Details of Training

Neural Nets

What next?

- Given an example (or group of examples), we know how to compute the derivative for each weight.
- How exactly do we update the weights?
- How often? (after each training data point? after all the training data points?)

What next? – Gradient Descent

- W_new = W_old - lr * derivative

- Classical approach – get derivative for entire data set, then take a step in that direction

- Pros: Each step is informed by all the data
- Cons: Very slow, especially as data gets big

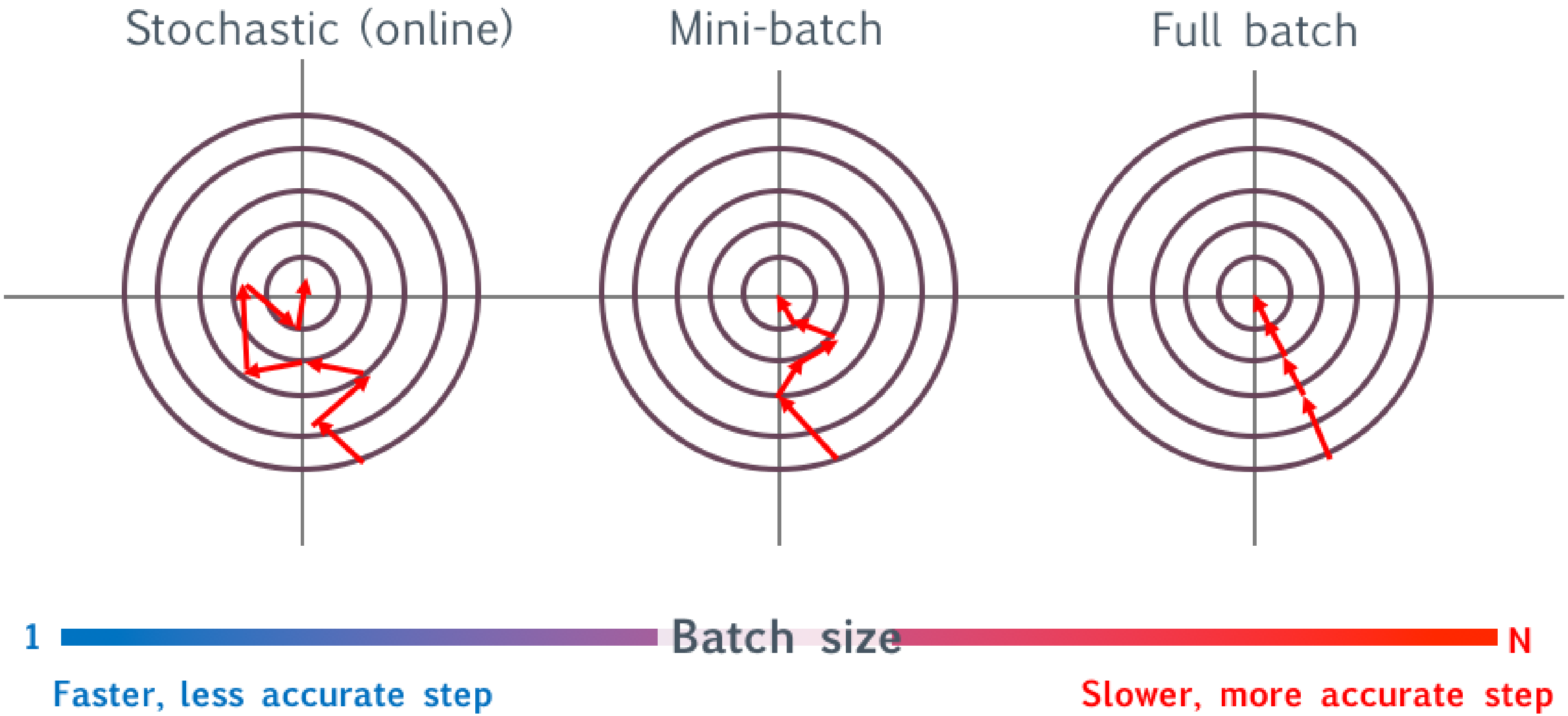
Another approach: Stochastic Gradient Descent

- Get derivative for just one point, and take a step in that direction
- Steps are “less informed” but you take more of them
- Should “balance out”
- Probably want a smaller step size
- Also helps “regularize”

Compromise approach: Mini-batch

- Get derivative for a ”small” set of points, then take a step in that direction
- Typical mini batch sizes are 16, 32
- Strikes a balance between two extremes

Comparison of Batching Approaches



Batching Terminology

- Full-batch: Use entire data set to compute gradient before updating
- Mini-batch: Use a smaller portion of data (but more than single example) to compute gradient before updating
- Stochastic Gradient Descent (SGD): Use a single example to compute gradient before updating (though sometimes people use SGD to refer to minibatch, also)

Batching Terminology

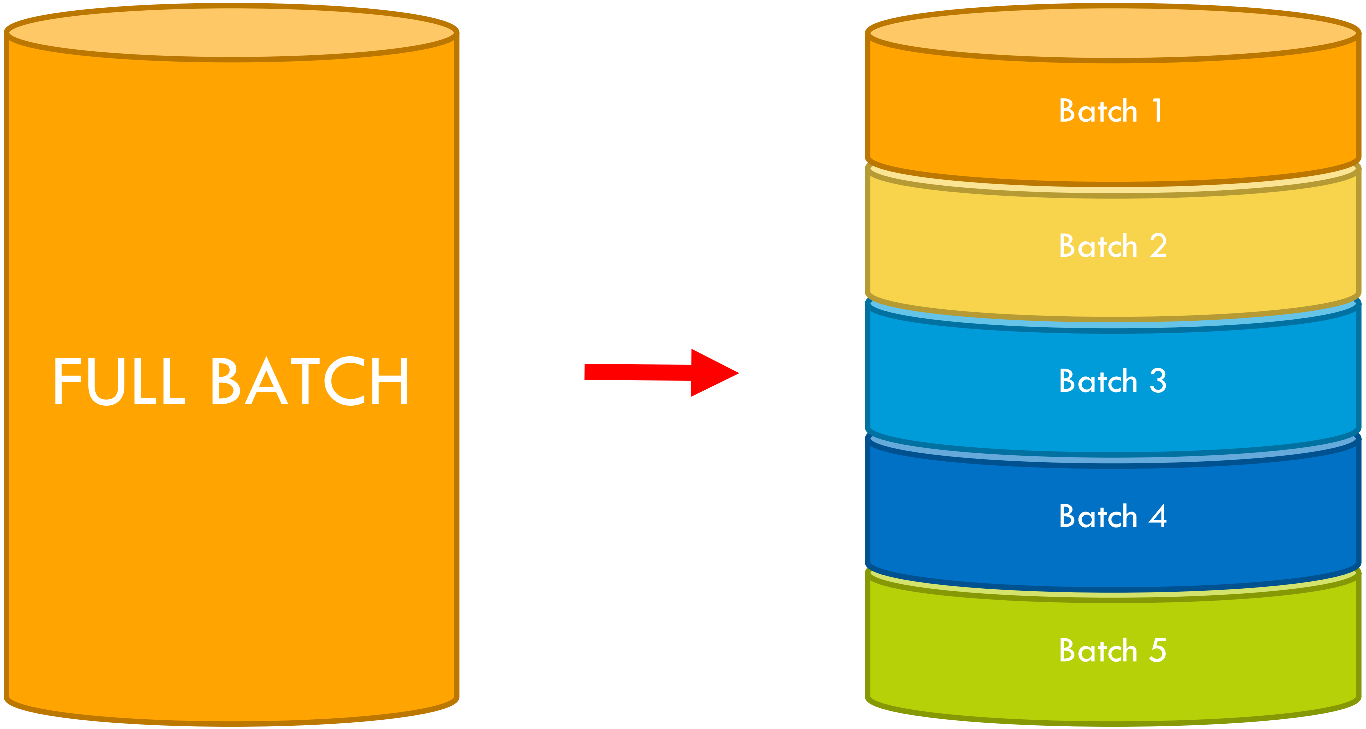
- An Epoch refers to a single pass through all of the training data.
- In full batch gradient descent, there would be one step taken per epoch.
- In SGD / Online learning, there would be n steps taken per epoch (n = training set size)
- In Minibatch there would be (n/batch size) steps taken per epoch
- When training, it is common to refer to the number of epochs needed for the model to be “trained”.

Note on Data Shuffling

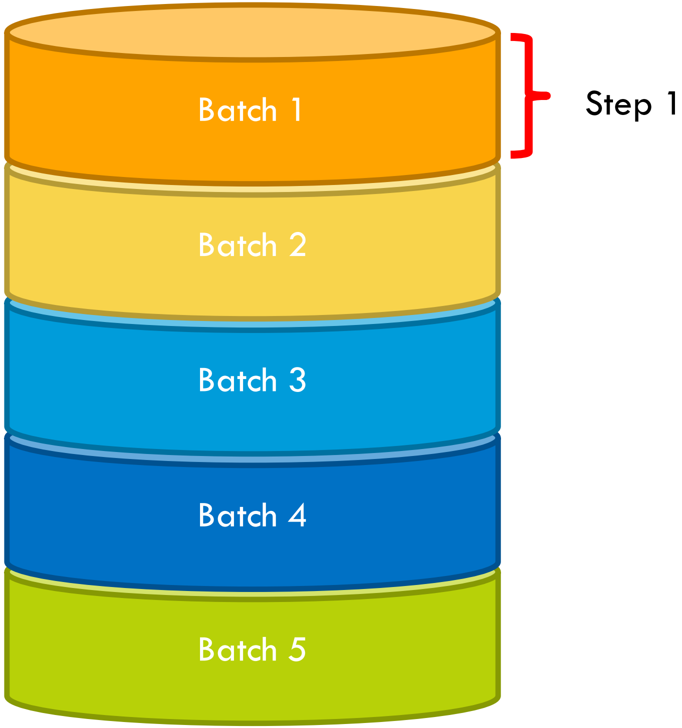
- To avoid any cyclical movement and aid convergence, it is recommended to shuffle the data after each epoch.

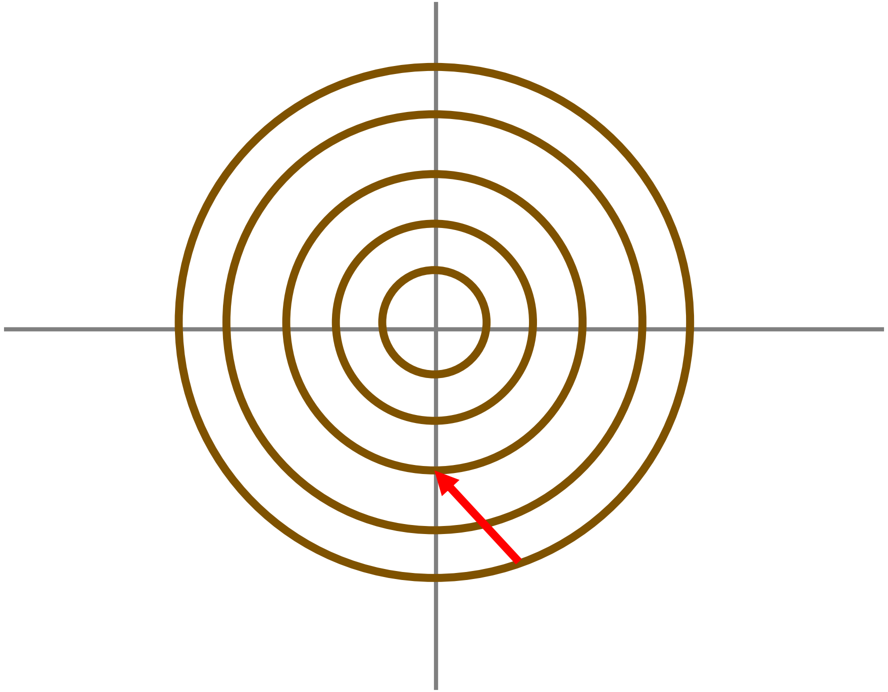
- This way, the data is not seen in the same order every time, and the batches are not the exact same ones.

Feedforward Neural Network



Training in Action





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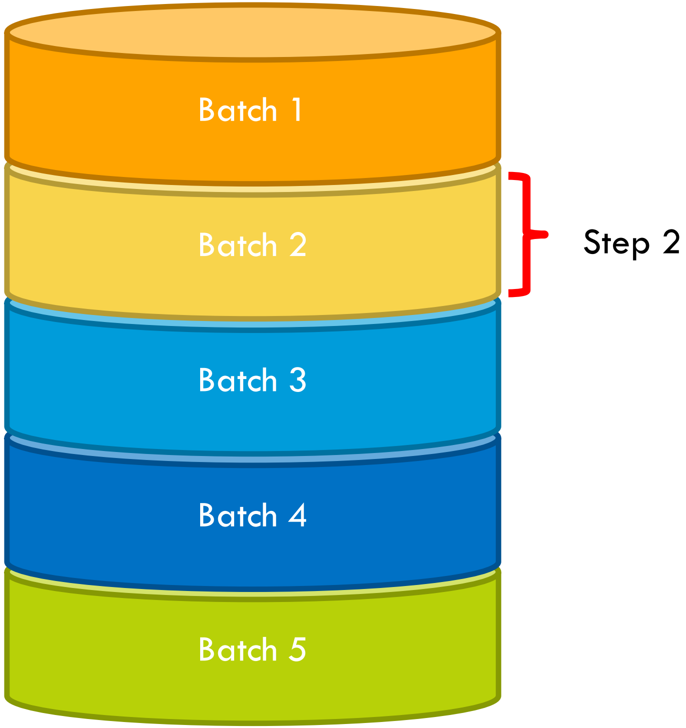

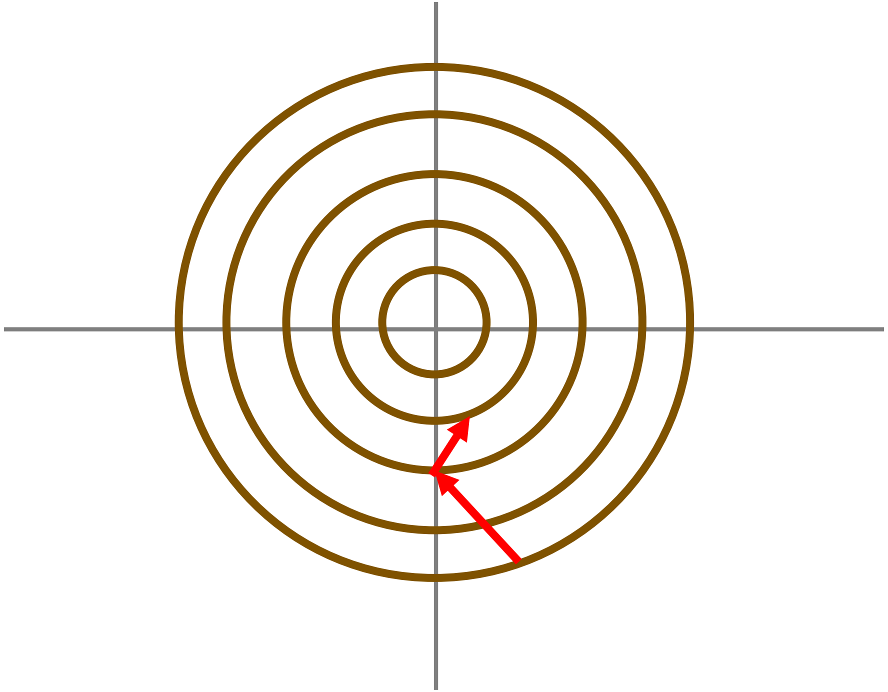

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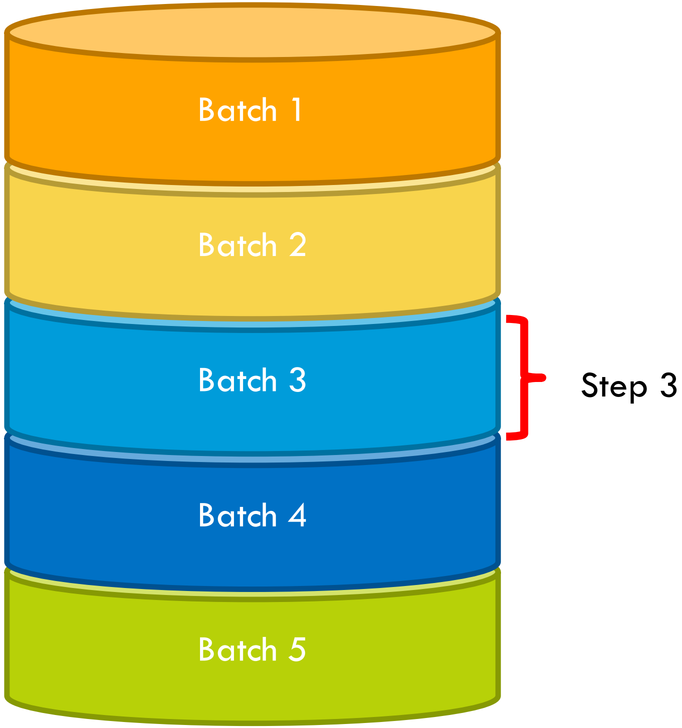
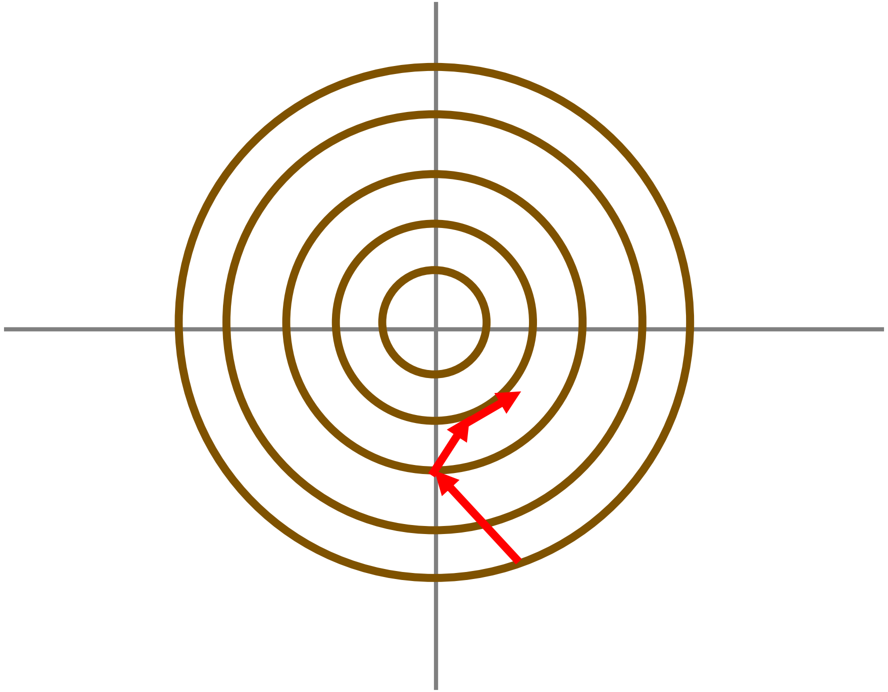
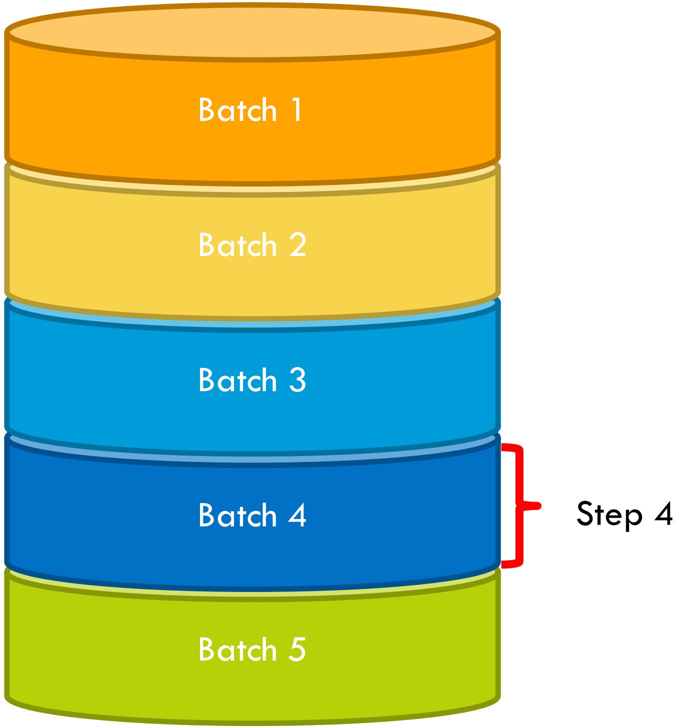
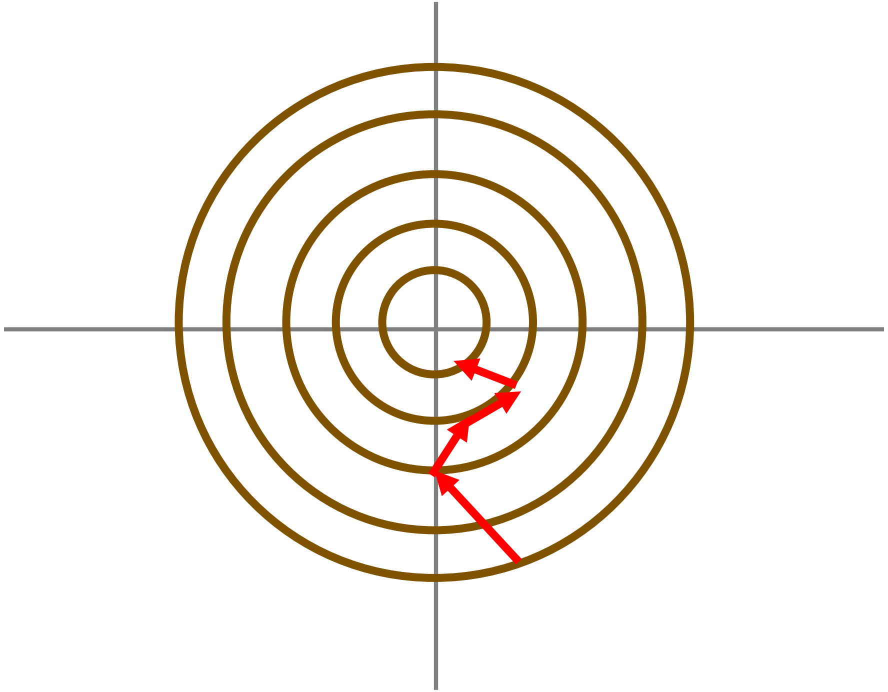




Training in Action





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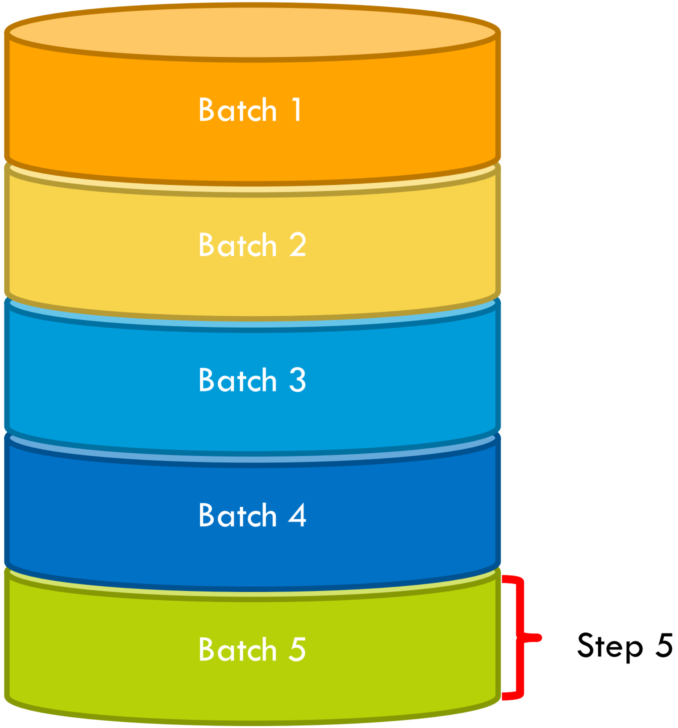

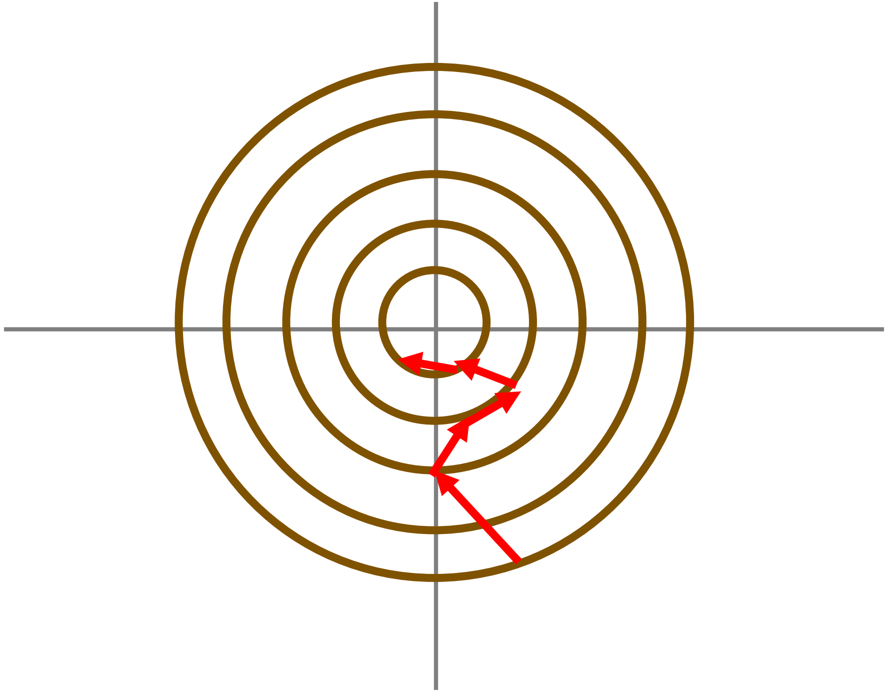

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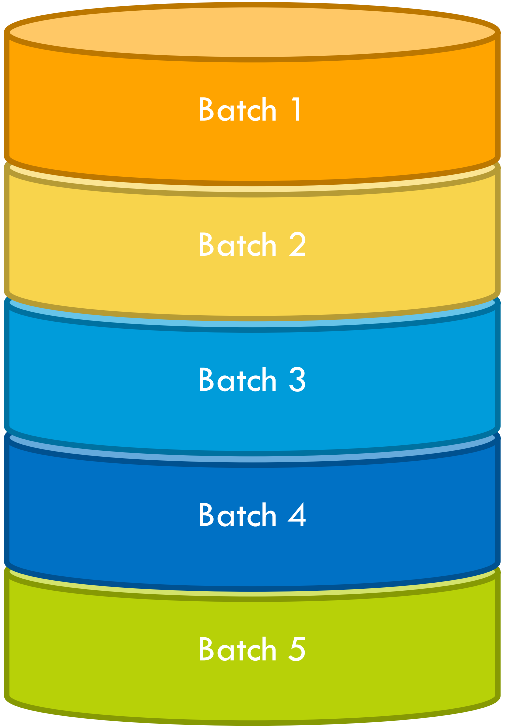
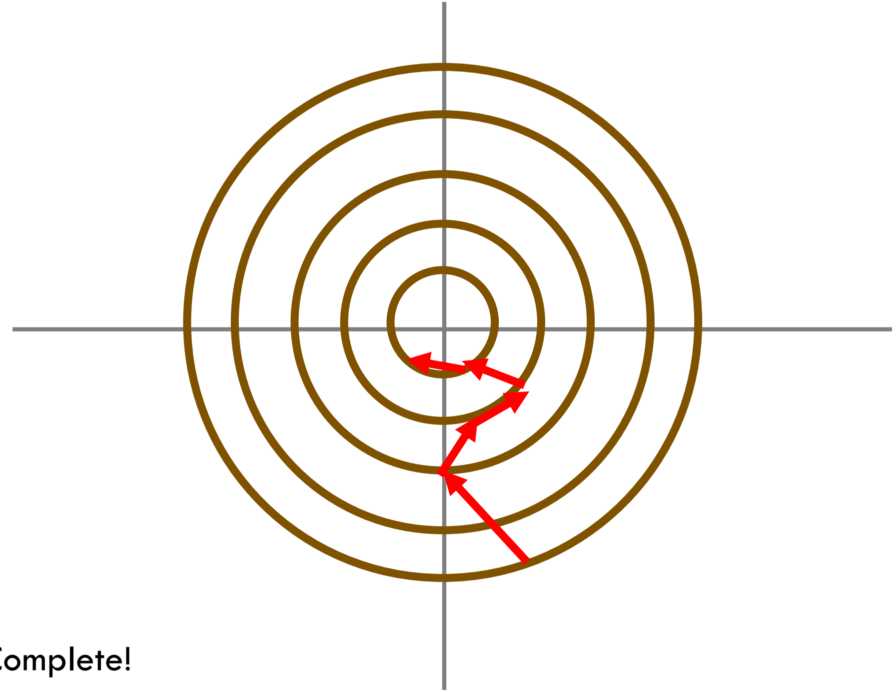
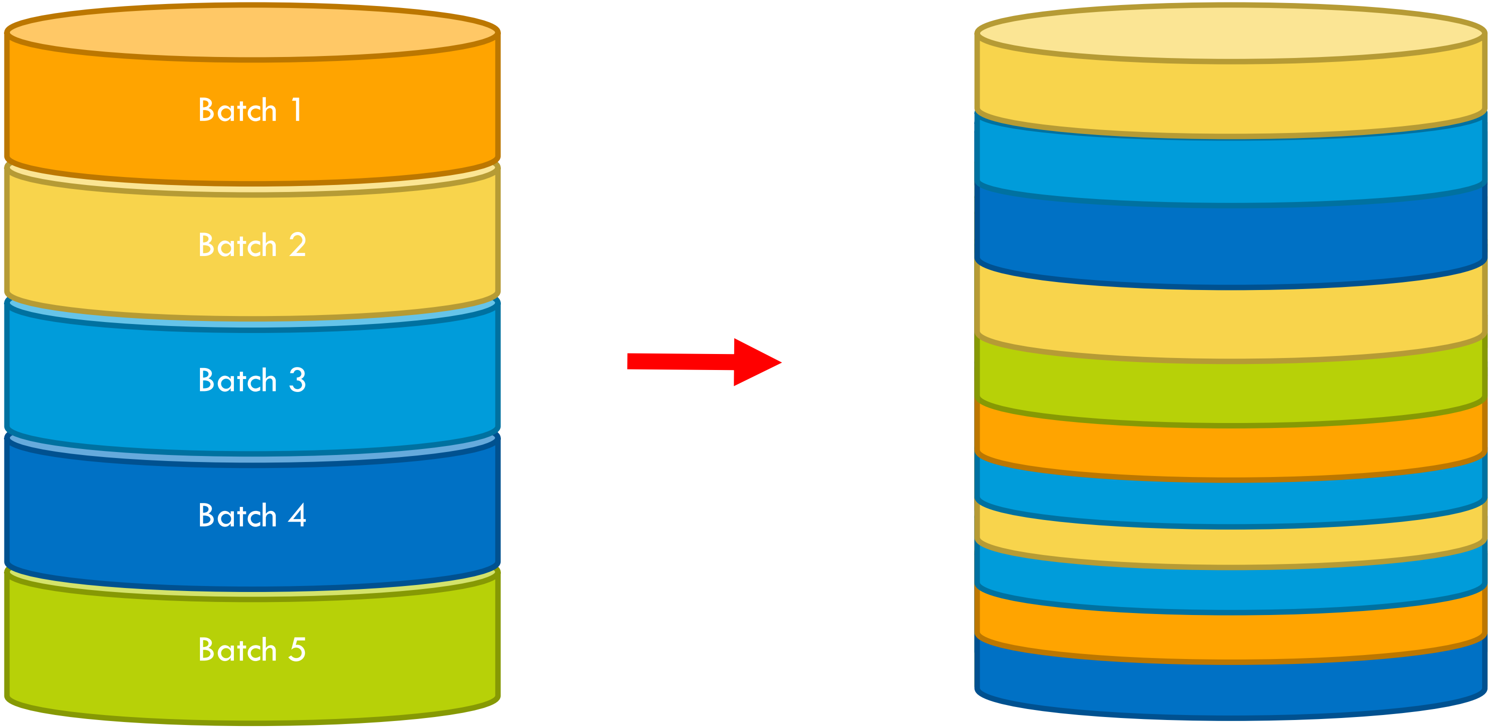


First Epoch Complete!



Shuffle the Data!



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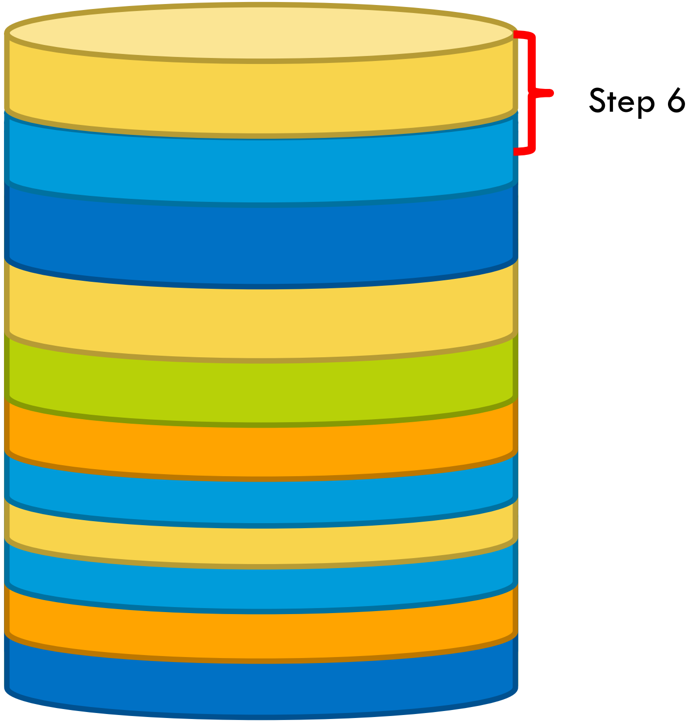
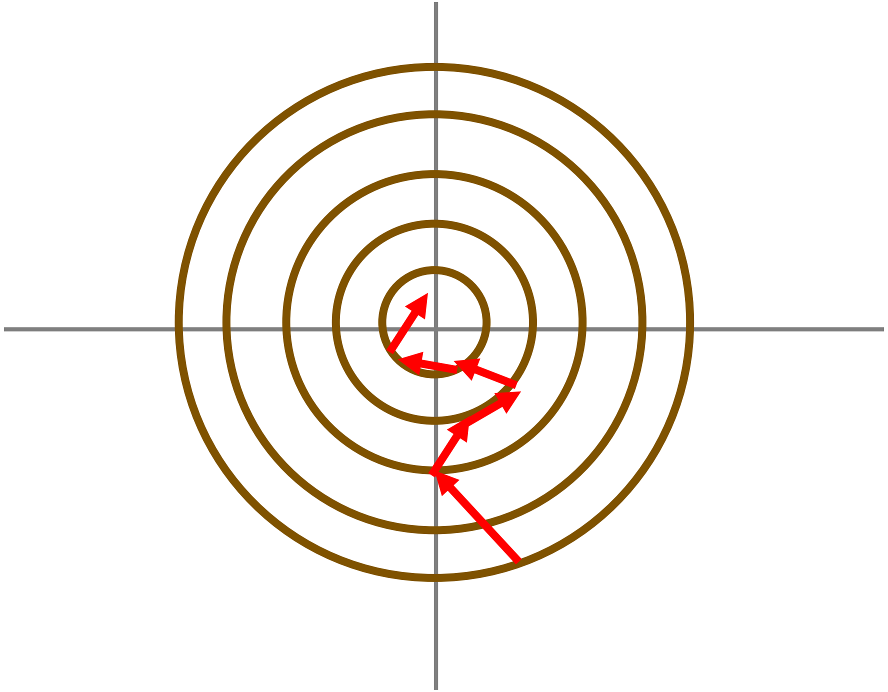




The Keras Package

- Keras allows easy construction, training, and execution of Deep Neural Networks
- Written in Python, and allows users to configure complicated models directly in Python
- Uses either Tensorflow or Theano “under the hood”
- Uses either CPU or GPU for computation
- Uses numpy data structures, and a similar command structure to scikit-learn (model.fit , model.predict, etc.)

Typical Command Structure in Keras

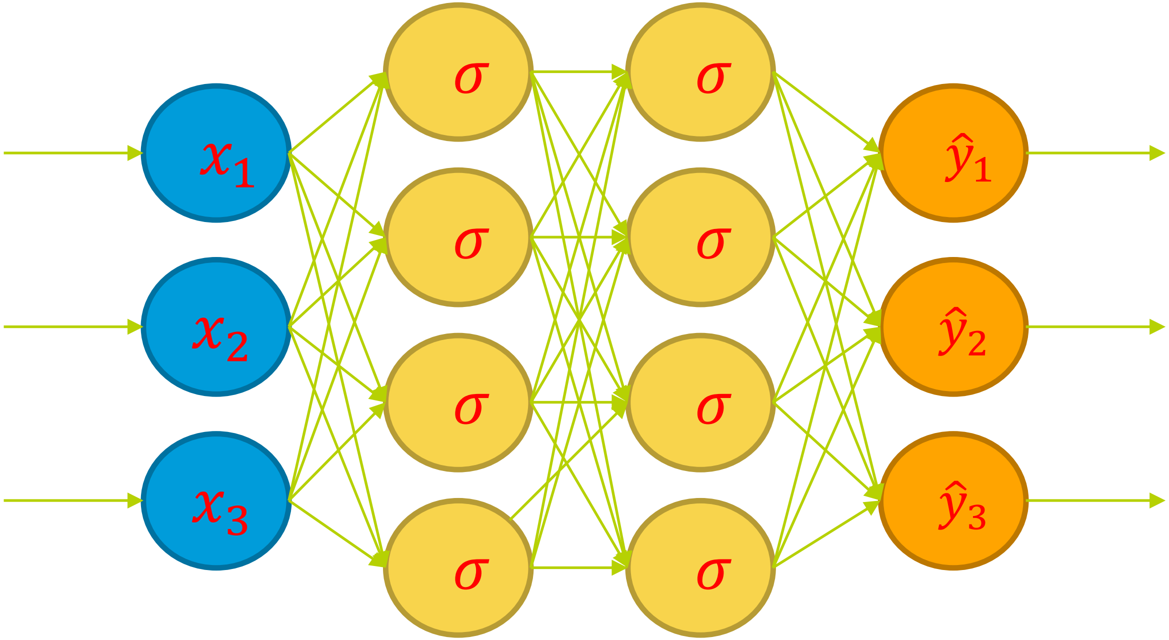
- Build the structure of your network.
- Compile the model, specifying your loss function, metrics, and optimizer (which includes the learning rate).
- Fit the model on your training data (specifying batch size, number of epochs)
- Predict on new data
- Evaluate your results

Building the model

- Keras provides two approaches to building the structure of your model:
- Sequential Model: allows a linear stack of layers – simpler and more convenient if model has this form
- Functional API: more detailed and complex, but allows more complicated architectures
- We will focus on the Sequential Model.

Running Example, this time in Keras

Let's build this Neural Network structure shown below in Keras:



Keras - Sequential Model

First, import the Sequential function and initialize your model object:

```
from keras.models import Sequential
model = Sequential()
```

Keras - Sequential Model

Then we add layers to the model one by one.

```
from keras.layers import Dense, Activation

# For the first layer, specify the input dimension
model.add(Dense(units=4, input_dim=3))

# Specify an activation function
model.add(Activation(sigmoid'))

# For subsequent layers, the input dimension is presumed from
# the previous layer
model.add(Dense(units=4))
model.add(Activation(sigmoid'))
model.add(Dense(units=3))
model.add(Activation('softmax'))
```

Multiclass Classification with Neural Networks

- For binary classification problems, we have a final layer with a single node and a sigmoid activation.
- This has many desirable properties
  - Gives an output strictly between 0 and 1
  - Can be interpreted as a probability
  - Derivative is “nice”
  - Analogous to logistic regression
- Is there a natural extension of this to a multiclass setting?

Multiclass Classification with Neural Networks

- Reminder: one hot encoding for categories
- Take a vector with length equal to the number of categories
- Represent each category with one at a particular position (and zero everywhere else)

$$\begin{bmatrix}1\\0\\0\end{bmatrix} \qquad \begin{bmatrix}0\\1\\0\end{bmatrix} \qquad \begin{bmatrix}0\\0\\1\end{bmatrix}$$

Cat Dog Toaster

Multiclass Classification with Neural Networks

- For multiclass classification problems, let the final layer be a vector with length equal to the number of possible classes.
- Extension of sigmoid to multiclass is the softmax function.
- $softmax(z_i) = \frac{e^{z_i}}{\sum_{k=1}^{K} e^{z_k}}$
- Yields a vector with entries that are between 0 and 1, and sum to 1

Multiclass Classification with Neural Networks

- For loss function use “categorical cross entropy”
- This is just the log-loss function in disguise

$$C.E. = -\sum_{i=1}^{n} y_i \log(\hat{y}_i)$$

- Derivative has a nice property when used with softmax

$$\frac{\partial C.E.}{\partial softmax} \cdot \frac{\partial softmax}{\partial z_i} = \hat{y}_i - y_i$$

Ways to scale inputs

- Linear scaling to the interval [0,1]

$$x_i = \frac{x_i - x_{min}}{x_{max} - x_{min}}$$

- Linear scaling to the interval [-1,1]

$$x_i = 2\left(\frac{x_i - \bar{x}}{x_{max} - x_{min}}\right) - 1$$

Ways to scale inputs

- Standardization (making variable approx. std. normal)

$$x_i = \frac{x_i - \bar{x}}{\sigma}; \qquad \sigma = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2}$$