INTRODUCTION

To Data Science

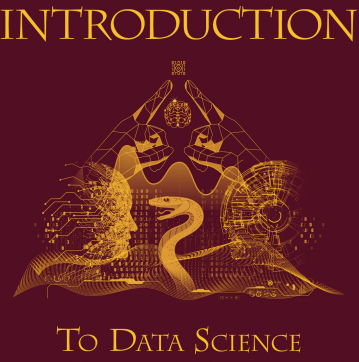
Demystifying Neural Networks

Intro to Data Science - Class 12

Giora Simchoni

gsimchoni@gmail.com and add #intro2ds in subject

Stat. and OR Department, TAU



Logistic Regression with Gradient Descent

INTRODUCTION

To Data Science

Reminder: Logistic Regression (I)

- Observe n pairs (x_i, y_i) $(i = 1, \ldots, n)$
- $y_i \in \{0, 1\}$ binary outcomes
- $x_i \in \mathbb{R}^q$ numeric predictors
- Model: $Y_i|X_i \sim Bernoulli(p_i)$, so: $E(Y_i|X_i = x_i) = P(Y_i = 1|X_i = x_i) = p_i$
- Choose some *link function* g and model *this* transformation of $E(Y_i|X_i = x_i)$
- Typically for this case g is the logit function:
  $g(E(Y_i|X_i = x_i)) = \text{logit}(p_i) = \log(\frac{p_i}{1-p_i}) = x_i'\beta$
- β a vector of q params

Reminder: Logistic Regression (II)

- And so we can write:
  $E(Y_i|X_i = x_i) = P(Y_i = 1|X_i = x_i; \beta) = p_i = g^{-1}(x_i\beta) = \frac{1}{1+e^{-x_i\beta}}$

- Once we get our estimate $\hat{\beta}$:

1. We could "explain" Y_i, the size and direction of each component of $\hat{\beta}$ indicating the contribution of that predictor to the *log-odds* of Y_i being 1
2. We could "predict" probability of new observation x_i having $Y_i = 1$ by fitting a probability $\hat{p}_i = \frac{1}{1+e^{-x_i\hat{\beta}}}$, where typically if $\hat{p}_i > 0.5$, or $x_i\hat{\beta} > 0$, we predict $\hat{Y}_i = 1$

Maximum Likelihood

- Under the standard Maximum Likelihood approach we assume Y_i are also *independent* and so their joint "likelihood" is:
  $L(\beta|X,y) = \prod_{i=1}^{n} P(Y_i|X;\beta) = \prod_{i=1}^{n} P(Y_i = 1|X;\beta)^{y_i} P(Y_i = 0|X;\beta)^{1-y_i}$
- But what is $P(Y_i = 1|X;\beta)$?
  $L(\beta|X,y) = \prod_{i=1}^{n} [g^{-1}(x_i\beta)]^{y_i} [1 - g^{-1}(x_i\beta)]^{1-y_i}$
- The $\hat{\beta}$ we choose is the vector maximizing $L(\beta|X,y)$

Maximum Likelihood (II)

- Take the log-likelihood which is easier to differentiate:
  $l(\beta|X,y) = \sum_{i=1}^{n} \ln P(Y_i|X;\beta) =$
  $\sum_{i=1}^{n} y_i \ln[g^{-1}(x_i\beta)] + (1-y_i)\ln[1-g^{-1}(x_i\beta)] =$
- This looks Ok but let us improve a bit just for easier differentiation:
  $\sum_{i=1}^{n} \ln[1-g^{-1}(x_i\beta)] + y_i \ln[\frac{g^{-1}(x_i\beta)}{1-g^{-1}(x_i\beta)}] = \sum_{i=1}^{n} -\ln[1+e^{x_i\beta}] + y_i x_i \beta$

Maximum Likelihood (III)

- Differentiate:
  $\frac{\partial l(\beta|X,y)}{\partial \beta_j} = \sum_{i=1}^{n} -\frac{1}{1+e^{x_i\beta}} e^{x_i\beta} x_{ij} + y_i x_{ij} = \sum_{i=1}^{n} x_{ij}(y_i - g^{-1}(x_i\beta))$
- Or in vector notation:
  $\frac{\partial l(\beta|X,y)}{\partial \beta} = X'(y - g^{-1}(X\beta))$, where X is the $n \times q$ data matrix.
- We would like to equate this with $\vec{0}$ and get $\hat{\beta}$ but there's no closed solution.
- At which point usually the Newton-Raphson method comes to the rescue.
- But let's look at simple gradient descent:

Gradient Descent

- Instead of maximizing log-likelihood, let's minimize negative log-likelihood $-l(\beta)$ (NLL)
- We'll start with an initial guess $\hat{\beta}_{t=0}$
- The partial derivatives vector of $-l(\beta)$ at point $\hat{\beta}_t$ (a.k.a the *gradient* $-\nabla l(\hat{\beta}_t)$) points to the direction of where $-l(\beta)$ has its steepest descent
- We'll go a small α step down that direction: $\hat{\beta}_{t+1} = \hat{\beta}_t - \alpha \cdot [-\nabla l(\hat{\beta}_t)]$
- We do this for I iterations or until some stopping rule indicating $\hat{\beta}$ has converged

Let's see that it works ! 😀

```
import numpy as np

n = 1000
q = 2
X = np.random.normal(size = n * q).reshape((n, q))
beta = [1.0, 2.0]
p = 1 / (1 + np.exp(-np.dot(X, beta)))
y = np.random.binomial(1, p, size = n)
```

See it in python!

You've already been Neural Network-ing!

INTRODUCTION

TO DATA SCIENCE

Call it a Neural Network

1. Call our $-l(\beta)$ “Cross Entropy”
2. Call $g^{-1}(X\beta)$ the “Sigmoid Function”
3. Call computing $\hat{p}_i$ and $-l(\hat{\beta})$ a “Forward Propagation” or “Feed Forward” step
4. Call the differentiation of $-l(\hat{\beta})$ a “Backward Propagation” step
5. Call our β vector $W_{(q+1)\text{x}1}$, a weight matrix (add intercept, call it “bias”)
6. Add *stochastic* gradient descent (SGD)
7. Draw a diagram with circles and arrows, call these “neurons”

And you have a Neural Network*.

*Ok, We’ll add some stuff later

Cross Entropy

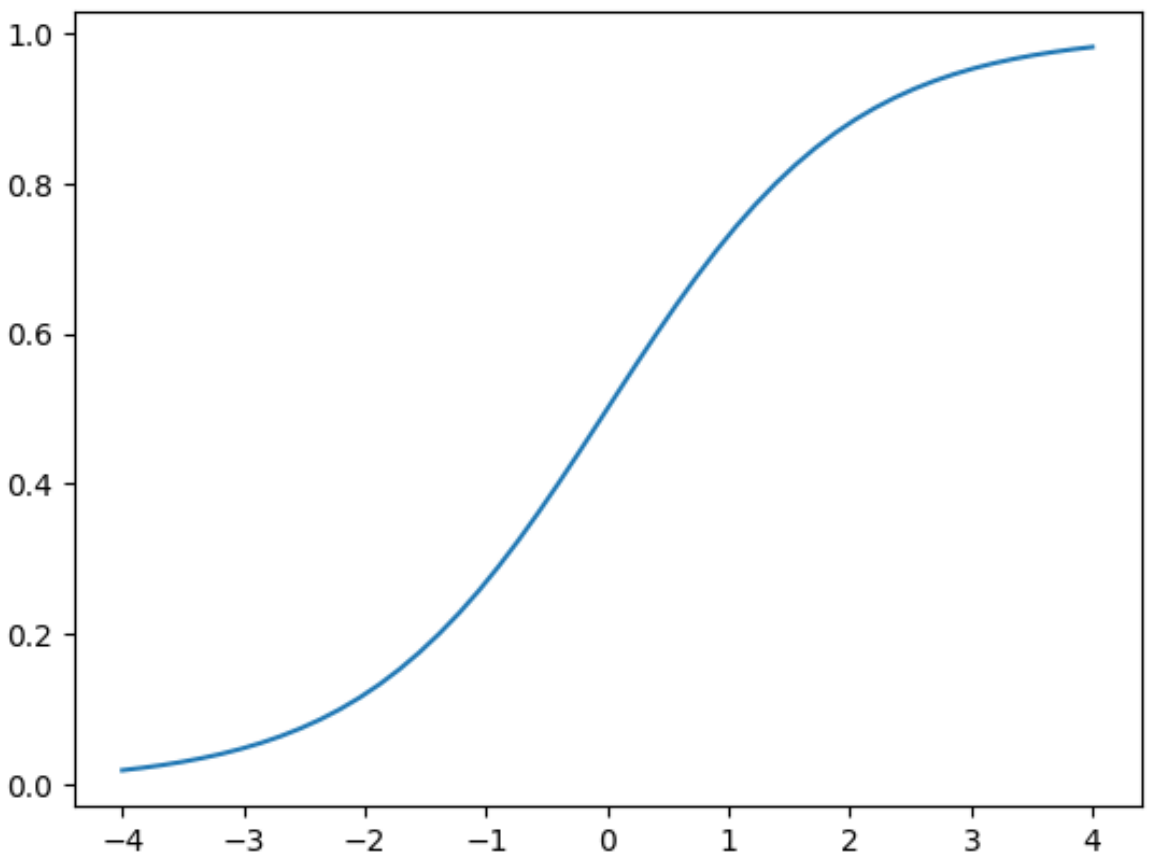
- For discrete probability distributions $P(X)$ and $Q(X)$ with the same support $x \in \mathcal{X}$ Cross Entropy could be seen as a metric of the "distance" between distributions:
  $H(P, Q) = -E_P[\log(Q)] = -\sum_{x \in \mathcal{X}} P(X = x) \log[Q(X = x)]$
- In case X has two categories, and $p_1 = P(X = x_1), p_2 = 1 - p_1$ and same for q_1, q_2:
  $H(P, Q) = -[p_1 \log(q_1) + (1 - p_1) \log(1 - q_1)]$
- If we let $p_1 = y_i$ and $q_1 = \hat{p}_i = g^{-1}(x_i\hat{\beta})$ we get:
  $H(y_i, \hat{p}_i) = -[y_i \log(\hat{p}_i) + (1 - y_i) \log(1 - \hat{p}_i)] =$
  $-[y_i \ln[g^{-1}(x_i\hat{\beta})] + (1 - y_i) \ln[1 - g^{-1}(x_i\hat{\beta})]]$
- Which is exactly the contribution of the $i\text{th}$ observation to the NLL $-l(\hat{\beta})$.

Sigmoid Function

If $g(p)$ is the logit function, its inverse would be the sigmoid function:

$$g(p) = logit(p) = \log(\frac{p}{1-p}); \;\; g^{-1}(z) = \sigma(z) = \frac{1}{1+e^{-z}}$$

So: $g^{-1}(g(p)) = \sigma(logit(p)) = p$



Forward/Backward Propagation

Recall that each iteration of gradient descent included:

1. Forward step: Calculating the NLL loss $-l(\hat{\beta})$
2. Backward step: Calculate the gradient $-\nabla l(\hat{\beta}_t)$
3. Gradient descent: $\hat{\beta}_{t+1} = \hat{\beta}_t - \alpha \cdot [-\nabla l(\hat{\beta}_t)]$

```
# forward step
p_hat = 1 / (1 + np.exp(-np.dot(X, beta_hat)))
nll = -np.sum(y * np.log(p_hat) + (1 - y) * np.log(1 - p_hat))
# backward step
grad = -np.dot(X.T, (y - p_hat))
# descent
beta_hat = beta_hat - alpha * grad
```

Why “Forward”, why “Backward”?…

Reminder: Chain Rule

In our case differentiating $l(\beta)$ analytically was manageable.

- As the NN architecture becomes more complex there is need to generalize this, and break down the derivative into (backward) steps.
- Recall that according to the Chain Rule, if $y = y(x) = f(g(h(x)))$ then: $y'(x) = f'(g(h(x)) \cdot g'(h(x)) \cdot h'(x)$
- Or if you prefer, if $z = z(x);\ u = u(z);\ y = y(u)$ then: $\frac{dy}{dx} = \frac{dy}{du} \cdot \frac{du}{dz} \cdot \frac{dz}{dx}$

Let's re-write $-l(\beta)$ as a composite function:

- Multiplying β by x_i will be $z_i = z(\beta) = x_i\beta$
- Applying the sigmoid g^{-1} will be $p_i = g^{-1}(z_i) = \frac{1}{1+e^{-z_i}}$
- Calculating the (minus) Cross Entropy will be:
  $l_i = l(p_i) = y_i \ln(p_i) + (1 - y_i) \ln(1 - p_i)$
- So one element of $-l(\beta)$ will be: $l_i(p_i(z_i(\beta)))$

Hence, Forward.

Now $-l(\beta)$ is the sum of (minus) cross entropies: $-l(\beta) = -\sum_i l_i(p_i(z_i(\beta)))$

And we could differentiate using the chain rule like so:

$$-\frac{\partial l(\beta)}{\partial \beta_j} = -\sum_i \frac{\partial l_i}{\partial p_i} \cdot \frac{\partial p_i}{\partial z_i} \cdot \frac{\partial z_i}{\partial \beta_j}$$

Hence, Backward.

Each of these is simpler to calculate:

$$\frac{\partial l_i}{\partial p_i} = \frac{y_i - p_i}{p_i(1-p_i)}$$

$$\frac{\partial p_i}{\partial z_i} = p_i(1-p_i)$$

$$\frac{\partial z_i}{\partial \beta_j} = x_{ij}$$

And so:

$$-\frac{\partial l(\beta)}{\partial \beta_j} = -\sum_i \frac{y_i - p_i}{p_i(1-p_i)} \cdot p_i(1-p_i) \cdot x_{ij}$$

Which is excatly what we got analytically but now we can write our gradient descent iteration as a list of forward/backward steps.

Implementing NN in python

```
def forward(X, y, beta_hat):
  z = np.dot(X, beta_hat)
  p_hat = 1 / (1 + np.exp(-z))
  l = y * np.log(p_hat) + (1 - y) * np.log(1 - p_hat)
  nll = -np.sum(l)
  return p_hat, nll

def backward(X, y, p_hat):
  dldz = y - p_hat
  dzdb = X.T
  grad = -np.dot(dzdb, dldz)
  return grad

def gradient_descent(alpha, beta_hat, grad):
  return beta_hat - alpha * grad

def optimize(X, y, alpha, beta_hat):
  p_hat, l = forward(X, y, beta_hat)
  grad = backward(X, y, p_hat)
  beta_hat = gradient_descent(alpha, beta_hat, grad)
```

```
def lr_nn(X, y, epochs):
  beta_hat = np.array([-2.5, -2.5])
  alpha = 0.001
  for i in range(epochs):
    l, beta_hat = optimize(X, y, alpha, beta_hat)
  return l, beta_hat
```

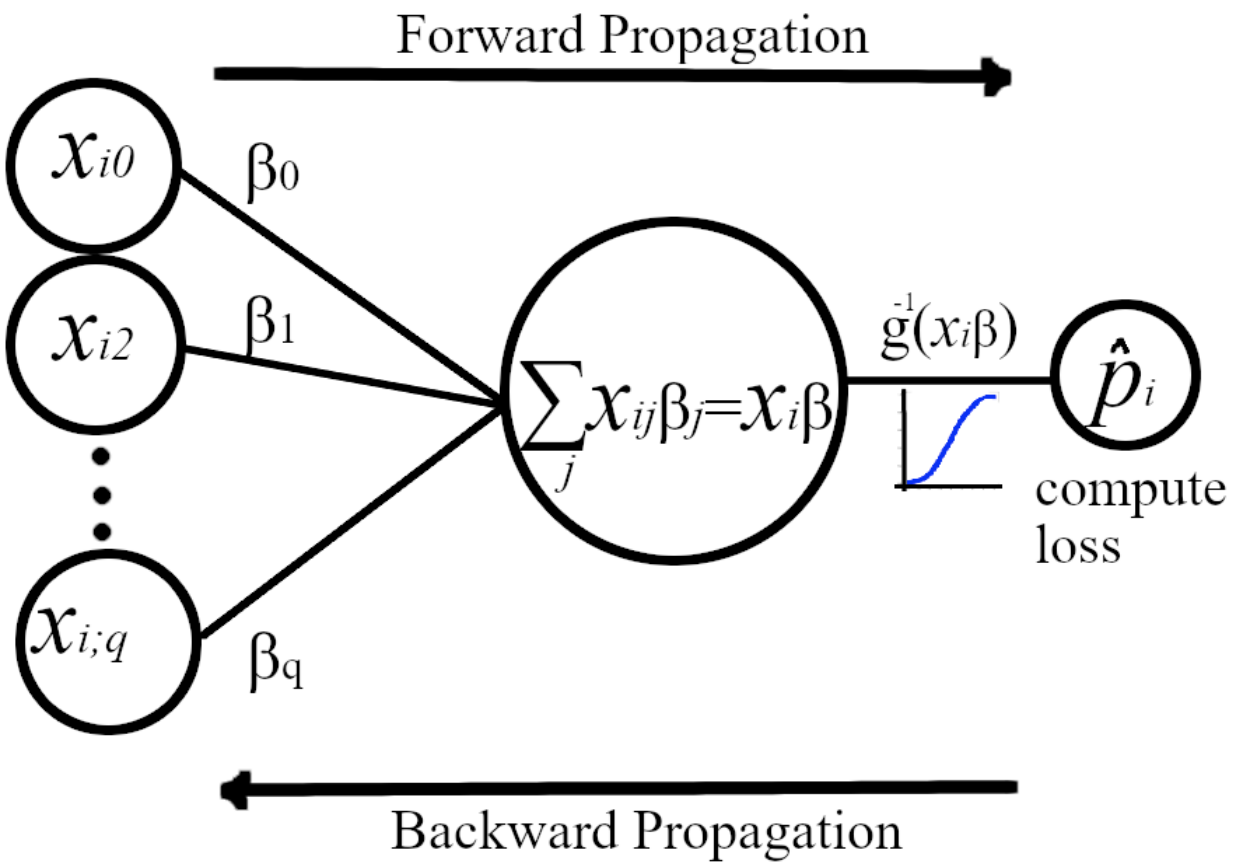
Adding *stochastic* gradient descent (SGD) on mini-batches:

```
def lr_nn(X, y, epochs):
  beta_hat = np.random.rand(X.shape[1])
  alpha = 0.001
  batch_size = 100
  n = X.shape[0]
  steps = int(n / batch_size)
  for i in range(epochs):
    print('epoch %d:' % i)
    permute = np.random.permutation(n)
    X_perm = X[permute, :]
    y_perm = y[permute]
    for j in range(steps):
      start = j * batch_size
      l, beta_hat = optimize(X_perm[start:start + batch_size, :],
                             y_perm[start:start + batch_size],
                             alpha, beta_hat)
      print('Trained on %d/%d, loss = %d' % (start + batch_size, n, l))
  return l, beta_hat

l, beta_hat = lr_nn(X, y, 50)
```

See it in python!

Put it in a Neural Network Diagram

Binary Logistic Regression, is in fact a single neuron firing a sigmoid probability-like number between 0 and 1, for each sample:



LR as NN in Keras

```
 1  from tensorflow.keras import Sequential
 2  from tensorflow.keras.layers import Dense
 3  from tensorflow.keras.optimizers import SGD
 4
 5  model = Sequential()
 6  model.add(Dense(1, input_shape=(X.shape[1], ),
 7    activation='sigmoid', use_bias=False))
 8  sgd = SGD(learning_rate=0.1)
 9  model.compile(loss='binary_crossentropy', optimizer=sgd)
10  model.fit(X, y, batch_size=100, epochs=50)
```

See it in python!

Is that it?

1. No 😃

2. > The knee-jerk response from statisticians was “What’s the big deal? A neural network is just another nonlinear model, not too different from many other generalizations of linear models”. While this may be true, neural networks brought a new energy to the field. They could be scaled up and generalized in a variety of ways… and innovative learning algorithms for massive data sets.”

(*Computer Age Statistical Inference* by Bradley Efron & Trevor Hastie, p. 352)

Add Classes

INTRODUCTION

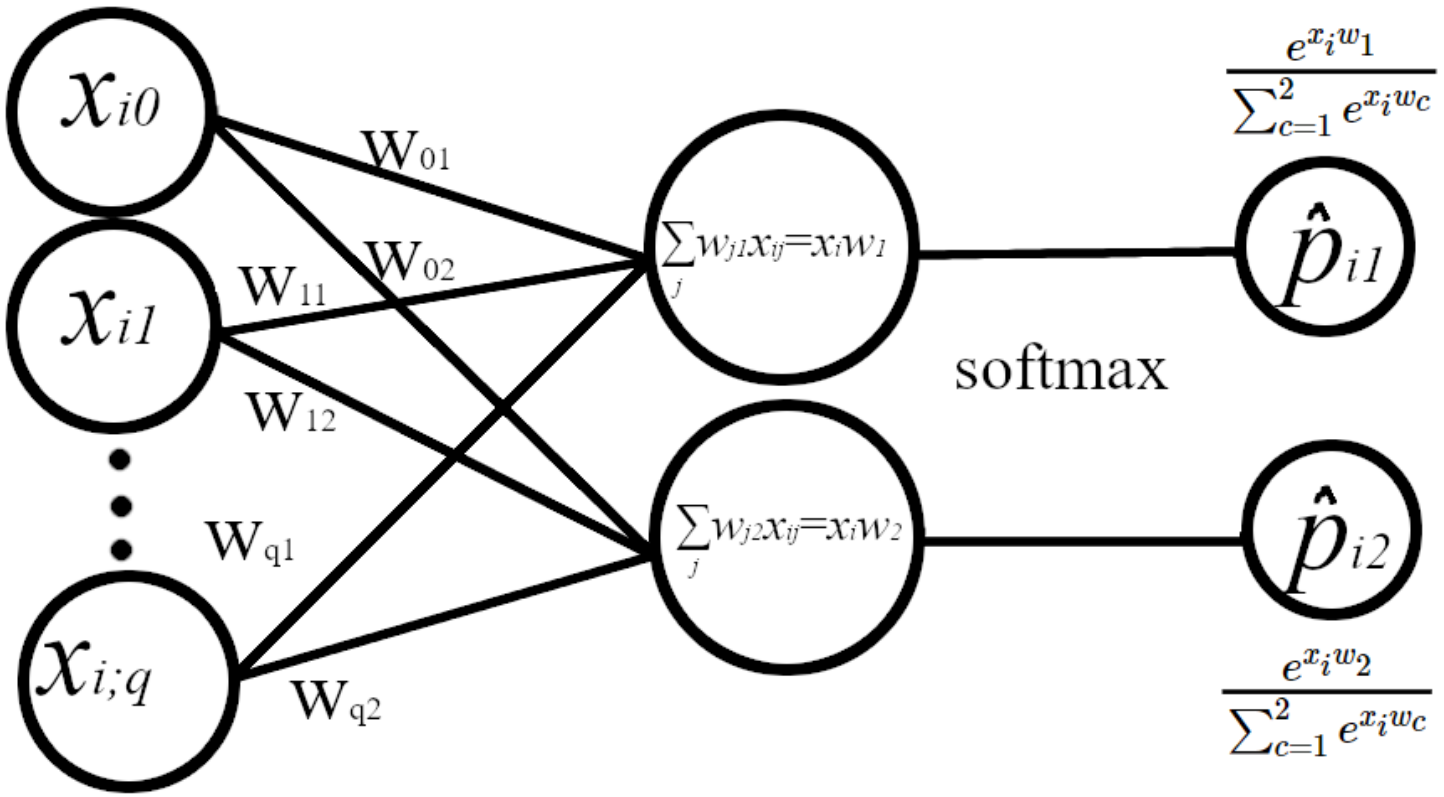
TO DATA SCIENCE

C Neurons for C Classes

- fit a β vector for each class (or let's start talking about W)
- have C neurons for C classes
- where the output layer is the *Softmax Function*, to make sure the fitted $\hat{p}$ sum up to 1:
  $\hat{p}_{i;c} = \text{softmax}(c, W_{(q+1)\text{x}C}, x_i) = \frac{e^{x_i w_c}}{\sum_{c=1}^{C} e^{x_i w_c}}$
  Where x_i is the ith row of X as before and w_c is the cth row of W^T (or cth column of W)

This would be equivalent to *multinomial logistic regression*!

So the architecture for 2 classes would be:



And in Keras we would do:

```
from tensorflow.keras.utils import to_categorical

y_categorical = to_categorical(y)
model = Sequential()
model.add(Dense(2, input_shape=(X.shape[1], ),
  activation='softmax', use_bias=False))
sgd = SGD(learning_rate=0.1)
model.compile(loss='categorical_crossentropy', optimizer=sgd)
model.fit(X, y_categorical, batch_size=100, epochs=50)
```

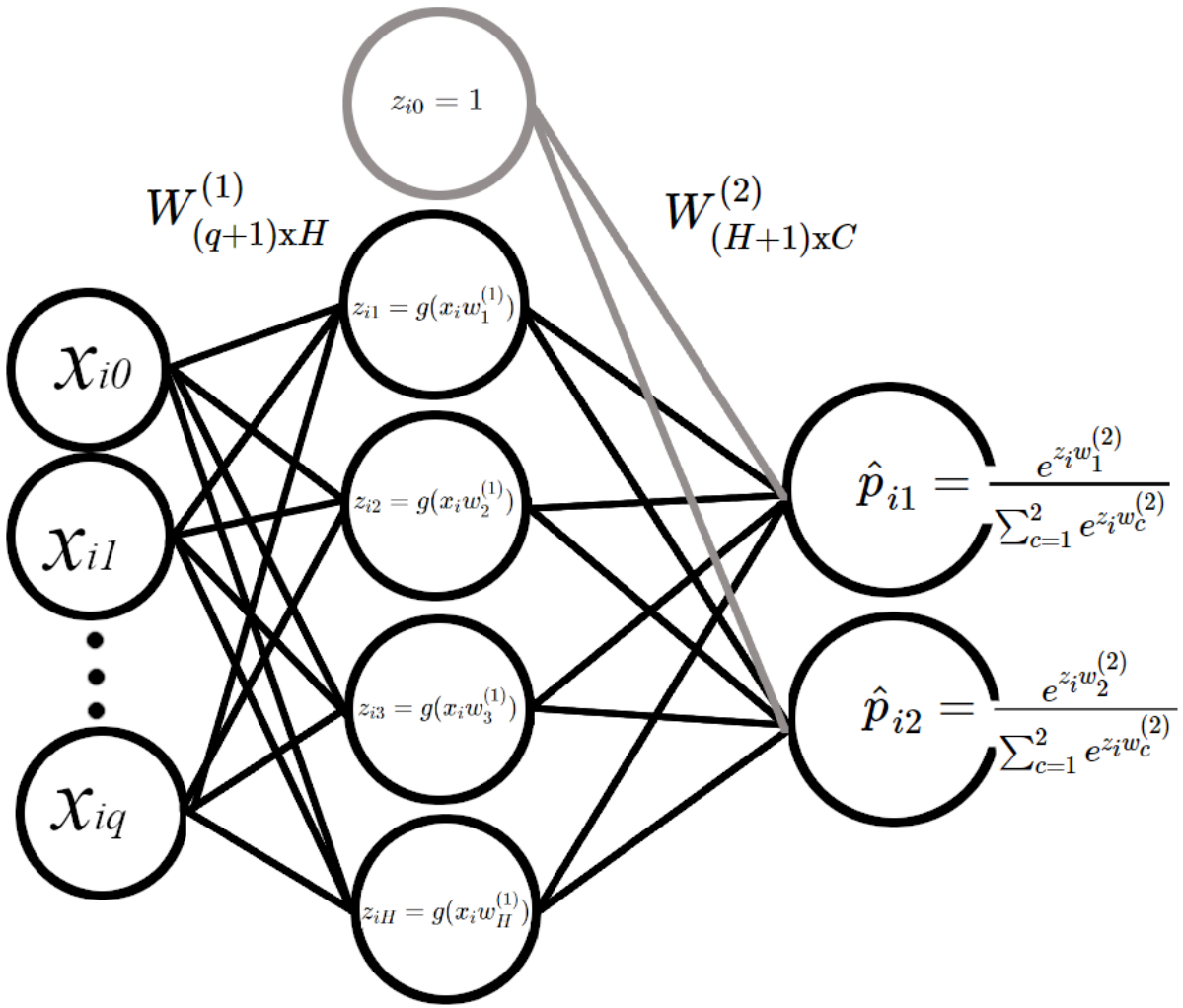
See it in python!

Add Hidden Layers

INTRODUCTION

TO DATA SCIENCE

Adding Hidden Layers



Where $g()$ is some non-linear *activation function*, e.g. sigmoid (but not often used).

- Notice we are not in Logistic Regression land anymore
- The bias term (intercept) is re-instated

```
model = Sequential()
model.add(Dense(4, input_shape=(X.shape[1], ), activation='sigmoid'))
model.add(Dense(2, activation='softmax'))
sgd = SGD(learning_rate=0.1)
model.compile(loss='categorical_crossentropy', optimizer=sgd)
```

This is the MLP (Multi-Layer Perceptron).

Guess how long it's been around.

Even now, the forward step is a simple formula:

$$\hat{p}_{n\times C} = softmax\{[1\vdots\sigma([1\vdots X]W^{(1)})]W^{(2)}\}$$

Call `model.summary()` and see that you can calculate the number of params yourself:

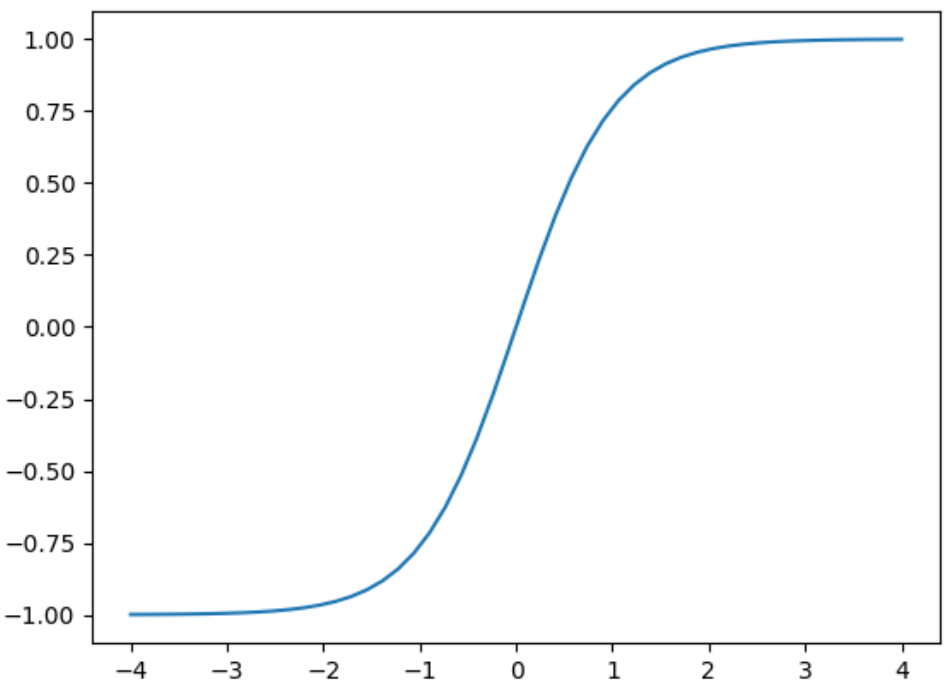
```
model.summary()
```

```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense (Dense)               (None, 4)                 12

 dense_1 (Dense)             (None, 2)                 10

=================================================================
Total params: 22
Trainable params: 22
Non-trainable params: 0
_________________________________________________________________
```

Activation Functions

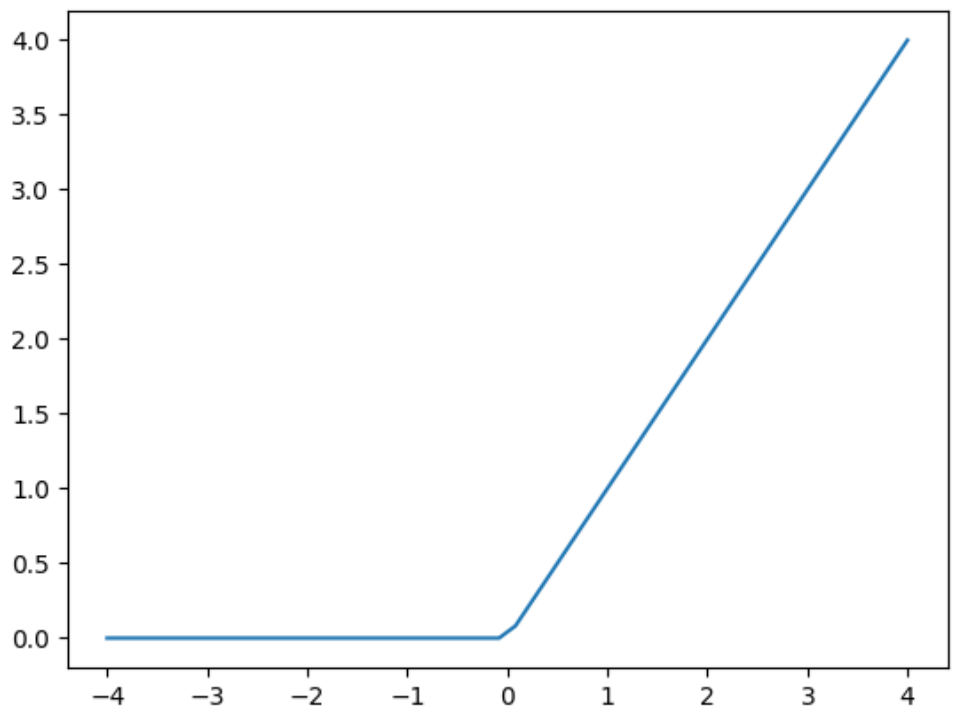
$g(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$

▶ Code



$g(z) = \text{ReLU}(z) = max(z, 0)$

▶ Code



What about linear activations?

See HW.

See it in python!

Add Regularization

INTRODUCTION

TO DATA SCIENCE

L1/L2 Regularization

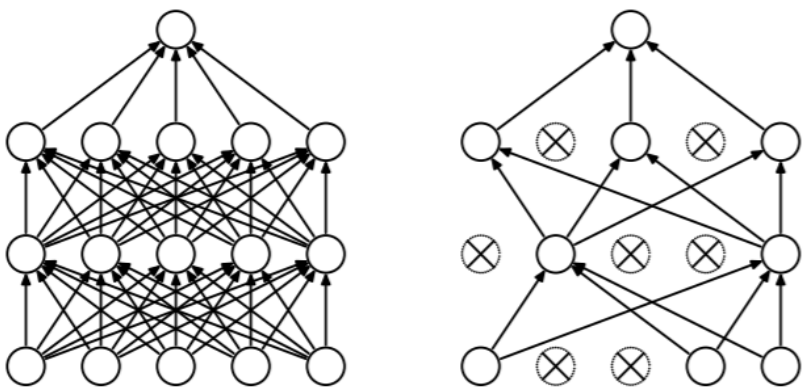
- You might have noticed neural networks intice you to add more and more params.
- Therefore, NN are infamous for overfitting the training data, and some kind of regularization is a must.
- Instead of minimizing some loss L (e.g. Cross Entropy) we add a penalty to the weights: $\min_W L(y, f(X; W)] + P(W)$
- Where $P(W)$ would typically be:
  - $P_{L_2}(W) = \lambda \sum_{ijk} (W_{ij}^{(k)})^2$
  - $P_{L_1}(W) = \lambda \sum_{ijk} |W_{ij}^{(k)}|$
  - or both (a.k.a Elastic Net, but not quite):
    $P_{L1L2}(W) = \lambda_1 \sum_{ijk} (W_{ij}^{(k)})^2 + \lambda_2 \sum_{ijk} |W_{ij}^{(k)}|$

L1/L2 Regularization in Keras:

```
from tensorflow.keras import regularizers

model = Sequential()
model.add(Dense(4, input_shape=(X.shape[1], ), activation='relu',
  kernel_regularizer=regularizers.l1(0.01),
  bias_regularizer=regularizers.l2(0.01)))
model.add(Dense(2, activation='softmax',
  kernel_regularizer=regularizers.l1_l2(l1=0.01, l2=0.01)))
sgd = SGD(learning_rate=0.1)
model.compile(loss='categorical_crossentropy', optimizer=sgd)
model.fit(X, y_categorical, batch_size=100, epochs=50, verbose=0)
```

Dropout

- How to take neurons with a grain of salt?
- During each epoch, individual neurons are either “dropped out” of the net with probability $1 - p$ (i.e. their weight is zero) or kept with probability p, so that a reduced network is left.



(a) Standard Neural Net

(b) After applying dropout.

During prediction no Dropout is performed, but neurons output is scaled by p to make it identical to their expected outputs at training time.

Why does it work?

- You could look at Dropout as an ensemble of neural networks! Each neuron can either count or not at each training step, so after 1K training steps you have virtually trained 1K slightly different models out of 2^N possible (where N is no. of neurons).
- Another explanation uses numerical analysis terms: with each epoch we "break" to randomly look at "close" solutions to the current optimal solution, this is increases our chances of reaching a global optimum
- Dropout in `Keras` (the `rate` parameter is the "fraction of the input units to drop"):

```
1  from tensorflow.keras.layers import Dropout
2
3  model = Sequential()
4  model.add(Dense(4, input_shape=(X.shape[1], ), activation='relu'))
5  model.add(Dropout(0.2))
6  model.add(Dense(2, activation='softmax'))
7  sgd = SGD(learning_rate=0.1)
8  model.compile(loss='categorical_crossentropy', optimizer=sgd)
9  model.fit(X, y_categorical, batch_size=100, epochs=50, verbose=0)
```

Early Stopping

Since NN are trained iteratively and are particularly useful on large datasets it is common to monitor the model performance using an additional validation set, or some of the training set. If you see no improvement in the model's performance (e.g. decrease in loss) for a few epochs - stop training.

```
 1  from tensorflow.keras.callbacks import EarlyStopping
 2
 3  model = Sequential()
 4  model.add(Dense(4, input_shape=(X.shape[1], ), activation='relu'))
 5  model.add(Dropout(0.2))
 6  model.add(Dense(2, activation='softmax'))
 7  sgd = SGD(learning_rate=0.1)
 8  callbacks = [EarlyStopping(monitor='val_loss', patience=5)]
 9  model.compile(loss='categorical_crossentropy', optimizer=sgd)
10
11  model.fit(X, y_categorical, batch_size=100, epochs=50,
12    validation_split=0.2, callbacks=callbacks)
```

Keras

INTRODUCTION

To Data Science

Keras is an API

- Keras is a high-level API “designed for human beings, not machines” developed by François Chollet
- It sits upon a popular DL backends such as Tensorflow, also by Google, and PyTorch by Meta

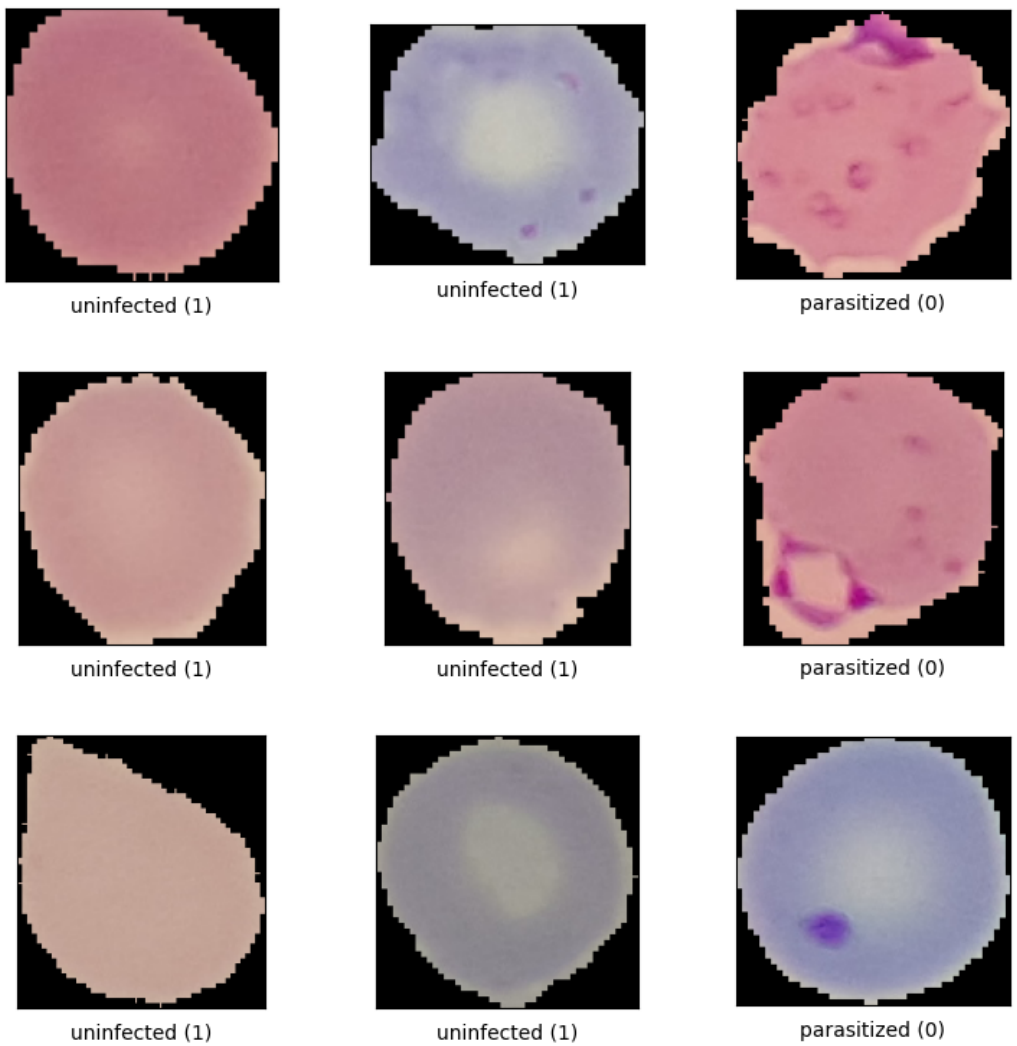
```
import tensorflow as tf
from tensorflow import keras
```

- “ease of use does not come at the cost of reduced flexibility”
- Seamless integration with the Pandasverse

Malaria!

- The Malaria dataset contains over 27K (processed and segmented) cell images with equal instances of parasitized and uninfected cells, from hundreds of patients in Bangaladesh. The images were taken by a mobile application that runs on a standard Android smartphone attached to a conventional light microscope. The goal is “reduce the burden for microscopists in resource-constrained regions and improve diagnostic accuracy”.
- This dataset is part of the `tensorflow_dataset` library which gives you easy access to dozens of varied datasets.
- Here we take only ~10% of the images as a Numpy array and resize them all to 100x100 pixels, for the sake of speed.

```
import tensorflow_datasets as tfds
from skimage.transform import resize

malaria, info = tfds.load('malaria', split='train', with_info=True)
fig = tfds.show_examples(malaria, info)
```



```
 1 from sklearn.model_selection import train_test_split
 2
 3 images = []
 4 labels = []
 5 for example in tfds.as_numpy(malaria):
 6   images.append(resize(example['image'], (100, 100)))
 7   labels.append(example['label'])
 8   if len(images) == 2500:
 9     break
10
11 X = np.array(images)
12 y = np.array(labels)
13
14 X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20, random_st
15
16 X_train = X_train.flatten().reshape((X_train.shape[0], -1))
17 X_test = X_test.flatten().reshape((X_test.shape[0], -1))
18
19 print(X_train.shape)
20 print(X_test.shape)
```

```
(2000, 30000)
(500, 30000)
```

```
from sklearn.linear_model import LogisticRegression

lr = LogisticRegression(penalty='none', max_iter=1000, random_state=42)
lr = lr.fit(X_train, y_train)

test_acc = lr.score(X_test, y_test)
print(f'Test accuracy for LR: {test_acc:.3f}')
```

```
Test accuracy for LR: 0.650
```

The `Sequential` API

```
from tensorflow import keras
from tensorflow.keras import Sequential
from tensorflow.keras.layers import Dense, Dropout

model = Sequential()
model.add(Dense(300, input_shape=(30000,), activation='relu', name='my_dense_layer'))
model.add(Dense(100, activation='relu'))
model.add(Dense(50, activation='relu'))
model.add(Dense(1, activation='sigmoid'))
```

Alternatively we could:

```
model = Sequential([
  Dense(300, input_shape=(30000,), activation='relu'),
  Dense(100, activation='relu'),
  Dense(50, activation='relu'),
  Dense(1, activation='sigmoid')
])
```

Make sure you get these numbers:

```
model.summary()
```

```
Model: "sequential_1"
_________________________________________________________________
 Layer (type)                 Output Shape              Param #
=================================================================
 my_dense_layer (Dense)       (None, 300)               9000300

 dense_2 (Dense)              (None, 100)               30100

 dense_3 (Dense)              (None, 50)                5050

 dense_4 (Dense)              (None, 1)                 51

=================================================================
Total params: 9,035,501
Trainable params: 9,035,501
Non-trainable params: 0
_________________________________________________________________
```

Are you at all worried?

Access layers and their weights:

```
model.layers
```

```
[<keras.layers.core.dense.Dense at 0x1be193375b0>,
 <keras.layers.core.dense.Dense at 0x1be19325fd0>,
 <keras.layers.core.dense.Dense at 0x1be1f660ca0>,
 <keras.layers.core.dense.Dense at 0x1be19337370>]
```

```
model.layers[0].name
```

```
'my_dense_layer'
```

```
W1, b1 = model.get_layer('my_dense_layer').get_weights()

print(W1.shape)
W1
```

```
(30000, 300)
```

```
array([[-0.00373691,  0.00533208,  0.00911605, ..., -0.00608832,
         0.0002673 ,  0.00754287],
       [ 0.00818818,  0.01370584,  0.00289636, ...,  0.0016083 ,
         0.00062872,  0.0125074 ],
       [ 0.00775008,  0.01029613,  0.00121749, ..., -0.00494439,
        -0.00866267,  0.00133855],
       ...,
       [-0.00981489, -0.00447228, -0.01358635, ...,  0.01322707,
        -0.0139491 , -0.0092314 ],
       [-0.00310255, -0.01183643,  0.0020827 , ..., -0.00384003,
         0.0108764 ,  0.0108641 ],
       [ 0.00948131,  0.01137586, -0.0029722 , ...,  0.00465663,
        -0.00467831,  0.00046353]], dtype=float32)
```

Compiling your model:

```
model.compile(loss="binary_crossentropy",
  optimizer="adam",
  metrics=["accuracy"])
```

For more initialization schemes, losses, metrics and optimizers:

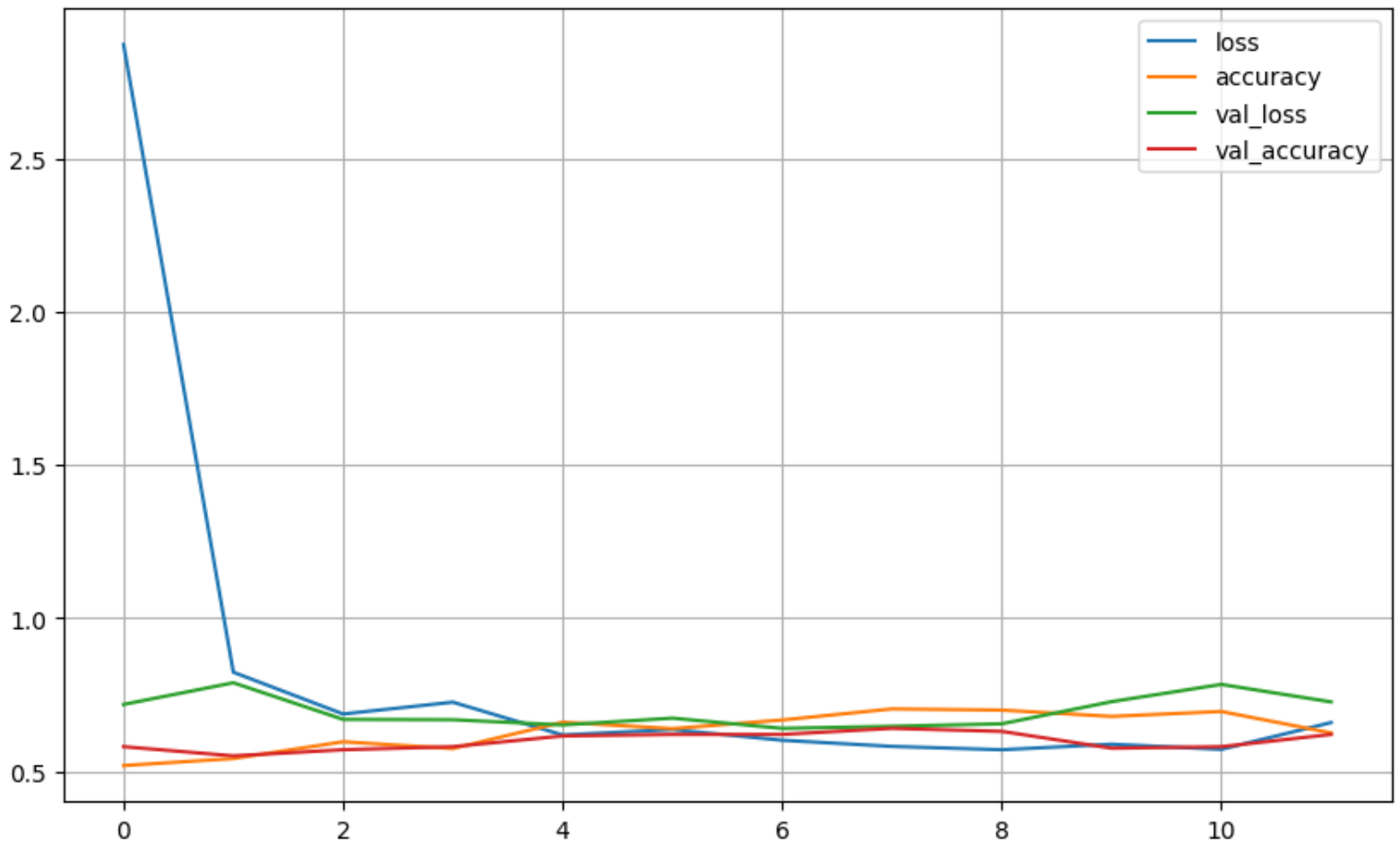
- https://keras.io/api/layers/initializers/
- https://keras.io/api/losses/
- https://keras.io/api/optimizers/
- https://keras.io/api/metrics/

Fitting the model:

```
from tensorflow.keras.callbacks import EarlyStopping

callbacks = [EarlyStopping(monitor='val_loss', patience=5,
  restore_best_weights=True)]

history = model.fit(X_train, y_train,
  batch_size=100, epochs=50,
  validation_split=0.1, callbacks=callbacks, verbose=0)
```

See later the `history` object's many fields.

```
import pandas as pd

pd.DataFrame(history.history).plot(figsize=(10, 6))
plt.grid(True)
plt.show()
```



Evaluate on test set:

```
test_loss, test_acc = model.evaluate(X_test, y_test, verbose=False)
print(f'Test accuracy for NN: {test_acc:.3f}')
```

```
Test accuracy for NN: 0.638
```

```
1  from sklearn.metrics import confusion_matrix
2
3  y_pred = (model.predict(X_test, verbose=0) > 0.5).astype(int).reshape(y_test.shape)
4  pd.DataFrame(
5    confusion_matrix(y_test, y_pred),
6    index=['true:yes', 'true:no'],
7    columns=['pred:yes', 'pred:no']
8  )
```

	pred:yes	pred:no
true:yes	160	102
true:no	79	159

It's OK to be underwhelmed.

Tuning params:

```
 1 from tensorflow.keras.layers import InputLayer
 2 from tensorflow.keras.optimizers import SGD
 3 from scikeras.wrappers import KerasClassifier
 4
 5 def malaria_model(n_hidden, n_neurons, lrt):
 6   model = Sequential()
 7   model.add(InputLayer(input_shape=(30000, )))
 8   for layer in range(n_hidden):
 9     model.add(Dense(n_neurons, activation='relu'))
10   model.add(Dense(1, activation='sigmoid'))
11   model.compile(loss="binary_crossentropy",
12     optimizer=SGD(learning_rate=lrt),
13     metrics=["accuracy"])
14   return model
15
16 keras_clf = KerasClassifier(model=malaria_model, n_hidden=1, n_neurons=30, lrt=3e-3
```

```
from scipy.stats import reciprocal
from sklearn.model_selection import RandomizedSearchCV

params = {
  'n_hidden': [0, 1, 2, 3],
  'n_neurons': np.arange(1, 100),
  'lrt': reciprocal(3e-4, 3e-2)
}

rnd_search_cv = RandomizedSearchCV(keras_clf, params, cv=5,
  n_iter=10)
rnd_search_cv.fit(X_train, y_train, epochs=50,
  validation_split=0.1, callbacks=callbacks)

print(f'Best test accuracy: {rnd_search_cv.best_score_:.2f}')
print(f'Best params: {rnd_search_cv.best_params_}')
```

```
Best test accuracy: 0.69
Best params: {'lrt': 0.0004918307063493132, 'n_hidden': 3, 'n_neurons': 17}
```

See also sklearn's `GridSearchCV()` and KerasTuner for a more robust solution.

Saving and restoring a model:

```
model.save('malaria.h5')
```

Then:

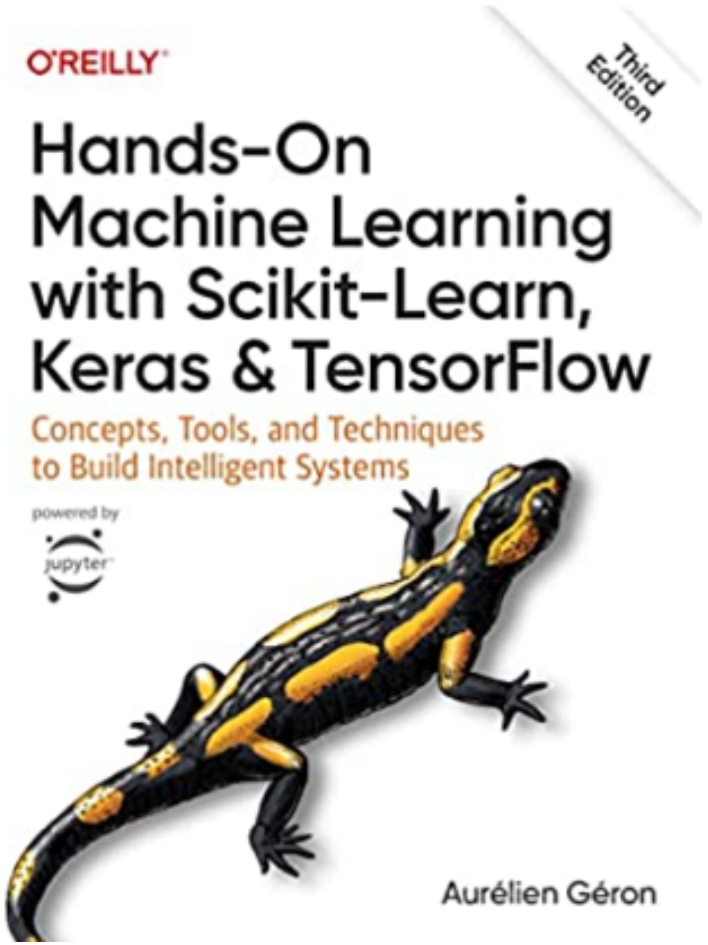
```
model = keras.models.load_model('malaria.h5')
model.predict(X_test[:3], verbose=0)
```

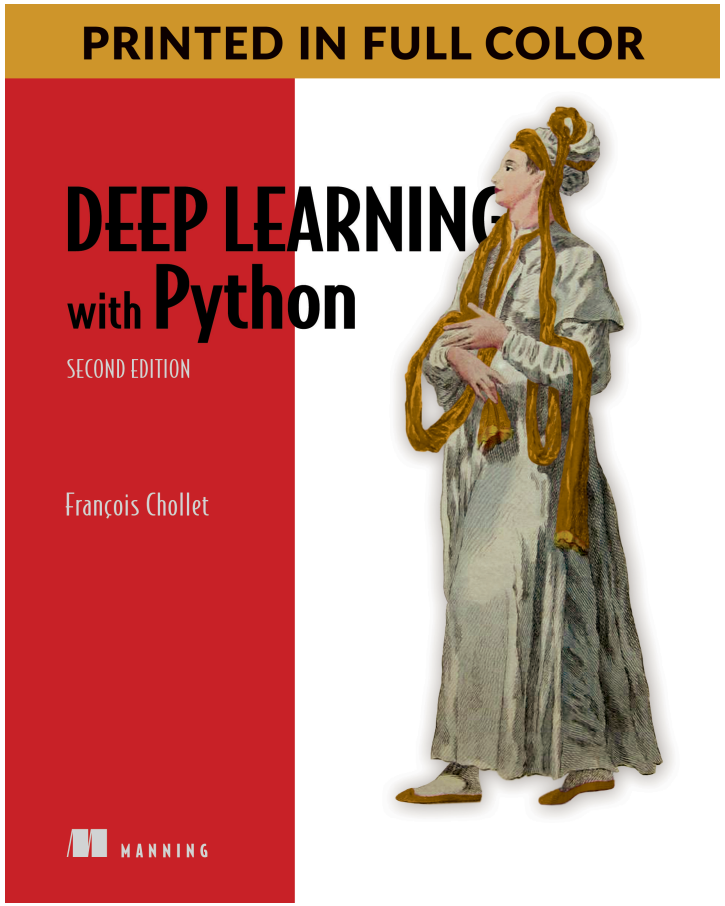
```
array([[0.47584853],
       [0.77716494],
       [0.3270011 ]], dtype=float32)
```

The HDF5 model saves the model's architecture and hyperparameters, and all weights matrices and biases.

Also see the `ModelCheckPoint()` callback.

Few Excellent Books





Intro to Data Science