# BST 261: Data Science II
# Lecture 2
## MLPs, Backpropagation, and coding neural networks in Python

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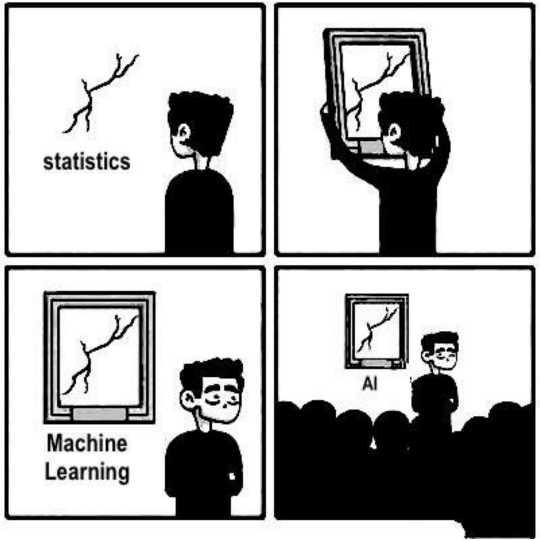
Harvard T.H. Chan School of Public Health
Spring 2 2021

# Recipe of the Day

[Blueberry scones with lemon glaze]

# Deep learning glossaries

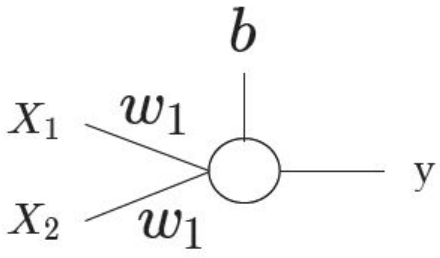
1. Google
2. WildML



# Perceptrons

# Perceptrons

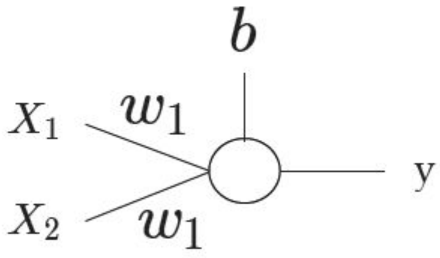
- Let’s put this all together
- Our first network will be a single neuron that will learn a simple function




| X1 | X2 | y |
|---|---|---|
| 0 | 0 | 0 |
| 0 | 1 | 1 |
| 1 | 0 | 1 |
| 1 | 1 | 1 |

# Perceptrons

- How do we make a prediction for each observation?




Assume the following values:

| w1 | w2 | b |
|---|---|---|
| 1 | -1 | -0.5 |

Observations

| X1 | X2 | y |
|---|---|---|
| 0 | 0 | 0 |
| 0 | 1 | 1 |
| 1 | 0 | 1 |
| 1 | 1 | 1 |

# Predictions

- For the first observation, $X_1 = 0, X_2 = 0, y = 0$
- First compute the weighted sum:

$$h = w_1 * X_1 + w_2 * X_2 + b$$

$$h = 1 * 0 + -1 * 0 + (-0.5)$$

$$h = -0.5$$

Assume the following values:

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Transform to a probability:

$$p = \frac{1}{1+\exp(-h)}$$

$$p = \frac{1}{1+\exp(-0.5)}$$

$$p = 0.38$$

Assume the following values:

| w1 | w2 | b |
|---|---|---|
| 1 | -1 | -0.5 |

*Note we are doing binary classification so we have to use the sigmoid activation function to calculate p

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$$p = 0.38$$

Round to get prediction:

$$\hat{y} = \text{round}(p)$$

$$\hat{y} = 0$$

Assume the following values:

| w1 | w2 | b |
|---|---|---|
| 1 | -1 | -0.5 |

# Predictions

$$h = w_1 * X_1 + w_2 * X_2 + b$$

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Complete the table:

| X1 | X2 | y | h | p | $\hat{y}$ |
|---|---|---|---|---|---|
| 0 | 0 | 0 | -0.5 | 0.38 | 0 |
| 0 | 1 | 1 | | | |
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Complete the table:

| X1 | X2 | y | h | p | $\hat{y}$ |
|---|---|---|---|---|---|
| 0 | 0 | 0 | -0.5 | 0.38 | 0 |
| 0 | 1 | 1 | -1.5 | 0.18 | 0 |
| 1 | 0 | 1 | 0.5 | 0.38 | 0 |
| 1 | 1 | 1 | -0.5 | 0.38 | 0 |

Assume the following values:

| w1 | w2 | b |
|---|---|---|
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# Performance

- Our network isn't so great
- How do we make it better?
- What does *better* mean?
  - Need to define a measure of performance
  - There are many ways

- Let's begin with squared error: $(y - p)^2$
- We need to find values for $w_1, w_2, b$ that make this error as small as possible.
- We need to **learn** values for $w_1, w_2, b$ such that the difference between the predicted and actual values is as small as possible.

# Learning From Data

How do we find the best values for $w_1, w_2, b$ ?

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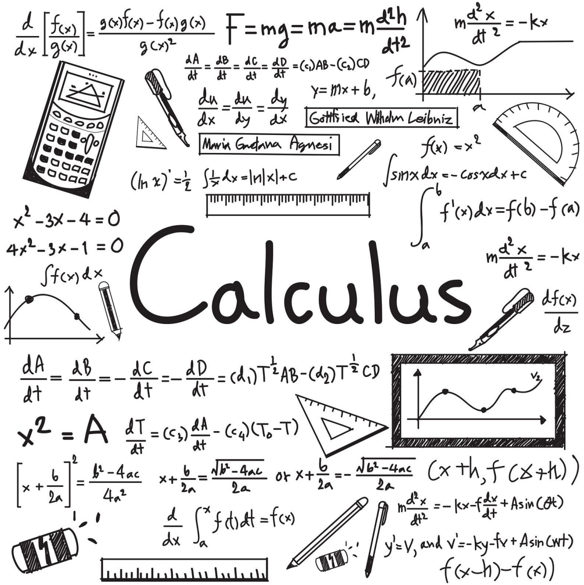

# Learning From Data

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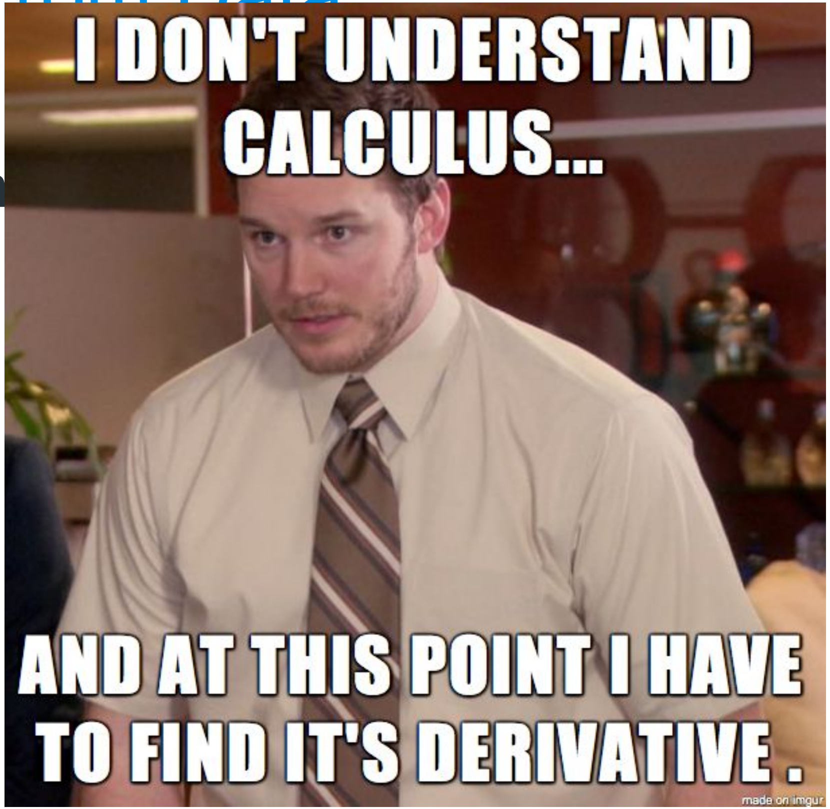
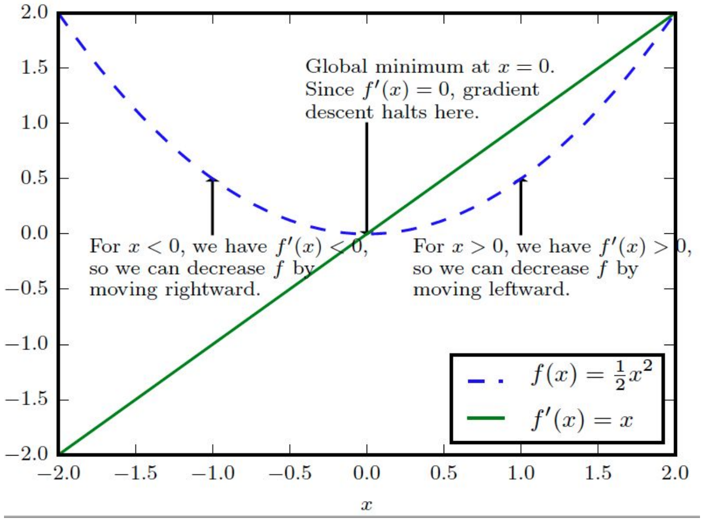


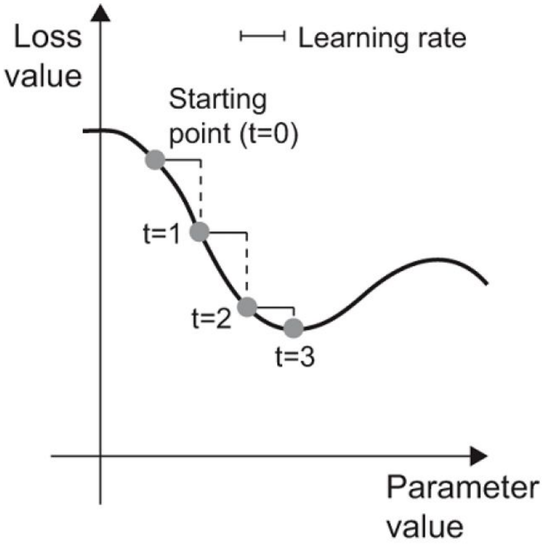
# Learning From Data

- Recall that the derivative of a function tells you how it is changing at any given location.
  - If the derivative is positive, it means it's going up
  - If the derivative is negative, it means it's going down

- Strategy:
  - Start with initial values for $w_1, w_2, b$
  - Take partial derivatives of the loss function with respect to $w_1, w_2, b$
  - Subtract the derivative (also called the **gradient**) from each
  - This is known as **gradient descent**

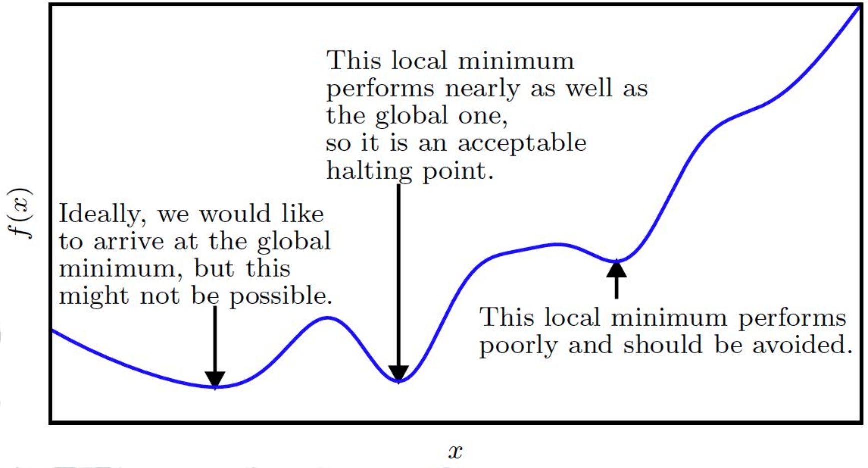
# Gradient-Based Optimization

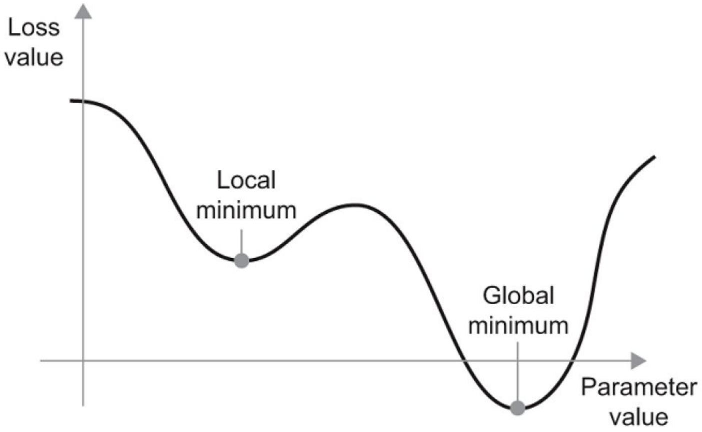


# Gradient-Based Optimization

- A point that obtains the absolute lowest value of *f(x)* is a global minimum
- There may be one global minimum or multiple global minima
- It is also possible for there to be local minima that are not globally optimal
- It is common in many settings to settle for a value *f* that is very low but not necessarily minimal



# Gradient-Based Optimization

- To minimize *f*, we would like to find the direction in which *f* decreases the fastest
- It can be shown that the gradient points directly uphill and the negative gradient directly downhill
- We can therefore decrease *f* by moving in the direction of the negative gradient
- For example, for a weight $w_i$

$$w_i^{\text{new}} = w_i^{\text{old}} - \eta g$$

where $\eta$ is the **learning rate** (how fast you want to move down the gradient), and $g$ is the gradient

# The Backpropagation Algorithm

**Learning representations by back-propagating errors**

**David E. Rumelhart*, Geoffrey E. Hinton† & Ronald J. Williams***

* Institute for Cognitive Science, C-015, University of California, San Diego, La Jolla, California 92093, USA
† Department of Computer Science, Carnegie-Mellon University, Pittsburgh, Philadelphia 15213, USA

**We describe a new learning procedure, back-propagation, for networks of neurone-like units. The procedure repeatedly adjusts the weights of the connections in the network so as to minimize a measure of the difference between the actual output vector of the net and the desired output vector. As a result of the weight adjustments, internal 'hidden' units which are not part of the input or output come to represent important features of the task domain, and the regularities in the task are captured by the interactions of these units. The ability to create useful new features distinguishes back-propagation from earlier, simpler methods such as the perceptron-convergence procedure[1].**

# The Backpropagation Algorithm

- Our perceptron performs the following computations:

$$h = w_1 * X_1 + w_2 * X_2 + b$$

$$p = \frac{1}{1+\exp(-h)}$$

- We want to minimize this quantity:

$$l = (y - p)^2$$

- We'll compute the gradients for each parameter by "backpropagating" errors through each component of the network

# The Backpropagation Algorithm

For $w_1$ we need to compute

$$\frac{\partial l}{\partial w_1}$$

To get there we will use the chain rule

$$\frac{\partial l}{\partial w_1} = \frac{\partial l}{\partial p} * \frac{\partial p}{\partial h} * \frac{\partial h}{\partial w_1}$$

This is "backprop"

Computations

$$h = w_1 * X_1 + w_2 * X_2 + b$$

$$p = \frac{1}{1+\exp(-h)}$$

Loss

$$l = (y - p)^2$$

# The Backpropagation Algorithm

$$\frac{\partial l}{\partial w_1} = \frac{\partial l}{\partial p} * \frac{\partial p}{\partial h} * \frac{\partial h}{\partial w_1}$$

$$\boxed{\frac{\partial l}{\partial p}} =$$

Computations

$$h = w_1 * X_1 + w_2 * X_2 + b$$

$$p = \frac{1}{1+\exp(-h)}$$

Loss

$$\boxed{l = (y-p)^2}$$

# The Backpropagation Algorithm

$$\frac{\partial l}{\partial w_1} = \frac{\partial l}{\partial p} * \frac{\partial p}{\partial h} * \frac{\partial h}{\partial w_1}$$

$$\boxed{\frac{\partial l}{\partial p}} = 2 * (p - y)$$

Computations

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$$p = \frac{1}{1+\exp(-h)}$$

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# The Backpropagation Algorithm

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Computations

$$h = w_1 * X_1 + w_2 * X_2 + b$$

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Computations

$$h = w_1 * X_1 + w_2 * X_2 + b$$

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Loss

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# The Backpropagation Algorithm

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$$\boxed{\frac{\partial h}{\partial w_1}} =$$

## Computations

$$\boxed{h = w_1 * X_1 + w_2 * X_2 + b}$$

$$\boxed{p = \frac{1}{1+\exp(-h)}}$$

## Loss

$$\boxed{l = (y - p)^2}$$

# The Backpropagation Algorithm

$$\frac{\partial l}{\partial w_1} = \frac{\partial l}{\partial p} * \frac{\partial p}{\partial h} * \frac{\partial h}{\partial w_1}$$

$$\boxed{\frac{\partial l}{\partial p}} = 2 * (p - y)$$

$$\boxed{\frac{\partial p}{\partial h}} = p * (1 - p)$$

$$\boxed{\frac{\partial h}{\partial w_1}} = X_1$$

Computations

$$\boxed{h = w_1 * X_1 + w_2 * X_2 + b}$$

$$\boxed{p = \frac{1}{1+\exp(-h)}}$$

Loss

$$\boxed{l = (y - p)^2}$$

Putting it all together:

$$\frac{\partial l}{\partial w_1} = 2 * (p - y) * p * (1 - p) * X_1$$

# Gradient Descent with Backprop

For some number of iterations:

1. Compute the gradient for $w_1$
2. Update $w_i^{\text{new}} = w_i^{\text{old}} - \eta g$
3. Repeat until "convergence"

Do this for each weight and bias term.

# Multilayer Perceptrons

# Perceptron → MLP

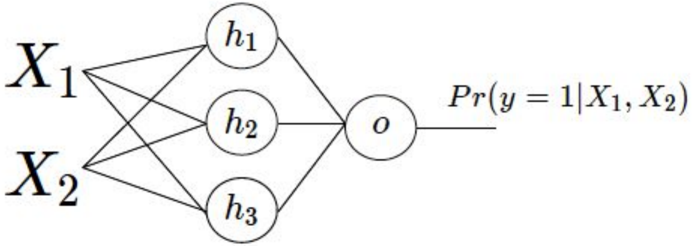
We can turn our perceptron model into a multilayer perceptron

- Instead of just one linear combination, we are going to take several, each with a different set of weights
- Each linear combination will be followed by a nonlinear activation
- Each of these nonlinear features will be fed into the logistic regression classifier (binary classifier)
- All of the weights are learned end-to-end via SGD

MLPs learn a set of nonlinear features directly from data - “feature engineering” is the hallmark of deep learning approaches

# Multilayer Perceptrons (MLPs)

Suppose we have the following MLP with 1 hidden layer that has 3 hidden units:




Each neuron in the hidden layer is going to do exactly the same thing as before.

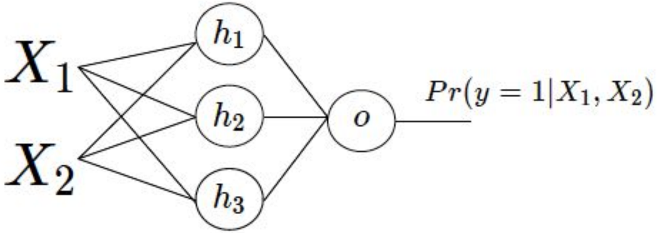
# Multilayer Perceptrons (MLPs)

Computations:

$$h_j = \phi(w_{1j} * X_1 + w_{2j} * X_2 + b_j)$$

$$o = b_o + \sum_{j=1}^{3} w_{oj} * h_j$$

$$p = \frac{1}{1+\exp(-o)}$$




*If we use a sigmoid activation function

Output layer weight derivatives

$$\frac{\partial l}{\partial w_{oj}} = \frac{\partial l}{\partial p} * \frac{\partial p}{\partial o} * \frac{\partial o}{\partial w_{oj}}$$

$$= (p - y) * p * (1 - p) * h_j$$

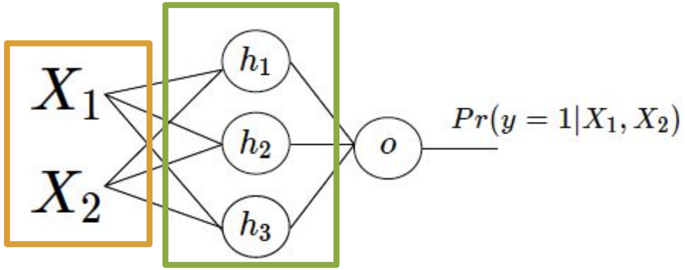
Hidden layer weight derivatives

$$\frac{\partial l}{\partial w_{1j}} = \frac{\partial l}{\partial p} * \frac{\partial p}{\partial o} * \frac{\partial o}{\partial h} * \frac{\partial h}{\partial w_{1j}}$$

$$= (p - y) * p * (1 - p) * h_j * (1 - h_j) * X_1$$

# Matrix Notation

Sum notation starts to get unwieldy quickly. We can use matrix notation to represent each calculation in a more concise way.




$$X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \quad W = \begin{bmatrix} w_{1,1} & w_{2,1} & w_{3,1} \\ w_{1,2} & w_{2,2} & w_{3,2} \end{bmatrix} \quad B = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

$$Z = W^T X + B \qquad H = \begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix} = \phi(Z)$$

# Notation

As the number of layers grows, the number of matrices grows and we have to add a superscript to denote the layer. We also have to add a superscript to denote which training example we are referencing.

Example notation for 1 weight in 1 hidden layer for 1 training example:

Training example *i*

Layer *l*

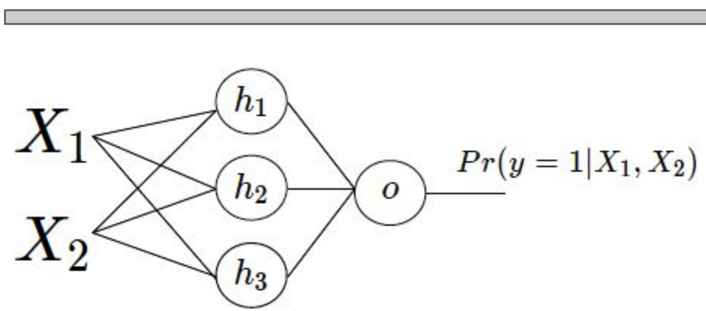
$$w_{j,k}^{[l](i)}$$

Hidden neuron *k*

Input feature *j*

# MLP Terminology

Forward pass = computing probability from input



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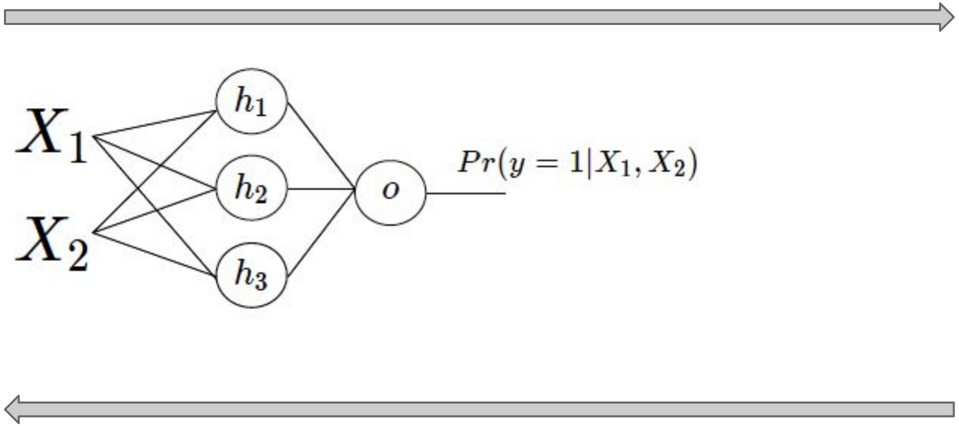
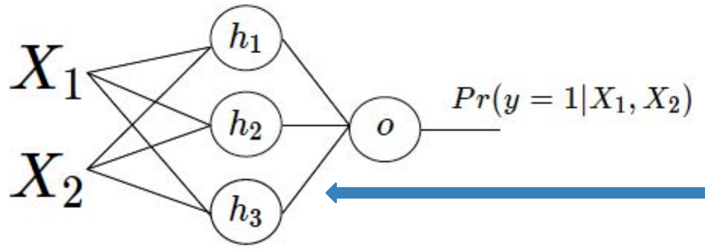
Forward pass = computing probability from input




Backward pass = computing derivatives from the output

# MLP Terminology

Forward pass = computing probability from input

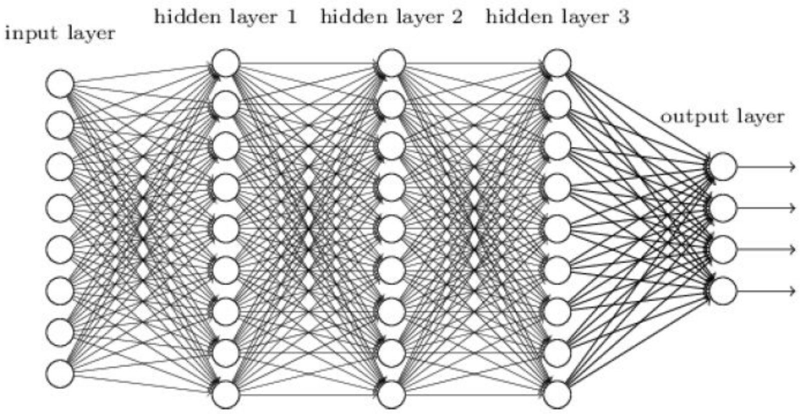



Hidden layers are also called "dense" layers or "fully connected" layers

Backward pass = computing derivatives from the output

# MLPs

Increasing the number of layers increases the flexibility of the model - but run the risk of overfitting

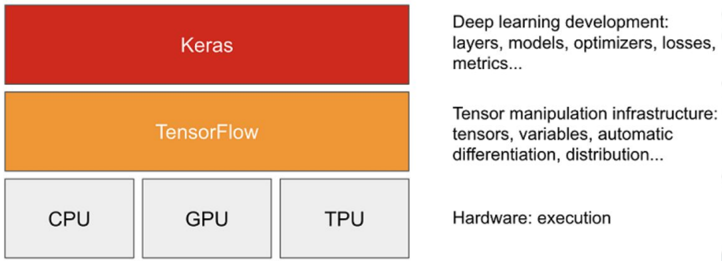


# Conclusions

- Backprop, perceptrons, and MLPs are the building blocks of neural nets
- You’ll get a chance to demonstrate your mastery in Problem Set 1
- We will use these concepts for the rest of the semester

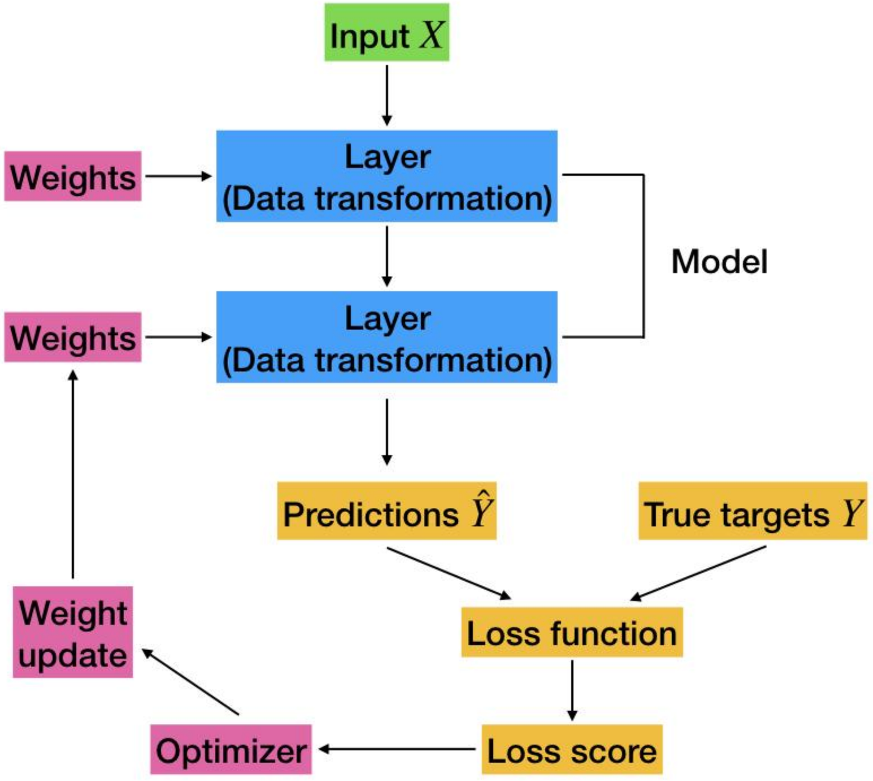
# Coding
# Neural Nets

# Keras and Tensorflow




- Keras is a model-level library that provides high-level building blocks for developing deep learning models
- It doesn’t handle low-level operations like matrix and tensor (n-dimensional matrix) multiplication and differentiation
  - It uses TensorFlow or Theano or CNTK (Microsoft Cognitive Toolkit) backends for this
  - We will be using TensorFlow
    - It is the most widely adopted, scalable and production ready
- Keras can run on both CPUs and GPUs
  - When running on CPUs, uses Eigen for tensor operations
  - When running on GPUs, uses the NVIDIA CUDA Deep Neural Network library (cuDNN)

# Neural Network Workflow



# Generic Feedforward Network

Elements needed:

1. Necessary libraries
2. Dataset split into training and test sets (validation as well if you have enough data)
3. **`models.Sequential()`**: defines a linear, or sequential architecture made up of a set of layers that will stack to create the network
4. **`layers.Dense()`**: specifies a fully connected layer
5. **`model.compile(optimizer, loss, metrics)`**: specifies how to execute the training of the network
6. **`model.fit(train_data, train_labels, epochs, batch_size)`**: fits the neural net using the training data, runs for a specified number of iterations (epochs) using batch_size number of training examples at a time

# Generic Feedforward Network

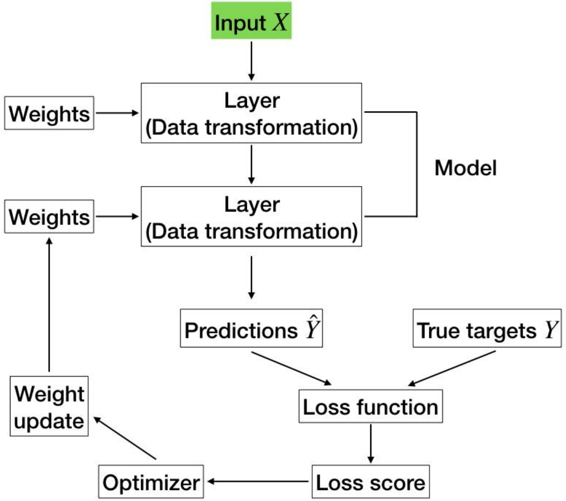
```python
# Import needed packages (not an exhaustive list)
import tensorflow as tf
from tensorflow import keras
from tensorflow.keras import layers

# Load data (will most likely be more complicated)
(x_train, y_train), (x_test, y_test) = load_data()

# Define model architecture
model = keras.Sequential([
  # Layer 1 (Hidden layer, fully connected)
  layers.Dense(c, activation='activation function'),
  # Layer 2 (Output layer, fully connected)
  layers.Dense(d, activation='output activation function')
])

# Define how to execute training
model.compile(optimizer='optimizing algorithm',
              loss='loss function',
              metrics=['performance metric'])

# Train the network
model.fit(x_train, y_train, epochs = e, batch_size = b)
```

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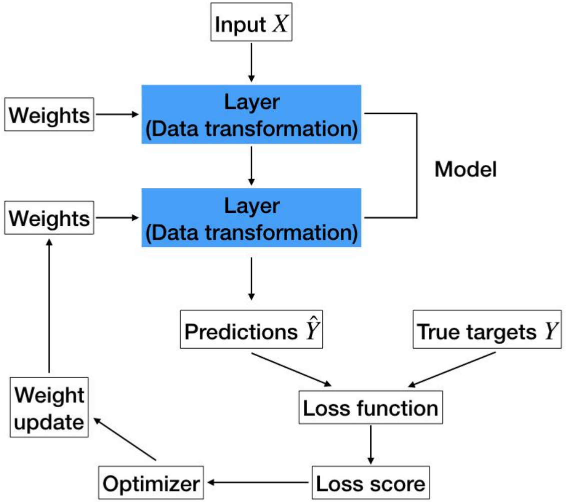


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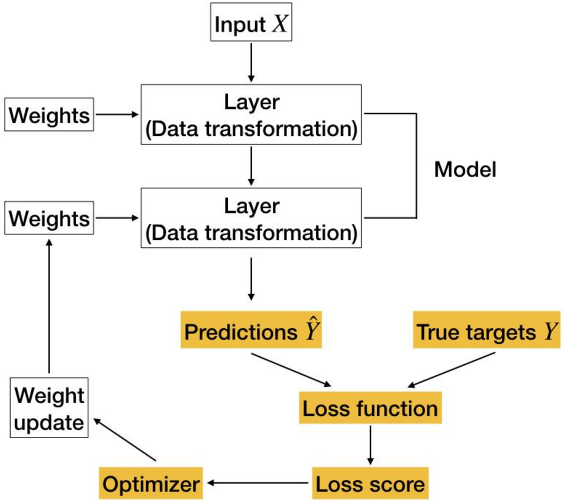


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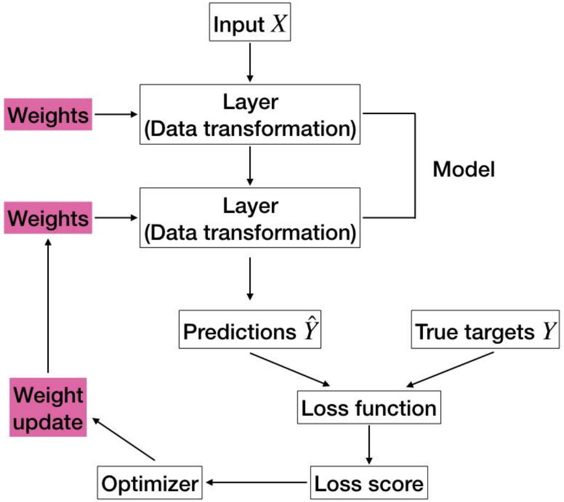


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```

# Generic Feedforward Network

**train_data**: training examples (matrix of feature vectors; $\mathbf{X}_{\mathbf{train}}$)

**train_labels**: training labels ($\mathbf{y}_{\mathbf{train}}$)

**test_data**: test examples used to measure performance of network ($\mathbf{X}_{\mathbf{test}}$)

**test_labels**: test set labels ($\mathbf{y}_{\mathbf{test}}$)

Optimizing algorithms: rmsprop, sgd, adagrad, adam, etc.

Loss function options: mse, mae, categorical_crossentropy, etc.

Performance measure options: accuracy, mae, etc.

Here:

- ***c*** = the number of hidden units (neurons) in a hidden layer
- ***d*** = the number of units (neurons) in the output layer
- ***e*** = the number of epochs (iterations) over entire training data set
- ***b*** = the batch size (how many training examples to optimize at once)

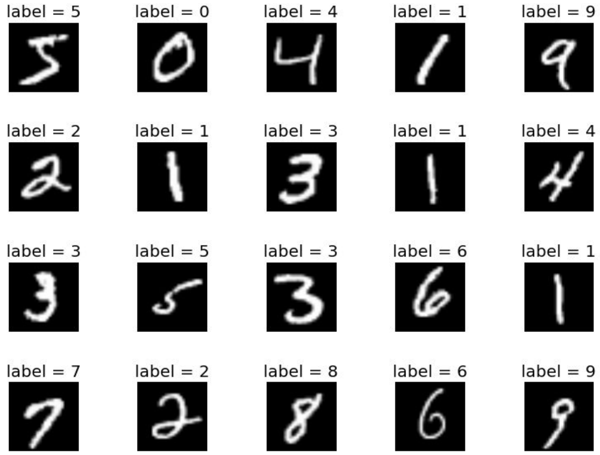
# MLPs in Python/Keras

# MNIST Data Example

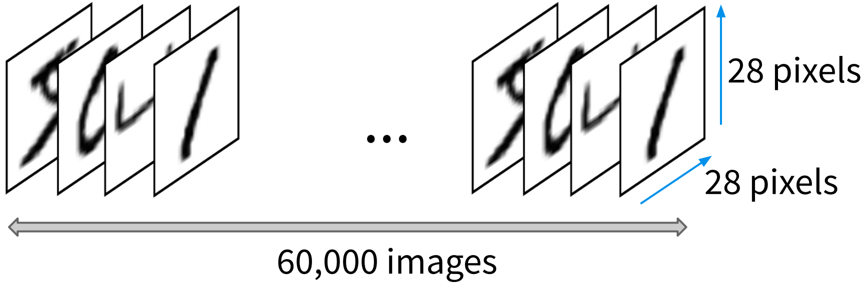
- The MNIST data set includes handwritten digits with corresponding labels

- Training set: 60,000 images of handwritten digits and corresponding labels
  - Each digit is represented as a 28 x 28 matrix of grayscale values 0 - 255
  - The entire training set is stored in a 3D tensor of shape (60000, 28, 28)
  - The corresponding image values are stored as a 1D tensor of values 0 - 9

- Testing set: 10,000 images with the same set up as the training set




Training Data



# MNIST Data Example

Data wrangling

- We’ll get into RGB images later, but for grayscale images, we need to first transform the matrix of values into a vector of values, and then normalize them to be between 0 and 1. It is not strictly necessary to normalize your inputs, but smaller numbers help speed up training and avoid getting stuck in local minima. This also ensures the gradients don’t “explode” or “vanish”
  - Reshape each image from a 28 x 28 matrix of grayscale values 0 - 255 to a vector of length 28*28 = 784 of values 0 - 1 (divide each by 255)

- We now have 10 classes (categories; the digits 0-9)
  - We need to have multiclass labels that tell the network which digit the example is
  - Reshape each corresponding image label to a vector of length 10 of values 0 or 1
  - Example: the digit 3 would be represented as [0, 0, 0, 1, 0, 0, 0, 0, 0, 0]
  - You can think of this as “dummy coding” the labels

# Activation and Loss Function Choices

| Task | Last-layer activation | Loss function |
|---|---|---|
| Binary classification | sigmoid | Binary cross-entropy |
| Multiclass, single-label classification | softmax | Categorical cross-entropy |
| Multiclass, multilabel classification | sigmoid | Binary cross-entropy |
| Regression to arbitrary values | None | Mean square error (MSE) |
| Regression to values between 0 and 1 | sigmoid | MSE or binary cross-entropy |

# Softmax function

$$\text{softmax}(\boldsymbol{z})_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

- Softmax units are used as outputs when predicting a discrete variable *y* with *j* possible values
- In this setting, which can be seen as a generalization of the Bernoulli distribution, we need to produce a vector $\hat{\mathbf{y}}$ with $\hat{y}_i = P(y = i|x)$
- We require that each $\hat{y}_i$ lie in the [0, 1] interval and that the entire vector sums to 1
- We first compute $z = w^T x + b$ as usual
- Here, $z_i = log[\tilde{P}(y = i|x)]$ represents an unnormalized log probability for class *i*
- The softmax function then exponentiates and normalizes *z* to obtain $\hat{\mathbf{y}}$

# Categorical cross-entropy

- In this case we want to maximize

$$log[P(y = i; z)] = log[\text{softmax}(z)_i] = z_i - log \sum_j exp(z_j)$$

- The first term shows that the input always has a direct contribution to the loss function

- Because $log \sum_j exp(z_j) \approx max_j z_j$ , the negative log-likelihood loss function always strongly penalizes the most active incorrect prediction

# MNIST Data Example

## Network Architecture

- Let’s start with 2 layers:
  - Hidden layer will have 512 hidden units and the **relu activation function**

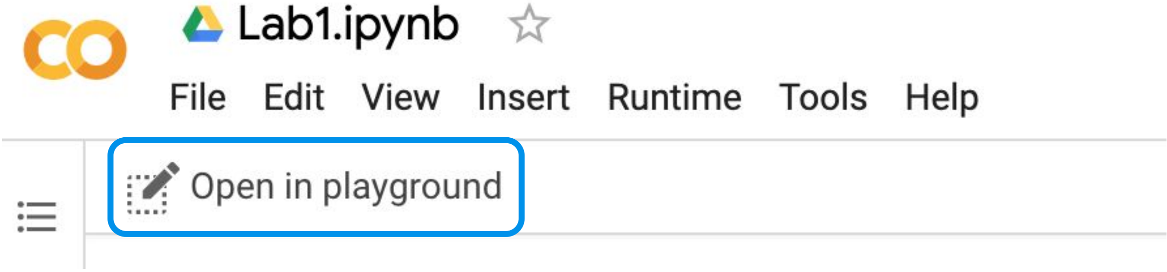
  - Output layer with 10 units (one for each possible digit) and the **softmax activation function** (this produces a vector of length 10, where each element is a probability between 0 and 1 of the image being classified as that digit)
  - Example: [0, 0.3, 0, 0, 0, 0, 0, 0.7, 0, 0] - the highest probability corresponds to a label of 7, so the network would classify this image as a 7

  - **rmsprop optimization algorithm**
  - **categorical_crossentropy loss function**
  - **accuracy performance measure** (the proportion of times the correct class is chosen)

# MNIST Data Example

[Colab link]

Step 1




Step 2