

```
In [1]: import torch, numpy as np, pandas as pd
```

Creating a Linear Model, Neural Net and Deep Learning Model from Scratch using Tabular Data

Introduction

In this notebook, I will be demonstrating my learning in creating neural networks (NNs) from scratch. I will be building on my knowledge by going through three distinct steps:

- . Build **linear model** from scratch.
- . Build simple **NN** from scratch.
- . Build a **deep learning** (DL) model from scratch.

While a similar task was previously completed for image classification using the MNIST dataset, this notebook will focus on the Titanic dataset, aiming to build a model that can predict the chance of survival.

Data Extraction and Cleaning

The data is contained in a csv file which we can open with Pandas.

```
In [2]: df = pd.read_csv('train.csv')
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 891 entries, 0 to 890
Data columns (total 12 columns):
#   Column          Non-Null Count  Dtype
---  -
0   PassengerId     891 non-null    int64
1   Survived        891 non-null    int64
2   Pclass          891 non-null    int64
3   Name            891 non-null    object
4   Sex             891 non-null    object
5   Age             714 non-null    float64
6   SibSp           891 non-null    int64
7   Parch           891 non-null    int64
8   Ticket          891 non-null    object
9   Fare            891 non-null    float64
10  Cabin           204 non-null    object
11  Embarked        889 non-null    object
dtypes: float64(2), int64(5), object(5)
memory usage: 83.7+ KB
```

We can see that some of the columns contain NaN values, which we will be unable to multiply by coefficients.

Let's replace the missing values with something - normally the mode is a good place to start.

```
In [3]: modes = df.mode().iloc[0] # we use .iloc to take first row, as it will replace all
df.fillna(modes, inplace=True)
```

Now we need to make sure that our data will be appropriate to feed through a model. A good place to start is with `.describe()` to see a summary, selecting numeric columns only to start with.

```
In [4]: df.describe(include=(np.number))
```

Out [4]:	PassengerId	Survived	Pclass	Age
count
mean
std
min
%
%
%
max

We need to do a bit of feature engineering to make our data fit for purpose.

Fare has many values between and but some massive values too. This will skew model, so we take the `log` to bring all values to a sensible range. This is generally a good technique for continuous variables involving *money* or *popn*.

```
In [5]: df['LogFare'] = np.log(df['Fare'] + 1) # we add 1 to avoid log(0)!
```

Clearly, we still have some issues - notably, the strings cannot be multiplied by coefficients! Let's fix them with numbers.

Pandas allows us to create new columns containing **dummy variables** which is a column that has a `1` where a particular column contains a particular value or `0` otherwise. This is very easy in using the `get_dummies` function - by default, this provides a n columns for n categories (even though technically we only need n-1 columns as you can derive the final column). However, this is useful as it means we do not need to worry about adding a constant term anymore as we don't need a separate intercept term to cover rows that aren't otherwise part of a column.

We will do this for all categorical variables, even `Pclass`, because as shown below, this has distinct values.

```
In [6]: # only 3 distinct values in Pclass
pclasses = sorted(df.Pclass.unique())
pclasses
```

```
Out [6]: [1, 2, 3]
```

```
In [7]: categorical = ['Pclass', 'Sex', 'Embarked']
df = pd.get_dummies(df, columns=categorical)
```

```
# get_dummies will automatically remove the original columns.
df.head()
```

Out [7]:

PassengerId	Survived	Name	Age	SibSp	Parch	Ticket	Fare
1	0	Braund, Mr. Owen Harris	22	1	0	A/502161	53.1
2	1	Cumings, Mrs. John Bradley (Florence Briggs Thayer)	38	1	0	PC 17599	51.66
3	0	Heikkinen, Miss. Laina	26	0	0	STON/O2 3510182	91.59
4	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	35	1	0	151601	53.1
5	0	Allen, Mr. William Henry	35	0	0	W 3692	51.66

Now, we have engineered both the independent and dependent variables we will use in the model. We will discard some of the remaining columns for the purpose of this notebook (which is focusing on creating a NN from scratch rather than effective data transformation).

However, it is worth noting that a lot can be done with the remaining columns. The best Kaggle model actually used *only* the name column to predict chance of survival!

In [8]: `df.drop(columns=["Fare", "PassengerId", "Name", "Ticket", "Cabin"], inplace=True)`
`df.head()`

Out [8]:

Survived	Age	SibSp	Parch	LogFare	Pclass_1	Pclass_2	Pclass_3	Sex
0	22	1	0	5.31	False	False	True	Male
1	38	1	0	5.17	True	False	False	Female
0	26	0	0	9.16	False	False	True	Female
1	35	1	0	5.31	True	False	False	Female
0	35	0	0	5.17	False	False	True	Male

The final step we want to do is **normalize** our data so that all the columns contain numbers from 1. We do this by dividing each column by its maximum value. This will prevent the model from being dominated by larger values such as *age*.

It is worth noting that I am practicing using Pandas here for data manipulation, but in practice (perhaps if working with more data) this would be much more efficient to perform in PyTorch, as we could **broadcasting** to rapidly perform divisions. However, this allows me to have all the data engineering together so I can focus on creating the models.

Also note, we are converting our boolean columns to floats, as this will enable matrix multiplication in PyTorch later.

```
In [9]: # PyTorch expects floats to perform matrix multiplications
indep_cols = df.columns[df.columns != "Survived"]
df[indep_cols] = df[indep_cols].astype(float)
```

```
In [10]: for col in df.columns:
df[col] = df[col]/df[col].max()
df.head()
```

```
Out[10]:
```

	Survived	Age	SibSp	Parch	LogFare	Pclass_	Pclass_	Pclass_
0	0	21.01	1	0	5.42	3	3	3
1	1	17.72	1	0	5.14	3	3	3
2	1	31.17	0	0	7.92	1	1	1
3	1	19.13	1	0	5.36	3	3	3
4	0	18.74	1	0	5.29	3	3	3

Now, we can start building models!

Linear Model

Compile Data

We will be using PyTorch to build our model, as PyTorch tensors can make use of the GPU to make fast calculations.

We start by turning our independent variables (predictors) and dependent variables (targets) into tensors.

```
In [11]: from torch import tensor

dep = tensor(df["Survived"])
indep = tensor(df[indep_cols].values)

indep.shape, dep.shape
```

```
Out[11]: (torch.Size([891, 12]), torch.Size([891]))
```

At this point, it is also important to split the data into **training** and **validation** sets, a topic I have in-depth about previously.

We can use fastai's `RandomSplitter` for this task as it will return distinct random selection of both training and validation sets.

```
In [12]: from fastai.data.transforms import RandomSplitter
train, val = RandomSplitter(seed=42)(df)
train, val
```

```
Out[12]: ((#713)
[788,525,821,253,374,98,215,313,281,305,701,812,76,50,387,47,516,564,434,117
(#178)
[303,778,531,385,134,476,691,443,386,128,579,65,869,359,202,187,456,880,705,
])
```

```
In [13]: trn_dep, val_dep = dep[train], dep[val]
trn_indep, val_indep = indep[train], indep[val]

trn_indep.shape, val_indep.shape, trn_dep.shape, val_dep.shape
```

```
Out[13]: (torch.Size([713, 12]),
torch.Size([178, 12]),
torch.Size([713]),
torch.Size([178]))
```

Finally, we need to turn our dependent variable into a column vector (rank-1 tensor) which we do by indexing the column dimension (which doesn't currently exist) with the special value `None` which tells PyTorch to add a new dimension here.

We are doing this as we will be using matrix multiplication and the predictions will be returned as rank-1 column vector.

```
In [14]: trn_dep = trn_dep[:,None]
val_dep = val_dep[:,None]
```

Initialise Coefficients

Now that we have our variables, we need to generate our (initially) random coefficients.

We need one coefficient for each independent variable and we will pick random numbers in the range $(-0.1, 0.1)$.

When we perform matrix multiplication between the coefficients and independent variables, we require `coeffs` to be a rank-1 column vector, hence, we add an extra dimension through the second argument of `torch.rand()`.

```
In [15]: def init_coeffs(n_coeff):
return (torch.rand(n_coeff, 1, dtype=torch.float64) * 0.1).requires_grad_
# I use dtype as I need to make sure the coeffs are the same data type
```

Calculating Predictions

Our predictions will be calculated by multiplying each row by the coefficients and adding them up.

The function `calc_preds` will use **broadcasting** to multiply each row of independent variable vector of coefficients. The sum of row of independent variables will be calculated and this will represent the prediction for these predictors.

But what about the `sigmoid` function? Well, this is a cool function that basically limits our prediction to be between `0` and `1` (since `0` means died and `1` means survived). Essentially whenever we are performing binary classification, we will use the sigmoid function as it improves the accuracy of the model substantially.

```
In [16]: def calc_preds(coeffs, indeps):  
         return torch.sigmoid((indeps*coeffs).sum(axis=1))
```

This function looks great! However, we can actually improve it further!

Multiplying elements together, then adding across rows is identical to doing a matrix-vector product. We can use the Python `@` operator to perform PyTorch optimised matrix products.

```
In [17]: def calc_preds(coeffs, indeps):  
         return torch.sigmoid(indeps@coeffs)
```

Calculating Loss

Once the predictions are made (initially on random coefficients) for each row of independent variables, we need to calculate the **loss**. The loss will allow us to update the coefficients (we will now refer to them as **parameters**).

`calc_loss` calls the `calc_preds` function and uses the **mean absolute error** for loss.

```
In [18]: def calc_loss(coeffs, indeps, deps):  
         return torch.abs(calc_preds(coeffs, indeps) - deps).mean()
```

Update Parameters

At this point, we have made predictions and calculated the loss. Now we need to use the loss as input to **stochastic gradient descent** (SGD) to update the parameters.

`update_coefs` uses the gradient (calculated by PyTorch as we used `requires_grad_` when initialising the parameters) of each coefficient to determine how to adjust it. It is adjusted by the **learning rate**, an important hyperparameter when designing a model.

We zero the coefficients to prevent the gradients from accumulating (the default behaviour of PyTorch).

```
In [19]: def update_coefs(coeffs, lr):  
         coeffs.sub_(coeffs.grad * lr)  
         coeffs.grad.zero_()
```

Training the Model

Now we have all of the important functions to:

- Initialise Coefficients

- . Calculate Predictions
- . Calculate Loss
- . Update Parameters

We will put this all together using `epoch` functions.

The first called `epoch` represents a single **epoch** which a full pass through all training data and our previously defined functions.

The second function called `train_model` will initialise the coefficients then call `epoch` for each epoch we want to perform.

```
In [20]: def epoch(coeffs, lr):
          loss = calc_loss(coeffs, trn_indep, trn_dep)
          loss.backward()
          with torch.no_grad():
              update_coefs(coeffs, lr)
          print(f"{loss:.3f}")
```

```
In [21]: def train_model(epochs, lr):
          torch.manual_seed(442)
          coefs = init_coefs(indep.shape[1])
          for i in range(epochs):
              epoch(coefs, lr=lr)
          return coefs
```

```
In [22]: coefs = train_model(15, 100)
```

```
0.515
0.323
0.288
0.204
0.200
0.198
0.197
0.197
0.196
0.196
0.196
0.195
0.195
0.195
0.195
```

Analyse Coefficients

We can write a quick function to see all of our coefficients for each independent variable. This will give us an idea of how our function works.

For example, we can see that a higher *age* is a strong predictor of death and a higher *class* (a higher class or a higher class) is a strong predictor of life by looking at the coefficients.

```
In [23]: def show_coefs():
          return dict(zip(indep_cols, coefs.requires_grad_(False)))
          show_coefs()
```

```
Out [23]: {'Age': tensor([-1.1208], dtype=torch.float64),
'SibSp': tensor([-0.8208], dtype=torch.float64),
'Parch': tensor([-0.3355], dtype=torch.float64),
'LogFare': tensor([0.4991], dtype=torch.float64),
'Pclass_1': tensor([3.3172], dtype=torch.float64),
'Pclass_2': tensor([1.2995], dtype=torch.float64),
'Pclass_3': tensor([-6.3529], dtype=torch.float64),
'Sex_female': tensor([8.2192], dtype=torch.float64),
'Sex_male': tensor([-10.0180], dtype=torch.float64),
'Embarked_C': tensor([1.2405], dtype=torch.float64),
'Embarked_Q': tensor([1.4383], dtype=torch.float64),
'Embarked_S': tensor([-4.3675], dtype=torch.float64)}
```

Calculating Metrics

Now we just need a **metric** to determine the quality of the model. We can see that the loss is going down, but loss is not suitable for evaluating how **accurate** the model is.

We will define a prediction of *death* as any value ≤ -0.5 and a prediction of *life* as any value > 0.5 .

We have our coefficients but we haven't used our validation set to determine how effective the model is. We will use the validation set to calculate accuracy.

```
In [24]: def accuracy(coeffs):
         return (val_dep.bool()==(calc_preds(coeffs, val_indep)>0.5)).float().mean()
         accuracy(coeffs)
```

```
Out [24]: tensor(0.8258)
```

Summary

We've now built a linear model that is performing very well! This model is not yet a NN but **it is the first step for creating a layer of a NN**, which we will be working on in the next section!

In reality, because this is a simple task and there is minimal data, a NN is unlikely to improve our performance, as an accuracy of 82.58% is very good. **However, for the purpose of learning, it is beneficial to see how our linear model integrates in a full NN.**

Neural Network

Now we will be creating a NN that will have **3 layers**. The first layer will take the independent variables as inputs and create **n activations** or outputs (after passing through an activation function). These **n** activations will be the input for the second layer which will output exactly **1** value, representing our prediction of survival or not.

Initialise Coefficients

Because our NN will have **3** layers, it will need **3** rank-**2** tensors of coefficients. We will redetermine the `init_coeffs` function for the NN.

By default, our `init_coeffs` function will produce `n_hidden` hidden units in the first layer, which are mapped to a single output in the second layer. If we increase the hidden units the network will be more flexible but slower and harder to train, so this is an important hyperparameter.

`layer1` will be a `n_hidden x n_hidden` tensor and when we matrix multiply our data by `layer1` we get `n_hidden` outputs. We divide each value by the number of hidden units as we want the coefficients to be inversely proportional to the number of hidden units. This prevents the weights from growing out of control.

`layer2` will be a `n_hidden x 1` tensor and we matrix multiply the activations from `layer1` to output a single prediction.

`const` is the bias for the final output layer. `layer2` has 'bias' already factored into the extra independent variables (discussed above).

Activations are the final output from `layer2` after passing through the activation function.

```
In [25]: def init_coeffs(n_coeff, n_hidden=20):
          layer1 = (torch.rand(n_coeff, n_hidden, dtype=torch.float64) - 0.5)/n_hidden
          layer2 = torch.rand(n_hidden, 1, dtype=torch.float64) - 0.2
          const = torch.rand(1, dtype=torch.float64)[0]
          return layer1.requires_grad_(), layer2.requires_grad_(), const.requires_grad_()
```

Calculate Predictions

We import `torch.nn.functional` so we can access the `relu` function from PyTorch.

Now we can really see the NN. Our `coeffs` are unpacked into their relevant variables.

We update `res` at each layer, initially multiplying our independent variables by `layer1`, we then employ the **activation function**, ReLU.

Then, the second layer takes `res` and multiplies by `layer2` adding the constant term. This gives our final hidden activations to a single prediction which we return after employing the `sigmoid` function (to map it to a value between 0 and 1).

```
In [26]: import torch.nn.functional as F

def calc_preds(coeffs, indeps):
    l1, l2, const = coeffs
    res = F.relu(indeps@l1)
    res = res@l2 + const
    return torch.sigmoid(res)
```

Update Coefficients

Once we have our prediction, we can update our coefficients. However, we need to update the coefficients in every layer, so we use a for loop.

```
In [27]: def update_coeffs(coeffs, lr):
          for layer in coeffs:
              layer.sub_(layer.grad * lr)
              layer.grad.zero_()
```

Train Model

Finally, the model can be trained, using many of the same functions used in the linear model. Th

`calc_loss` function remains the same as does the `epoch` and `train_model` functions.

```
In [28]: coeffs = train_model(30, 20)
```

[illegible]

```
In [29]: accuracy(coeffs)
```

```
Out[29]: tensor(0.8258)
```

Summary

We see minimal improvement by employing a NN in this situation; however, we can easily see how a linear model easily translates to a NN simply by adding layers and activation functions.

Deep Learning

Initialise Coefficients

Because the NN above only uses a single hidden layer, it does not count as "deep learning". However, we can easily extend the logic from above to add an arbitrary number of layers.

As we can see, `sizes` starts with a dimension of `n_coeff`, representing the number of coefficients needed for each independent variable. It takes our defined `hidden` layer dimensions and maps them to a single output (our prediction).

Next, we define our `layers` and `consts`.

To help demonstrate my understanding we can run through what `layers` looks like. It is a list of tensors. The first tensor has random values and shape `n_coeff x hidden[0]`. The second tensor is `hidden[0] x hidden[1]` as it takes the `hidden[0]` outputs from layer 0 and maps it to `hidden[1]` outputs. The third tensor is `hidden[1] x 1` as it takes the `hidden[1]` outputs from layer 1 and maps it to a single prediction.

`consts` consists of `hidden` tensors too, all with a single random constant term.

```
In [30]: def init_coeffs(n_coeff):
    hidden = [10, 10] # this will represent the size of each hidden layer
    sizes = [n_coeff] + hidden + [1]
    n = len(sizes)

    layers = [(torch.rand(sizes[i], sizes[i + 1], dtype=torch.float64) - 0.5) * 0.1 for i in range(n - 1)]
    consts = [(torch.rand(1, dtype=torch.float64) - 0.5) * 0.1 for i in range(n)]

    for l in layers + consts:
        l.requires_grad_()

    return layers, consts
```

Calculate Predictions

Now we can alter our `calc_preds` function to be suitable for deep learning.

The main difference is we loop through each layer performing the matrix multiplication and activation. A key thing to notice is that we use the ReLU function after each linear transformation *unless* we are at the final layer, in which case we use the sigmoid function to ensure our final prediction falls between 0 and 1.

```
In [31]: def calc_preds(coeffs, indeps):
    layers, consts = coeffs

    n = len(layers)

    res = indeps

    for i, l in enumerate(layers):
        res = res @ l + consts[i]
        if i != n - 1:
            res = F.relu(res)

    return torch.sigmoid(res)
```

Update Coefficients

Again, only a minor change is required here, ensuring we perform SGD on each parameter (both weights and bias).

```
In [32]: def update_coeffs(coeffs, lr):  
        layers, consts = coeffs  
        for l in layers + consts:  
            l.sub_(l.grad * lr)  
            l.grad.zero_()
```

Train Model

Finally, we can train our model and check its accuracy!

```
In [33]: coeffs = train_model(20, 4)
```

```
0.554  
0.484  
0.407  
0.345  
0.314  
0.293  
0.212  
0.201  
0.218  
0.213  
0.194  
0.194  
0.193  
0.193  
0.193  
0.193  
0.193  
0.193  
0.193  
0.193  
0.193
```

```
In [34]: accuracy(coeffs)
```

```
Out[34]: tensor(0.8258)
```

Conclusion

In this notebook, we have seen the gradual build of a deep learning neural network from a primitive model. Other than understanding how neural networks really work (which is pretty cool!) there's a few other takeaways from this notebook:

- **Sometimes simple solutions work.** We actually saw no improvement from our initial linear model. While it was great to demonstrate my understanding of NNs, they're not always necessary depending on the data available.
- **There's no need to build NNs from scratch.** By using pretrained models and curated architectures we can get better results much easier. Throughout this notebook, particularly with initialising random coefficients, we had to multiply or divide our parameters by arbitrary numbers which is not ideal, and there are more evidenced-based approaches to selecting appropriate initial parameters, that other architectures have researched and put in place.

However, overall, this notebook did not intend to produce the best results but to demonstrate how models are built and how DL is conducted on a basic, yet low-level. As such, I feel I have a deep understanding of how NNs work.