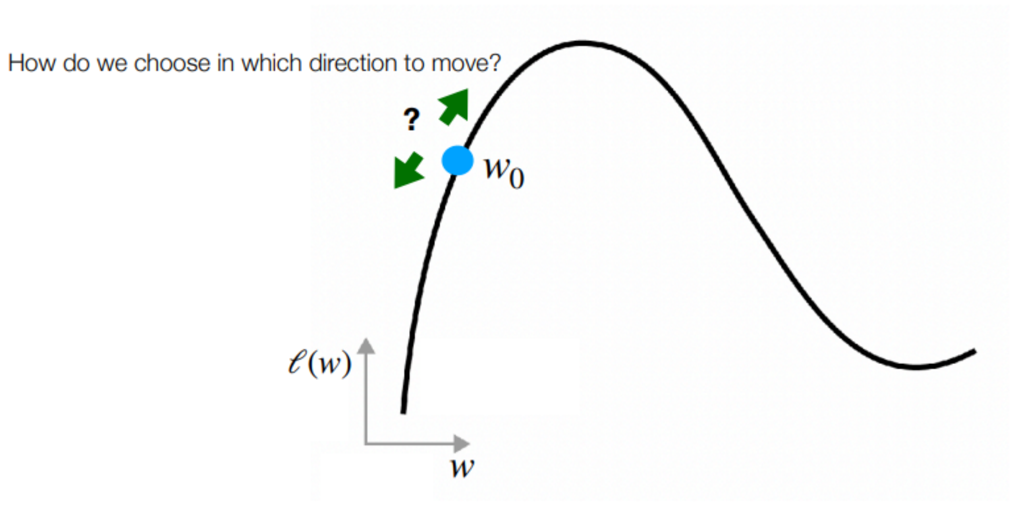
> Invented in 1847 by French mathematician Louis-Augustin Cauchy
>
> It is an optimization technique that powers modern neural networks

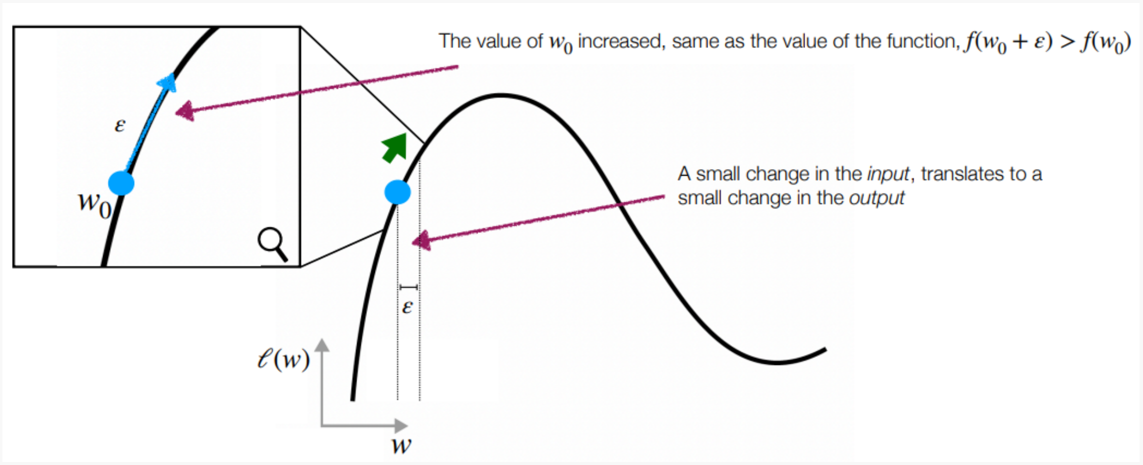


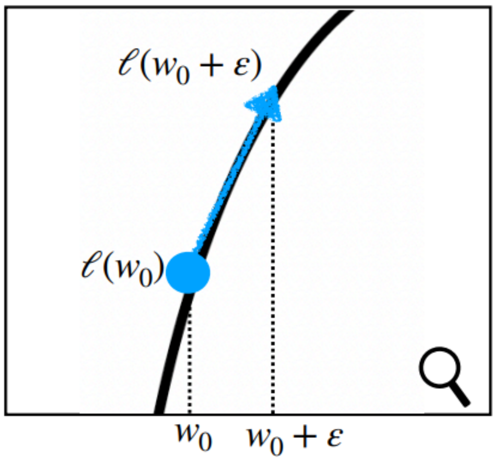
- Core idea: The “**gradient**” encodes information about what **small change to each coefficient** (i.e. positive or negative) will **decrease the loss the most**
- Using that information, you can change the coefficients iteratively until finding **a minimum value** for the loss

How






The value of w_0 increased, same as the value of the function, $f(w_0+\varepsilon) > f(w_0)$
ε
w_0
A small change in the *input*, translates to a small change in the *output*
ε
$\ell(w)$
w



The rate of change rc is defined as:

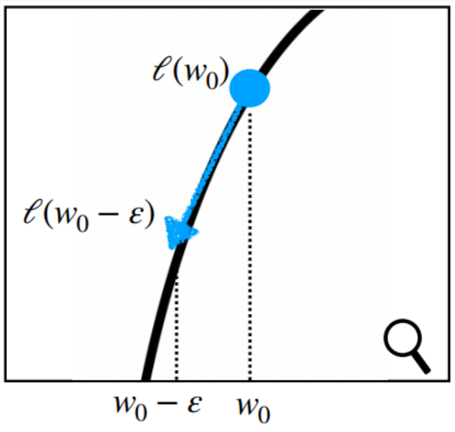
$$rc = \frac{\ell(w_0+\varepsilon)-\ell(w_0)}{w_0+\varepsilon-w_0}$$

In this case, $rc > 0$ and we should have decreased the value of w_0, i.e. subtract a positive number.

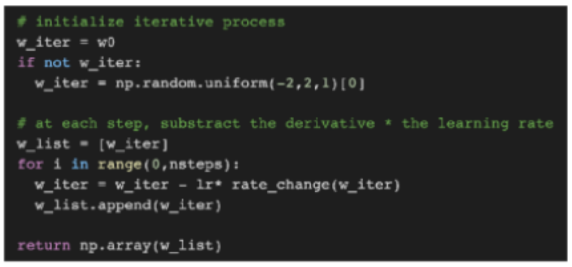
What happens if we go the other way (downhill)?

$$rc = \frac{\ell(w_0+\varepsilon)-\ell(w_0)}{w_0-\varepsilon-w_0} = \frac{\ell(w_0)-\ell(w_0-\varepsilon)}{\varepsilon}$$

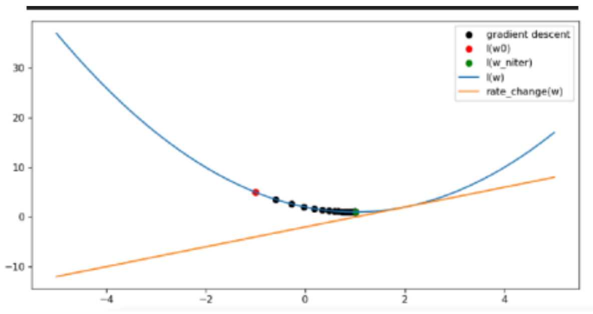
In this case $\ell(w_0) > \ell(w_0+\varepsilon)$ so $rc > 0$. We are going in the right direction, and we should indeed decrease x_0.



Naive Gradient Descent



```
# initialize iterative process
w_iter = w0
if not w_iter:
  w_iter = np.random.uniform(-2,2,1)[0]

# at each step, substract the derivative * the learning rate
w_list = [w_iter]
for i in range(0,nsteps):
  w_iter = w_iter - lr* rate_change(w_iter)
  w_list.append(w_iter)

return np.array(w_list)
```



Given a function $l(w)$ that you want to minimize with respect to w, do:

1. Initialize $w_{iter} = w_0$ in a random point
2. In a loop, do:

  - $w_{iter} = w_{iter} - lr \cdot rc$
  - where $rc = \frac{l(w_{iter}+\epsilon) - l(w_{iter})}{\epsilon}$
  - lr: **learning rate** (or **step size** in optimization)
3. Repeat step 2 until reach N iterations

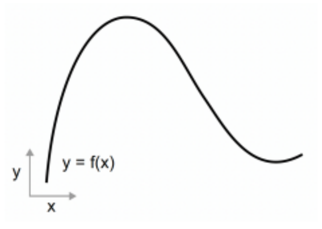
3. Gradient

What is Gradient?

$$rc = \frac{\ell(w_0+\varepsilon) - \ell(w_0)}{\varepsilon} \quad \xrightarrow[\varepsilon\to 0]{} \quad \nabla\ell(w_0)$$

When ε is very small (almost 0), rc becomes the gradient of $\ell(w)$.

1D → N-dim parameters



- The 2D plots so far
  - parameter space on x-axis (1-dim param)
  - loss function on y-axis
- Actual neural network models have **many parameters** (like, thousands or millions or billions)
  - parameter space is **N-dim** (i.e. w is a N-dim array)
  - loss function `y=f(input, w)`

GD in Tensors

When working with tensors, GD is applied to each element of the tensor in the same way as before.

$$W_{iter} = W_{iter} - lr\,.\,\nabla\ell(W_{iter})$$

To know the value of $l(W_{iter})$ we need to do a forward pass, so actually $l(W_{iter}) = l(W_{iter}, X)$ where is the input data.

Stochastic Gradient Descent

We can't fit all the data in memory at once to compute the gradient. We use **batches of data** instead

Stochastic Gradient Descent (SGD) is **GD over batches**.

$$W_{iter} = W_{iter} - lr\,.\,\nabla \ell(X_{iter}, W_{iter})$$

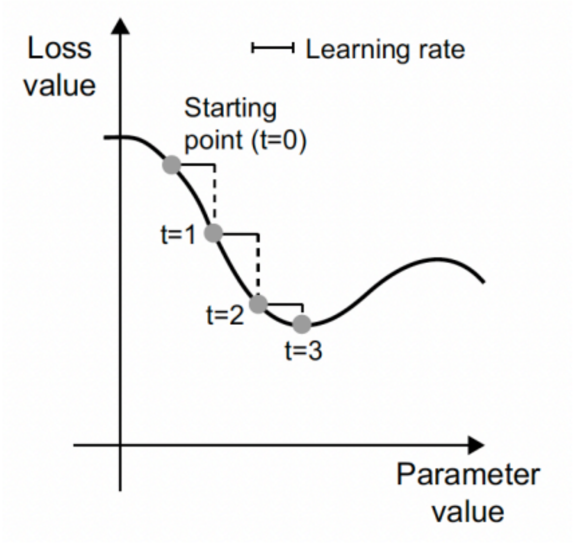
- where $l(X_{iter}, W_{iter})$ is the loss over one batch of data X_{iter}

Variants and Extensions of SGD

Many variants and extensions of SGD incorporating many tricks

- SGD with momentum
- RMSprop
- Adam, AdamW
- Adagrad

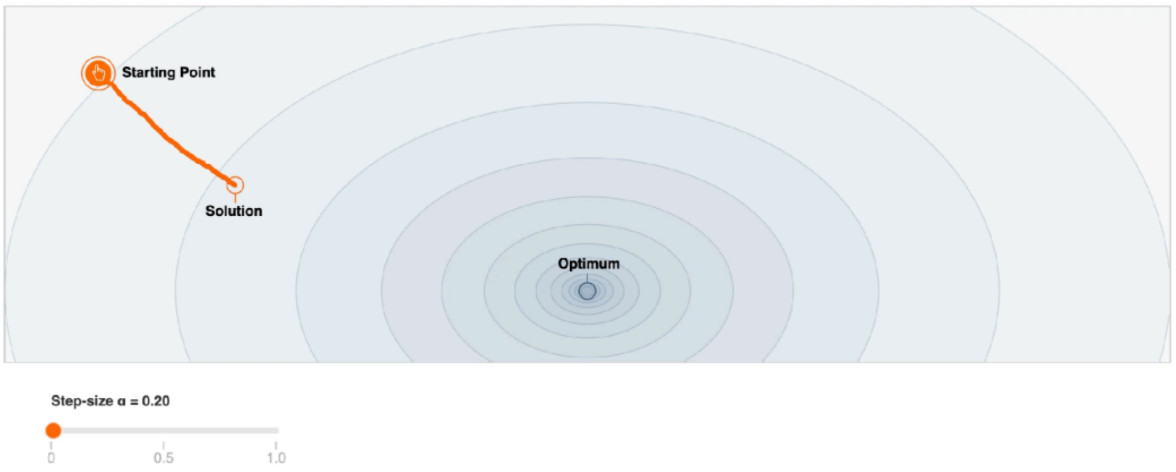
Learning Rate (aka step size)



$$W_{iter} = W_{iter} - \boxed{lr\,.}\,\nabla \ell(X_{iter}, W_{iter})$$

- If **too big**, SGD might not converge (find the minimum)

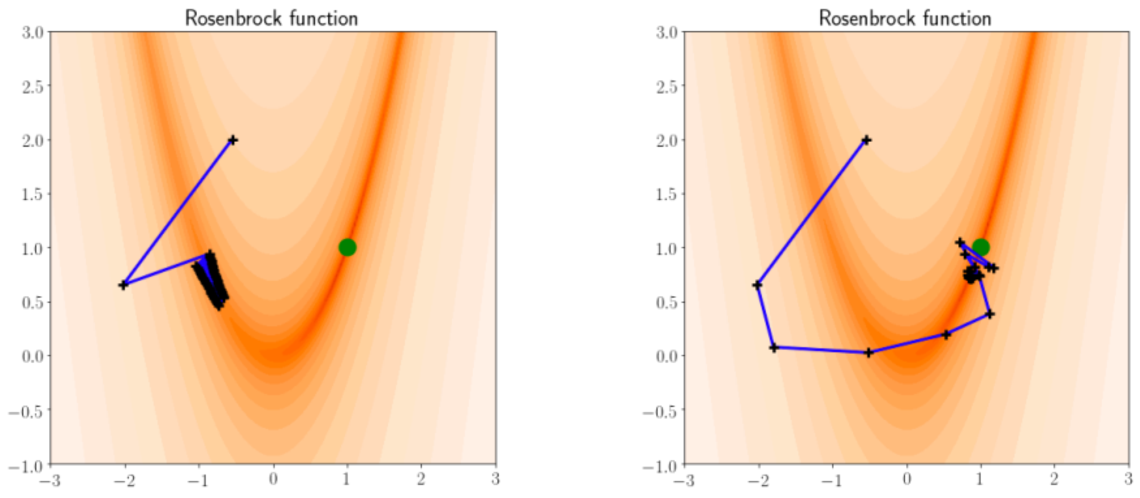
- If **too small**, SGD will take a lot of iterations (and time) to converge. If number of iterations is not enough, it won't find the solution.
- Safe bet: **start with a biggish and a few iterations, observe a batch of validation data and tune it**.



Momentum

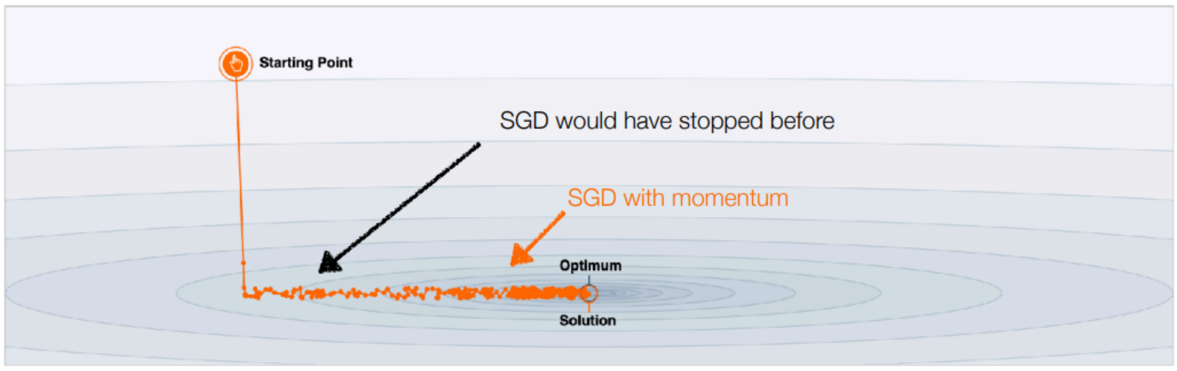
In DNNs there are many "valleys" where SGD can get stuck, and momentum helps it to "keep going".

$$W_{iter} = W_{iter} - lr\,.\,\nabla \ell(X_{iter}, W_{iter}) + \beta(W_{iter} - W_{iter-1})$$

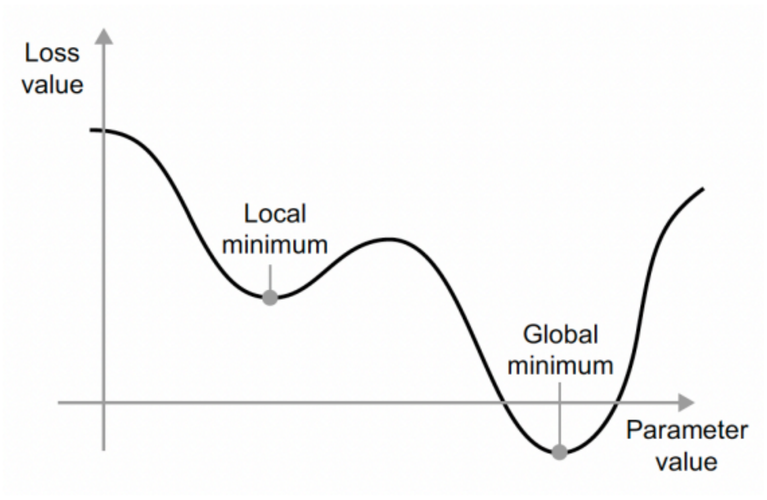


Gradient Descent

Gradient Descent with momentum



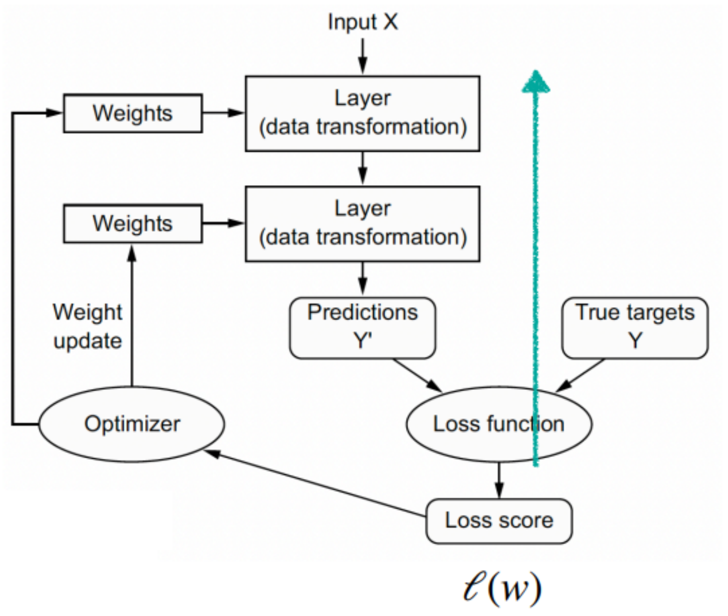
Local Minimum



- SGD is not infallible
- Momentum typically helps in this cases, but also not infallible
- Good news: local minimums in DNNs are not that bad

Backpropagation

Backpropagation is a clever trick to compute the gradient of the loss with respect to the parameters through multiple layers (=deep learning models!)



- **Main idea**: all the **gradients** of the tensor operations in the network **are known** in advance by TensorFlow, Keras, PyTorch. Backpropagation combines the gradients of each layer to form the gradient of the loss.

Takeaways

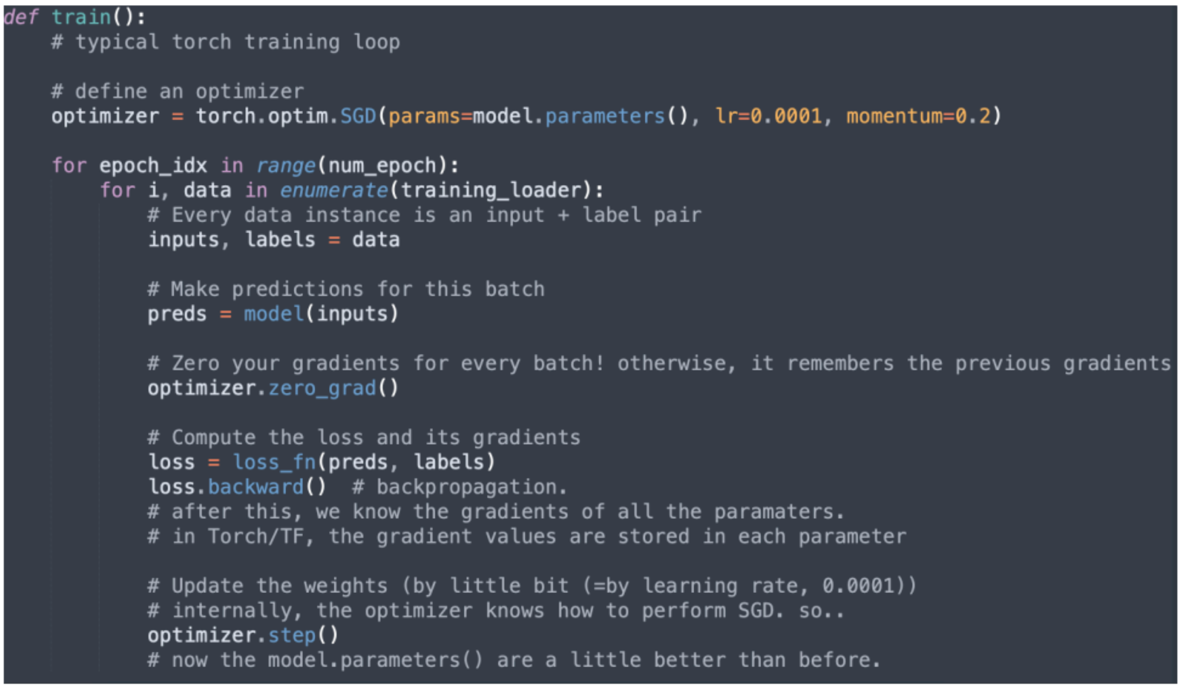
- SGD is very sensitive to the learning rate. Momentum often helps
- What is important when choosing an optimizer?
  - Choose an optimizer with momentum and some trick for adjusting the learning rate (e.g. Adam)
  - Choose a **big learning rate to start with** (e.g. 0.01 with Adam).

        - If network doesn’t converge, make it smaller.
        - Bigger lr speeds things up.
        - Always monitor the loss!.
    - Choose **a small number of epochs to start** (e.g. 10) and a small part of the data.
        - If SGD (or variants) converges, augment the data and/or epochs until you reach the size of your problem.
        - If it doesn’t converge, you needs more epochs

4. Remember these terms

- Training loop
- Batches
- Optimizer
- Loss function
- Gradient
- Gradient Descent
- Stochastic Gradient Descent (SGD)
- Learning rate
- Number of iterations
- Momentum
- Back propagation
- Convergence
- Global minimum
- Local minimum

Training in a nutshell



```python
def train():
    # typical torch training loop

    # define an optimizer
    optimizer = torch.optim.SGD(params=model.parameters(), lr=0.0001, momentum=0.2)

    for epoch_idx in range(num_epoch):
        for i, data in enumerate(training_loader):
            # Every data instance is an input + label pair
            inputs, labels = data

            # Make predictions for this batch
            preds = model(inputs)

            # Zero your gradients for every batch! otherwise, it remembers the previous gradients
            optimizer.zero_grad()

            # Compute the loss and its gradients
            loss = loss_fn(preds, labels)
            loss.backward()  # backpropagation.
            # after this, we know the gradients of all the paramaters.
            # in Torch/TF, the gradient values are stored in each parameter

            # Update the weights (by little bit (=by learning rate, 0.0001))
            # internally, the optimizer knows how to perform SGD. so..
            optimizer.step()
            # now the model.parameters() are a little better than before.
```