Review Session:
Deep Learning Fundamentals

What we will cover today

- Deep learning basics
    - Defining a neural network architecture
    - Defining a loss function
    - Optimizing the loss function

- Model implementation using deep learning frameworks

- Neural network design choices

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What you are expected to know for the class:

- Definition and conceptual understanding of how the main components of different types of neural networks work
- Framework of training a deep learning model
- Conceptual understanding and trade-offs among design choices
- Good practices and techniques for effectively developing deep learning models for different biomedical tasks

What is not expected:

- Remembering / deriving complicated mathematical derivations of gradients, backpropagation, specific optimization methods (Adam, etc.), learning rate schedulers, etc.
- Mathematical details of design choices such as batch normalization, dropout (scaling), etc. Instead you are expected to understand them conceptually, understand trade-offs, and understand how to make good choices about using them

From lecture: Machine learning framework

Data-driven learning of a mapping from input to output

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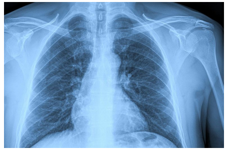
Data-driven learning of a mapping from input to output

Traditional machine learning approaches

Input → **Feature extractor** → **Machine learning model** → **Output**

(e.g., )

(e.g., color and texture histograms)

(e.g., support vector machines and random forests)

(e.g., presence or not or disease)

From lecture: Deep learning (a type of machine learning)

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Traditional machine learning

Input

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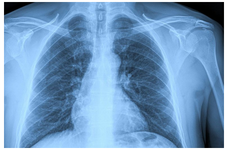

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Feature extractor

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Machine learning model

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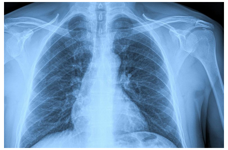
(e.g., )

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Deep learning

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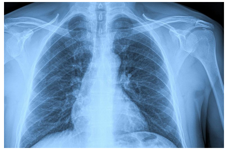
(e.g., )

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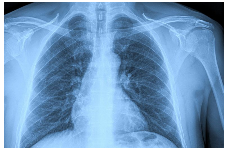
(e.g., )

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Deep learning

Directly learns what are useful (and better!) features from the training data

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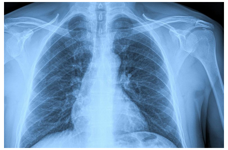
(e.g., )

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Defining a neural network architecture

Our first architecture: a single-layer, fully connected neural network

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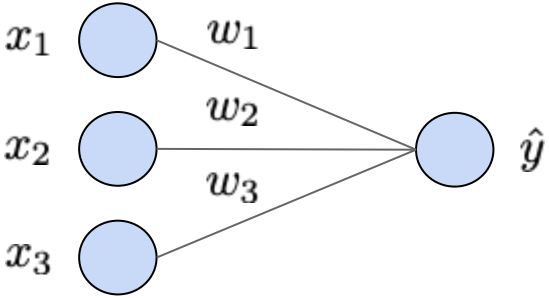
Output:
$$\hat{y} = w_1x_1 + w_2x_2 + w_3x_3 + b$$
$$= w^Tx + b$$



From lecture: let us consider a regression task

Let us consider the task of **regression**: predicting a single real-valued output from input data

Model input: data vector $x = [x_1, x_2, ..., x_N]$

Model output: prediction (single number) $\hat{y}$

Example: predicting hospital length-of-stay from clinical variables in the electronic health record

$x =$ [age, weight, …, temperature, oxygen saturation]

$\hat{y} =$ length-of-stay (days)

Example: predicting expression level of a target gene from the expression levels of N landmark genes

$x \in \mathcal{R}^N =$ expression levels of N landmark genes

$\hat{y} =$ expression level of target gene

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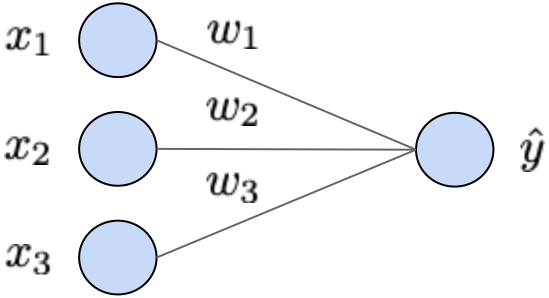

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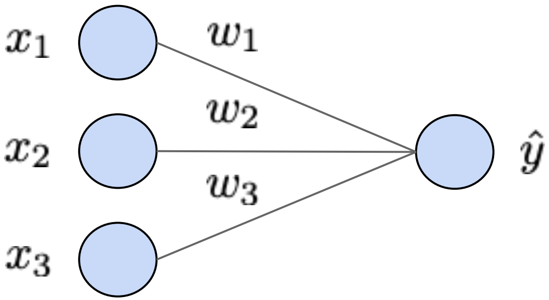

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bias term (allows constant shift)

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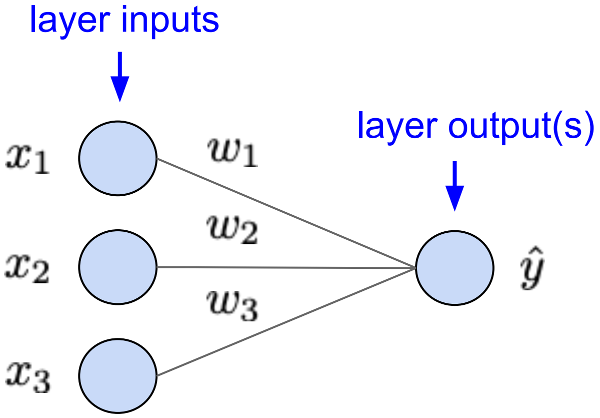

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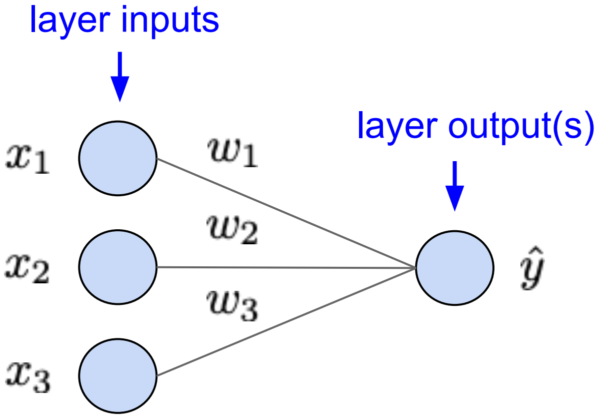

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Neural network parameters:

$$W = \{[w_1, w_2, w_3], b\}$$

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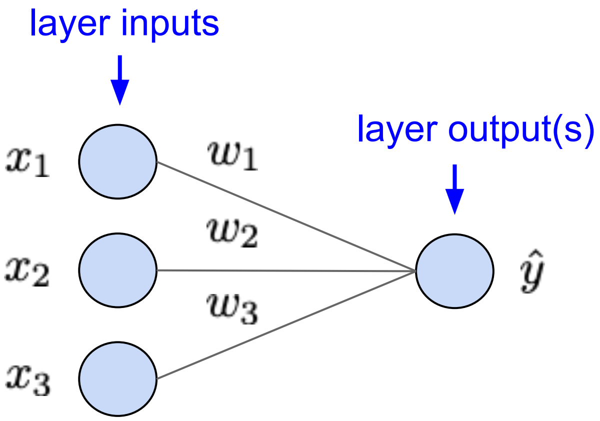

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layer “weights”

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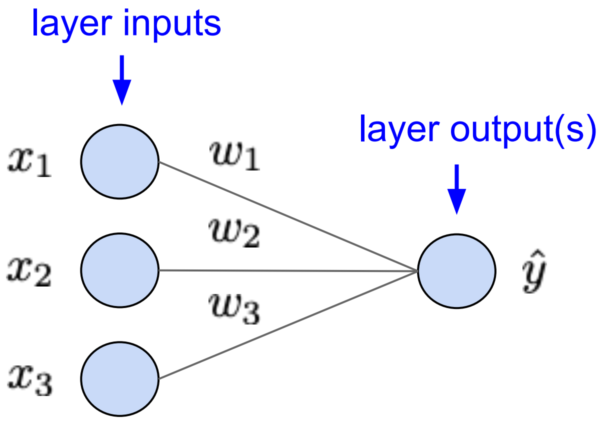

layer inputs

layer output(s)

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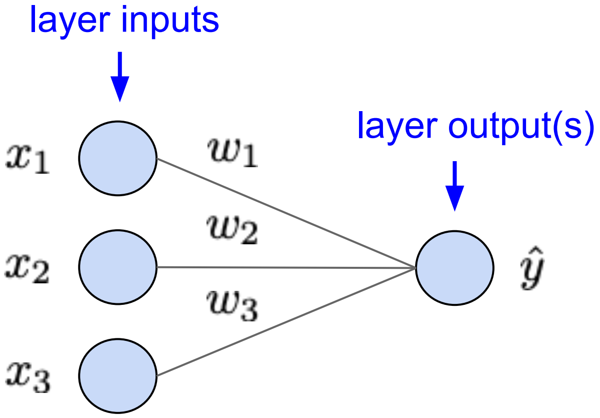

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Caveats of our first (simple) neural network architecture:

- Single layer still "shallow", not yet a "deep" neural network. Will see how to stack multiple layers.
- Also equivalent to a linear regression model! But useful base case for deep learning.

Defining a loss function

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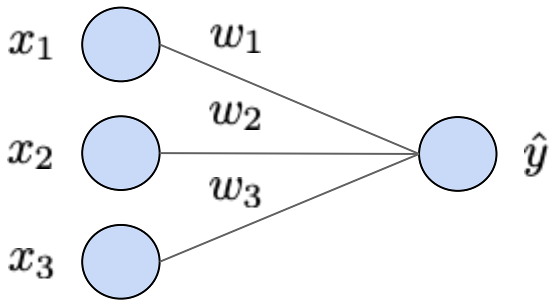

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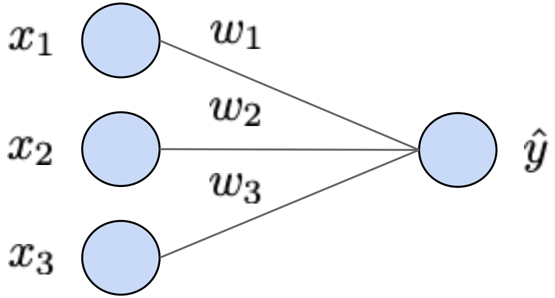

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Loss functions are quantitative measures of how satisfactory the model predictions are (i.e., how “good” the model parameters are).

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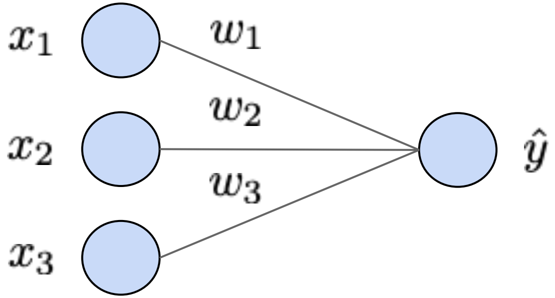

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We will use the mean square error (MSE) loss which is standard for regression.

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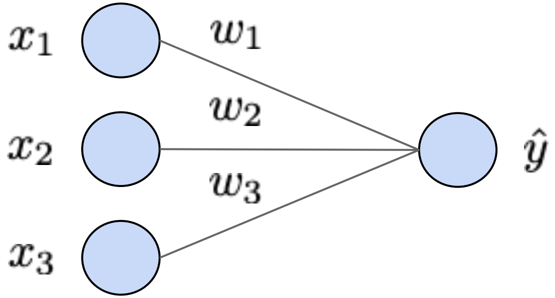

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MSE loss for a single example x^i, when the prediction is $\hat{y}^i$ and the correct (ground truth) output is y^i:

$$L^i(W) = (\hat{y}^i - y^i)^2$$

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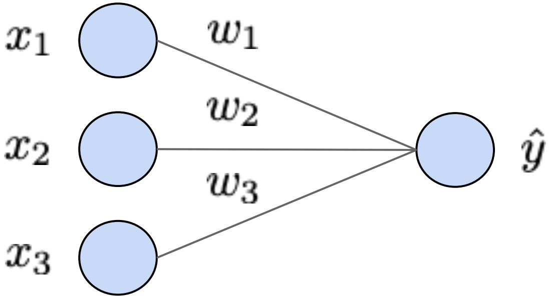

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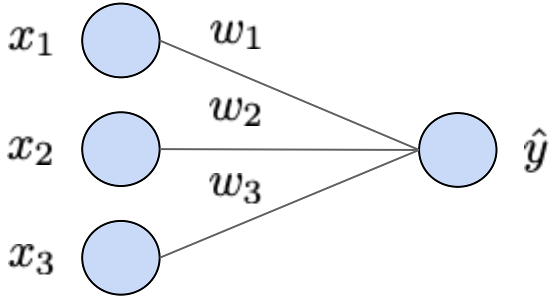

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MSE loss over a set of examples $i = \{1, \ldots, M\}$: $L = \frac{1}{M}\sum_i L^i(W)$

Optimizing the loss function: gradient descent

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“Loss landscape”: the value of the loss function at every value of the model parameters

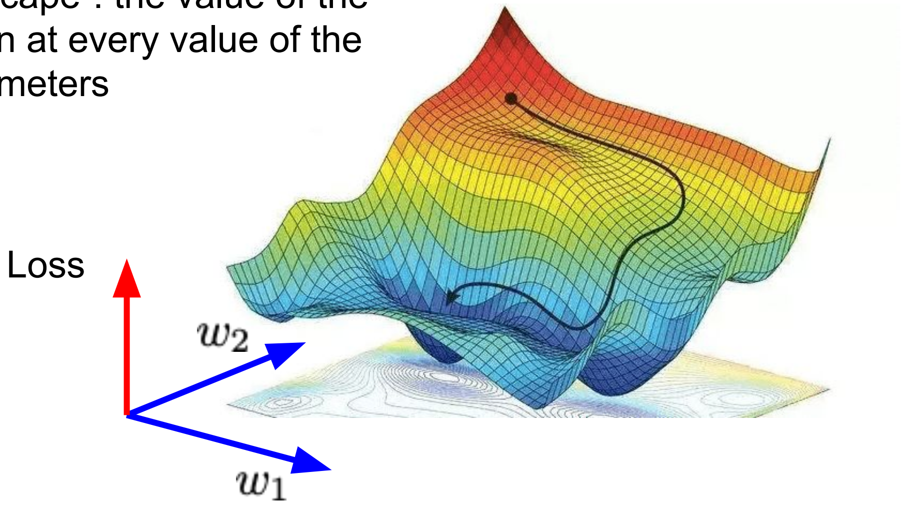

Figure credit: https://easyai.tech/wp-content/uploads/2019/01/tiduxiajiang-1.png

Optimizing the loss function: gradient descent

Goal: find the “best” values of the model parameters that minimize the loss function

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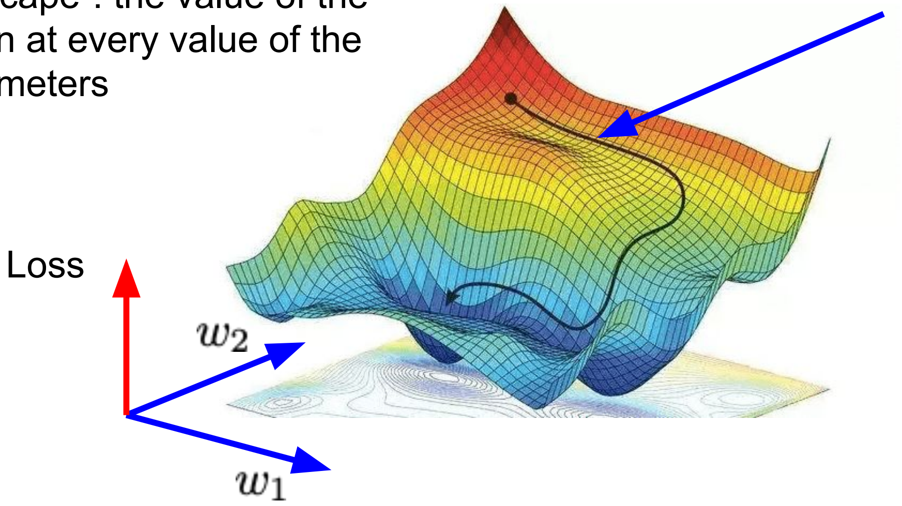
Main idea: iteratively update the model parameters, to take steps in the local direction of steepest (negative) slope, i.e., the negative gradient



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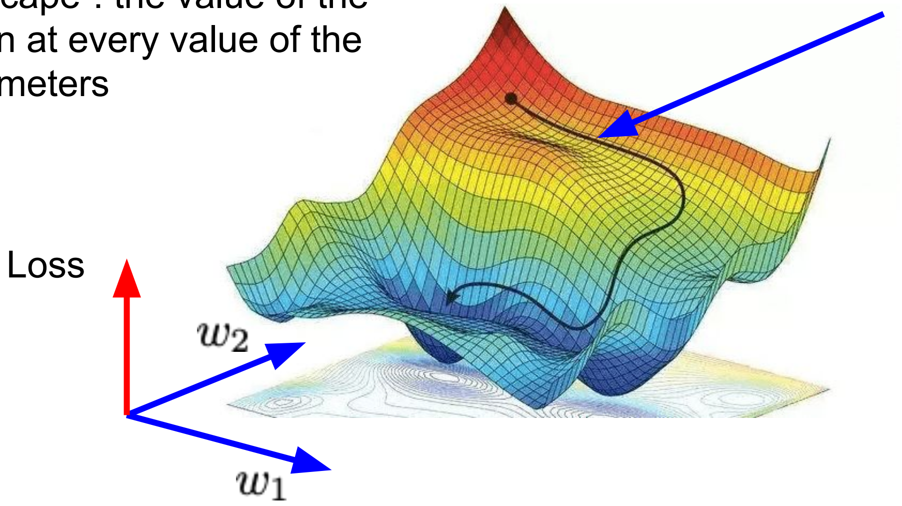

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We will be able to use gradient descent to iteratively optimize the complex loss function landscapes corresponding to deep neural networks!

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Review from calculus: derivatives and gradients

The **derivative** of a function is a measure of local slope.

Ex: $f(x) = x^2$ $\frac{\partial f}{\partial x} = 2x$

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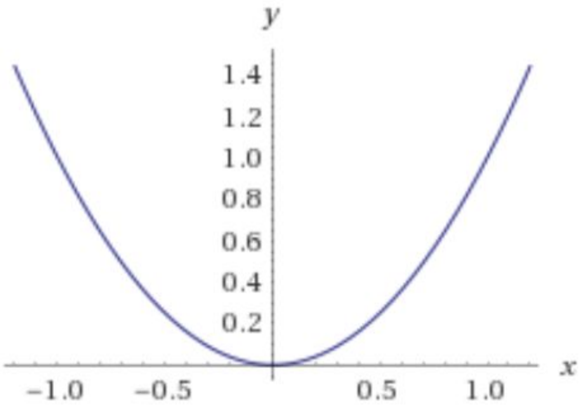

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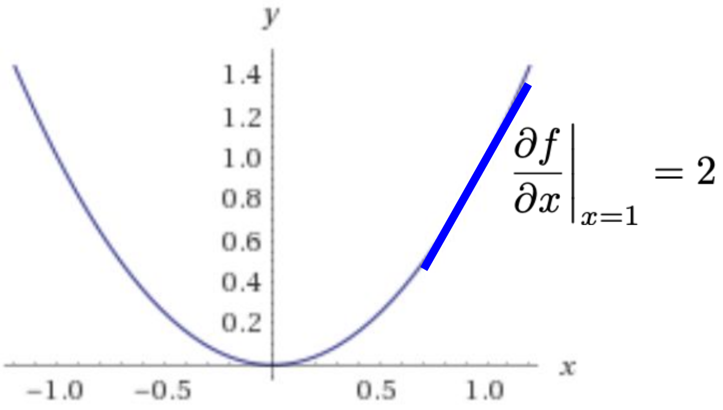

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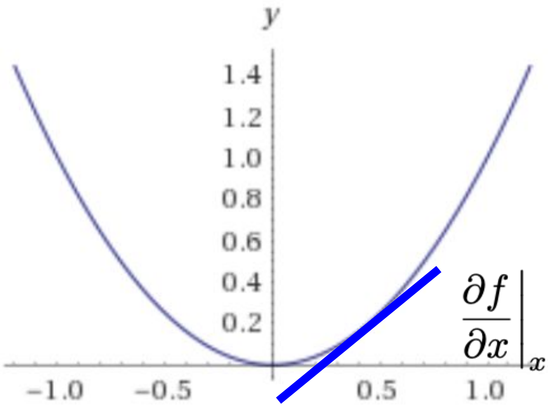
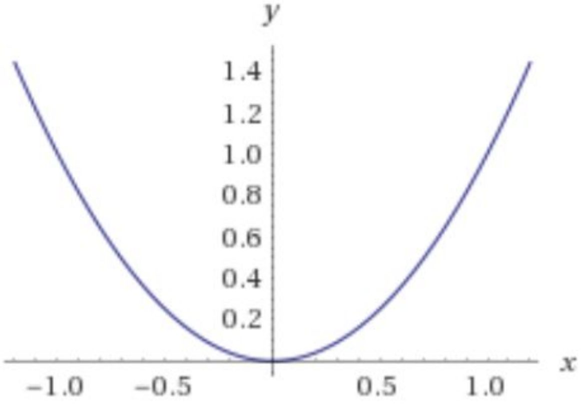


$$\left.\frac{\partial f}{\partial x}\right|_{x=0.5} = 1$$

Review from calculus: derivatives and gradients



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The **gradient** of a function of multiple variables is the vector of partial derivatives of the function with respect to each variable.

Ex: $f(x_1, x_2) = 3{x_1}^2 + {x_2}^2$ $\qquad$ $\nabla f_x = [6x_1, 2x_2]$

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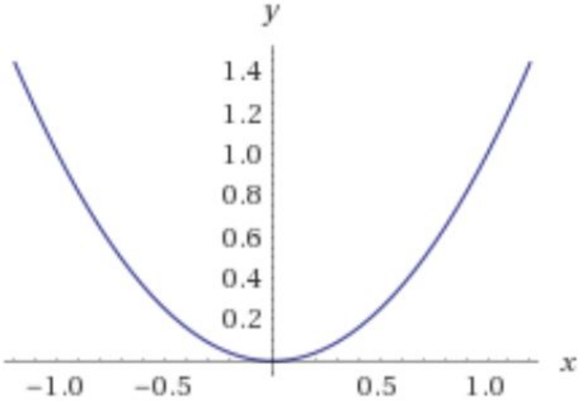

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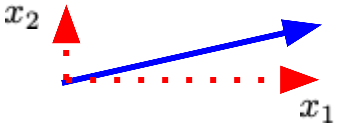
The gradient evaluated at a particular point is the direction of steepest ascent of the function.

$$\nabla f_x \Big|_{x_1=1, x_2=1} = [6, 2]$$



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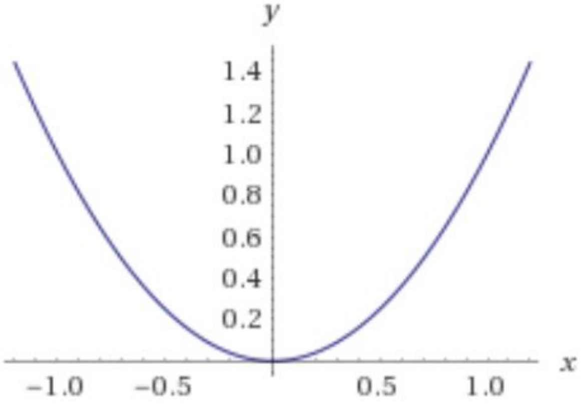

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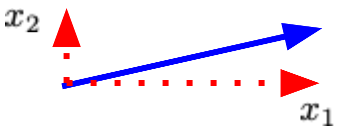

The negative of the gradient is the direction of steepest descent -> direction we want to move in the loss function landscape!

Gradient descent algorithm

Let the gradient of the loss function with respect to the model parameters w be:

$$\nabla L_W = \left[\frac{\partial L}{\partial w_1}, \frac{\partial L}{\partial w_2}, ..., \frac{\partial L}{\partial w_K} \right]$$

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For ease of notation, rewrite parameter b as w_0 corresponding to $x_0 = 1$:

$$\hat{y} = w_0 x_0 + w_1 x_1 + w_2 x_2 + w_3 x_3$$
$$W = \{[w_0, w_1, w_2, w_3]\}$$

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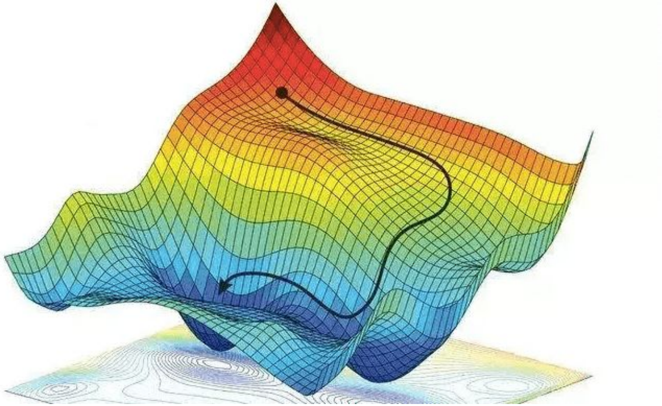
Then we can minimize the loss function by iteratively updating the model parameters ("taking steps") in the direction of the negative gradient, until convergence:

$$W := W - \alpha \nabla L_W$$



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$$\hat{y} = w_0x_0 + w_1x_1 + w_2x_2 + w_3x_3$$
$$W = \{[w_0, w_1, w_2, w_3]\}$$

Then we can minimize the loss function by iteratively updating the model parameters ("taking steps") in the direction of the negative gradient, until convergence:

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"Step size" hyperparameter (design choice) indicating how big of a step in the negative gradient direction we want to take at each update.
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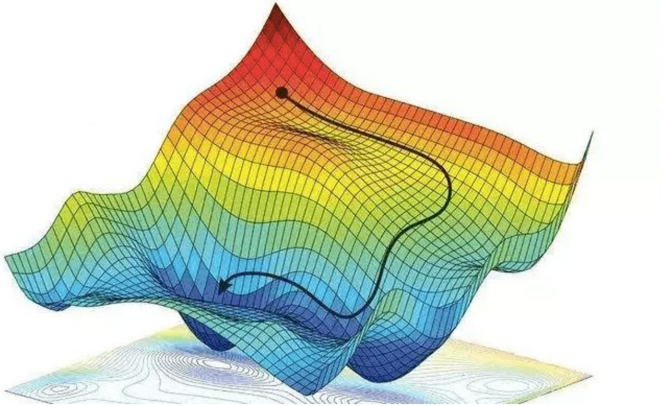
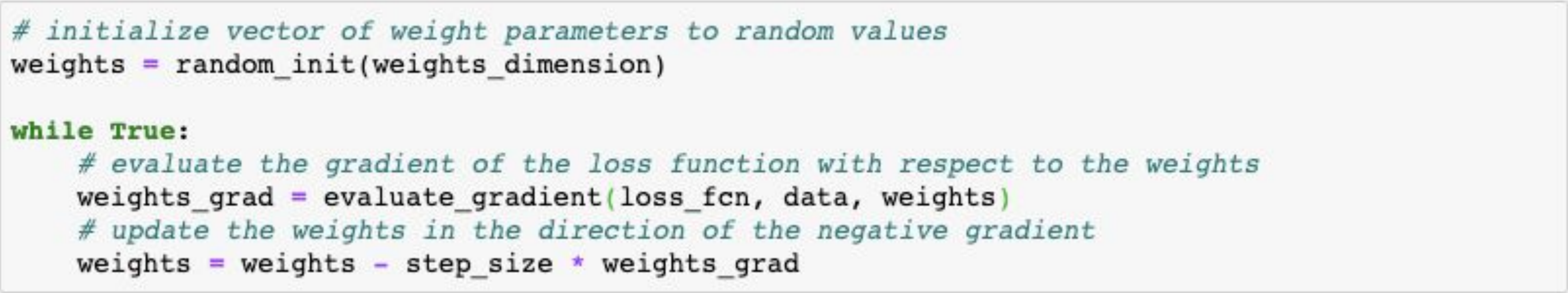


Gradient descent algorithm: in code



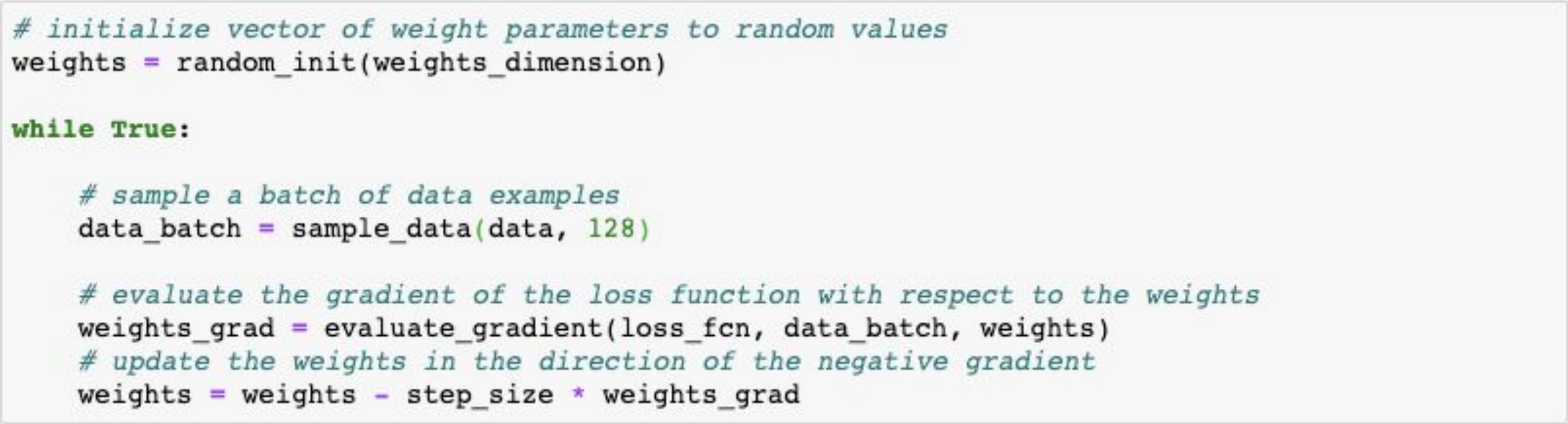
```
# initialize vector of weight parameters to random values
weights = random_init(weights_dimension)

while True:
    # evaluate the gradient of the loss function with respect to the weights
    weights_grad = evaluate_gradient(loss_fcn, data, weights)
    # update the weights in the direction of the negative gradient
    weights = weights - step_size * weights_grad
```

Stochastic gradient descent (SGD)

Evaluating gradient involves iterating over all data examples, which can be slow!

In practice, usually use stochastic gradient descent: **estimate gradient over a sample of data examples** (usually as many as can fit on GPU at one time, e.g. 32, 64, 128)



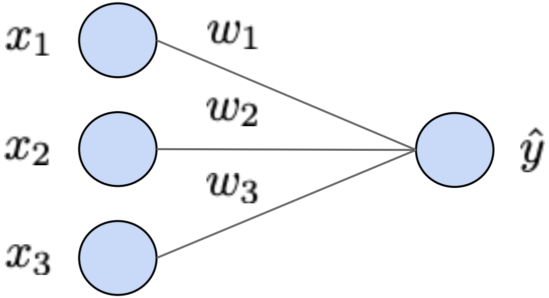
```
# initialize vector of weight parameters to random values
weights = random_init(weights_dimension)

while True:

    # sample a batch of data examples
    data_batch = sample_data(data, 128)

    # evaluate the gradient of the loss function with respect to the weights
    weights_grad = evaluate_gradient(loss_fcn, data_batch, weights)
    # update the weights in the direction of the negative gradient
    weights = weights - step_size * weights_grad
```

Optimizing the loss function: our example



Output: $$\hat{y} = w_1x_1 + w_2x_2 + w_3x_3 + b$$
$$= w^Tx + b$$

Neural network parameters:

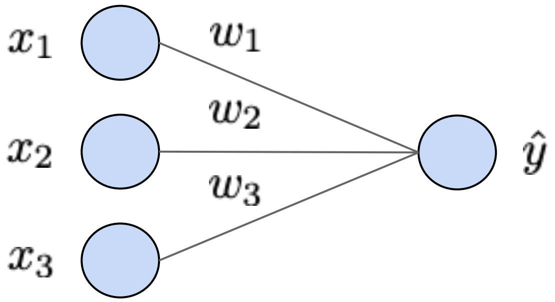
$$W = \{[w_1, w_2, w_3], b\}$$

Loss function:

Per-example: $L^i(W) = (\hat{y}^i - y^i)^2$

Over M examples: $L = \frac{1}{M}\sum_i L^i(W)$

Optimizing the loss function: our example



Output: $\hat{y} = w_1 x_1 + w_2 x_2 + w_3 x_3 + b$

$$= w^T x + b$$

Neural network parameters:

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Per-example: $L^i(W) = (\hat{y}^i - y^i)^2$

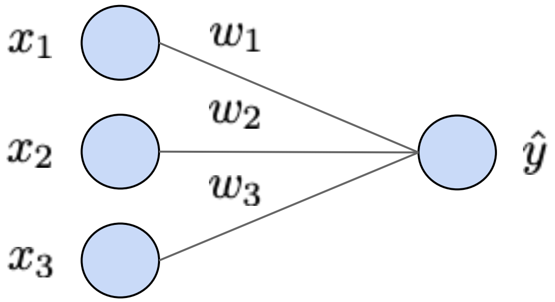
Over M examples: $L = \frac{1}{M} \sum_i L^i(W)$

Gradient of loss w.r.t. weights:

Partial derivative of loss w.r.t. kth weight:

$$\frac{\partial L^i}{\partial w_k} = \frac{\partial L^i}{\partial \hat{y}^i} \frac{\partial \hat{y}^i}{\partial w_k} = 2(\hat{y}^i - y^i) x_k^i$$

Optimizing the loss function: our example



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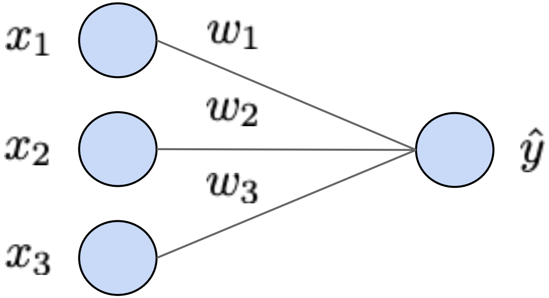
Gradient of loss w.r.t. weights:

Partial derivative of loss w.r.t. kth weight:

Chain rule

$$\frac{\partial L^i}{\partial w_k} = \frac{\partial L^i}{\partial \hat{y}^i}\frac{\partial \hat{y}^i}{\partial w_k} = 2(\hat{y}^i - y^i)x_k^i$$

Optimizing the loss function: our example



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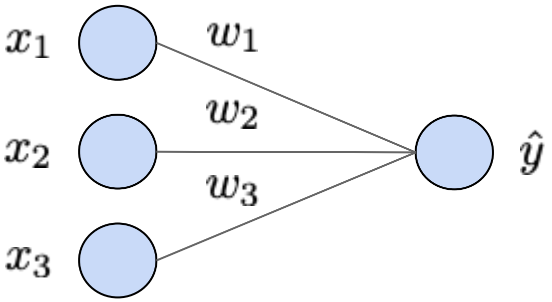
Over M examples

$$\frac{\partial L}{\partial w_k} = \frac{1}{M} \sum_i \frac{\partial L^i}{\partial w_k} = \frac{1}{M} \sum_i 2(\hat{y}^i - y^i) x_k^i$$

Optimizing the loss function: our example



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$= w^Tx + b$

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$$\frac{\partial L}{\partial w_k} = \frac{1}{M}\sum_i \frac{\partial L^i}{\partial w_k} = \frac{1}{M}\sum_i 2(\hat{y}^i - y^i)x_k^i$$

Full gradient expression:

$$\nabla L_W = \left[\frac{\partial L}{w_0}, \ldots, \frac{\partial L}{w_3}\right] = \boxed{\frac{1}{M}\sum_i 2(\hat{y}^i - y^i)x^i}$$

Gradient descent algorithm

Let the gradient of the loss function with respect to the model parameters w be:

$$\nabla L_W = \left[\frac{\partial L}{\partial w_1}, \frac{\partial L}{\partial w_2}, \ldots, \frac{\partial L}{\partial w_K}\right]$$

For ease of notation, rewrite parameter b as w_0 corresponding to $x_0 = 1$:

$$\hat{y} = w_0 x_0 + w_1 x_1 + w_2 x_2 + w_3 x_3$$

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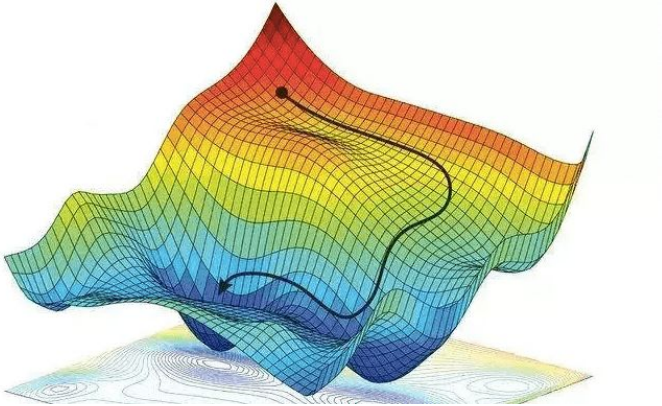
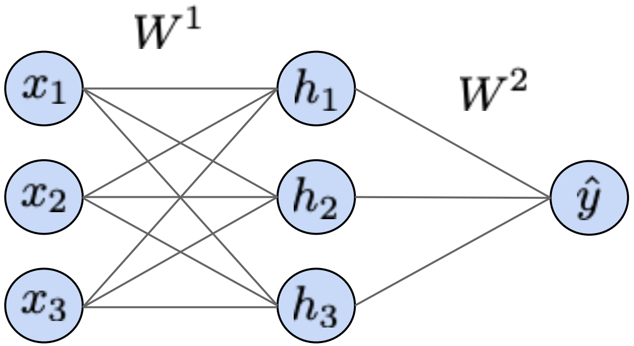


Remember from lecture: a two-layer fully-connected neural network



Output: $h = \sigma(W^1 x + b^1)$

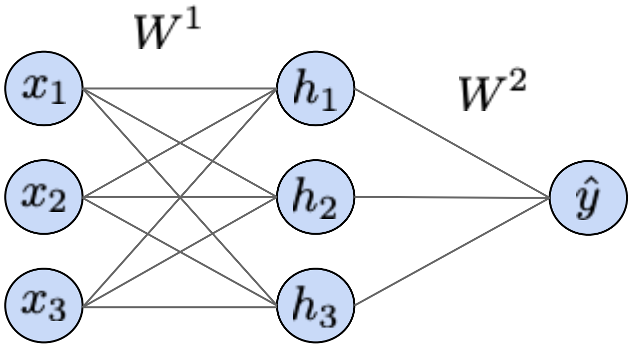
$\hat{y} = W^2 h + b^2$

$$W^1 = \begin{bmatrix} w^1_{11} & w^1_{12} & w^1_{13} \\ w^1_{21} & w^1_{22} & w^1_{23} \\ w^1_{31} & w^1_{32} & w^1_{33} \end{bmatrix} \quad b^1 = \begin{bmatrix} b^1_1 \\ b^1_2 \\ b^1_3 \end{bmatrix}$$

$$W^2 = \begin{bmatrix} w^2_{11} & w^2_{12} & w^2_{13} \end{bmatrix} \quad b^2 = \begin{bmatrix} b^2_1 \end{bmatrix}$$

Now: a two-layer fully-connected neural network

$$\sigma(a) = \frac{1}{1+e^{-a}}$$



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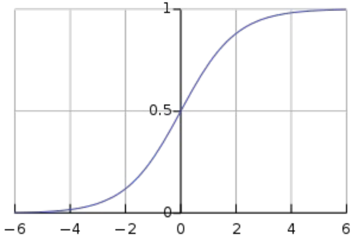

Sigmoid “activation function”

$$W^1 = \begin{bmatrix} w^1_{11} & w^1_{12} & w^1_{13} \\ w^1_{21} & w^1_{22} & w^1_{23} \\ w^1_{31} & w^1_{32} & w^1_{33} \end{bmatrix} \quad b^1 = \begin{bmatrix} b^1_1 \\ b^1_2 \\ b^1_3 \end{bmatrix}$$

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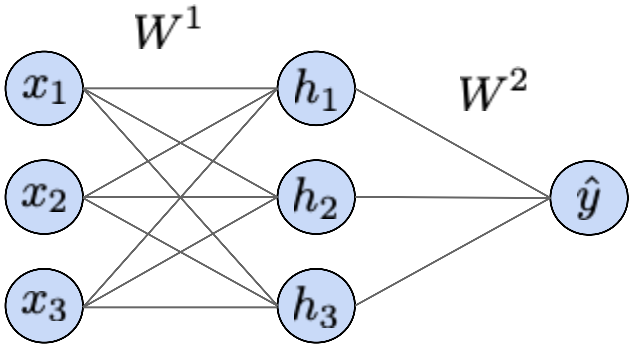
Now: a two-layer fully-connected neural network



Output: $h = \sigma(W^1 x + b^1)$

$\hat{y} = W^2 h + b^2$

Full function expression:

$$\hat{y} = W^2(\sigma(W^1 x + b^1)) + b^2$$

$$W^1 = \begin{bmatrix} w^1_{11} & w^1_{12} & w^1_{13} \\ w^1_{21} & w^1_{22} & w^1_{23} \\ w^1_{31} & w^1_{32} & w^1_{33} \end{bmatrix} \quad b^1 = \begin{bmatrix} b^1_1 \\ b^1_2 \\ b^1_3 \end{bmatrix}$$

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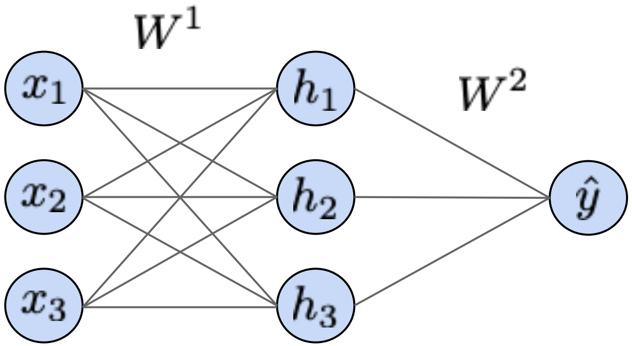
Now: a two-layer fully-connected neural network



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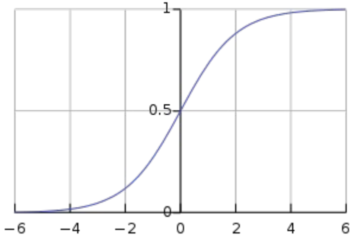
$$\sigma(a) = \frac{1}{1 + e^{-a}}$$

Full function expression:

$$\hat{y} = W^2(\sigma(W^1 x + b^1)) + b^2$$

Activation functions introduce non-linearity into the model -- allowing it to represent highly complex functions.



Sigmoid "activation function"

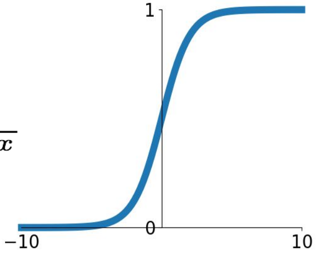
Common activation functions

You can find these in Keras:
https://keras.io/layers/advanced-activations/

You will see these extensively, typically after linear or convolutional layers.
They add nonlinearity to allow the model to express complex nonlinear functions.

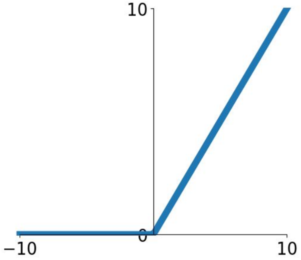
Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



ReLU

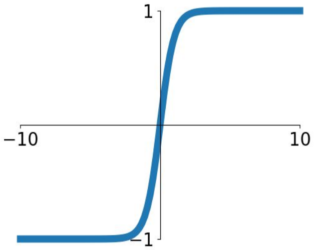
$$\max(0, x)$$



and many more...

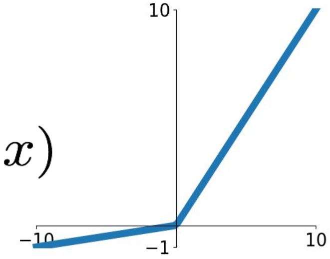
Tanh

$$\tanh(x)$$



Leaky ReLU

$$\max(0.1x, x)$$



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Typical in modern CNNs and MLPs

Sigmoid

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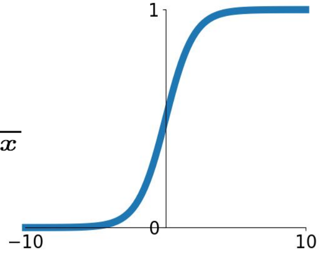

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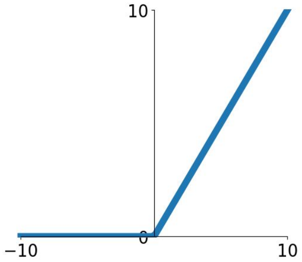

and many more...

Tanh

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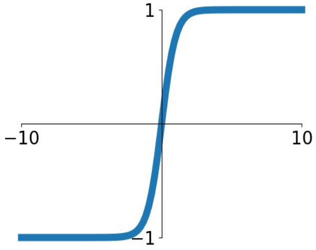

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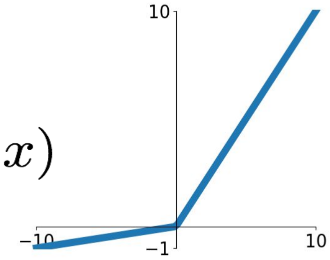

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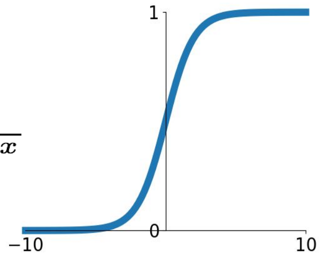

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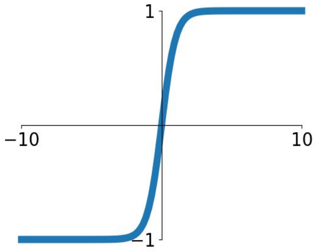
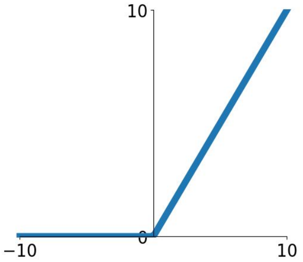
$$\tanh(x)$$



Will see in recurrent neural networks. Also used in early MLPs and CNNs.

ReLU

$$\max(0, x)$$



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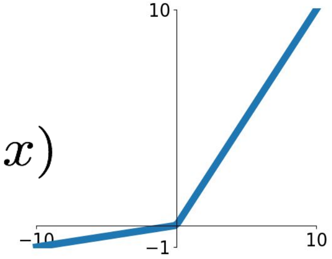
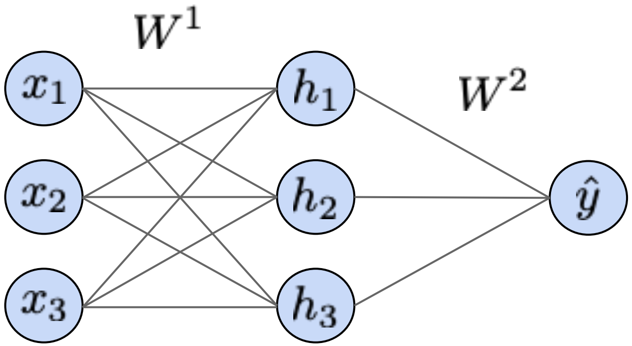


and many more...

Now: a two-layer fully-connected neural network



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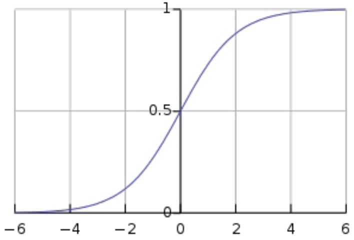
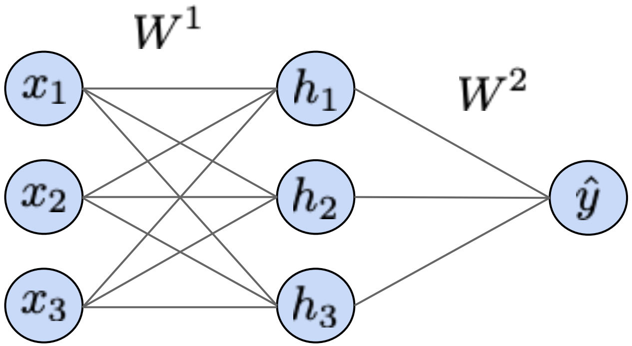


Sigmoid “activation function”

Activation functions introduce non-linearity into the model -- allowing it to represent highly complex functions.

A **fully-connected neural network** (also known as multi-layer perceptron) is a stack of [affine transformation + activation function] layers. There may not be an activation function in the last layer.

Now: a two-layer fully-connected neural network



Output: $\hat{y} = W^2(\sigma(W^1 x + b^1)) + b^2$

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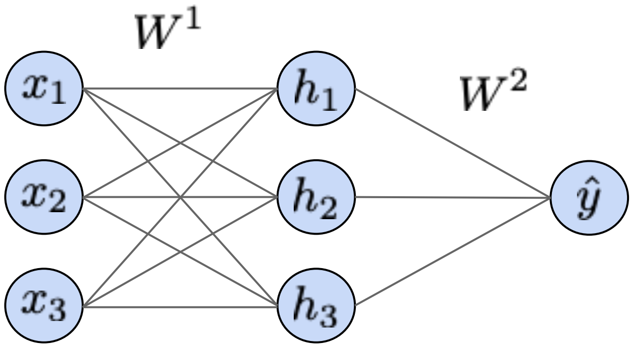
Now: a two-layer fully-connected neural network



Output: $\hat{y} = W^2(\sigma(W^1 x + b^1)) + b^2$

Neural network parameters:

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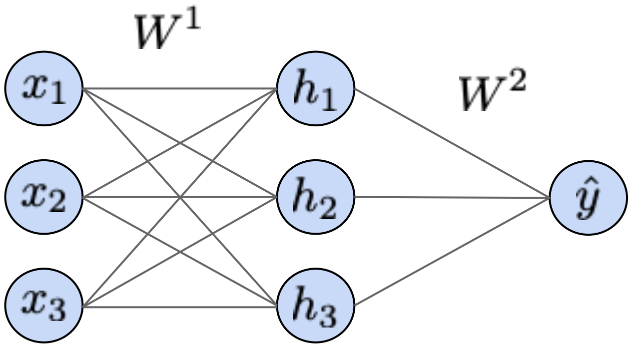

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Neural network parameters:

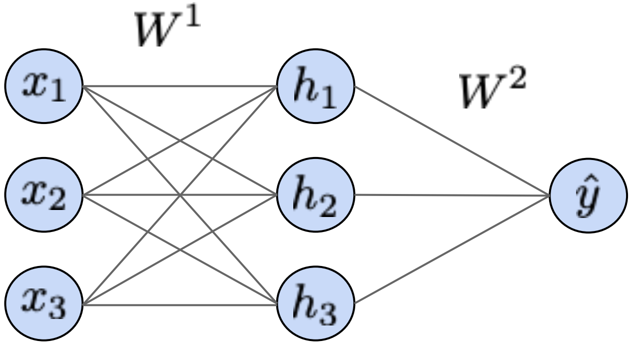
$$W = \{W^1, b^1, W^2, b^2\}$$

Loss function (regression loss, same as before)**:**

Per-example: $L^i(W) = (\hat{y}^i - y^i)^2$

Over M examples: $L = \frac{1}{M}\sum_i L^i(W)$

Now: a two-layer fully-connected neural network



$$W^1 = \begin{bmatrix} w^1_{11} & w^1_{12} & w^1_{13} \\ w^1_{21} & w^1_{22} & w^1_{23} \\ w^1_{31} & w^1_{32} & w^1_{33} \end{bmatrix} \quad b^1 = \begin{bmatrix} b^1_1 \\ b^1_2 \\ b^1_3 \end{bmatrix}$$

$$W^2 = \begin{bmatrix} w^2_{11} & w^2_{12} & w^2_{13} \end{bmatrix} \quad b^2 = \begin{bmatrix} b^2_1 \end{bmatrix}$$

Output: $\hat{y} = W^2(\sigma(W^1 x + b^1)) + b^2$

Neural network parameters:

$$W = \{W^1, b^1, W^2, b^2\}$$

Loss function (regression loss, same as before)**:**

Per-example: $L^i(W) = (\hat{y}^i - y^i)^2$

Over M examples: $L = \frac{1}{M} \sum_i L^i(W)$

Gradient of loss w.r.t. weights:

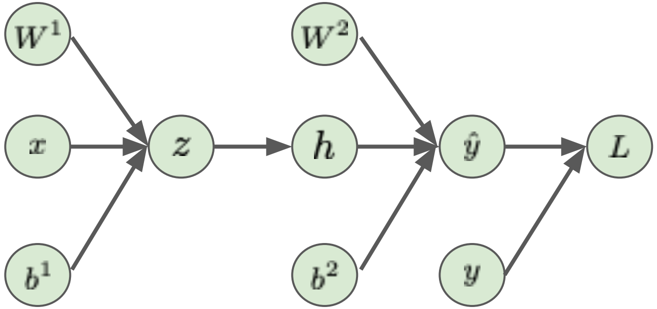
Function more complex -> now much harder to derive the expressions! Instead… computational graphs and backpropagation.

Computing gradients with backpropagation

Computing gradients with backpropagation

Network output: $\hat{y} = W^2(\sigma(W^1 x + b^1)) + b^2$

Think of computing loss function as staged computation of intermediate variables:



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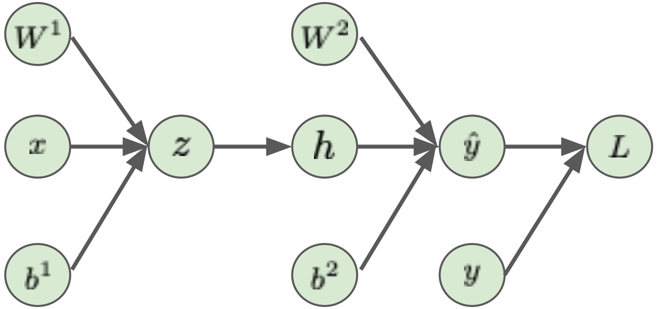

"Forward pass": $z = W^1x + b^1$

$$h = \sigma(z)$$

$$\hat{y} = W^2h + b^2$$

$$L = (\hat{y} - y)^2$$

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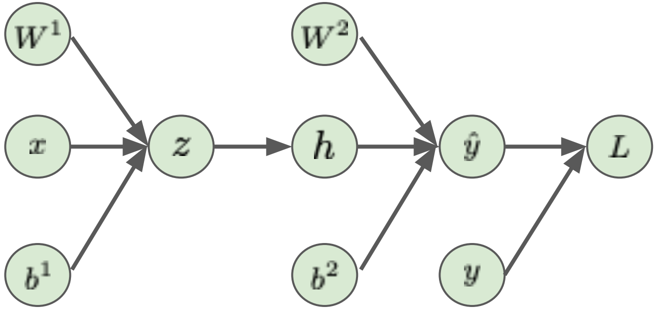

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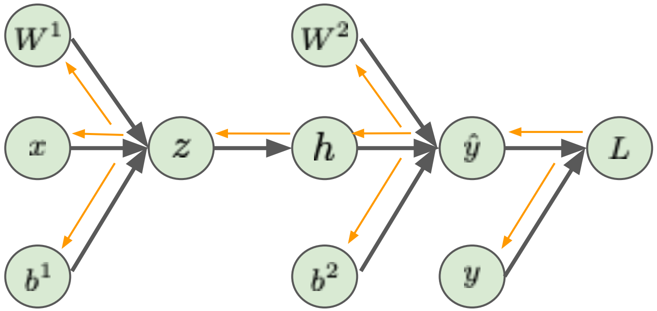

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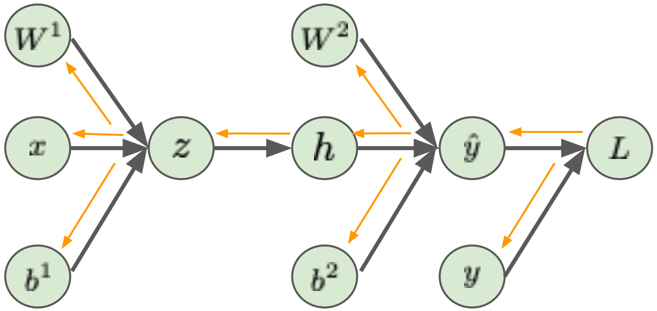

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Plug in from earlier computations via chain rule

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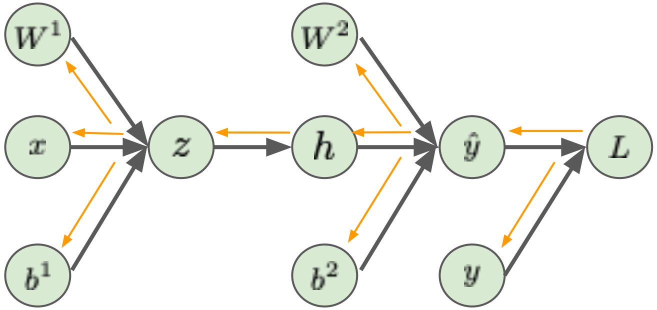

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Plug in from earlier computations via chain rule

Local gradients to derive

Computing gradients with backpropagation

Key idea: Don’t mathematically derive entire math expression for e.g. dL / dW^1. By writing it as nested applications of the chain rule, only have to derive simple “local” gradients representing relationships between connected nodes of the graph (e.g. dH / dW^1).

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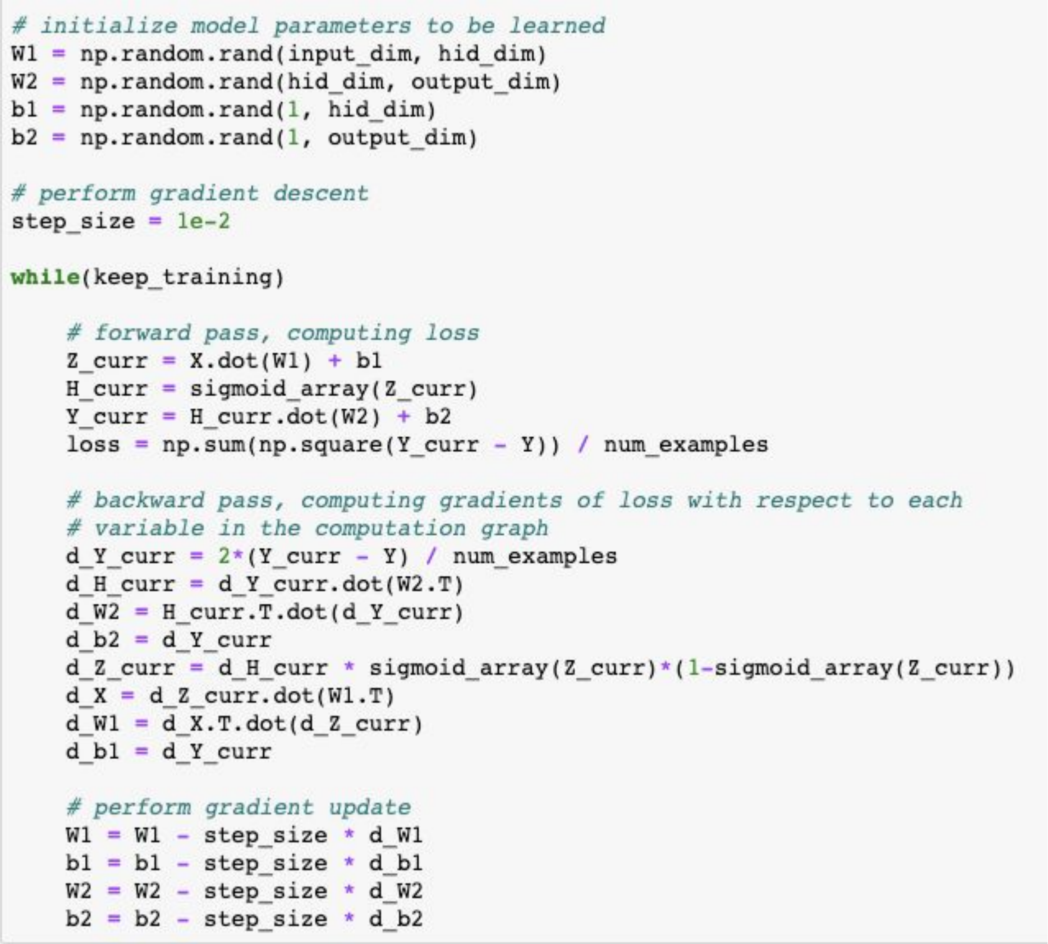
Can use more or less intermediate variables to control how difficult local gradients are to derive!

Training our two-layer neural network in code, using backpropagation



```
# initialize model parameters to be learned
W1 = np.random.rand(input_dim, hid_dim)
W2 = np.random.rand(hid_dim, output_dim)
b1 = np.random.rand(1, hid_dim)
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# perform gradient descent
step_size = 1e-2

while(keep_training)

    # forward pass, computing loss
    Z_curr = X.dot(W1) + b1
    H_curr = sigmoid_array(Z_curr)
    Y_curr = H_curr.dot(W2) + b2
    loss = np.sum(np.square(Y_curr - Y)) / num_examples

    # backward pass, computing gradients of loss with respect to each
    # variable in the computation graph
    d_Y_curr = 2*(Y_curr - Y) / num_examples
    d_H_curr = d_Y_curr.dot(W2.T)
    d_W2 = H_curr.T.dot(d_Y_curr)
    d_b2 = d_Y_curr
    d_Z_curr = d_H_curr * sigmoid_array(Z_curr)*(1-sigmoid_array(Z_curr))
    d_X = d_Z_curr.dot(W1.T)
    d_W1 = d_X.T.dot(d_Z_curr)
    d_b1 = d_Y_curr

    # perform gradient update
    W1 = W1 - step_size * d_W1
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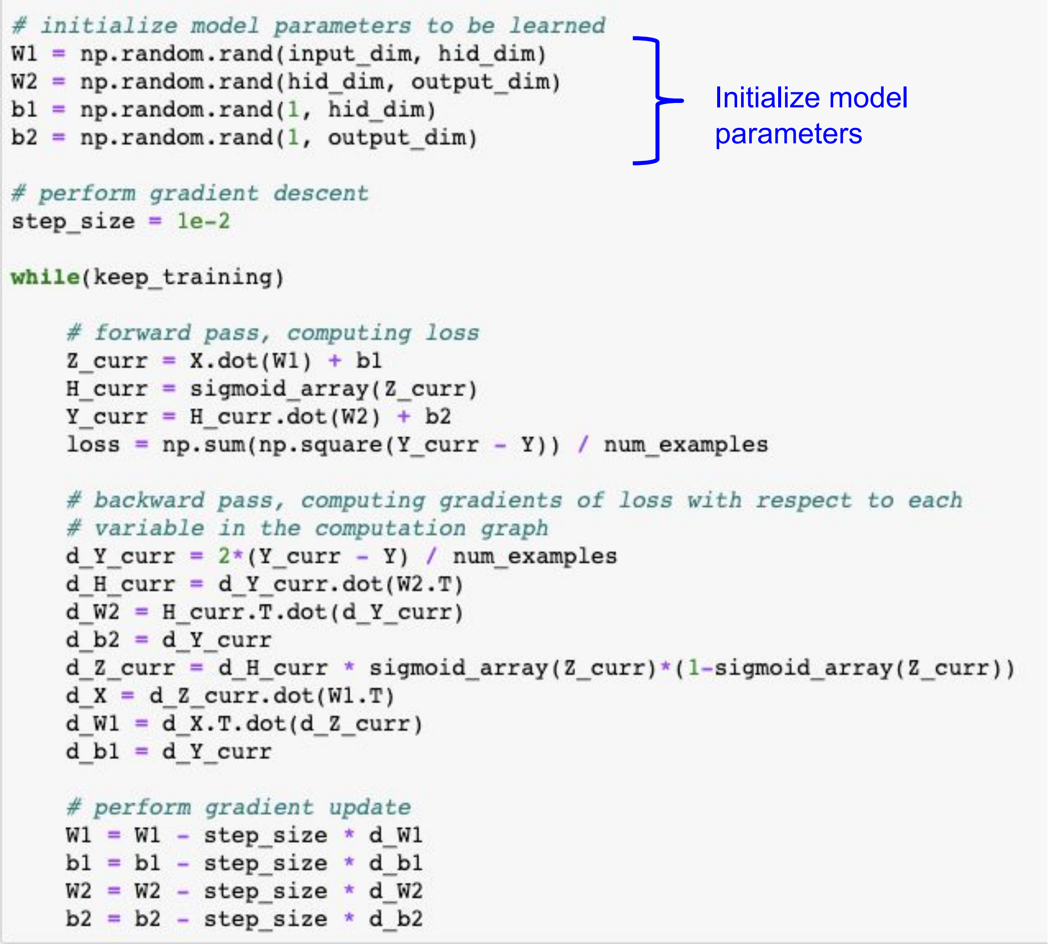

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```
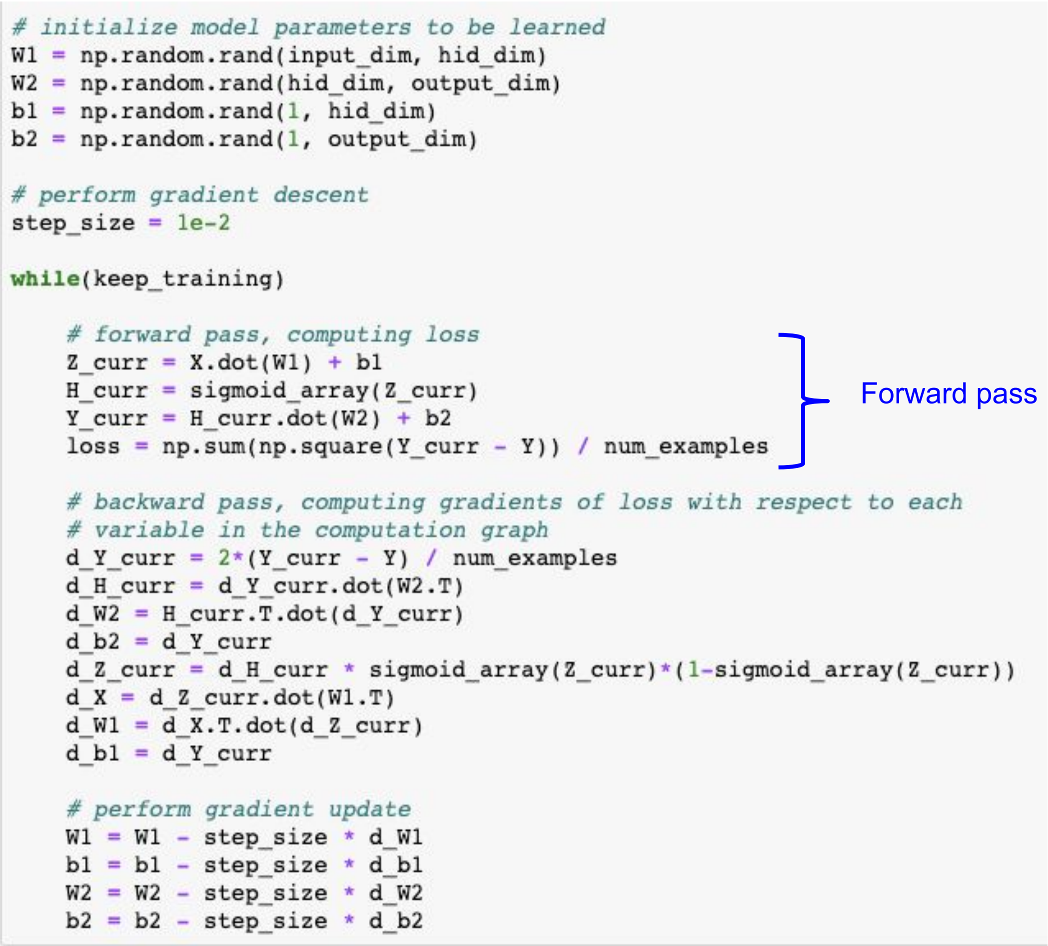

Initialize model parameters

Training our two-layer neural network in code, using backpropagation



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    d_W1 = d_X.T.dot(d_Z_curr)
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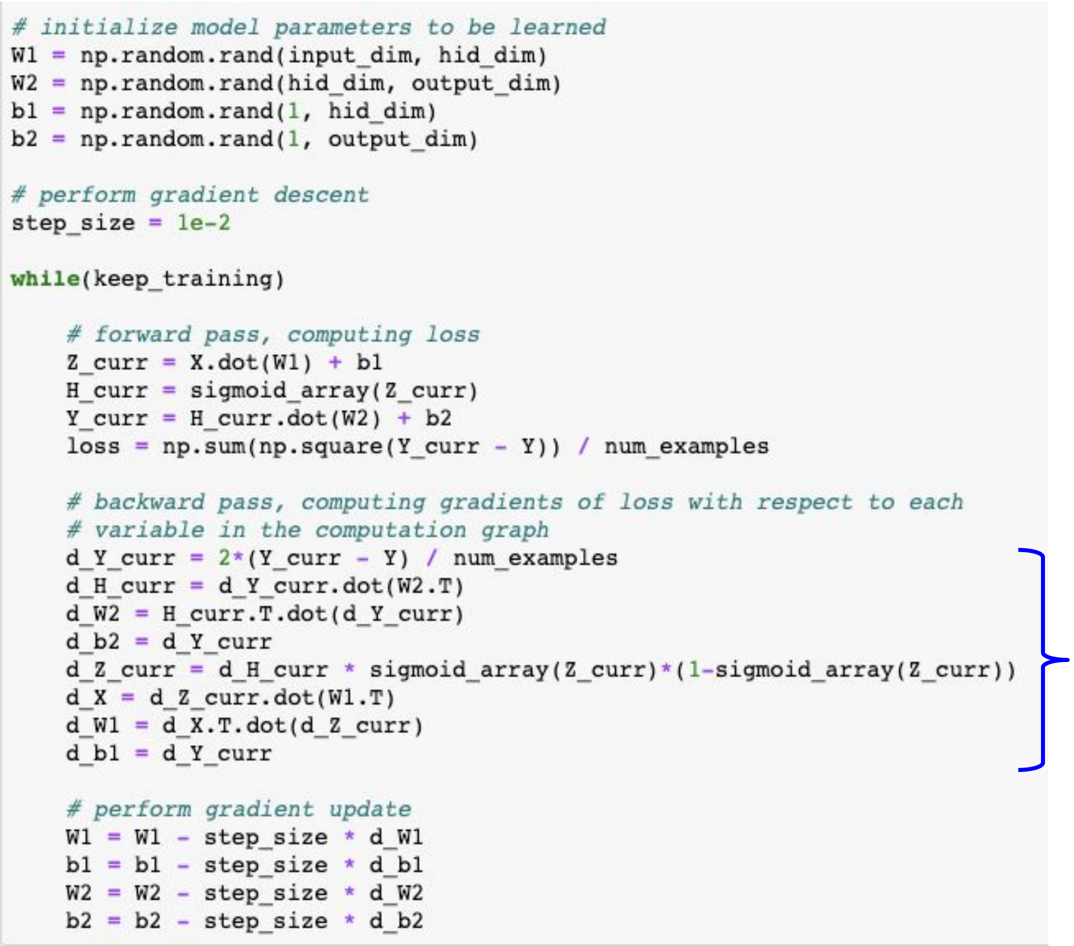
Forward pass

Training our two-layer neural network in code, using backpropagation



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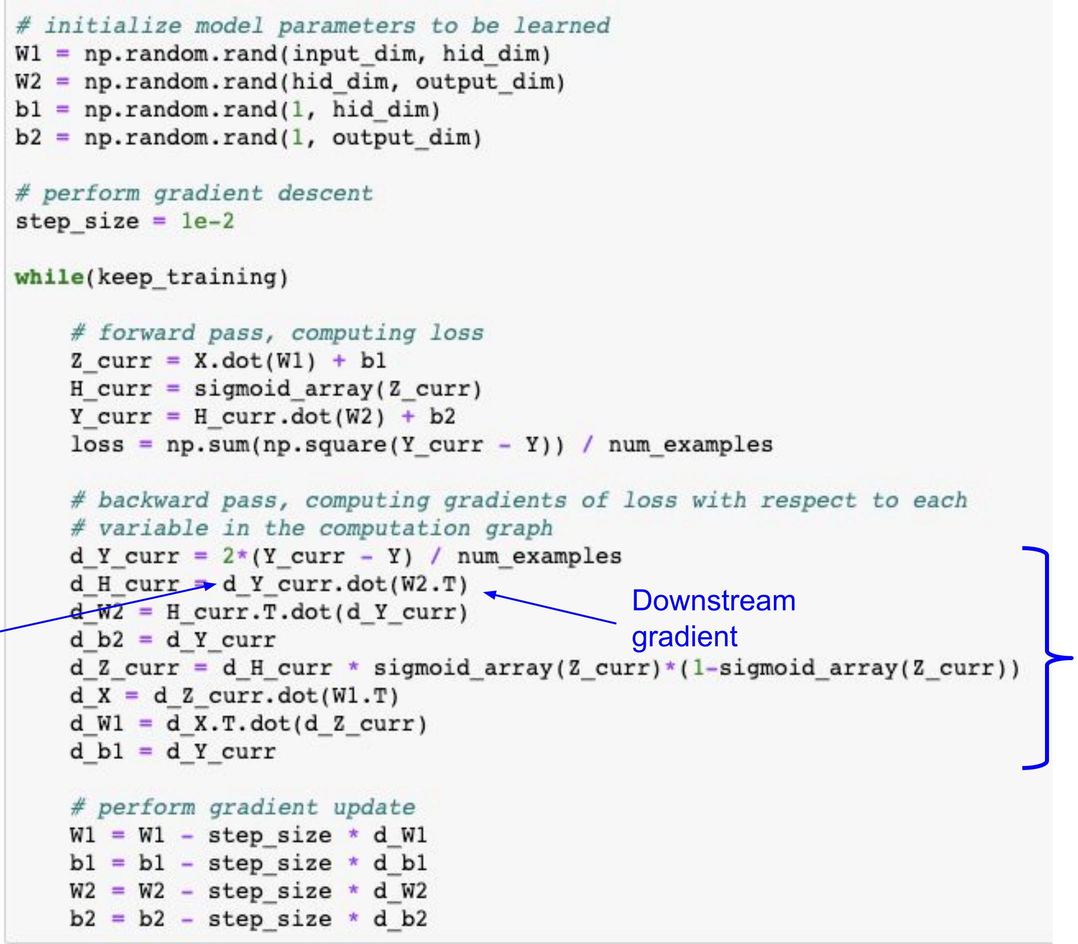
```

Backward pass

Training our two-layer neural network in code, using backpropagation



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```
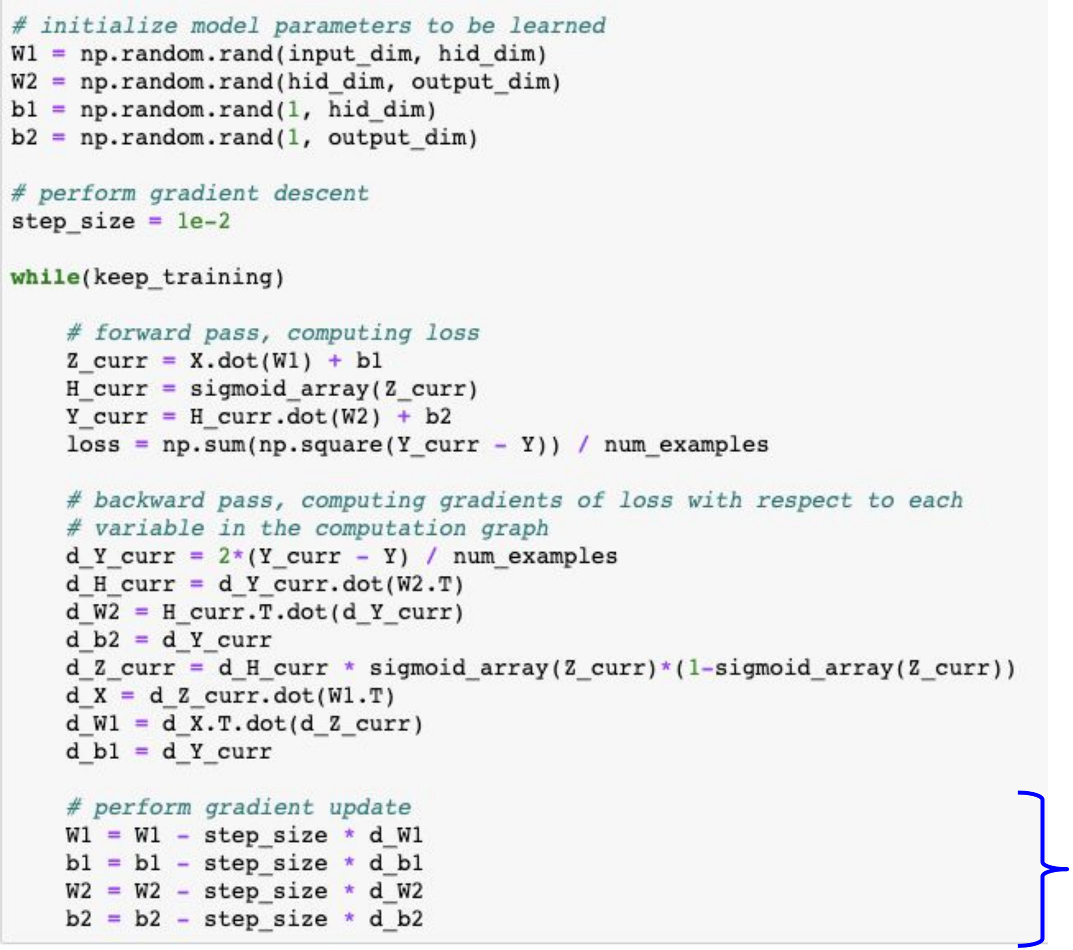

Upstream gradient

Downstream gradient

Backward pass

Training our two-layer neural network in code, using backpropagation



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Gradient update

Deep learning software frameworks

- Makes our lives easier by providing implementations and higher-level abstractions of many components for deep learning, and running them on GPUs:
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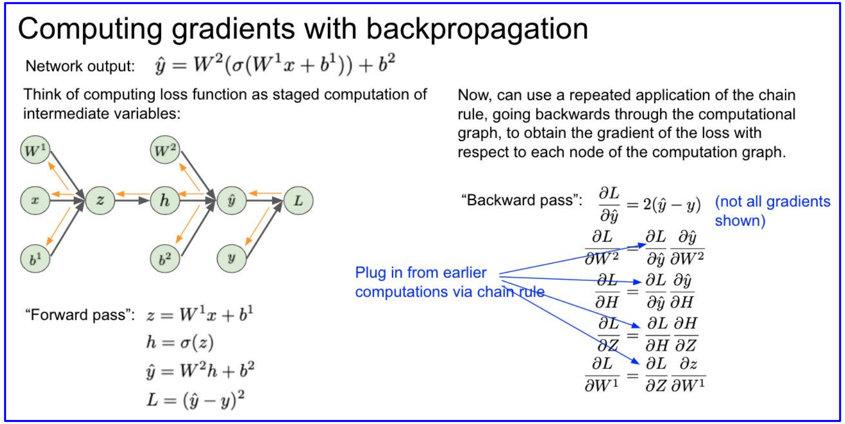

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Plug in from earlier computations via chain rule

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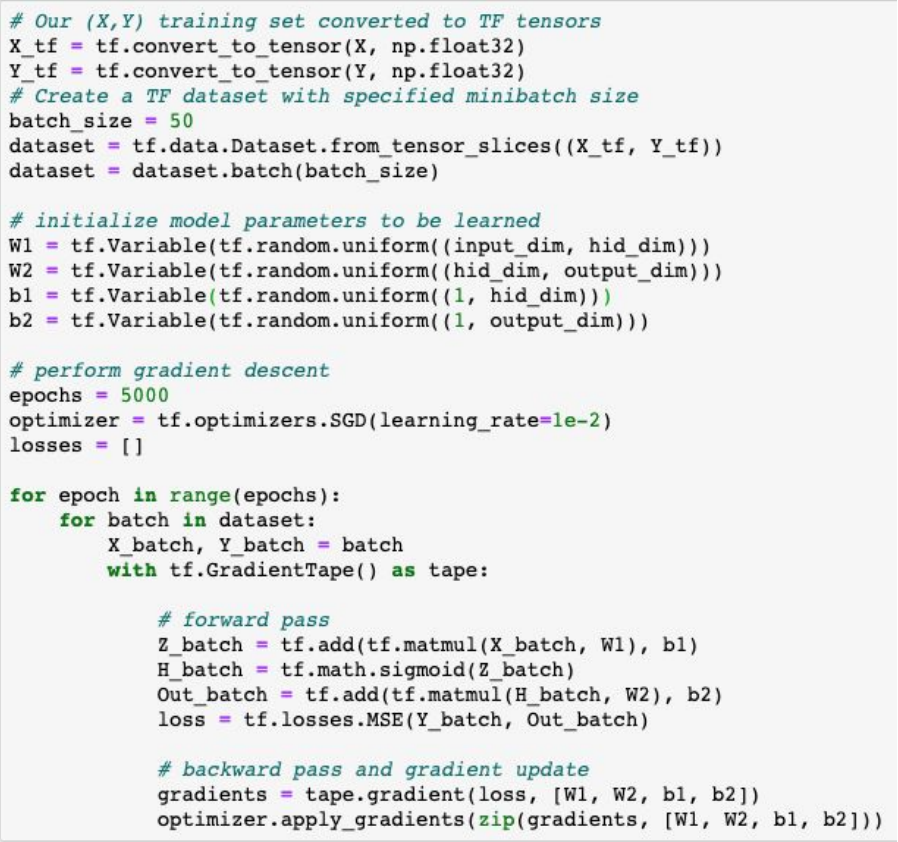
- More next Friday, Oct 7, during the Tensorflow review section.

Training our two-layer neural network in code, in Tensorflow 2.0



```python
# Our (X,Y) training set converted to TF tensors
X_tf = tf.convert_to_tensor(X, np.float32)
Y_tf = tf.convert_to_tensor(Y, np.float32)
# Create a TF dataset with specified minibatch size
batch_size = 50
dataset = tf.data.Dataset.from_tensor_slices((X_tf, Y_tf))
dataset = dataset.batch(batch_size)

# initialize model parameters to be learned
W1 = tf.Variable(tf.random.uniform((input_dim, hid_dim)))
W2 = tf.Variable(tf.random.uniform((hid_dim, output_dim)))
b1 = tf.Variable(tf.random.uniform((1, hid_dim)))
b2 = tf.Variable(tf.random.uniform((1, output_dim)))

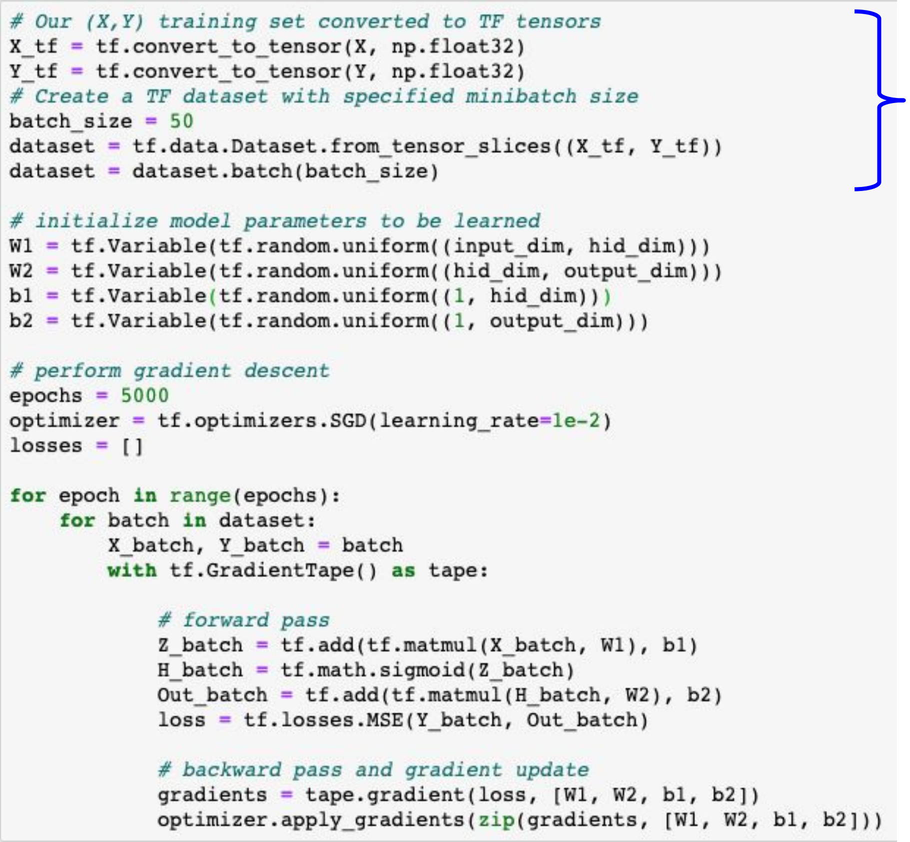
# perform gradient descent
epochs = 5000
optimizer = tf.optimizers.SGD(learning_rate=1e-2)
losses = []

for epoch in range(epochs):
    for batch in dataset:
        X_batch, Y_batch = batch
        with tf.GradientTape() as tape:

            # forward pass
            Z_batch = tf.add(tf.matmul(X_batch, W1), b1)
            H_batch = tf.math.sigmoid(Z_batch)
            Out_batch = tf.add(tf.matmul(H_batch, W2), b2)
            loss = tf.losses.MSE(Y_batch, Out_batch)

            # backward pass and gradient update
            gradients = tape.gradient(loss, [W1, W2, b1, b2])
            optimizer.apply_gradients(zip(gradients, [W1, W2, b1, b2]))
```

Training our two-layer neural network in code, in Tensorflow 2.0



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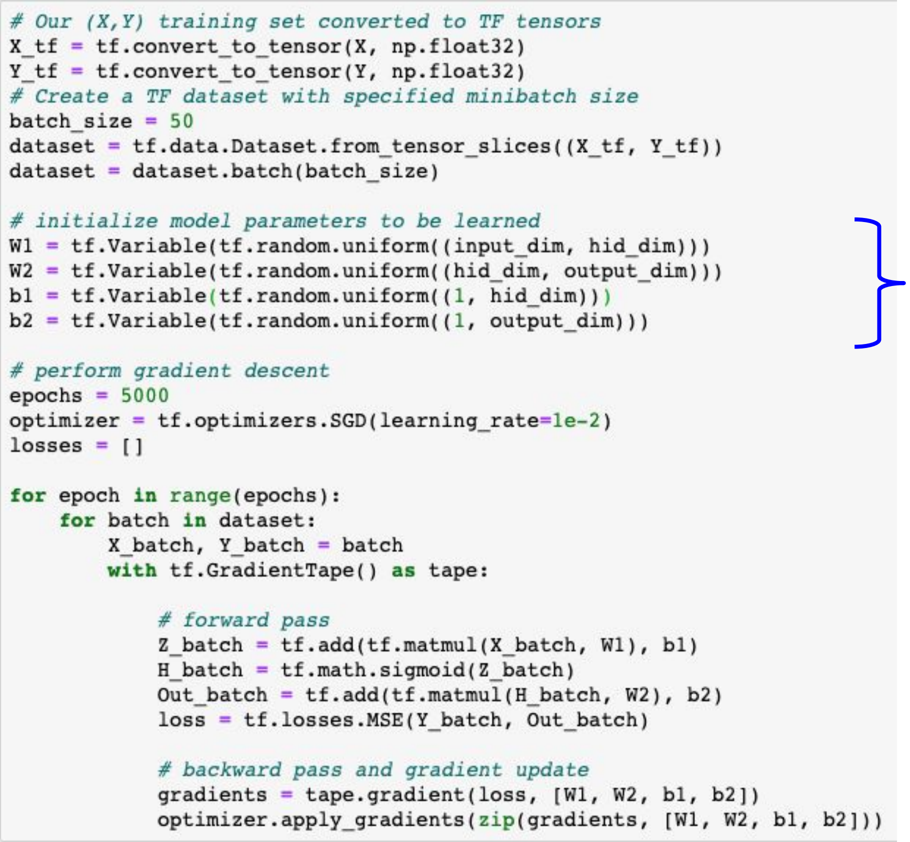
            Z_batch = tf.add(tf.matmul(X_batch, W1), b1)
            H_batch = tf.math.sigmoid(Z_batch)
            Out_batch = tf.add(tf.matmul(H_batch, W2), b2)
            loss = tf.losses.MSE(Y_batch, Out_batch)

            # backward pass and gradient update
            gradients = tape.gradient(loss, [W1, W2, b1, b2])
            optimizer.apply_gradients(zip(gradients, [W1, W2, b1, b2]))
```

Convert data to TF tensors, create a TF dataset

Training our two-layer neural network in code, in Tensorflow 2.0



```
# Our (X,Y) training set converted to TF tensors
X_tf = tf.convert_to_tensor(X, np.float32)
Y_tf = tf.convert_to_tensor(Y, np.float32)
# Create a TF dataset with specified minibatch size
batch_size = 50
dataset = tf.data.Dataset.from_tensor_slices((X_tf, Y_tf))
dataset = dataset.batch(batch_size)

# initialize model parameters to be learned
W1 = tf.Variable(tf.random.uniform((input_dim, hid_dim)))
W2 = tf.Variable(tf.random.uniform((hid_dim, output_dim)))
b1 = tf.Variable(tf.random.uniform((1, hid_dim)))
b2 = tf.Variable(tf.random.uniform((1, output_dim)))

# perform gradient descent
epochs = 5000
optimizer = tf.optimizers.SGD(learning_rate=1e-2)
losses = []

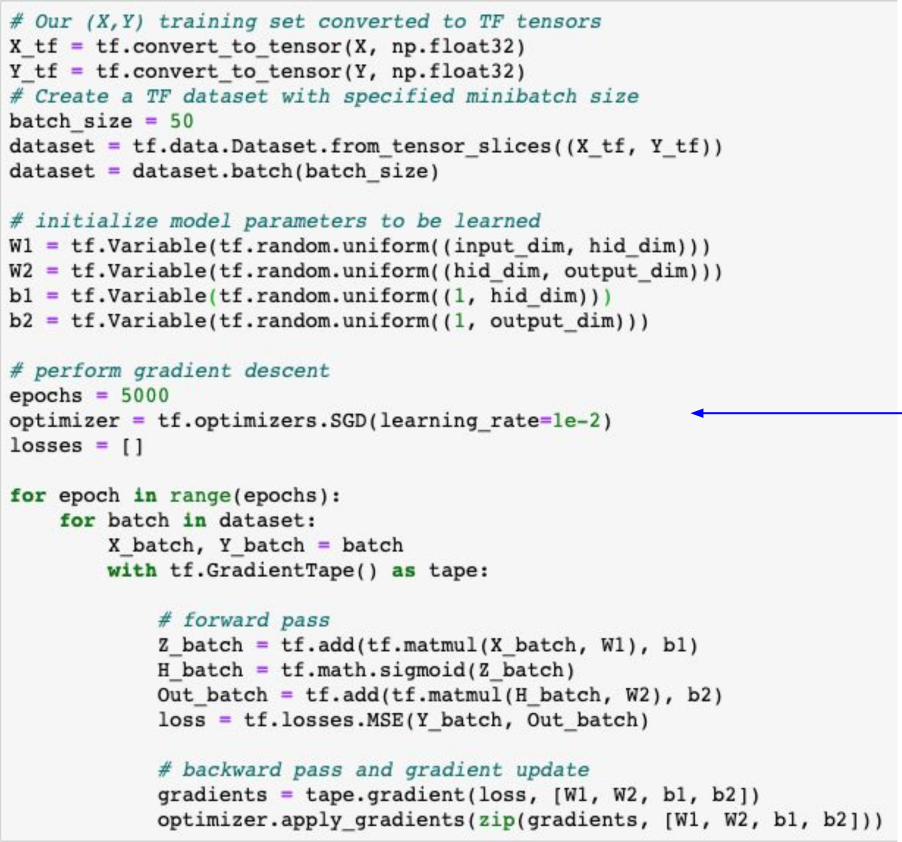
for epoch in range(epochs):
    for batch in dataset:
        X_batch, Y_batch = batch
        with tf.GradientTape() as tape:

            # forward pass
            Z_batch = tf.add(tf.matmul(X_batch, W1), b1)
            H_batch = tf.math.sigmoid(Z_batch)
            Out_batch = tf.add(tf.matmul(H_batch, W2), b2)
            loss = tf.losses.MSE(Y_batch, Out_batch)

            # backward pass and gradient update
            gradients = tape.gradient(loss, [W1, W2, b1, b2])
            optimizer.apply_gradients(zip(gradients, [W1, W2, b1, b2]))
```

Initialize parameters to be learned as tf.Variable -> allows them to receive gradient updates during optimization

Training our two-layer neural network in code, in Tensorflow 2.0



```
# Our (X,Y) training set converted to TF tensors
X_tf = tf.convert_to_tensor(X, np.float32)
Y_tf = tf.convert_to_tensor(Y, np.float32)
# Create a TF dataset with specified minibatch size
batch_size = 50
dataset = tf.data.Dataset.from_tensor_slices((X_tf, Y_tf))
dataset = dataset.batch(batch_size)

# initialize model parameters to be learned
W1 = tf.Variable(tf.random.uniform((input_dim, hid_dim)))
W2 = tf.Variable(tf.random.uniform((hid_dim, output_dim)))
b1 = tf.Variable(tf.random.uniform((1, hid_dim)))
b2 = tf.Variable(tf.random.uniform((1, output_dim)))

# perform gradient descent
epochs = 5000
optimizer = tf.optimizers.SGD(learning_rate=1e-2)
losses = []

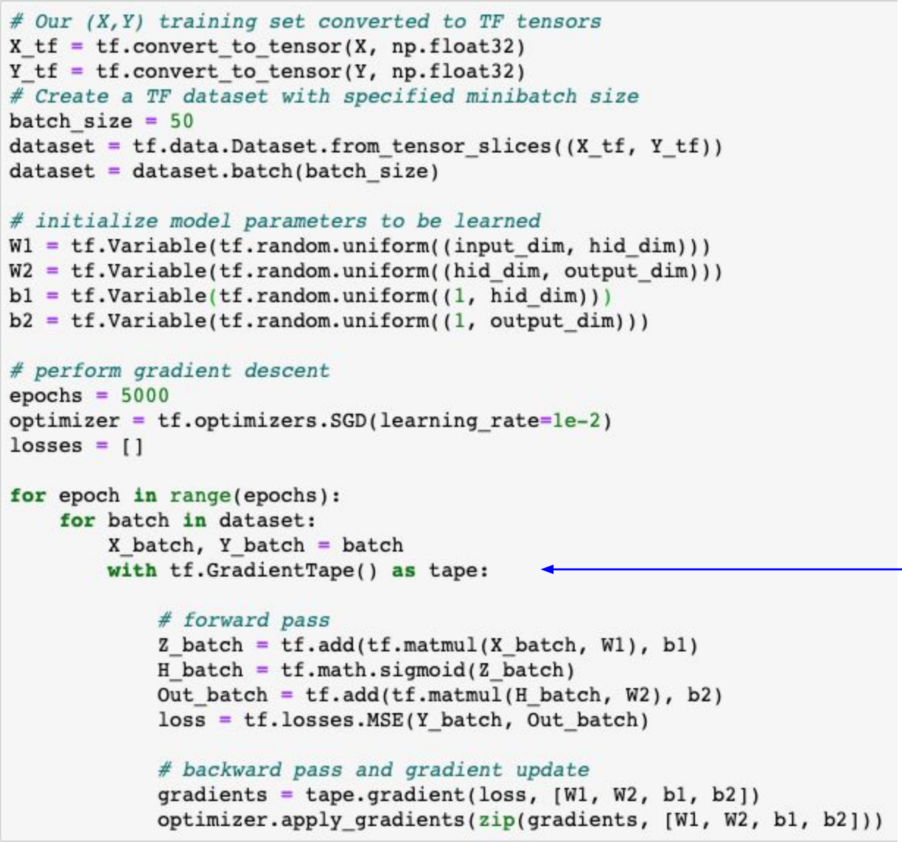
for epoch in range(epochs):
    for batch in dataset:
        X_batch, Y_batch = batch
        with tf.GradientTape() as tape:

            # forward pass
            Z_batch = tf.add(tf.matmul(X_batch, W1), b1)
            H_batch = tf.math.sigmoid(Z_batch)
            Out_batch = tf.add(tf.matmul(H_batch, W2), b2)
            loss = tf.losses.MSE(Y_batch, Out_batch)

            # backward pass and gradient update
            gradients = tape.gradient(loss, [W1, W2, b1, b2])
            optimizer.apply_gradients(zip(gradients, [W1, W2, b1, b2]))
```

Initialize a TF optimizer

Training our two-layer neural network in code, in Tensorflow 2.0



```
# Our (X,Y) training set converted to TF tensors
X_tf = tf.convert_to_tensor(X, np.float32)
Y_tf = tf.convert_to_tensor(Y, np.float32)
# Create a TF dataset with specified minibatch size
batch_size = 50
dataset = tf.data.Dataset.from_tensor_slices((X_tf, Y_tf))
dataset = dataset.batch(batch_size)

# initialize model parameters to be learned
W1 = tf.Variable(tf.random.uniform((input_dim, hid_dim)))
W2 = tf.Variable(tf.random.uniform((hid_dim, output_dim)))
b1 = tf.Variable(tf.random.uniform((1, hid_dim)))
b2 = tf.Variable(tf.random.uniform((1, output_dim)))

# perform gradient descent
epochs = 5000
optimizer = tf.optimizers.SGD(learning_rate=1e-2)
losses = []

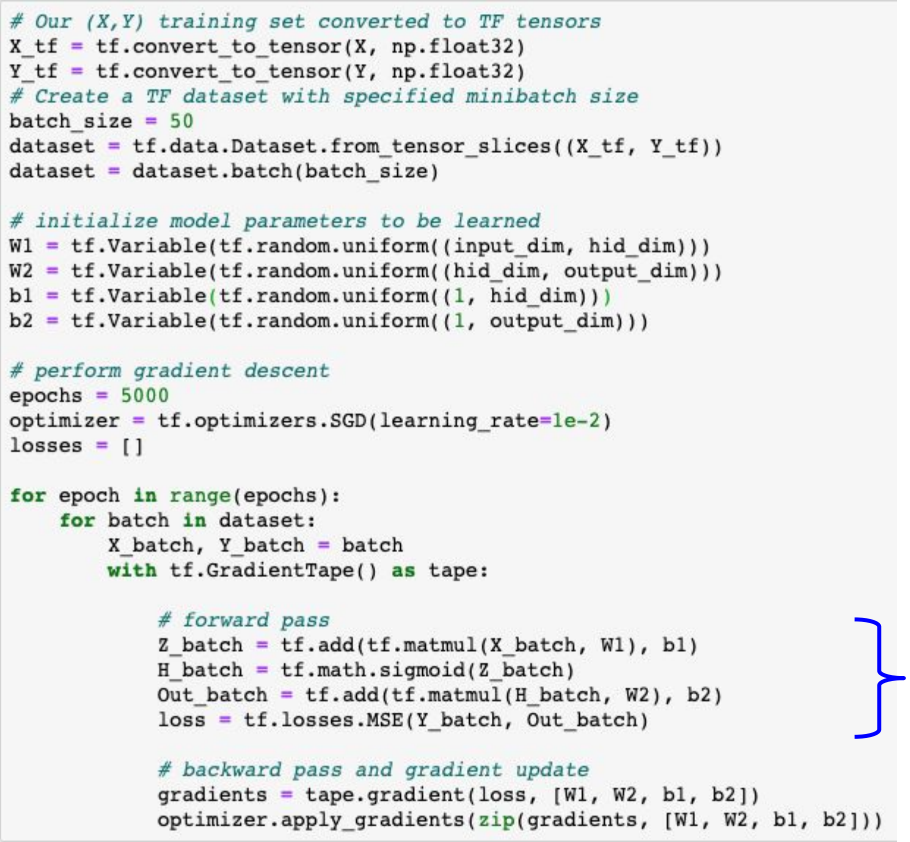
for epoch in range(epochs):
    for batch in dataset:
        X_batch, Y_batch = batch
        with tf.GradientTape() as tape:

            # forward pass
            Z_batch = tf.add(tf.matmul(X_batch, W1), b1)
            H_batch = tf.math.sigmoid(Z_batch)
            Out_batch = tf.add(tf.matmul(H_batch, W2), b2)
            loss = tf.losses.MSE(Y_batch, Out_batch)

            # backward pass and gradient update
            gradients = tape.gradient(loss, [W1, W2, b1, b2])
            optimizer.apply_gradients(zip(gradients, [W1, W2, b1, b2]))
```

All operations defined under the gradient tape will be used to construct a computational graph

Training our two-layer neural network in code, in Tensorflow 2.0



```
# Our (X,Y) training set converted to TF tensors
X_tf = tf.convert_to_tensor(X, np.float32)
Y_tf = tf.convert_to_tensor(Y, np.float32)
# Create a TF dataset with specified minibatch size
batch_size = 50
dataset = tf.data.Dataset.from_tensor_slices((X_tf, Y_tf))
dataset = dataset.batch(batch_size)

# initialize model parameters to be learned
W1 = tf.Variable(tf.random.uniform((input_dim, hid_dim)))
W2 = tf.Variable(tf.random.uniform((hid_dim, output_dim)))
b1 = tf.Variable(tf.random.uniform((1, hid_dim)))
b2 = tf.Variable(tf.random.uniform((1, output_dim)))

# perform gradient descent
epochs = 5000
optimizer = tf.optimizers.SGD(learning_rate=1e-2)
losses = []

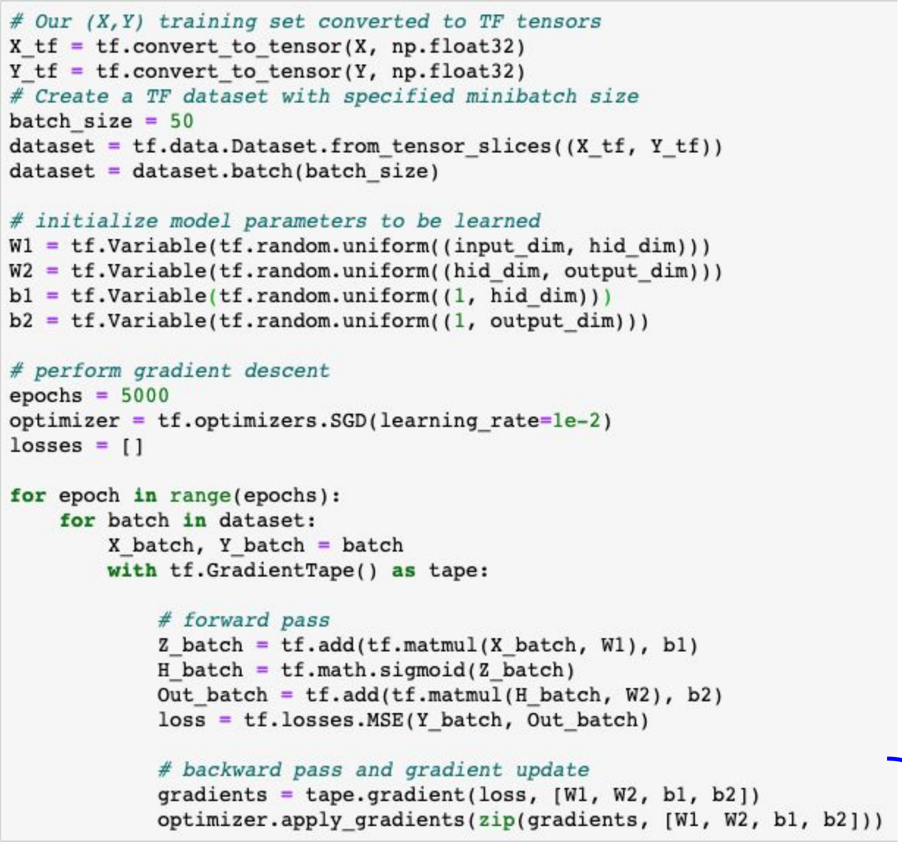
for epoch in range(epochs):
    for batch in dataset:
        X_batch, Y_batch = batch
        with tf.GradientTape() as tape:

            # forward pass
            Z_batch = tf.add(tf.matmul(X_batch, W1), b1)
            H_batch = tf.math.sigmoid(Z_batch)
            Out_batch = tf.add(tf.matmul(H_batch, W2), b2)
            loss = tf.losses.MSE(Y_batch, Out_batch)

            # backward pass and gradient update
            gradients = tape.gradient(loss, [W1, W2, b1, b2])
            optimizer.apply_gradients(zip(gradients, [W1, W2, b1, b2]))
```

The computational graph for our two-layer neural network

Training our two-layer neural network in code, in Tensorflow 2.0



```
# Our (X,Y) training set converted to TF tensors
X_tf = tf.convert_to_tensor(X, np.float32)
Y_tf = tf.convert_to_tensor(Y, np.float32)
# Create a TF dataset with specified minibatch size
batch_size = 50
dataset = tf.data.Dataset.from_tensor_slices((X_tf, Y_tf))
dataset = dataset.batch(batch_size)

# initialize model parameters to be learned
W1 = tf.Variable(tf.random.uniform((input_dim, hid_dim)))
W2 = tf.Variable(tf.random.uniform((hid_dim, output_dim)))
b1 = tf.Variable(tf.random.uniform((1, hid_dim)))
b2 = tf.Variable(tf.random.uniform((1, output_dim)))

# perform gradient descent
epochs = 5000
optimizer = tf.optimizers.SGD(learning_rate=1e-2)
losses = []

for epoch in range(epochs):
    for batch in dataset:
        X_batch, Y_batch = batch
        with tf.GradientTape() as tape:

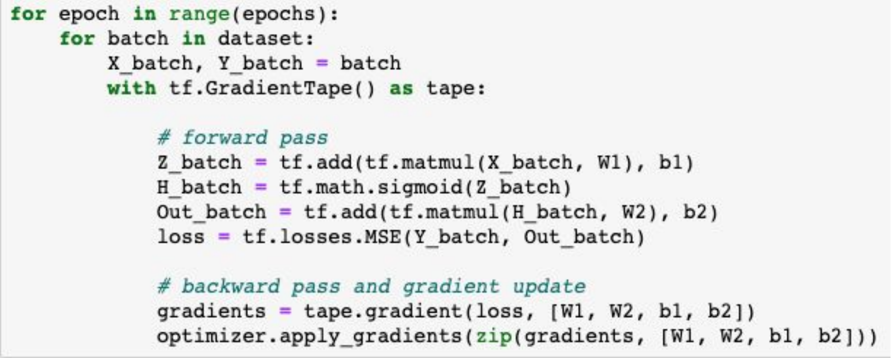
            # forward pass
            Z_batch = tf.add(tf.matmul(X_batch, W1), b1)
            H_batch = tf.math.sigmoid(Z_batch)
            Out_batch = tf.add(tf.matmul(H_batch, W2), b2)
            loss = tf.losses.MSE(Y_batch, Out_batch)

            # backward pass and gradient update
            gradients = tape.gradient(loss, [W1, W2, b1, b2])
            optimizer.apply_gradients(zip(gradients, [W1, W2, b1, b2]))
```

Evaluate gradients using automatic differentiation and perform gradient update

Also high level libraries built on top of Tensorflow, that provide even easier-to-use APIs:

In Tensorflow 2.0:

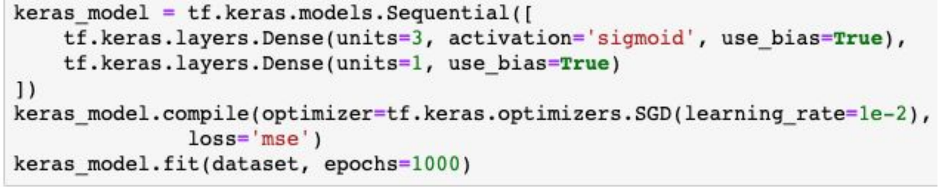


```
for epoch in range(epochs):
    for batch in dataset:
        X_batch, Y_batch = batch
        with tf.GradientTape() as tape:

            # forward pass
            Z_batch = tf.add(tf.matmul(X_batch, W1), b1)
            H_batch = tf.math.sigmoid(Z_batch)
            Out_batch = tf.add(tf.matmul(H_batch, W2), b2)
            loss = tf.losses.MSE(Y_batch, Out_batch)

            # backward pass and gradient update
            gradients = tape.gradient(loss, [W1, W2, b1, b2])
            optimizer.apply_gradients(zip(gradients, [W1, W2, b1, b2]))
```

In Keras:

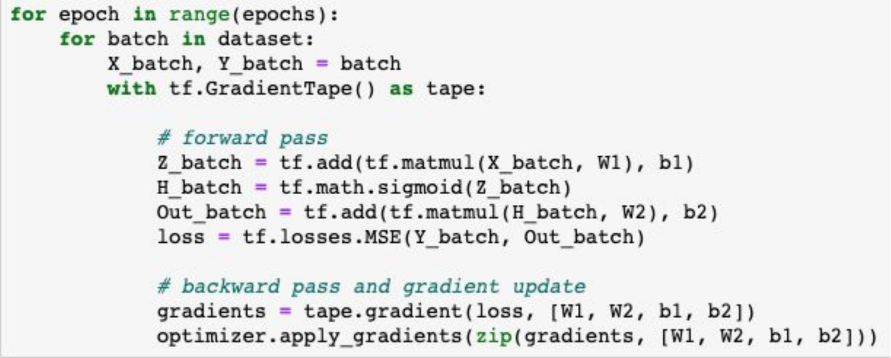


```
keras_model = tf.keras.models.Sequential([
    tf.keras.layers.Dense(units=3, activation='sigmoid', use_bias=True),
    tf.keras.layers.Dense(units=1, use_bias=True)
])
keras_model.compile(optimizer=tf.keras.optimizers.SGD(learning_rate=1e-2),
              loss='mse')
keras_model.fit(dataset, epochs=1000)
```

Also high level libraries built on top of Tensorflow, that provide even easier-to-use APIs:

Stack of layers

In Tensorflow 2.0:

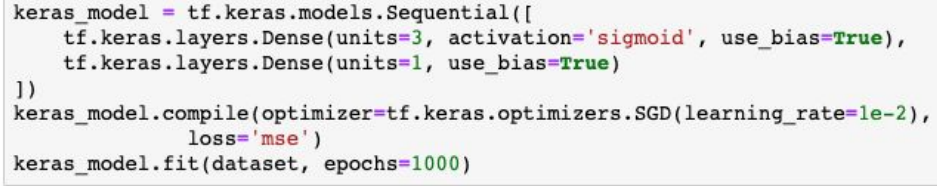


```
for epoch in range(epochs):
    for batch in dataset:
        X_batch, Y_batch = batch
        with tf.GradientTape() as tape:

            # forward pass
            Z_batch = tf.add(tf.matmul(X_batch, W1), b1)
            H_batch = tf.math.sigmoid(Z_batch)
            Out_batch = tf.add(tf.matmul(H_batch, W2), b2)
            loss = tf.losses.MSE(Y_batch, Out_batch)

            # backward pass and gradient update
            gradients = tape.gradient(loss, [W1, W2, b1, b2])
            optimizer.apply_gradients(zip(gradients, [W1, W2, b1, b2]))
```

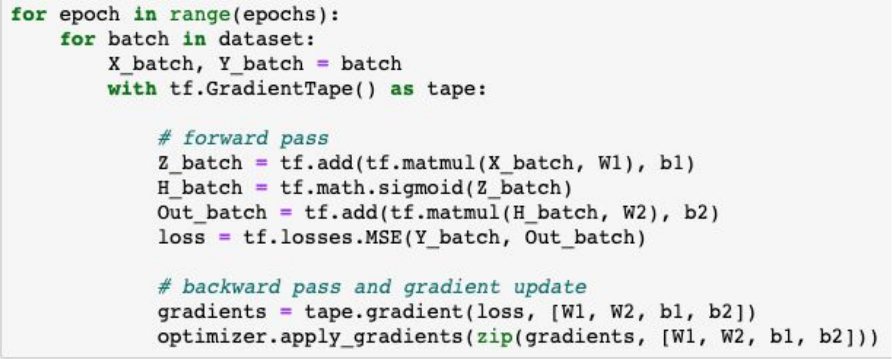
In Keras:



```
keras_model = tf.keras.models.Sequential([
    tf.keras.layers.Dense(units=3, activation='sigmoid', use_bias=True),
    tf.keras.layers.Dense(units=1, use_bias=True)
])
keras_model.compile(optimizer=tf.keras.optimizers.SGD(learning_rate=1e-2),
              loss='mse')
keras_model.fit(dataset, epochs=1000)
```

Also high level libraries built on top of Tensorflow, that provide even easier-to-use APIs:

In Tensorflow 2.0:



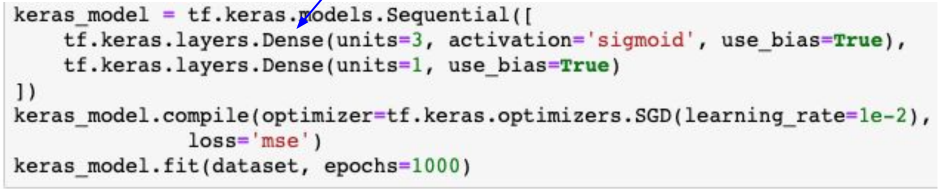
```
for epoch in range(epochs):
    for batch in dataset:
        X_batch, Y_batch = batch
        with tf.GradientTape() as tape:

            # forward pass
            Z_batch = tf.add(tf.matmul(X_batch, W1), b1)
            H_batch = tf.math.sigmoid(Z_batch)
            Out_batch = tf.add(tf.matmul(H_batch, W2), b2)
            loss = tf.losses.MSE(Y_batch, Out_batch)

            # backward pass and gradient update
            gradients = tape.gradient(loss, [W1, W2, b1, b2])
            optimizer.apply_gradients(zip(gradients, [W1, W2, b1, b2]))
```

In Keras:

Fully-connected layer

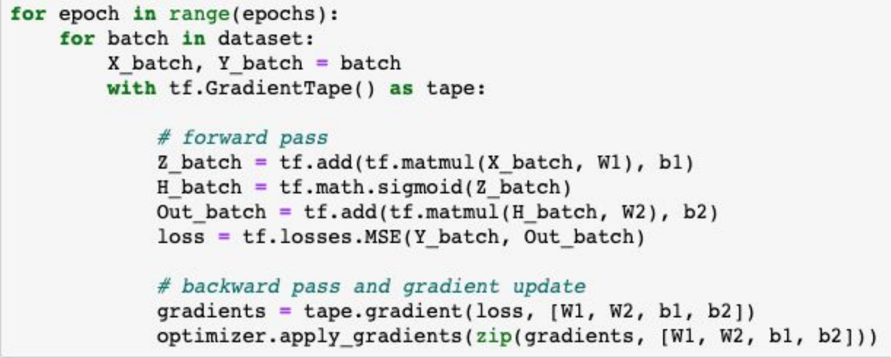


```
keras_model = tf.keras.models.Sequential([
    tf.keras.layers.Dense(units=3, activation='sigmoid', use_bias=True),
    tf.keras.layers.Dense(units=1, use_bias=True)
])
keras_model.compile(optimizer=tf.keras.optimizers.SGD(learning_rate=1e-2),
              loss='mse')
keras_model.fit(dataset, epochs=1000)
```

Also high level libraries built on top of Tensorflow, that provide even easier-to-use APIs:

Activation function and bias configurations included!

In Tensorflow 2.0:

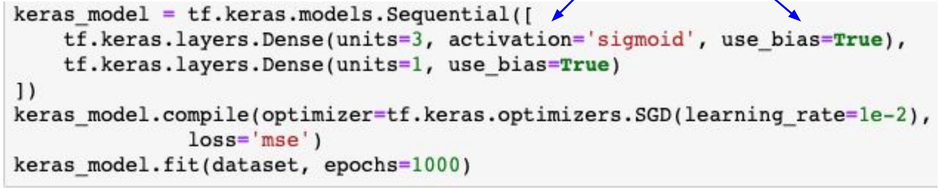


```
for epoch in range(epochs):
    for batch in dataset:
        X_batch, Y_batch = batch
        with tf.GradientTape() as tape:

            # forward pass
            Z_batch = tf.add(tf.matmul(X_batch, W1), b1)
            H_batch = tf.math.sigmoid(Z_batch)
            Out_batch = tf.add(tf.matmul(H_batch, W2), b2)
            loss = tf.losses.MSE(Y_batch, Out_batch)

            # backward pass and gradient update
            gradients = tape.gradient(loss, [W1, W2, b1, b2])
            optimizer.apply_gradients(zip(gradients, [W1, W2, b1, b2]))
```

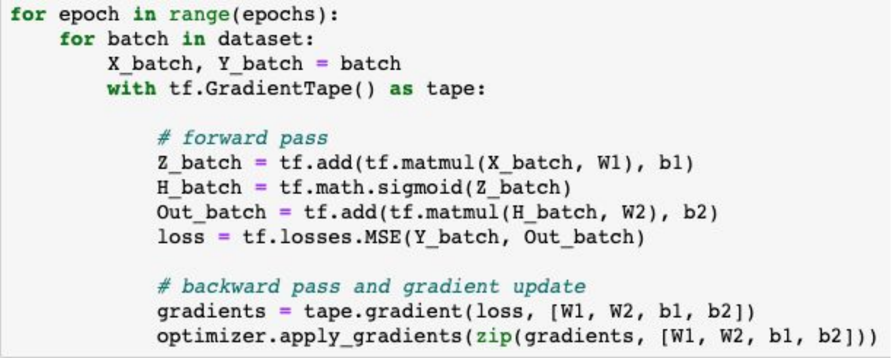
In Keras:



```
keras_model = tf.keras.models.Sequential([
    tf.keras.layers.Dense(units=3, activation='sigmoid', use_bias=True),
    tf.keras.layers.Dense(units=1, use_bias=True)
])
keras_model.compile(optimizer=tf.keras.optimizers.SGD(learning_rate=1e-2),
          loss='mse')
keras_model.fit(dataset, epochs=1000)
```

Also high level libraries built on top of Tensorflow, that provide even easier-to-use APIs:

In Tensorflow 2.0:

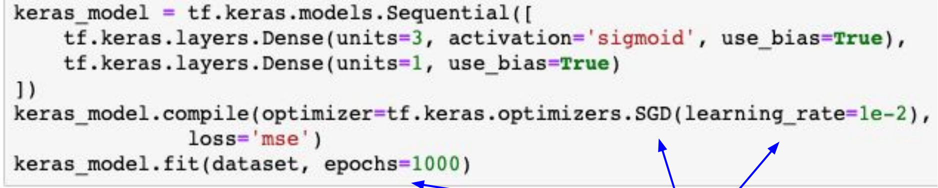


```
for epoch in range(epochs):
    for batch in dataset:
        X_batch, Y_batch = batch
        with tf.GradientTape() as tape:

            # forward pass
            Z_batch = tf.add(tf.matmul(X_batch, W1), b1)
            H_batch = tf.math.sigmoid(Z_batch)
            Out_batch = tf.add(tf.matmul(H_batch, W2), b2)
            loss = tf.losses.MSE(Y_batch, Out_batch)

            # backward pass and gradient update
            gradients = tape.gradient(loss, [W1, W2, b1, b2])
            optimizer.apply_gradients(zip(gradients, [W1, W2, b1, b2]))
```

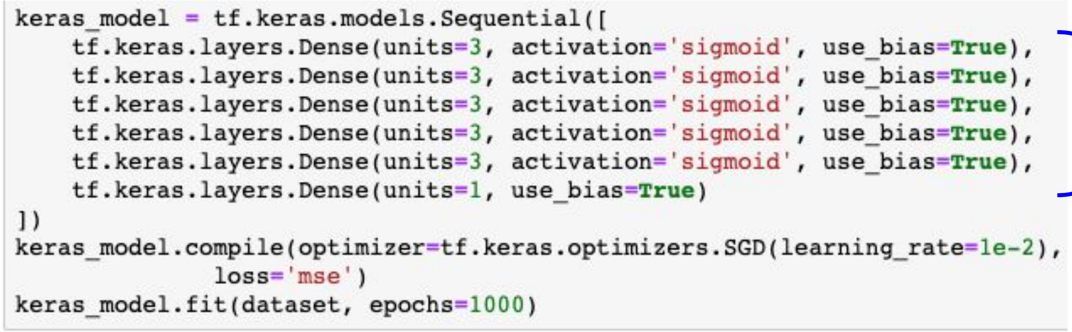
In Keras:



```
keras_model = tf.keras.models.Sequential([
    tf.keras.layers.Dense(units=3, activation='sigmoid', use_bias=True),
    tf.keras.layers.Dense(units=1, use_bias=True)
])
keras_model.compile(optimizer=tf.keras.optimizers.SGD(learning_rate=1e-2),
              loss='mse')
keras_model.fit(dataset, epochs=1000)
```

Specify hyperparameters for the training procedure

Training more complex neural networks is a straightforward extension

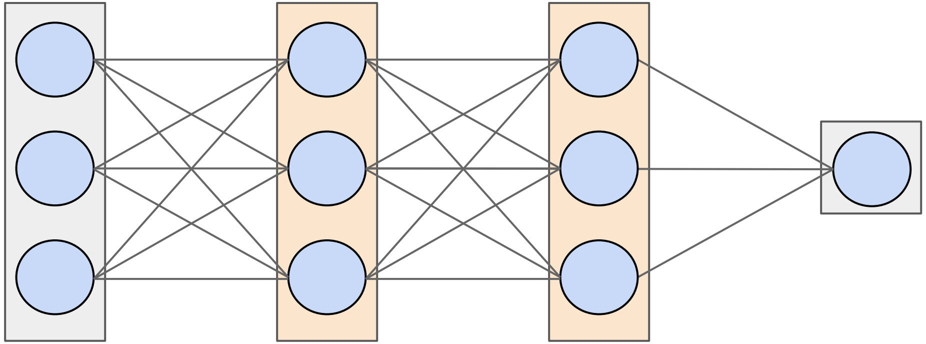


```
keras_model = tf.keras.models.Sequential([
    tf.keras.layers.Dense(units=3, activation='sigmoid', use_bias=True),
    tf.keras.layers.Dense(units=3, activation='sigmoid', use_bias=True),
    tf.keras.layers.Dense(units=3, activation='sigmoid', use_bias=True),
    tf.keras.layers.Dense(units=3, activation='sigmoid', use_bias=True),
    tf.keras.layers.Dense(units=3, activation='sigmoid', use_bias=True),
    tf.keras.layers.Dense(units=1, use_bias=True)
])
keras_model.compile(optimizer=tf.keras.optimizers.SGD(learning_rate=1e-2),
              loss='mse')
keras_model.fit(dataset, epochs=1000)
```

Now a 6-layer network

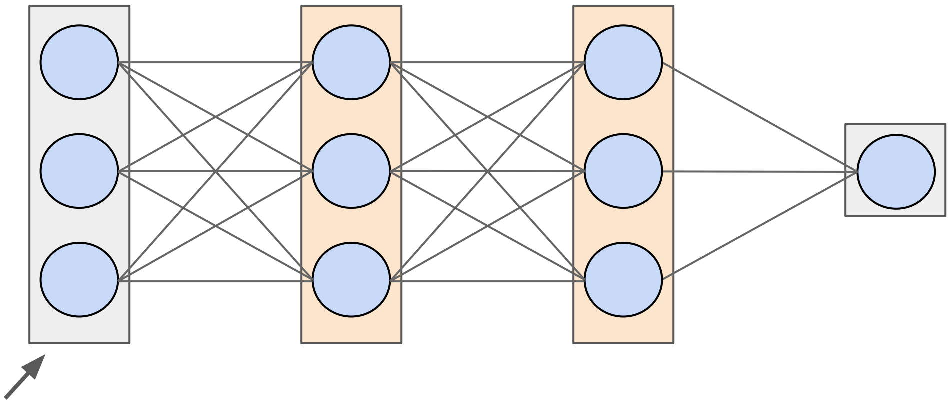
“Deep learning”

Can continue to stack more layers to get deeper models!



“Deep learning”

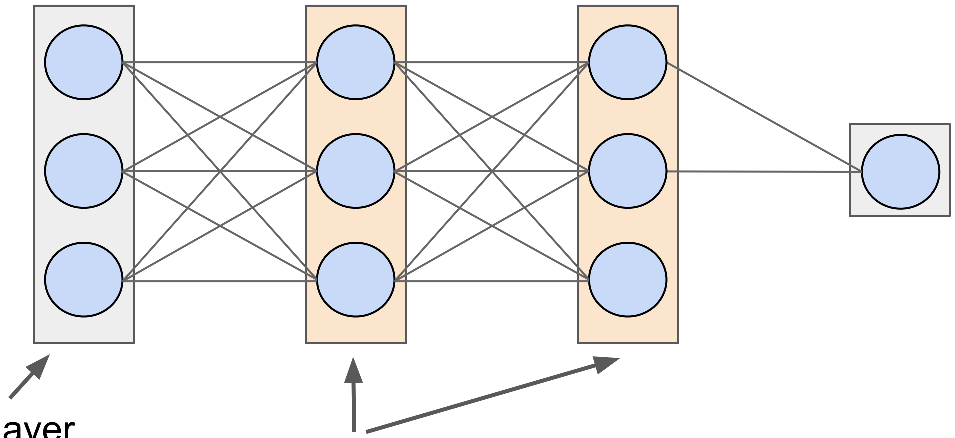
Can continue to stack more layers to get deeper models!



Input layer

“Deep learning”

Can continue to stack more layers to get deeper models!

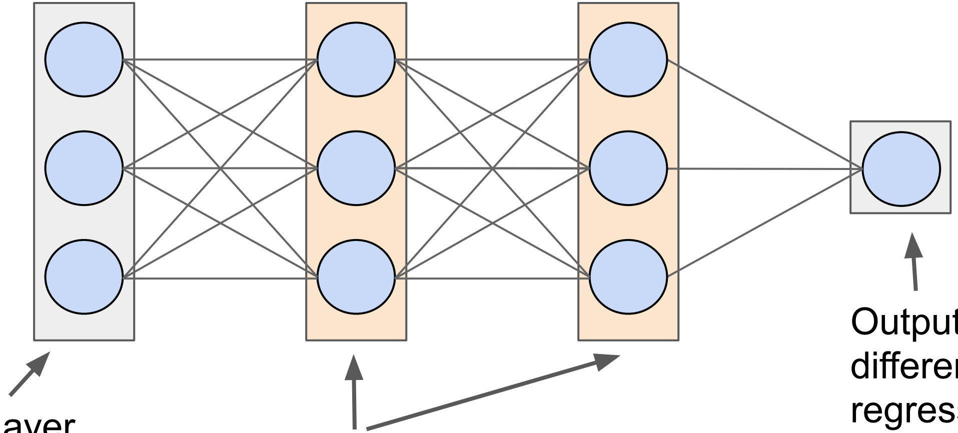


Input layer

“Hidden” layers - will see lots of diversity in size (# neurons), type (linear, convolutional, etc.), and activation function (sigmoid, ReLU, etc.)

"Deep learning"

Can continue to stack more layers to get deeper models!



Input layer

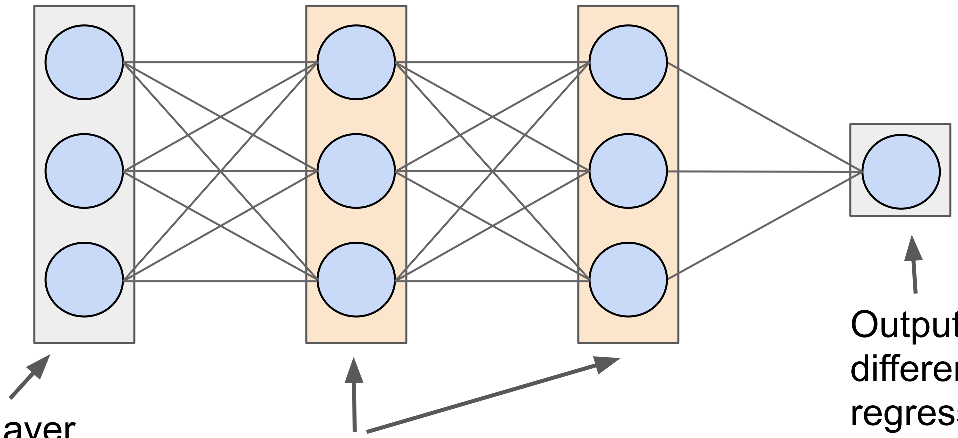
"Hidden" layers - will see lots of diversity in size (# neurons), type (linear, convolutional, etc.), and activation function (sigmoid, ReLU, etc.)

Output layer - will differ for different types of tasks (e.g. regression). Should match with loss function.

“Deep learning”

Can continue to stack more layers to get deeper models!

Vanilla fully-connected neural networks (MLPs) usually pretty shallow -- otherwise too many parameters! ~2-3 layers. Can have wide range in size of layers (16, 64, 256, 1000, etc.) depending on how much data you have.



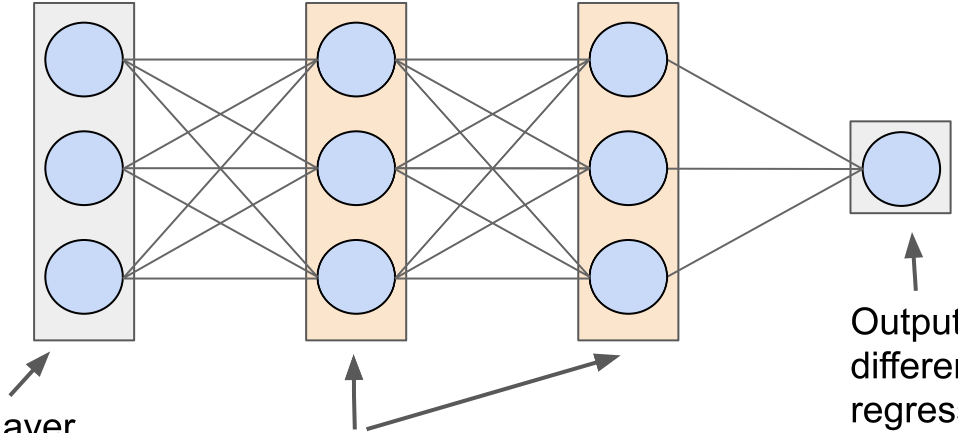
Input layer

“Hidden” layers - will see lots of diversity in size (# neurons), type (linear, convolutional, etc.), and activation function (sigmoid, ReLU, etc.)

Output layer - will differ for different types of tasks (e.g. regression). Should match with loss function.

“Deep learning”

Can continue to stack more layers to get deeper models!



Input layer

“Hidden” layers - will see lots of diversity in size (# neurons), type (linear, convolutional, etc.), and activation function (sigmoid, ReLU, etc.)

Output layer - will differ for different types of tasks (e.g. regression). Should match with loss function.

Vanilla fully-connected neural networks (MLPs) usually pretty shallow -- otherwise too many parameters! ~2-3 layers. Can have wide range in size of layers (16, 64, 256, 1000, etc.) depending on how much data you have.

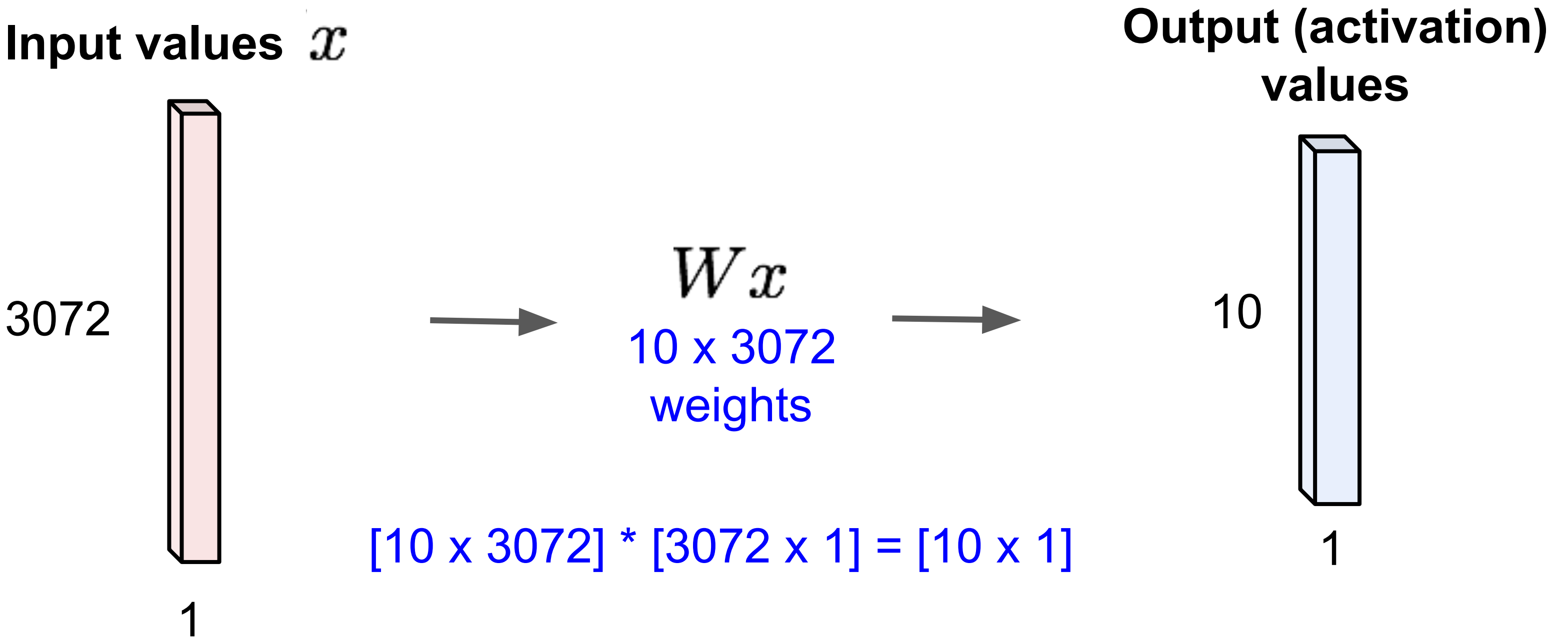
Will see different classes of neural networks (e.g. CNNs) that leverage structure in data to reduce parameters + increase network depth

What we’ve seen so far

- Defining a neural network architecture, neural network components
- How to train a neural network
    - Loss function
    - Gradient descent algorithm
    - Computing complex gradients with backpropagation (computational graphs)
    - Implementing and training neural networks in code
        - Deep learning frameworks

Revisiting fully connected networks vs. convolutional networks (from lecture)

From lecture: fully connected neural network layers



Input values x

3072

1

Wx

10 x 3072

weights

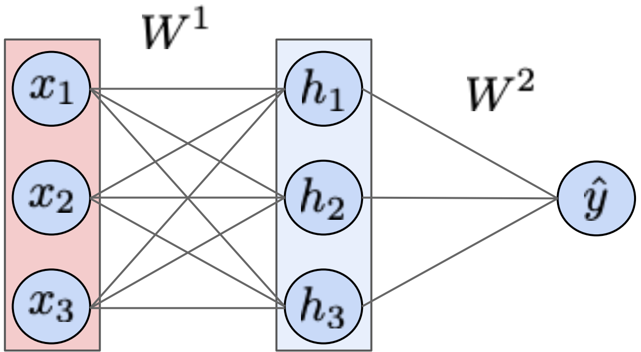
Output (activation) values

10

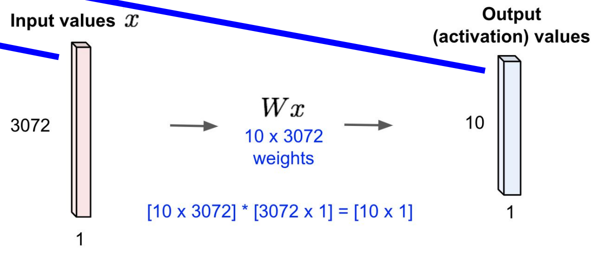
1

[10 x 3072] * [3072 x 1] = [10 x 1]

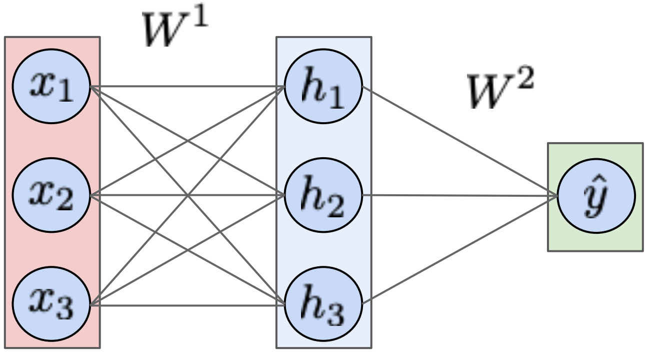
From lecture: Simple two-layer fully-connected neural network



Each layer has the same structure we just saw, but this is a different example with different dimensions



Simple two-layer fully-connected neural network



$$W^1 = \begin{bmatrix} w^1_{11} & w^1_{12} & w^1_{13} \\ w^1_{21} & w^1_{22} & w^1_{23} \\ w^1_{31} & w^1_{32} & w^1_{33} \end{bmatrix} \quad b^1 = \begin{bmatrix} b^1_1 \\ b^1_2 \\ b^1_3 \end{bmatrix}$$

$$W^2 = \begin{bmatrix} w^2_{11} & w^2_{12} & w^2_{13} \end{bmatrix} \quad b^2 = \begin{bmatrix} b^2_1 \end{bmatrix}$$

Output: $\hat{y} = W^2(\sigma(W^1 x + b^1)) + b^2$

Neural network parameters:

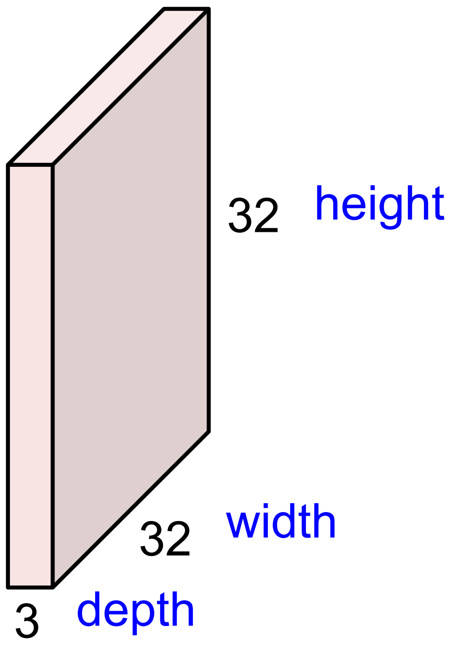
$$W = \{W^1, b^1, W^2, b^2\}$$

"weights" "biases"

Often refer to all parameters together as just "weights". Bias is implicitly assumed.

Now: Convolutional layer

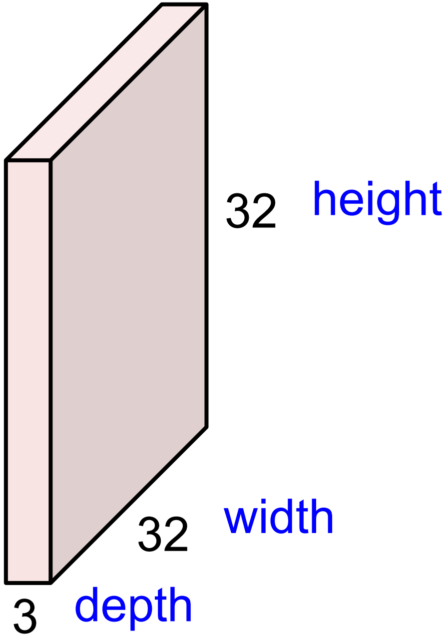
32x32x3 image -> preserve spatial structure



Slide credit: CS231n

Convolutional layer

32x32x3 image -> preserve spatial structure

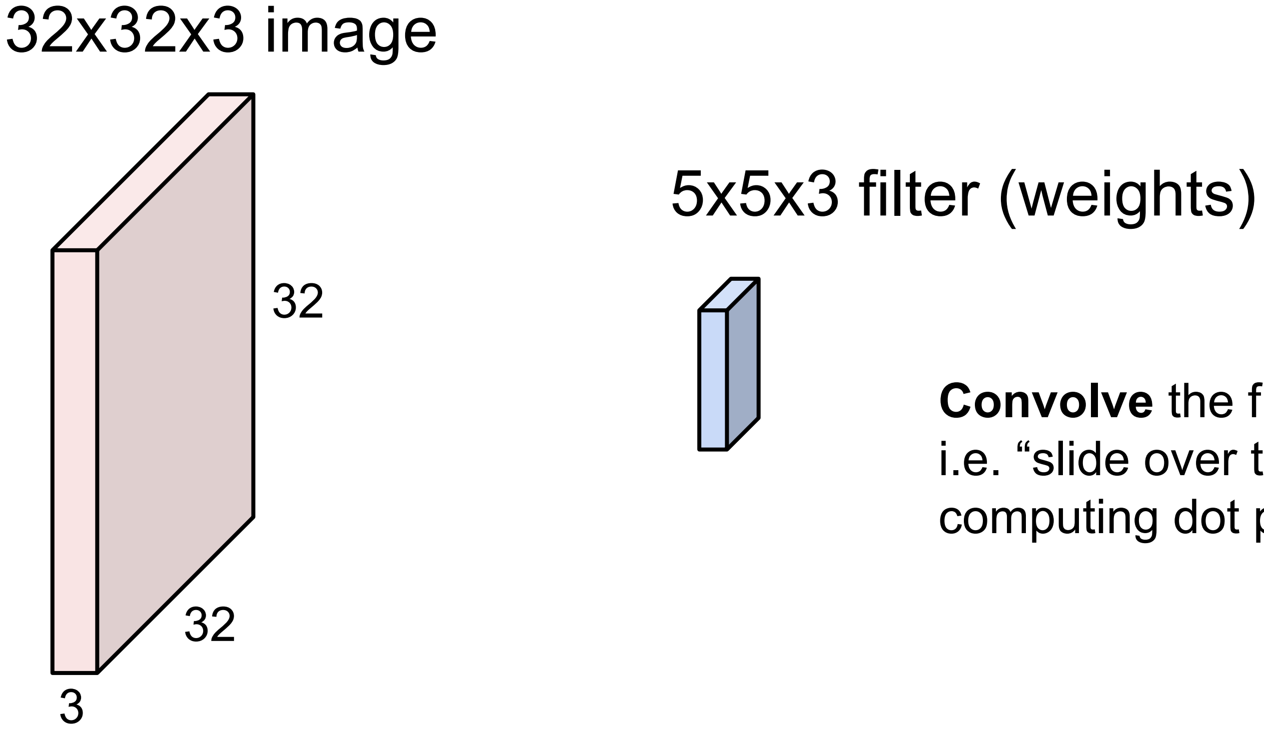


Input now has spatial height and width dimensions!

In contrast to fully-connected layers, want to preserve spatial structure when processing with a convolutional layer

Slide credit: CS231n

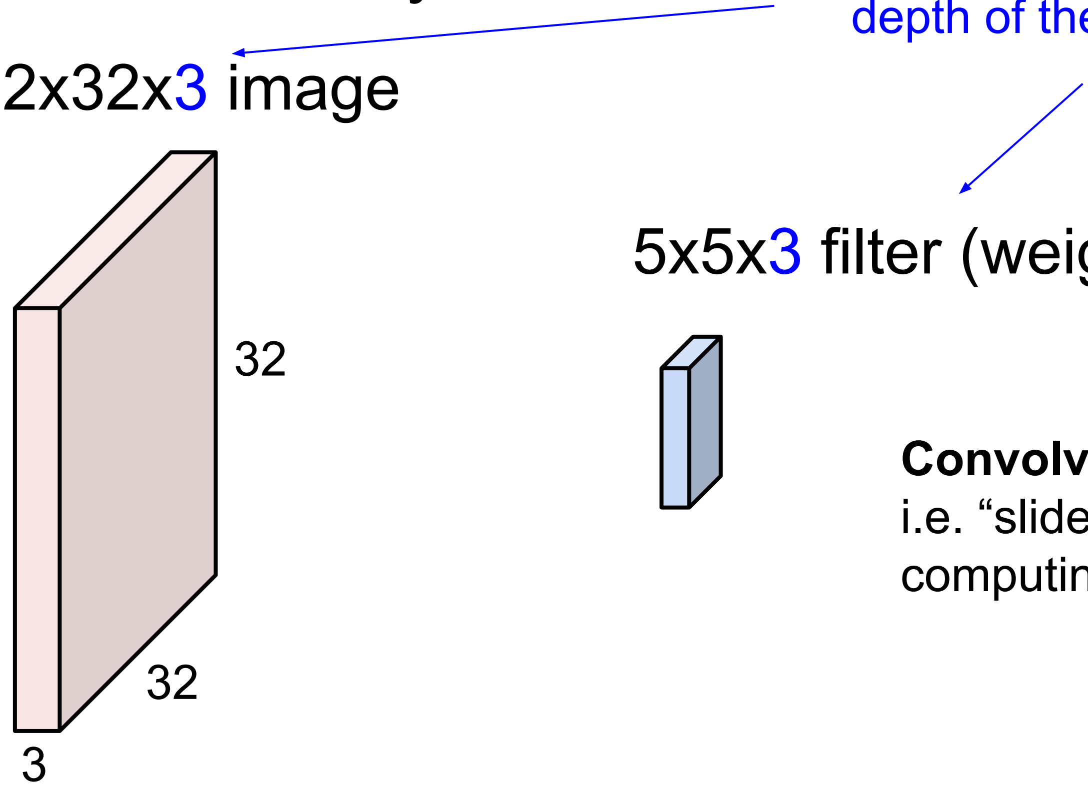
Convolutional layer



Convolve the filter with the image
i.e. “slide over the image spatially,
computing dot products”

Slide credit: CS231n

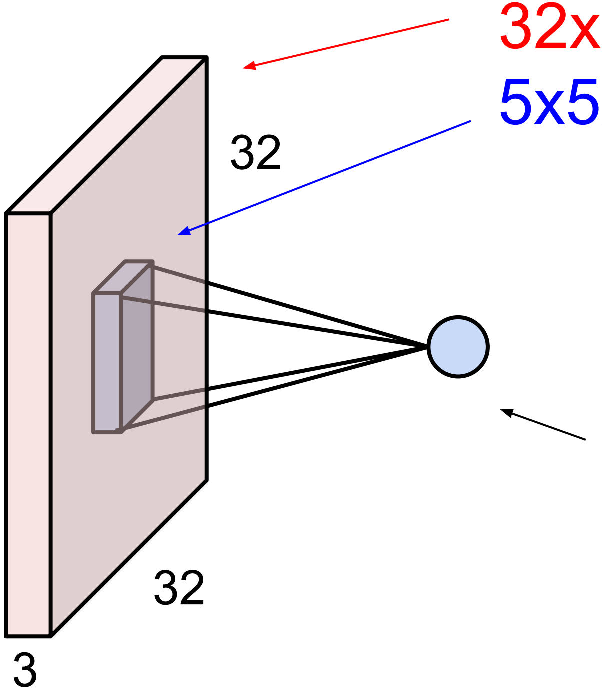
Convolutional layer



Convolve the filter with the image i.e. “slide over the image spatially, computing dot products”

Slide credit: CS231n

Convolutional layer



32x32x3 image

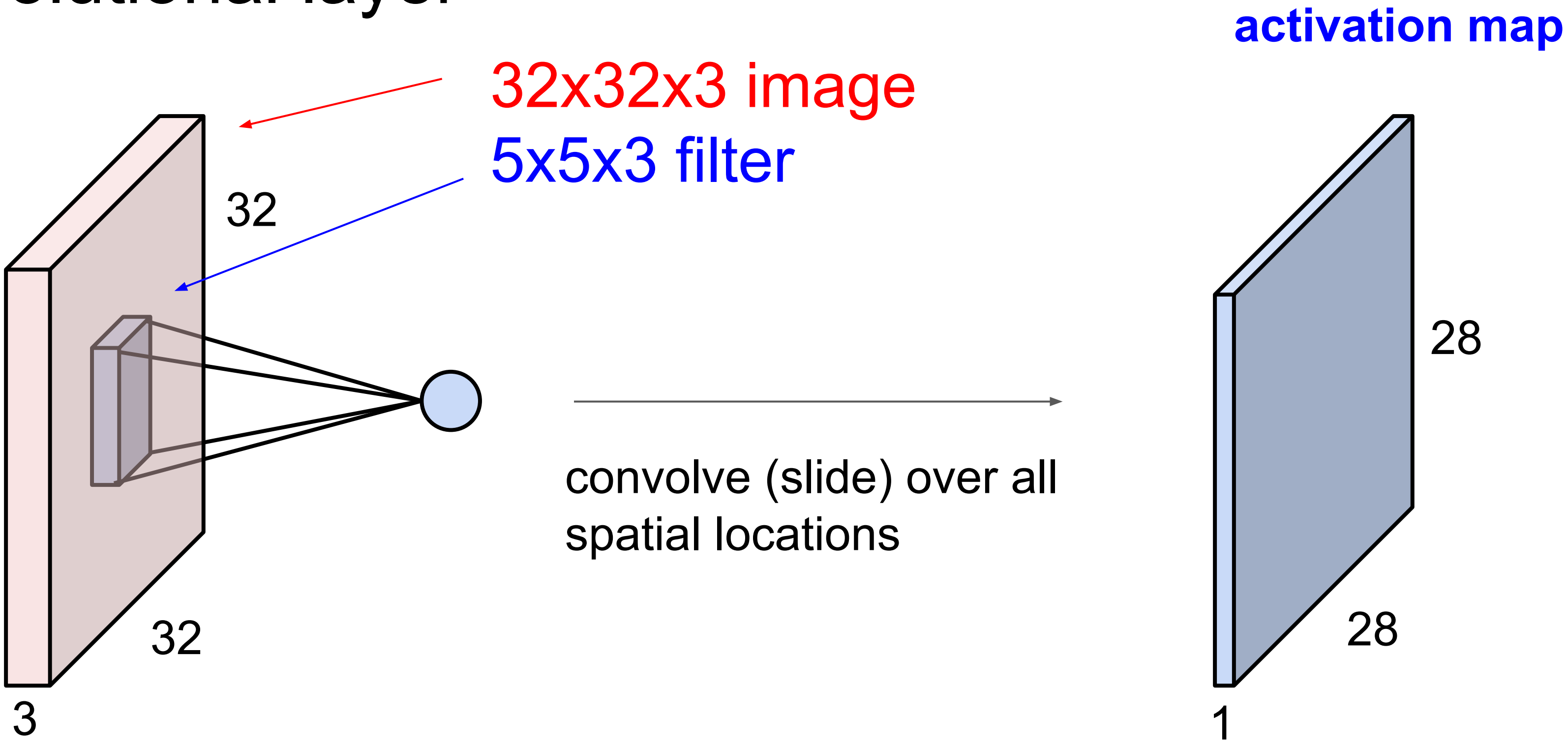
5x5x3 filter w

1 number:
the result of taking a dot product between the filter and a small 5x5x3 chunk of the image
(i.e. 5*5*3 = 75-dimensional dot product + bias)

$$w^T x + b$$

Slide credit: CS231n

Convolutional layer

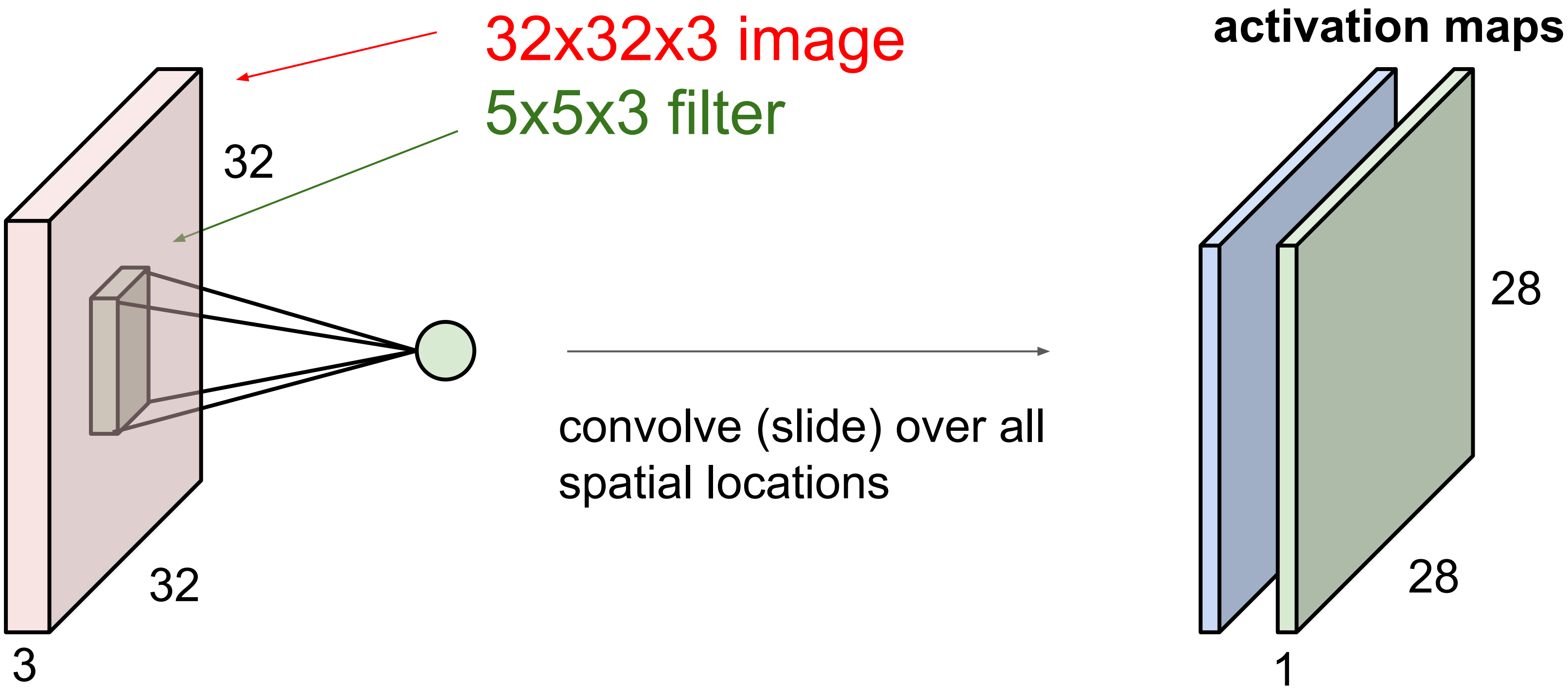


convolve (slide) over all spatial locations

Slide credit: CS231n

Convolutional layer

consider a second, green filter



32x32x3 image

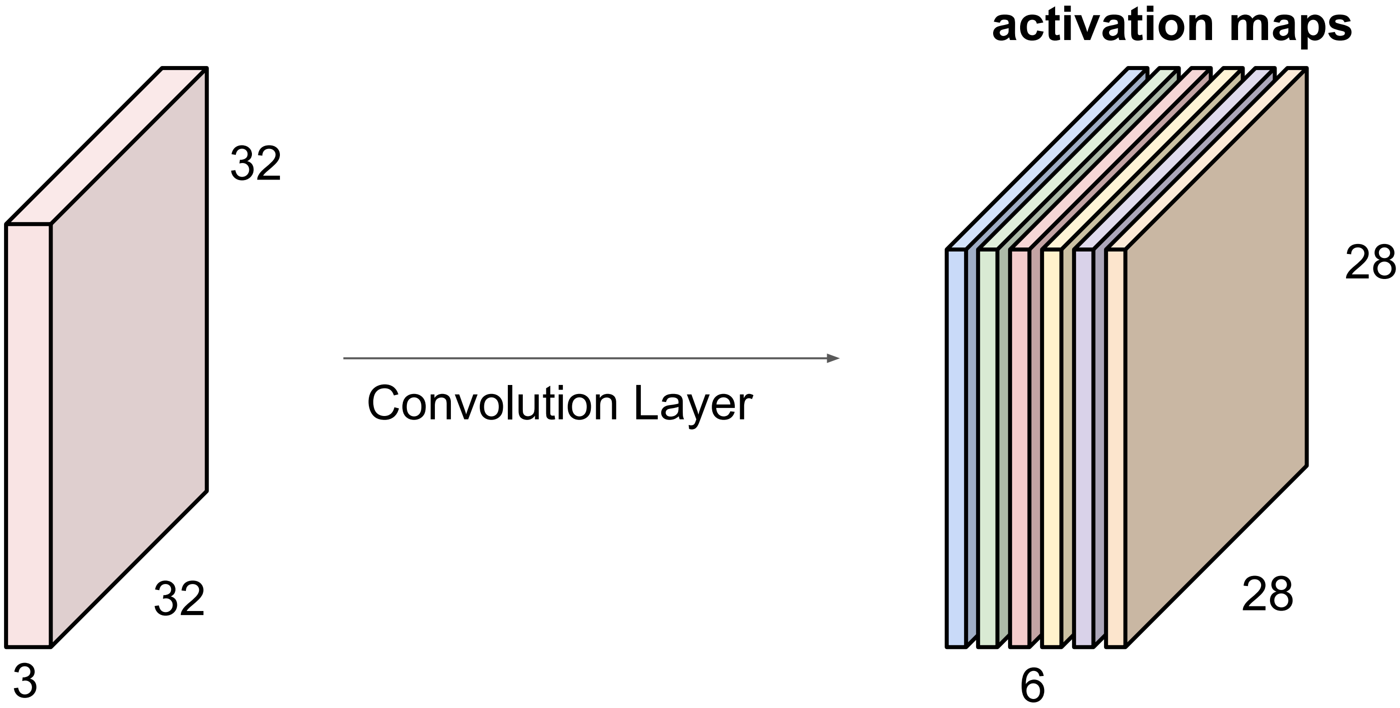
5x5x3 filter

activation maps

convolve (slide) over all spatial locations

Slide credit: CS231n

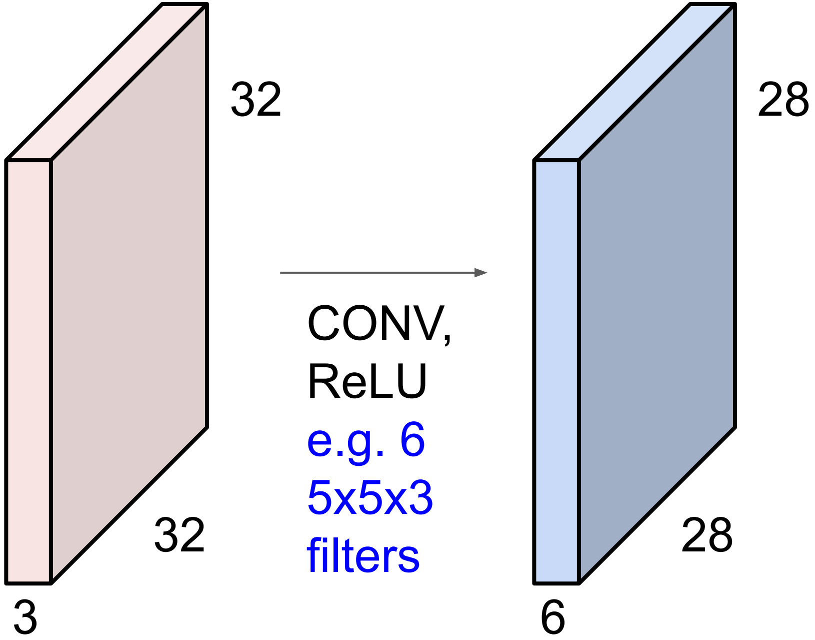
For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:



We stack these up to get a "new image" of size 28x28x6!

Slide credit: CS231n

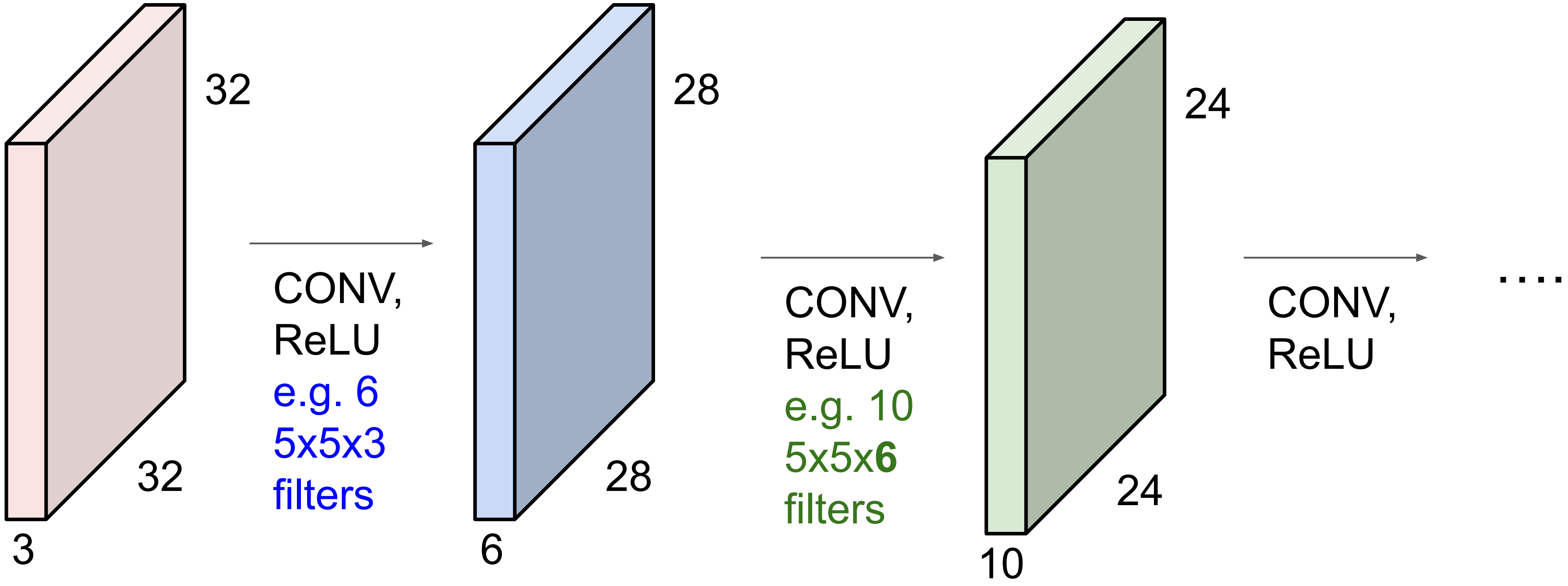
Preview: ConvNet (or CNN) is a sequence of Convolution Layers, interspersed with activation functions



CONV,
ReLU
e.g. 6
5x5x3
filters

Slide credit: CS231n

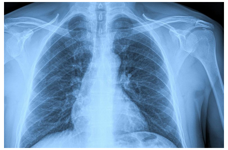
Preview: ConvNet (or CNN) is a sequence of Convolution Layers, interspersed with activation functions

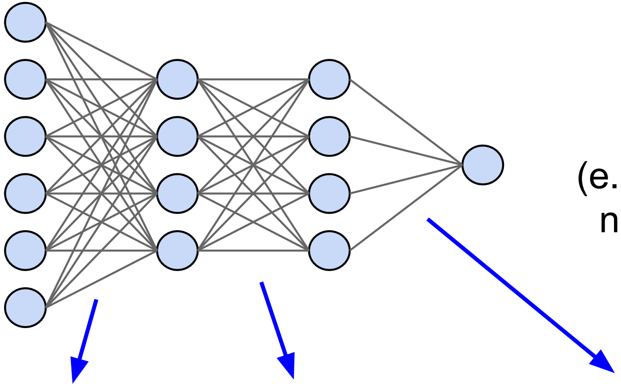


Slide credit: CS231n

Hierarchical structure of neural networks

Input

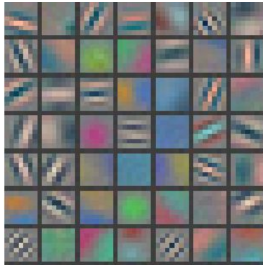
(e.g., )



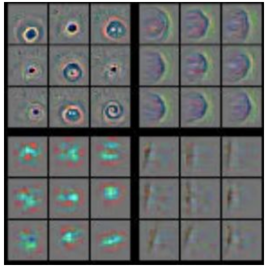
Output

(e.g., presence or not or disease)

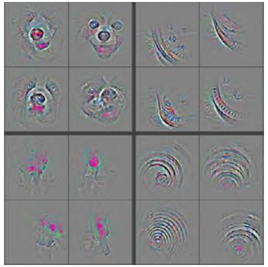
Hierarchical structure of neural networks allows compositional extraction of increasingly complex features



Low-level features



Mid-level features



High-level features

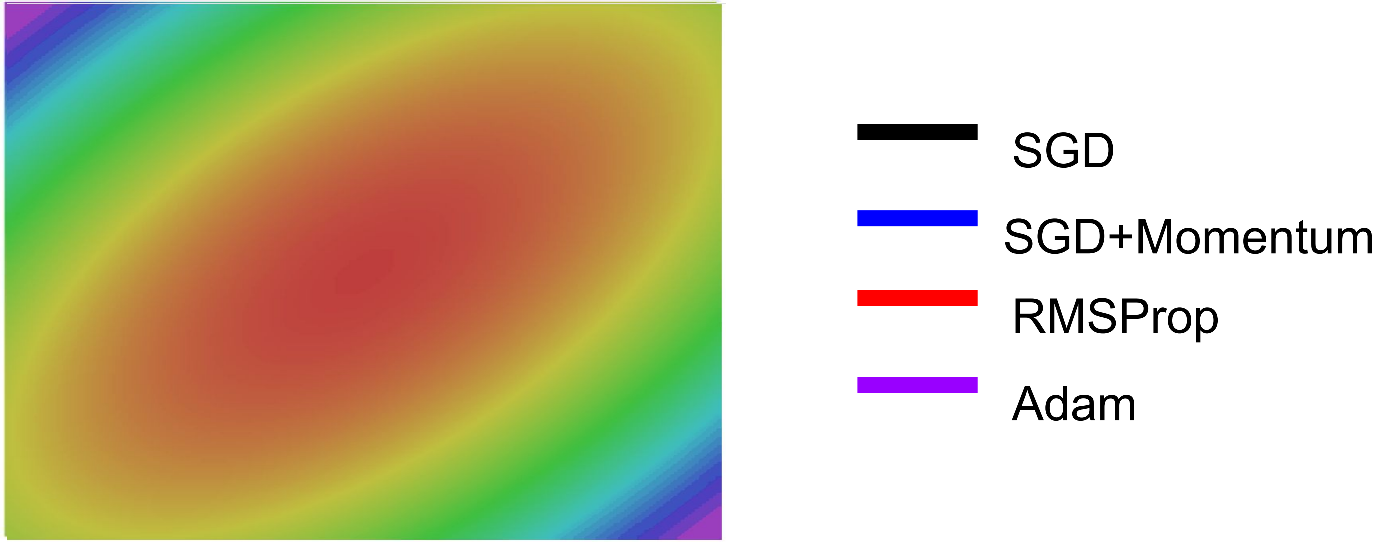
Feature visualizations from Zeiler and Fergus 2013

Neural network design choices, tips and tricks

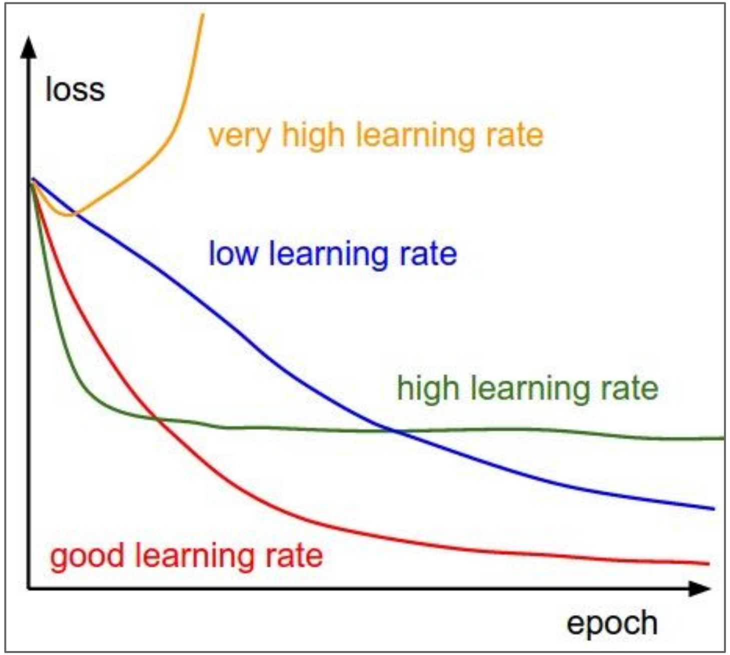
Training hyperparameters: control knobs for the art of training neural networks

Optimization methods: SGD, SGD with momentum, RMSProp, Adam

- **Adam** is a good default choice in many cases; it often works ok even with constant learning rate
- **SGD+Momentum** can outperform Adam but may require more tuning of LR and schedule



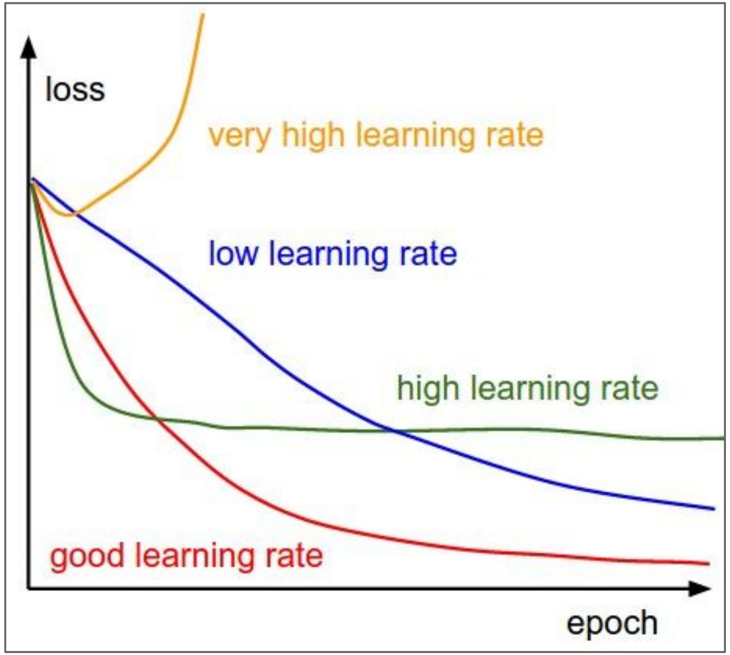
SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.



Q: Which one of these learning rates is best to use?

Slide credit: CS231n

SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.



Q: Which one of these learning rates is best to use?

A: All of them! Start with large learning rate and decay over time

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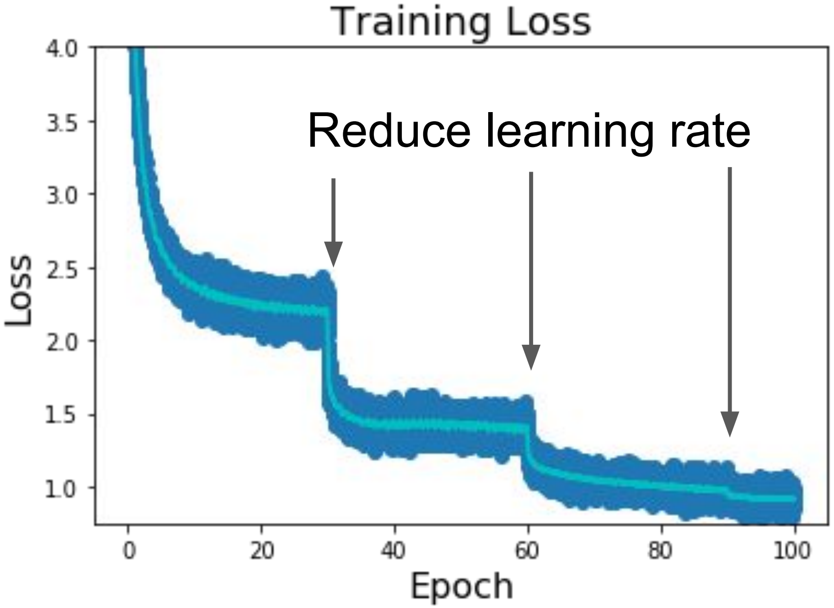
Learning rate decay

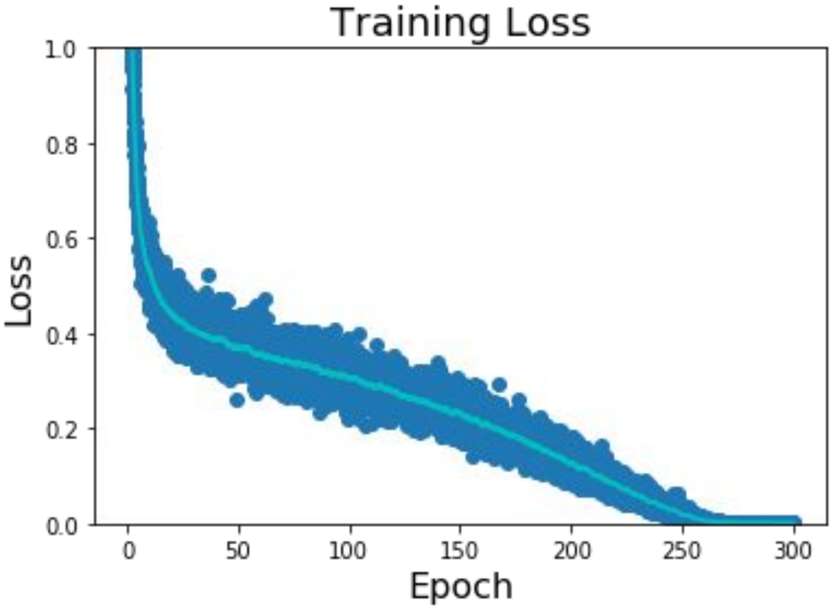


Reduce learning rate

Step: Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

Slide credit: CS231n

Learning rate decay



Step: Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

Fancy decay schedules like cosine, linear, inverse sqrt.

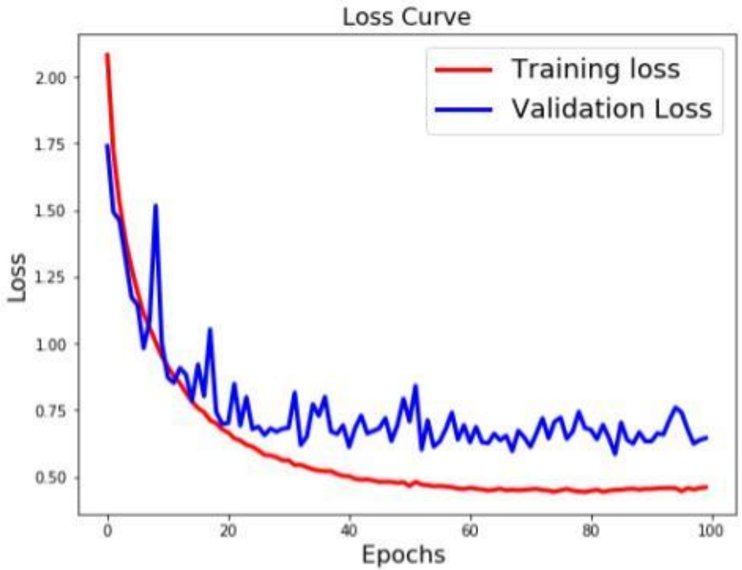
Empirical rule of thumb: If you increase the batch size by N, also scale the initial learning rate by N.

Loshchilov and Hutter, “SGDR: Stochastic Gradient Descent with Warm Restarts”, ICLR 2017
Radford et al, “Improving Language Understanding by Generative Pre-Training”, 2018
Feichtenhofer et al, “SlowFast Networks for Video Recognition”, arXiv 2018
Child at al, “Generating Long Sequences with Sparse Transformers”, arXiv 2019

Slide credit: CS231n

Monitor learning curves

Also useful to plot performance on final metric



Periodically evaluate validation loss

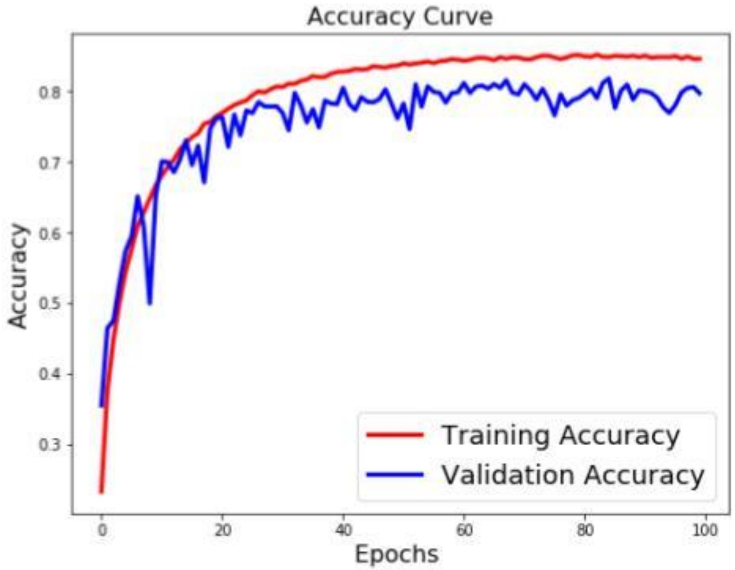


Figure credit: https://www.learnopencv.com/wp-content/uploads/2017/11/cnn-keras-curves-without-aug.jpg

Monitor learning curves

Training loss can be noisy. Using a scatter plot or plotting moving average can help better visualize trends.

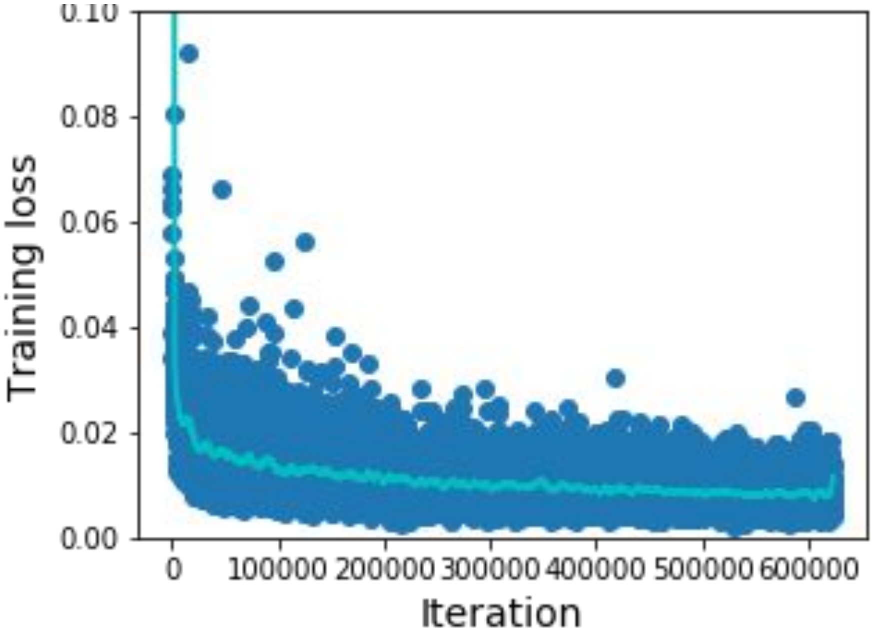
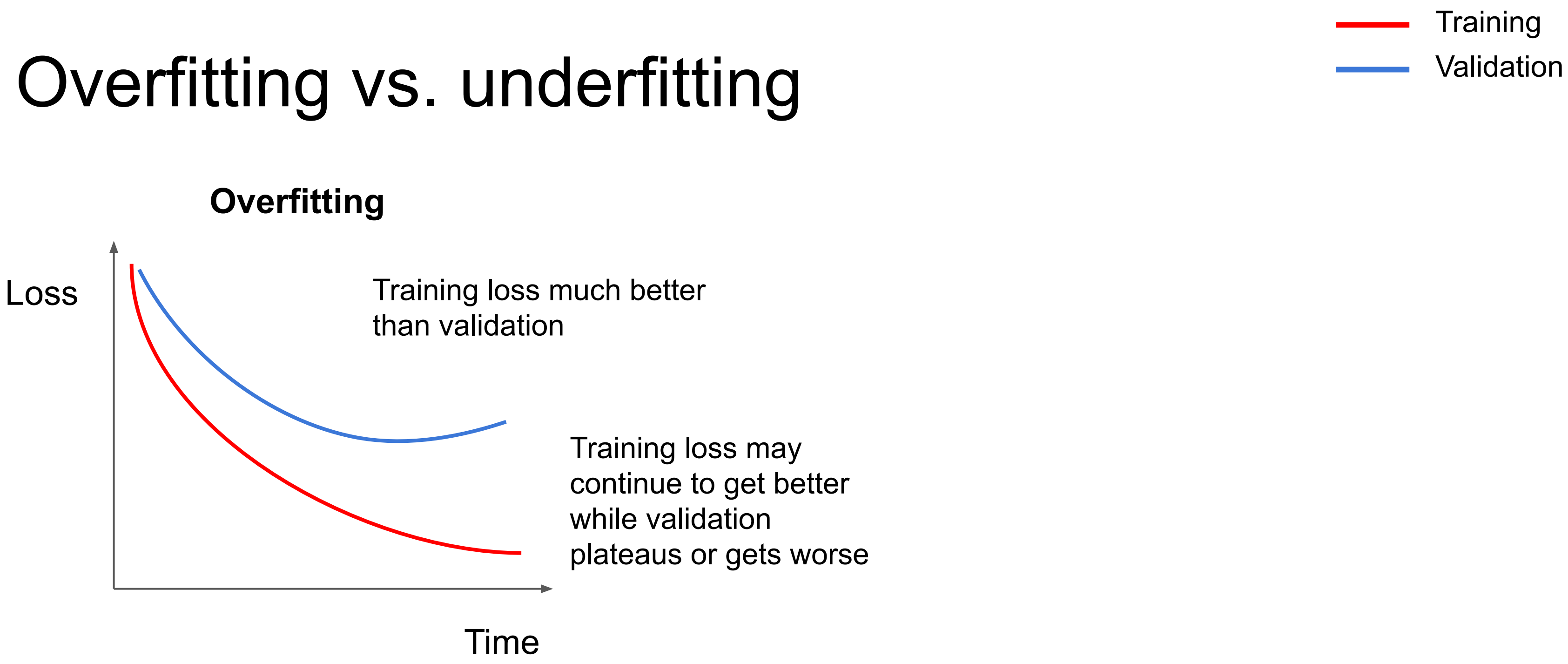


Figure credit: CS231n

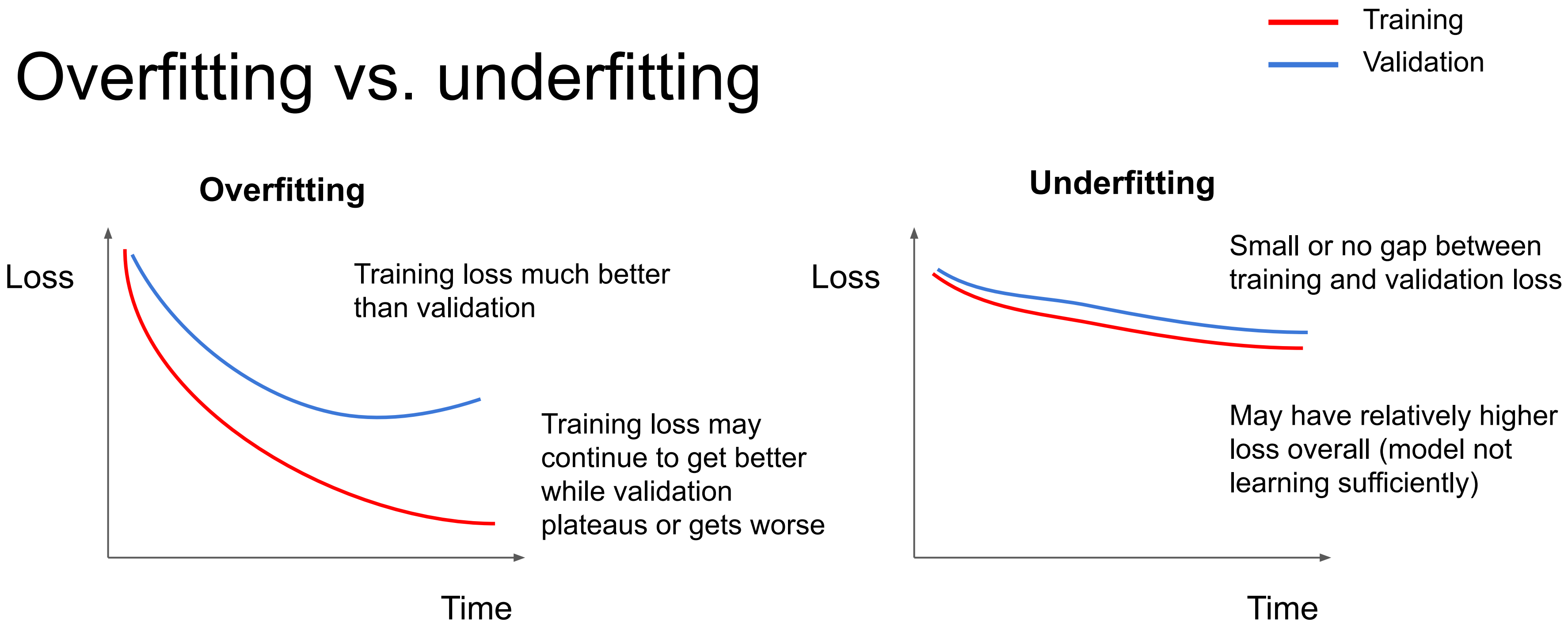
Overfitting vs. underfitting



Training loss much better than validation

Training loss may continue to get better while validation plateaus or gets worse

Overfitting vs. underfitting



Training loss much better than validation

Training loss may continue to get better while validation plateaus or gets worse

Small or no gap between training and validation loss

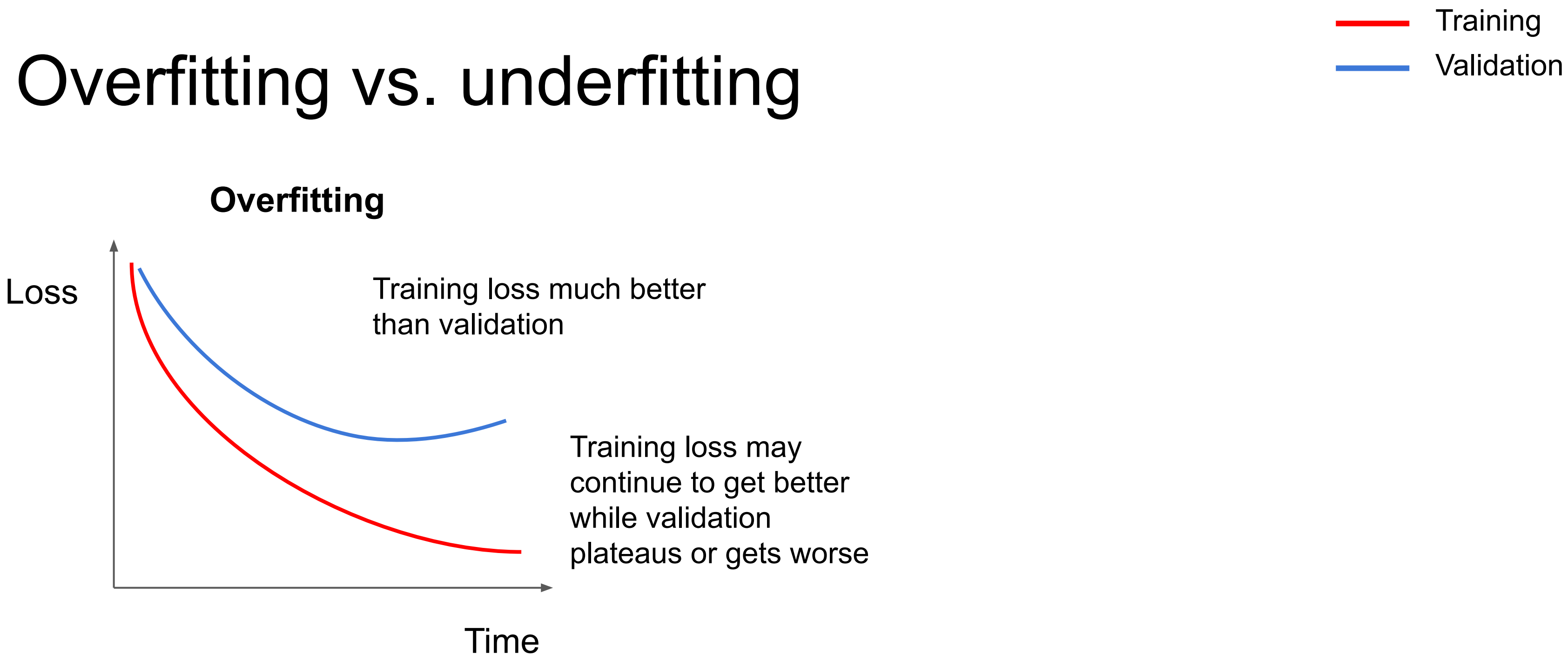
May have relatively higher loss overall (model not learning sufficiently)

Overfitting vs. underfitting

Question:

- What are some ways to combat overfitting?
- What are some ways to combat underfitting?

Overfitting vs. underfitting



Training loss much better than validation

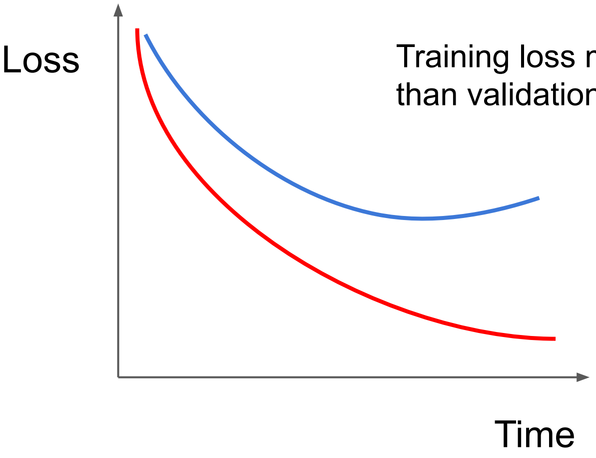
Training loss may continue to get better while validation plateaus or gets worse

Model is “overfitting” to the training data. Best strategy: Increase data or regularize model. Second strategy: decrease model capacity (make simpler)

Overfitting vs. underfitting

🟥 Training
🟦 Validation

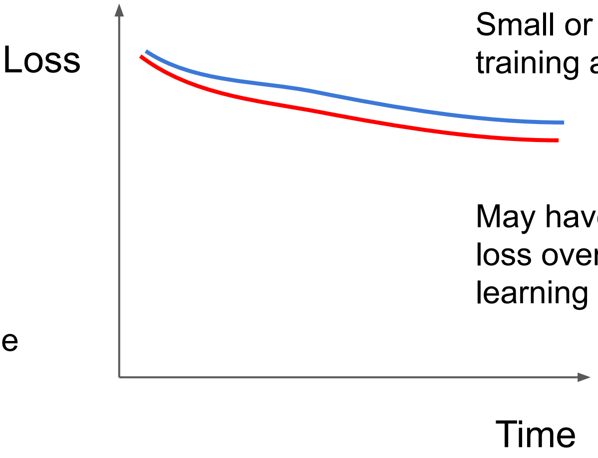
Overfitting



Training loss much better than validation

Training loss may continue to get better while validation plateaus or gets worse

Underfitting



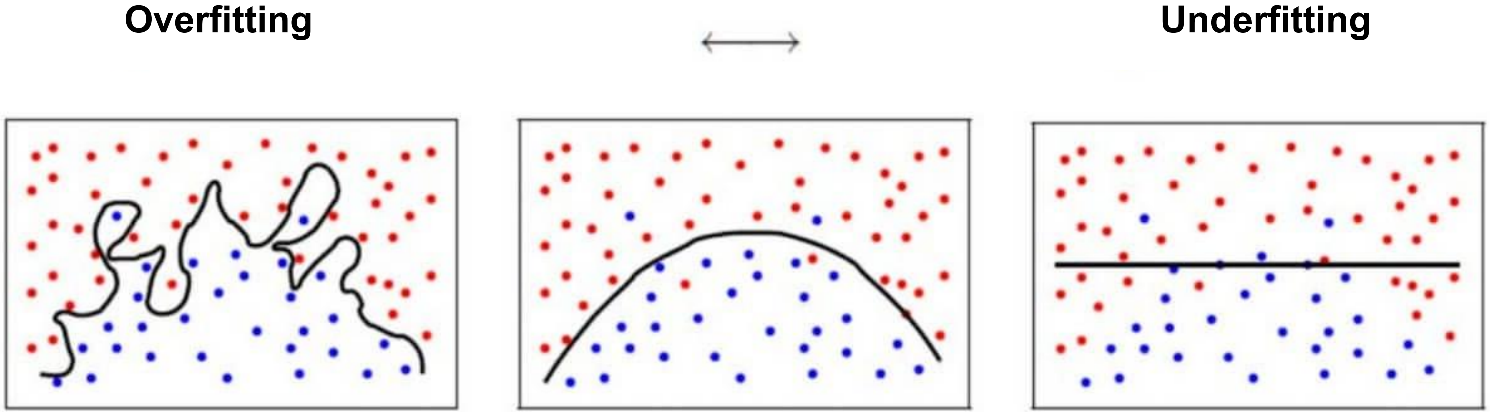
Small or no gap between training and validation loss

May have relatively higher loss overall (model not learning sufficiently)

Model is “overfitting” to the training data. Best strategy: Increase data or regularize model. Second strategy: decrease model capacity (make simpler)

Model is not able to sufficiently learn to fit the data well. Best strategy: Increase complexity (e.g. size) of the model. Second strategy: make problem simpler (easier task, cleaner data)

Overfitting vs. underfitting: more intuition

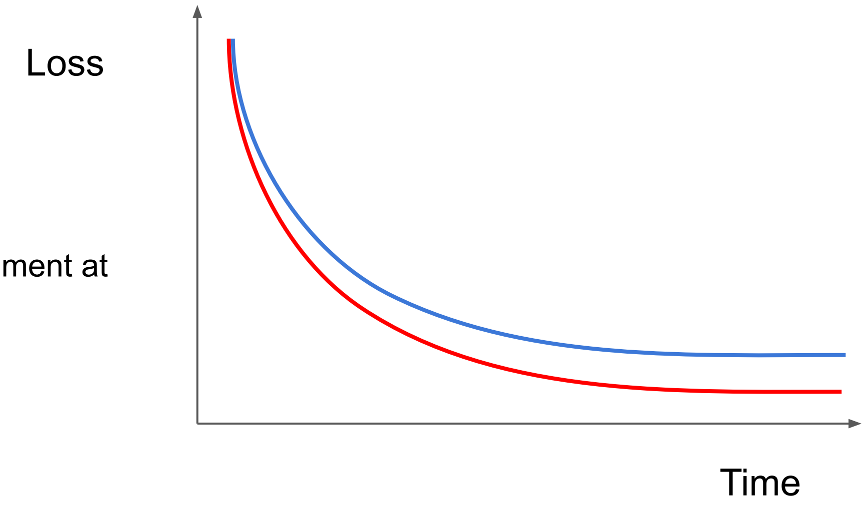


Overfitting

Underfitting

Figure credit: https://qph.fs.quoracdn.net/main-qimg-412c8556aacf7e25b86bba63e9e67ac6-c

Healthy learning curves



Steep improvement at beginning

Continue to gradually improve

Healthy learning curves

Steep improvement at beginning

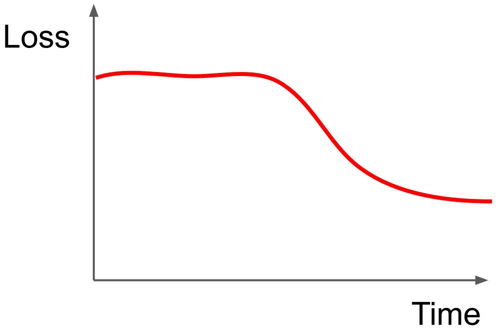
Continue to gradually improve

In practice, models with best final metric (e.g. accuracy) often have slight overfitting.

Intuition: slightly push complexity of model to the highest that the data can handle

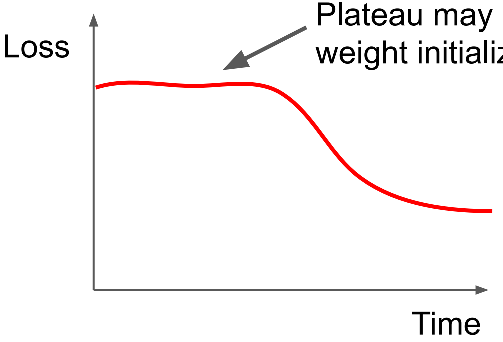
🟥 Training
🟦 Validation

More debugging



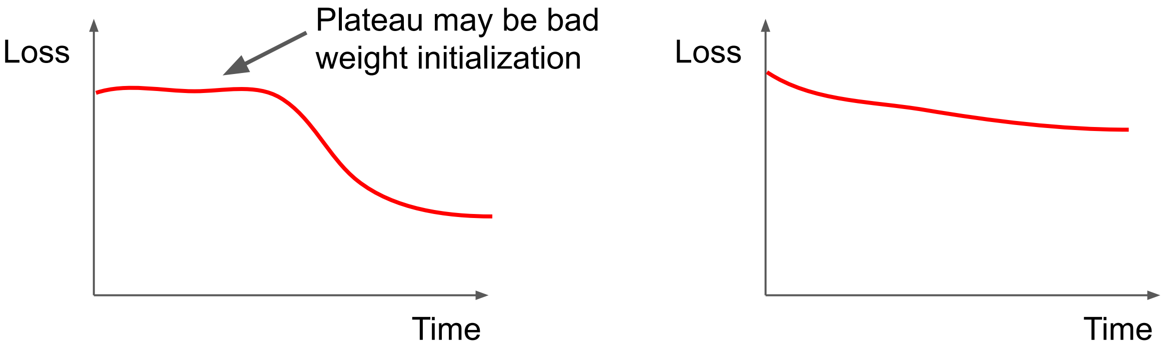
More debugging

🟥 Training
🟦 Validation



Plateau may be bad weight initialization

More debugging



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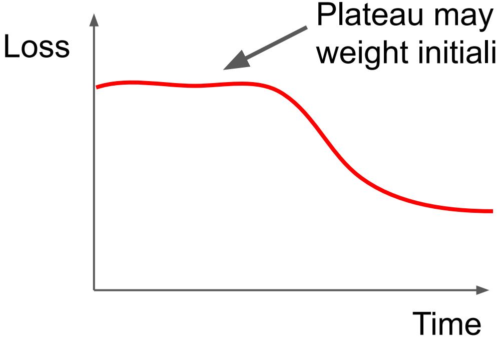
More debugging

🟥 Training
🟦 Validation



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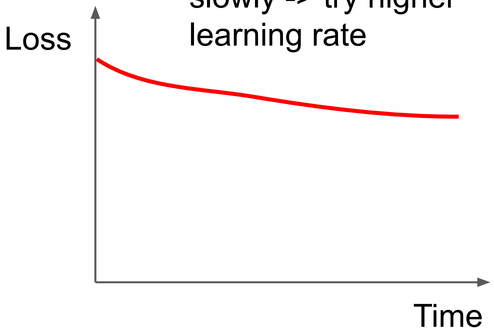
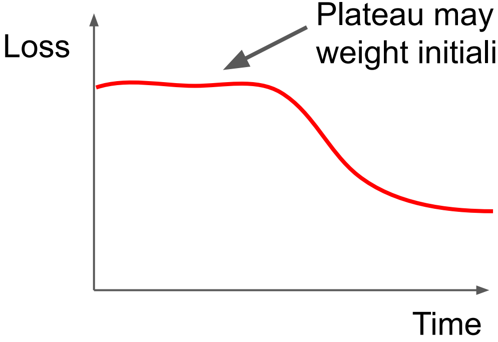


Loss decreasing but slowly -> try higher learning rate

🟥 Training
🟦 Validation

More debugging



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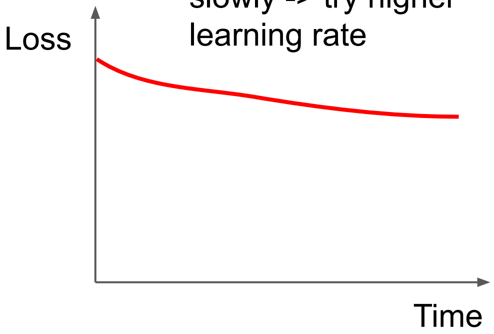

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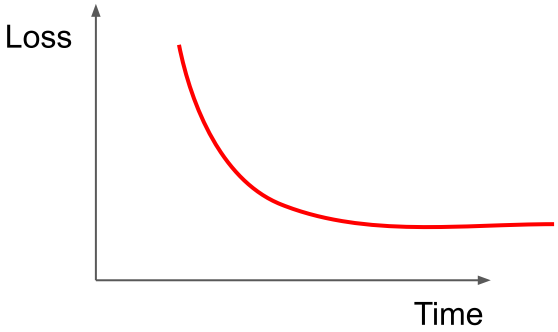
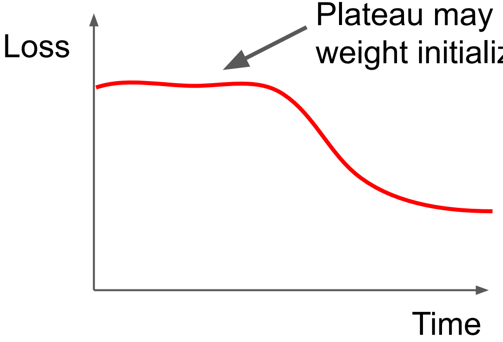


More debugging

🟥 Training
🟦 Validation



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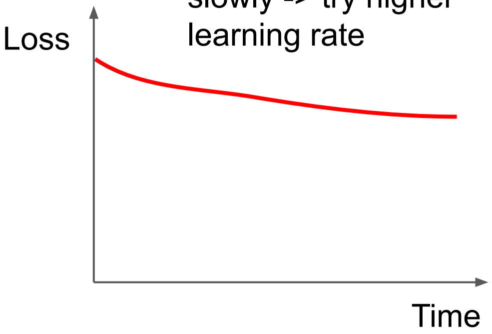

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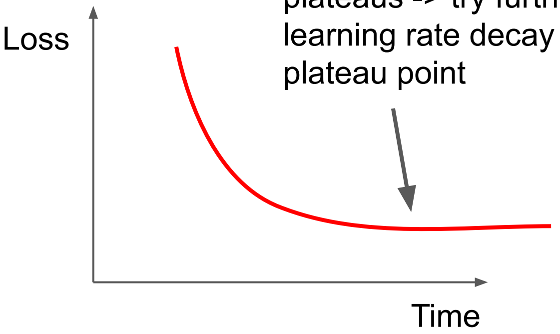
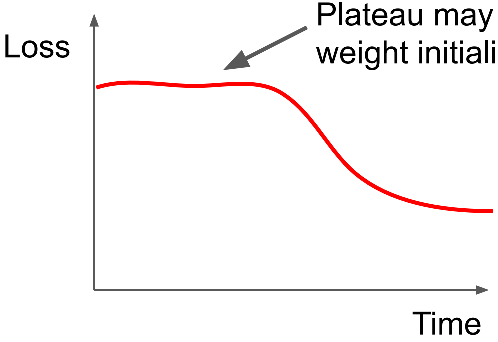


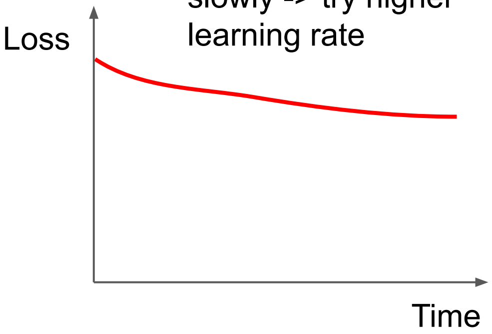
Healthy loss curve plateaus -> try further learning rate decay at plateau point

More debugging

🟥 Training
🟦 Validation



Plateau may be bad weight initialization



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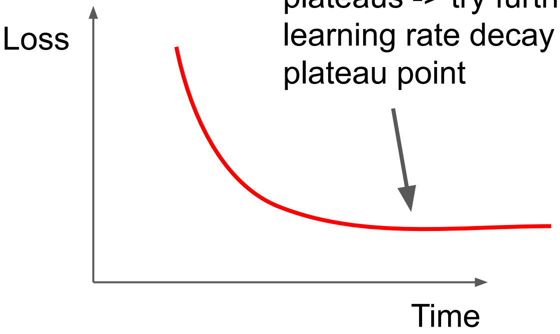

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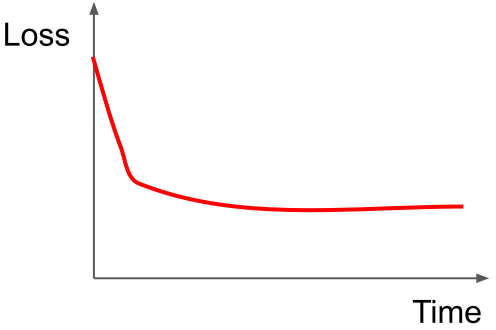
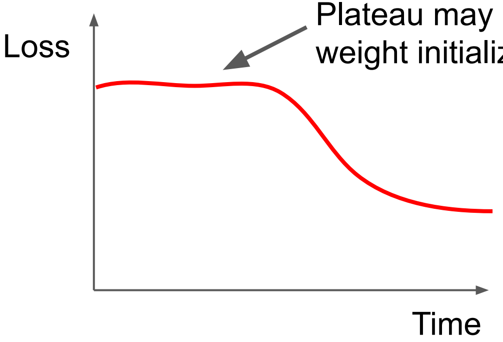


More debugging

🟥 Training
🟦 Validation



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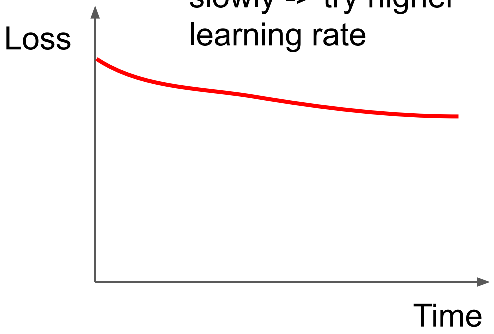
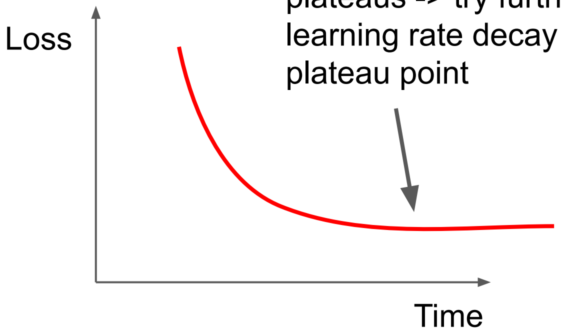
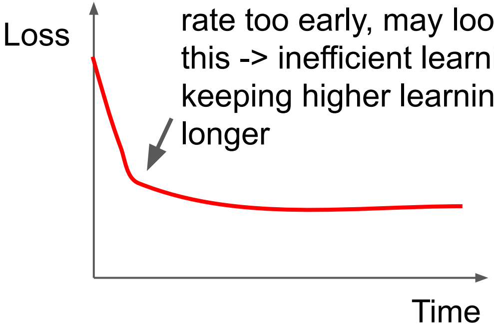


Loss decreasing but slowly -> try higher learning rate



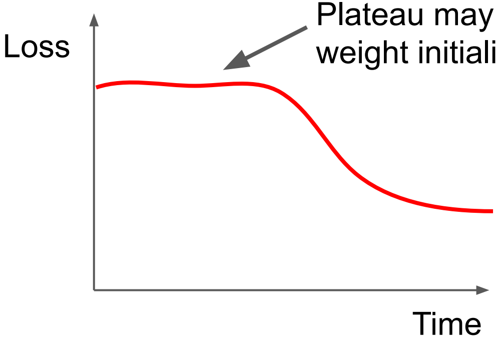
Healthy loss curve plateaus -> try further learning rate decay at plateau point



If you further decay learning rate too early, may look like this -> inefficient learning vs. keeping higher learning rate longer

More debugging

— Training
— Validation



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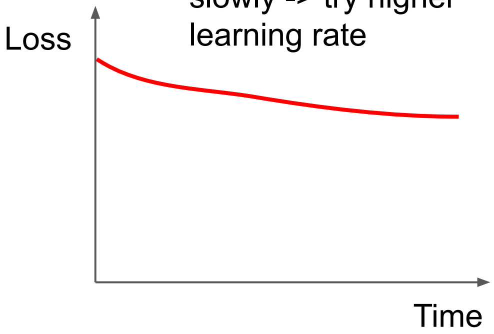
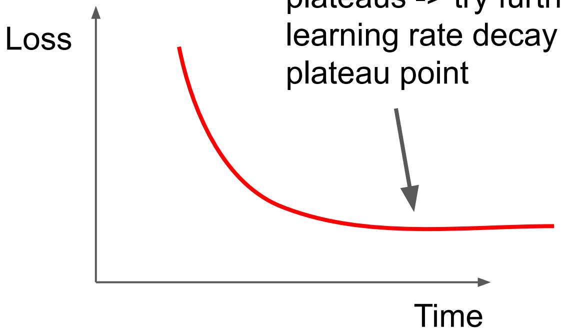
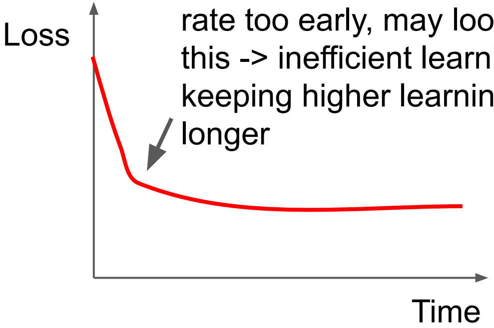


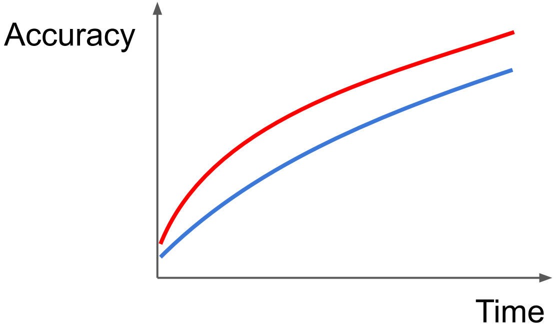
Loss decreasing but slowly -> try higher learning rate



Healthy loss curve plateaus -> try further learning rate decay at plateau point

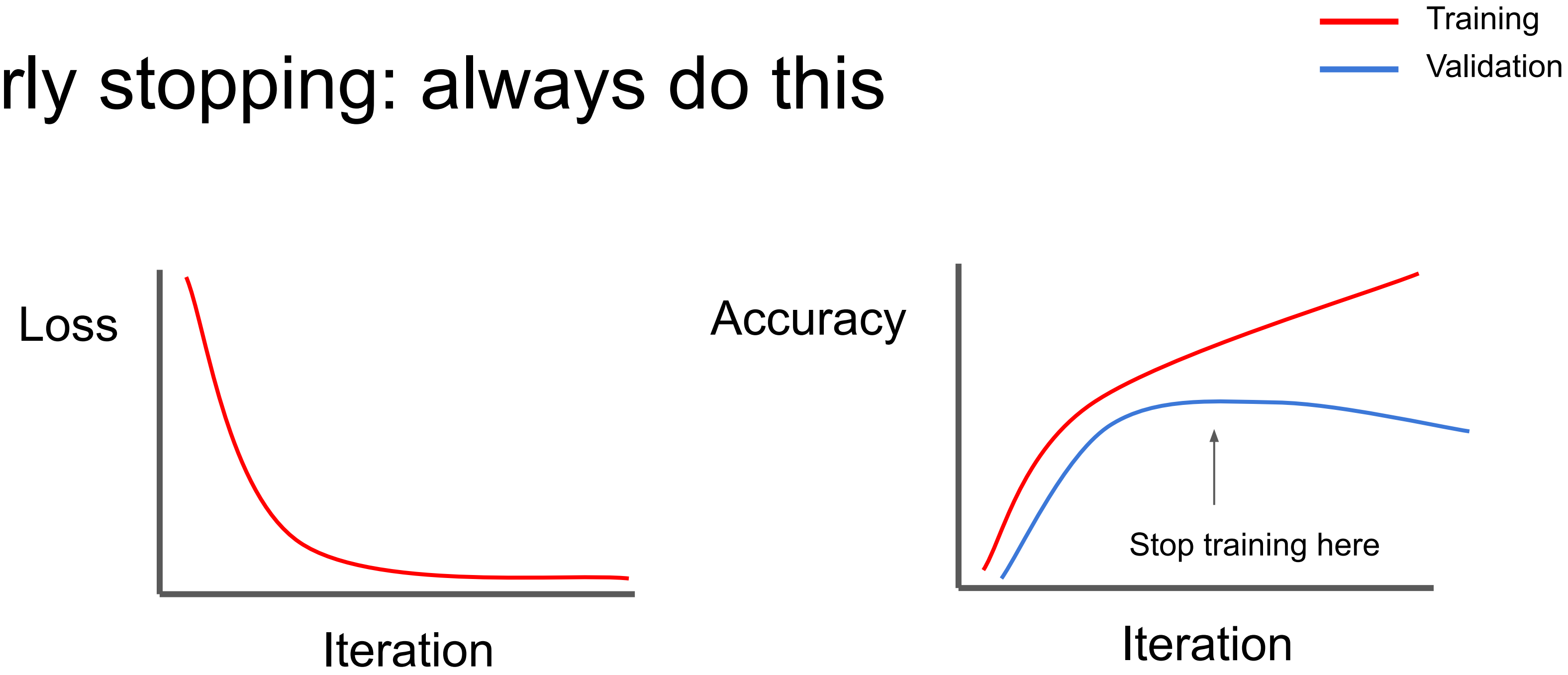


If you further decay learning rate too early, may look like this -> inefficient learning vs. keeping higher learning rate longer



Final metric is still improving -> keep training!

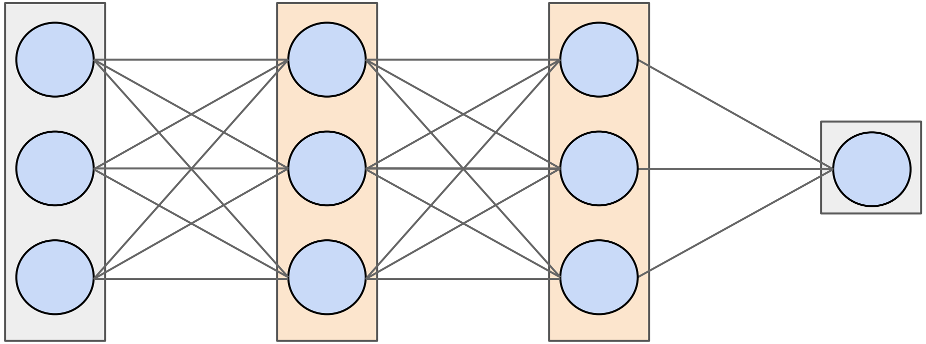
Early stopping: always do this



Stop training the model when accuracy on the validation set decreases
Or train for a long time, but always keep track of the model snapshot that worked best on val.

Slide credit: CS231n

Design choices: network architectures



Major design choices:

- Architecture type (ResNet, DenseNet, etc. for CNNs)
- Depth (# layers)
- For MLPs, # neurons in each layer (hidden layer size)
- For CNNs, # filters, filter size, filter stride in each layer
- Look at argument options in Tensorflow when defining network layers

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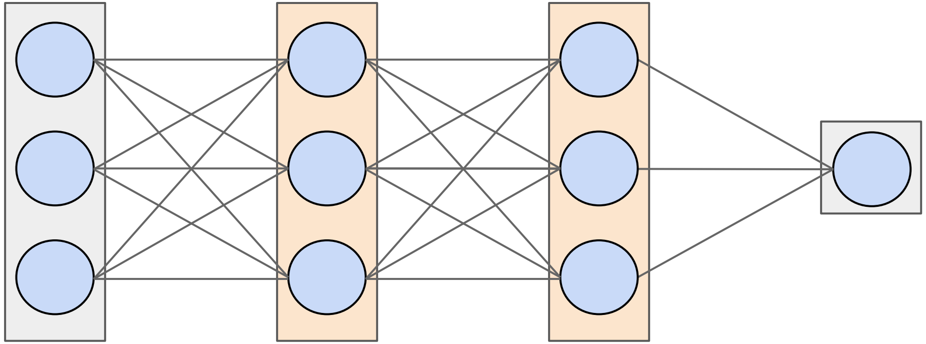

If trying to make network bigger (when underfitting) or smaller (when overfitting), network depth and hidden layer size best to adjust first. Don’t waste too much time early on fiddling with choices that only minorly change architecture.

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Remember optimizing loss functions, which express how well model fit training data, e.g.:

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$$L = \frac{1}{M} \sum_i \underset{\substack{\uparrow \\ \text{Data loss}}}{(\hat{y}^i - y^i)^2} + \overset{\substack{\text{importance of reg. term} \\ \swarrow}}{\lambda} \underset{\substack{\uparrow \\ \text{Regularization} \\ \text{loss}}}{R(W)}$$

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Data loss

Regularization loss

Examples

L2 regularization: $R(W) = \sum_k \sum_l W_{k.l}^2$ (weight decay)

L1 regularization: $R(W) = \sum_k \sum_l |W_{k,l}|$

Elastic net (L1 + L2): $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

https://www.tensorflow.org/api_docs/python/tf/keras/regularizers

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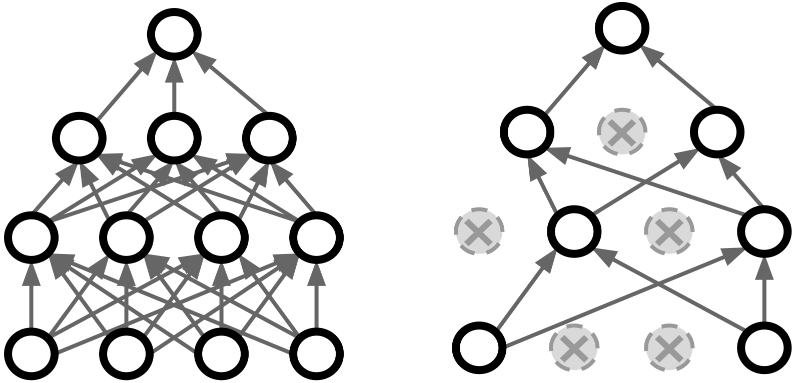
Next: implicit regularizers that do not add an explicit term; instead do something implicit in network to prevent it from fitting too well to training data

Design choices: regularization (dropout)

First example of an implicit regularizer.
During training, at each iteration of forward pass randomly set some neurons to zero (i.e., change network architecture such that paths to some neurons are removed).



During testing, all neurons are active. But scale neuron outputs by dropout probability p, such that expected output during training and testing match.

Srivastava et al, “Dropout: A simple way to prevent neural networks from overfitting”, JMLR 2014. Figure credit: CS231n.

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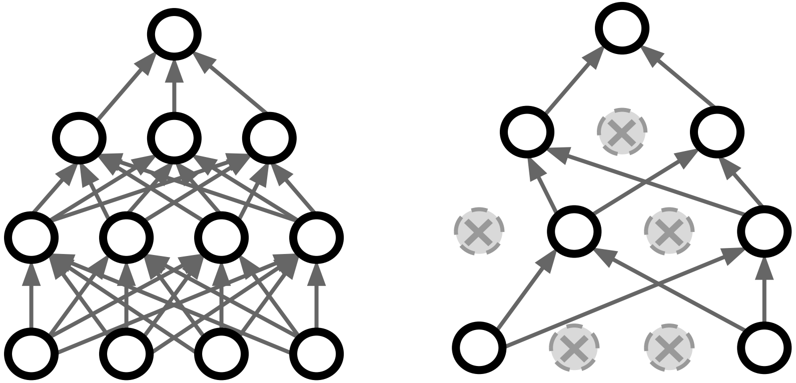

Probability of "dropping out" each neuron at a forward pass is hyperparameter p. 0.5 and 0.9 are common (high!).

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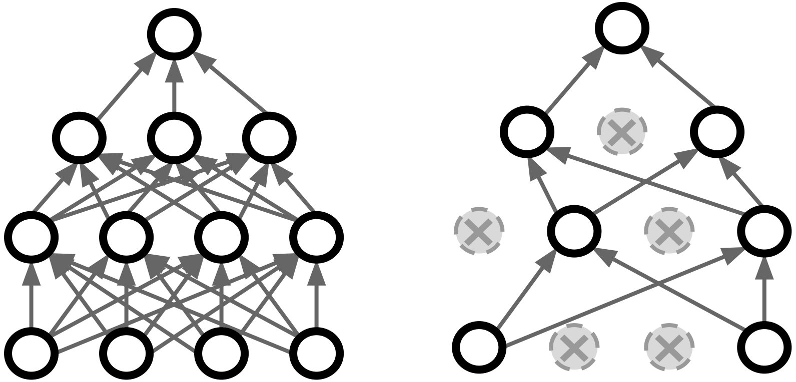

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Intuition: dropout is equivalent to training a large ensemble of different models that share parameters.

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Design choices: regularization (batch normalization)

Another example of an implicit regularizer.
Insert BN layers after FC or conv layers, before activation function.
During training, at each iteration of forward pass normalize neuron activations by mean and variance of minibatch. Also learn scale and shift parameter to get final output.

$$\mu_j = \frac{1}{N}\sum_{i=1}^{N} x_{i,j}$$

$$\sigma_j^2 = \frac{1}{N}\sum_{i=1}^{N}(x_{i,j} - \mu_j)^2$$

$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}}$$

$$y_{i,j} = \gamma_j \hat{x}_{i,j} + \beta_j$$

During testing, normalize by a fixed mean and variance computed from the entire training set. Use learned scale and shift parameters.

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Intuition: batch normalization allows keeping the weights in a healthy range. Also some randomness at training due to different effect from each minibatch sampling -> regularization!

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Design choices: data augmentation

Augment effective training data size by simulating more diversity from existing data. Random combinations of:

- Translation and scaling
- Distortion
- Image color adjustment
- Etc.

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- Etc.

Think about the domain of your data: what makes sense as realistic augmentation operations?

Design choices: weight initialization

Default initializer for most Keras layers is uniform distribution with a Xavier / Glorot normalization

```
    @interfaces.legacy_dense_support
    def __init__(self, units,
                 activation=None,
                 use_bias=True,
                 kernel_initializer='glorot_uniform',
                 bias_initializer='zeros',
                 kernel_regularizer=None,
                 bias_regularizer=None,
                 activity_regularizer=None,
                 kernel_constraint=None,
                 bias_constraint=None,
                 **kwargs):
        if 'input_shape' not in kwargs and 'input_dim' in kwargs:
            kwargs['input_shape'] = (kwargs.pop('input_dim'),)
        super(Dense, self).__init__(**kwargs)
```

Glorot and Bengio, “Understanding the difficulty of training deep feedforward neural networks”, AISTAT 2010

Hyperparameter search

Step 1: Find LR that makes loss go down
Step 2: Define coarse grid of hyperparameter options, train for ~1-5 epochs
Step 3: Refine grid, train longer
Step 4: Look at loss curves
Step 5: GOTO step 3

Slide credit: CS231n

Hyperparameter search

Useful debugging / sanity check: restrict to a very small dataset first (e.g. 1 or 2 minibatches). You should be able to severely overfit and drive the loss to 0.

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Aside: For LR, should sample e^x for x in Uniform [-5, 0]!

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Random search vs. grid search

Random Search for Hyper-Parameter Optimization
Bergstra and Bengio, 2012

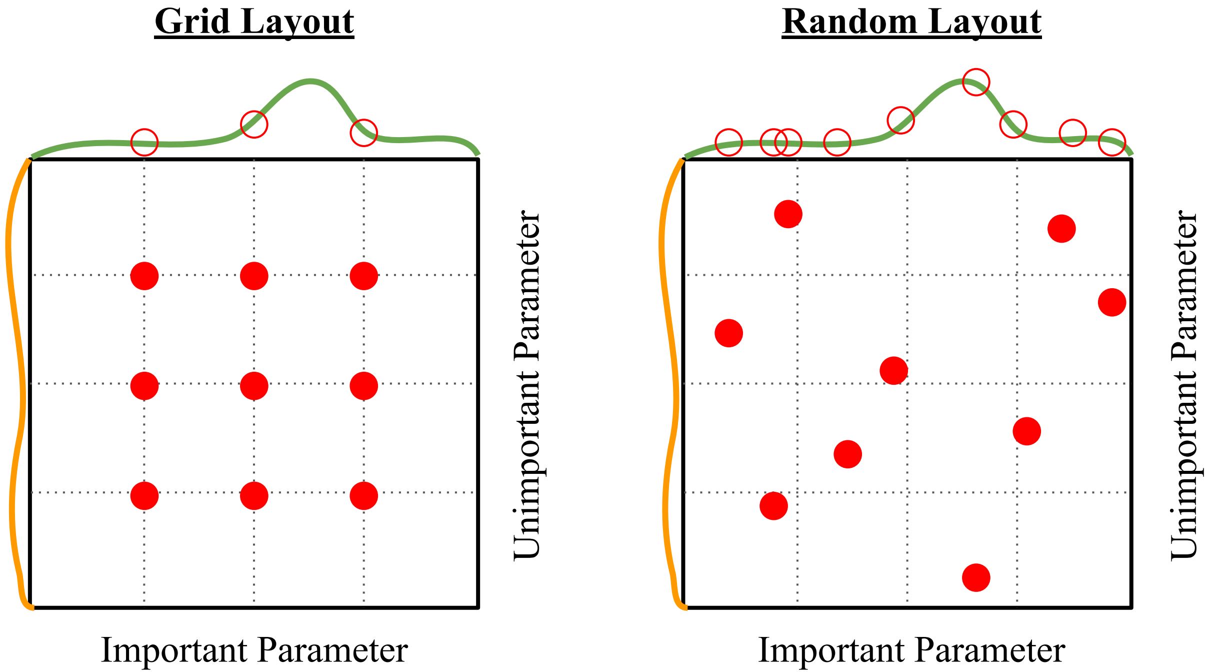

Illustration of Bergstra et al., 2012 by Shayne Longpre, copyright CS231n 2017

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Model inference

Maximizing test-time performance: apply data augmentation operations

Main idea: apply model on multiple variants of a data example, and then take average or max of scores

Can use data augmentation operations we saw during training! E.g.:

- Evaluate at different translations and scales
- Common approach for images: evaluate image crops at 4 corners and center, + horizontally flipped versions -> average 10 scores

Model ensembles

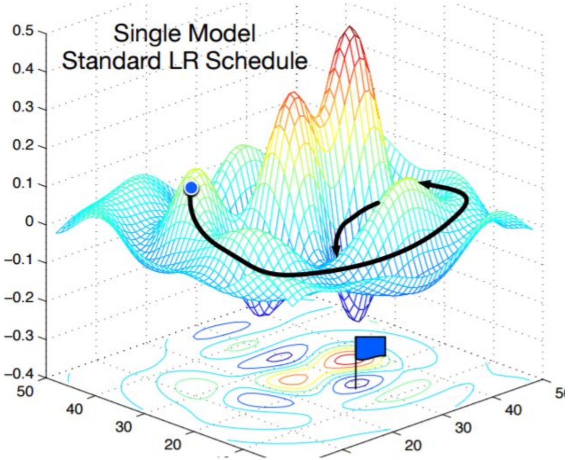
1. Train multiple independent models
2. At test time average their results

Enjoy 2% extra performance

Slide credit: CS231n

Model ensembles: tips and tricks

Instead of training independent models, use multiple snapshots of a single model during training!



Loshchilov and Hutter, “SGDR: Stochastic gradient descent with restarts”, arXiv 2016
Huang et al, “Snapshot ensembles: train 1, get M for free”, ICLR 2017
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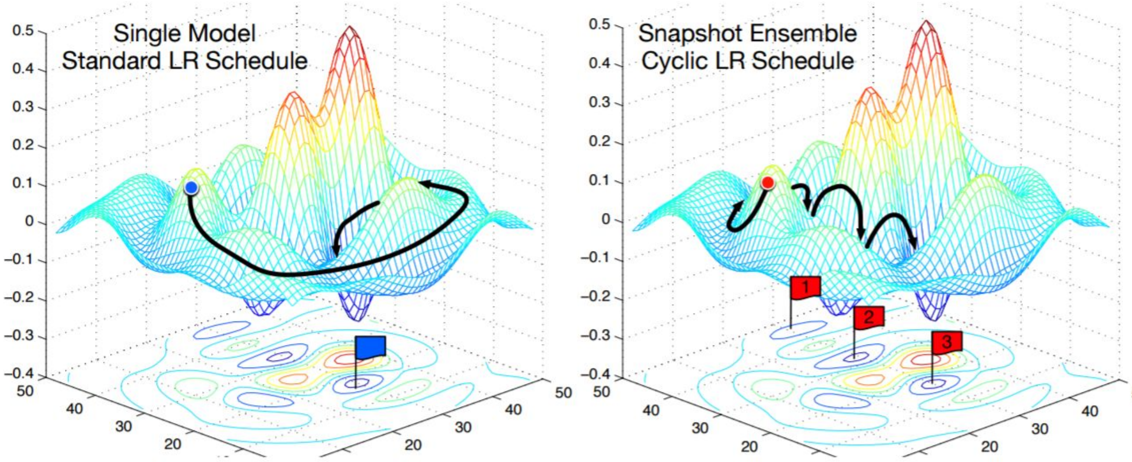

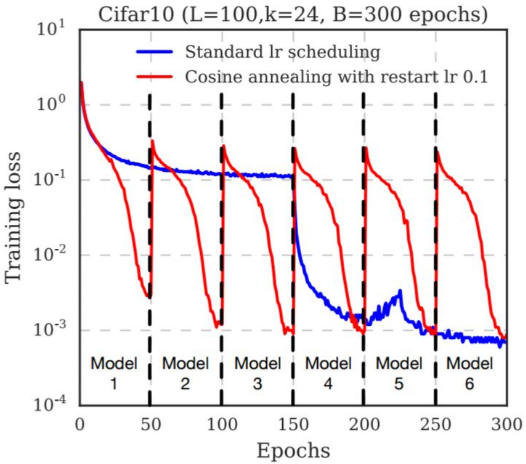

Cyclic learning rate schedules can make this work even better!

Loshchilov and Hutter, “SGDR: Stochastic gradient descent with restarts”, arXiv 2016
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Summary

- Overview of deep learning fundamentals and training neural networks
- Next Friday’s section will provide an in-depth tutorial on Tensorflow