How does the NN ”learn” the transformations ?

The matrix $\mathbf{W}$ contains the "patterns" that serve to recognize the synthetic features created by each layer

- $\mathbf{W}_{(l),j}$ are the weights /pattern for feature $\mathbf{y}_{(l),j}$

How are these patterns discovered ?

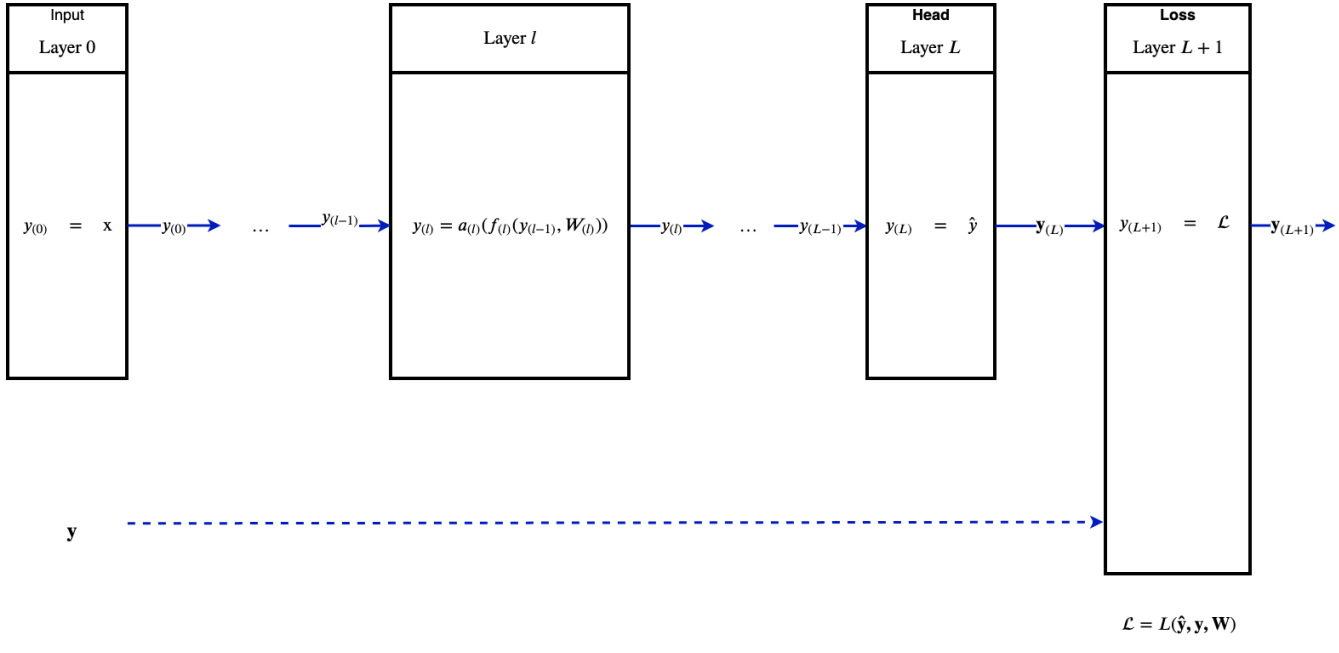
The answer is: exactly as we did in Classical Machine Learning

- Define a loss function that is parameterized by $\mathbf{W}$:
$$\mathcal{L} = L(\hat{\mathbf{y}}, \mathbf{y}; \mathbf{W})$$
  - Per example loss $\mathcal{L}^{(\mathbf{i})}$
  - Average loss $\mathcal{L} = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}^{(\mathbf{i})}$
- Our goal is to find $\mathbf{W}^*$ the "best" set of weights
$$\mathbf{W}^* = \underset{W}{\operatorname{argmin}}\, L(\hat{\mathbf{y}}, \mathbf{y}; \mathbf{W})$$
- Find $\mathbf{W}^*$ using Gradient Descent !

Very much in spirit of the multi-layer architecture

- We add a new layer (L+1) to compute the loss $\mathcal{L}$!

Additional Loss Layer (L+1)



Gradient Descent review

Gradient Descent is an iterative method for finding the minimum of a function. <!--EdX: Omit this from EdX: can't refer to prior course

- See the Gradient Descent lecture (Gradient_Descent.ipynb) in the Classical ML part of the course for more details -->

Let's review Gradient Descent using our current notation

- We start with an initial guess for $\mathbf{W}$ and iteratively improve it.
- Compute the loss $\mathcal{L}$ given the current $\mathbf{W}$
    - Average loss of the m examples in the training examples
- Compute the gradient

$$\frac{\partial \mathcal{L}}{\partial W}$$

- Update $\mathbf{W}$ in the direction of the *negative* of the gradient
- Scaled by a learning rate α

$$\mathbf{W} = \mathbf{W} - \alpha * \frac{\partial \mathcal{L}}{\partial W}$$

A unit change in $\mathbf{W}$ *increases* $\mathcal{L}$ by $\frac{\partial \mathcal{L}}{\partial W}$

- That's why there is a negative sign: we proceed in the direction *opposite* the one that increases $\mathcal{L}$
- We move only a fraction $\alpha \leq 1$ of the (negative) of the gradient
- To avoid the possibility of over-shooting the minimum

$\mathbf{W}$ is a multi-dimensional vector, not a scalar

- So the gradient is multi-dimensional
- We will formally discuss Matrix Gradients in a later lecture
    - For now: we compute the derivative with respect to each element of $\mathbf{W}$ and arrange in a matrix

The loss $\mathcal{L}$ is averaged over all m training examples.

This can be expensive to compute.

We can approximate $\mathcal{L}$ by *sampling* from the m training examples

- Choose a *random subset (of size $m' \leq m$)* of examples: $I = \{i_1, \ldots, i_{m'}\}$
- Approximate $\mathcal{L}$ on I

$$\mathcal{L} \approx \frac{1}{|I|} \sum_{i \in I} \mathcal{L}^{(\mathbf{i})}$$

Minibatch gradient descent

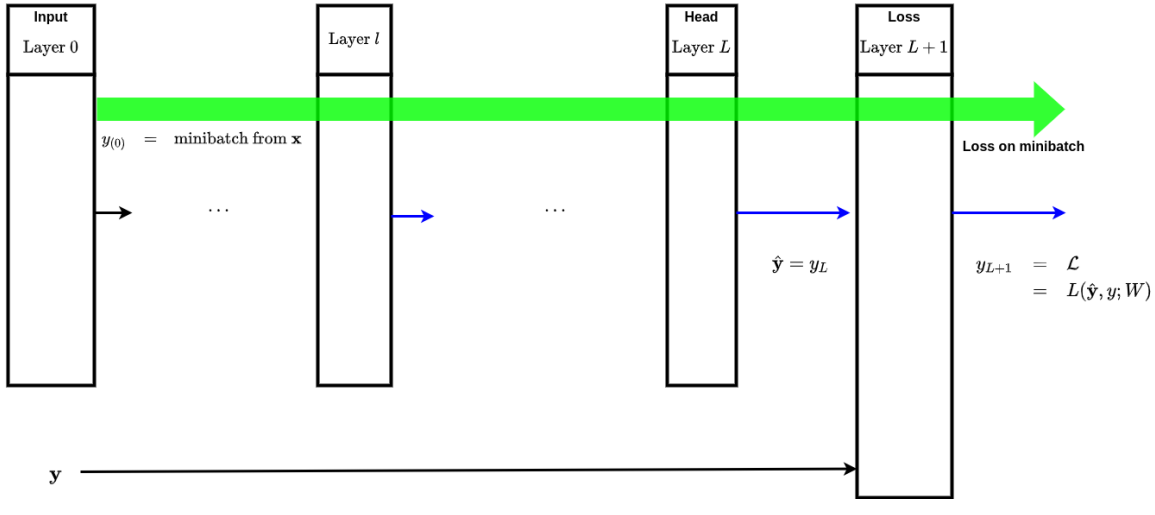
- Divides the m training examples
- Into $b = m/m'$ disjoint batches of $m' \leq m$ examples each

- Iterates over the batches
    - Approximate the loss on the current batch
    - Update $\mathbf{W}$ according to

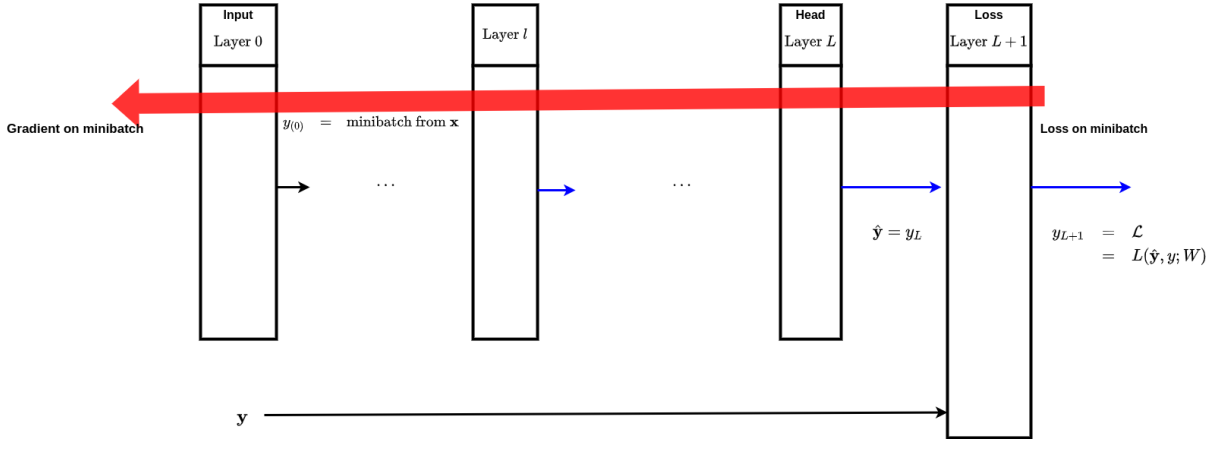
$$\mathbf{W} = \mathbf{W} - \alpha * \frac{\partial \mathcal{L}}{\partial W}$$

    - Repeat until all the batches have been processed

Minibatch: Forward Pass
From minibatch to Loss



Minibatch: Backwards Pass
From minibatch Loss to Gradient



Thus, Minibatch Gradient Descent

- Examines *all* m training examples
- In batches of size $m' \leq m$
- Resulting in $b = m/m'$ updates to $\mathbf{W}$ for each complete pass through the m training examples

Minibatch Gradient Descent is faster than a single batch of size m

- Update $\mathbf{W}$ b times, rather than once
- A complete pass through the b mini-batches is called an *epoch*

The Training loop

A single epoch of Gradient Descent encounters all m examples and makes b updates

We may need additional epochs to continue to drive down the Loss.

This iterative process is called the *training loop*.

Here is some pseudo-code:

initialize(W) # Training loop to implement mini-batch SGD for epoch in range(n_epochs):` for X_batch, y_batch in next_batch(X_train, y_train, batch_size, shuffle=True): # Forward pass y = NN(X_batch) # Loss calculation loss = loss_fn(y, y_batch) # Backward pass grads = gradient(loss, W) # Update W = W - grads * learning_rate

It used to be the case that this fairly standard training loop was coded for each problem.

Just as `sklearn` wrapped common code into a high-level API

- We will use a toolkit that hides the training loop behind a high level API

Scaling the inputs

Many times in this course we have pointed out that some models are *scale sensitive*.

Neural Networks are not *mathematically* sensitive but tend to be so *in practice*.

It is *highly recommended* to scale your data so their absolute values are around 1.0 or at least somewhat small.

Gradient Descent is the root of the problem:

- Two features on different scales can cause the optimizer to favor one over the other
- Activations can *saturate*
    - Output of dot product (Dense layer) is in the "flat* area of the activation
    - Zero derivative: no learning
- The Cost/Loss may be large in initial epochs when the target values are too different from the dot products
    - *Large* gradients: unstable learning
    - Weights are typically initialized to values less than 1.0, leading to small dot products

Remember: if you re-scale the inputs, you will need to invert the transformation when communicating the results.

In [4]:
```
print("Done")
```

```
Done
```