Neural networks

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About

Linear function approximation with SGD

From linear regression to neural networks

Practical aspects

Conclusion

About

- We will try to get a practical understanding of neural networks
  - The topic is massive
- The field has changed names a number of times
  - Connectionist systems
  - Neural networks
  - Deep learning
- They are all the same stuff, different name
  - Re-branding

Linear function approximation

- One of the simplest ways to do a prediction
- In case we have a single variable/feature/co-variate, we are trying to learn
  - $\hat{f}_w(x) = w_1 x + w_0$
- w_0 is often called the bias
- x is a sample from the data
- Let's load some data

Data loading

```
df_linear = pd.DataFrame()
```

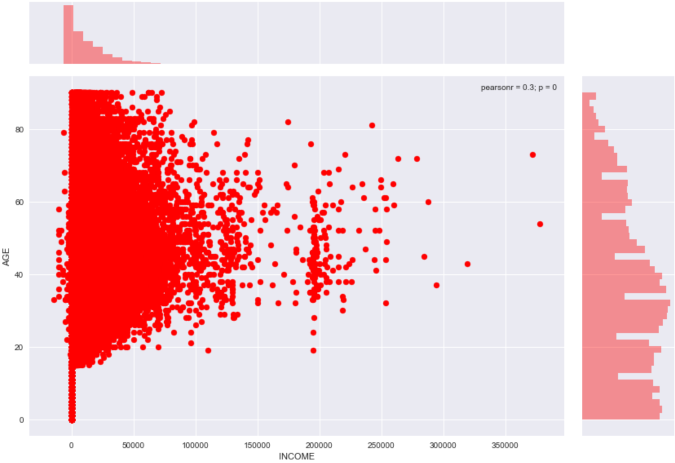
```
df_linear["AGE"] = df[["AGE"]].copy()
df_linear["INCOME"] = df[["INCOME" + str(i) for i in range(1,8)]].sum(axis = 1)

df_linear["YEARSCH"] = df[["YEARSCH"]].copy()
df_linear["ENGLISH"] = df[["ENGLISH"]].copy()
df_linear["FERTIL"] = df[["FERTIL"]].copy()
df_linear["YRSSERV"] = df[["YRSSERV"]].copy()
```

Is there another way we could have done the same?

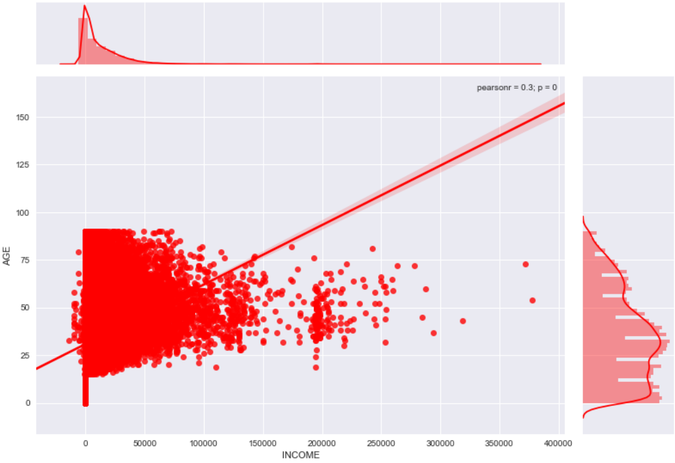
Visualisation

```
g = sns.jointplot("INCOME", "AGE", data=df_linear, color = "r")
```



Visualisation - linear regression

```
g = sns.jointplot("INCOME", "AGE", data=df_linear, color = "r", kind="reg")
```



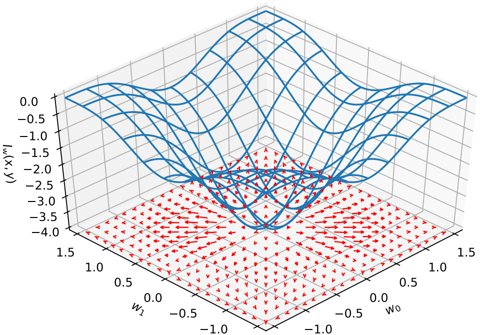
Stochastic gradient descent (SGD)

- Let's define a cost function $J_w(x, y)$, which signifies how far we are from the solution
- We have seen such cost functions before in terms of evaluating prediction
  - $J_w(x, y) = \frac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - \hat{f}_w \left(x^{(i)} \right) \right)^2$
- For just one example we have:
  - $J_w(x^{(0)}, y^{(0)}) = \left(y^{(0)} - \hat{f}_w \left(x^{(i)} \right) \right)^2$

$$w = w - \eta \cdot \nabla_w J_w(x, y)$$

Gradients

The gradient $\nabla_w J_w(x, y)$ is the direction of steepest descent[1]



$$\nabla_w J_w(x, y) \equiv \left[\frac{\partial J_w(x,y)}{\partial w_0}, \frac{\partial J_w(x,y)}{\partial w_1}, \ldots, \frac{\partial J_w(x,y)}{\partial w_n}\right]$$

[1] `https://commons.wikimedia.org/wiki/File:Gradient_Visual.svg`

Find the gradient

```
from sympy import Function, Symbol, latex, init_printing

y0,y1,y2 = symbols('y^(0),y^(1),y^(2)')
x0, x1, x2, x = symbols('x^(0), x^(1), x^(2), x')

f = (x*w1 + w0)

w0,w1 = symbols('w0, w1')

mse = ((f.subs(x, x0) - y0 )**2 )


mse.diff(w0)
mse.diff(w1)
```

$$\frac{\partial J_w(x,y)}{\partial w_0} = 2\left(w_0 + w_1 x^{(0)} - y^{(0)}\right)$$

$$\frac{\partial J_w(x,y)}{\partial w_1} = 2x^{(0)}\left(w_0 + w_1 x^{(0)} - y^{(0)}\right)$$

Some simplifications

$$[w_0, w_1] = [w_0, w_1] - \eta \cdot \left[\frac{\partial J_w(x,y)}{\partial w_0}, \frac{\partial J_w(x,y)}{\partial w_1}\right]$$

$$[w_0, w_1] =$$
$$[w_0, w_1] - \eta \cdot \left[2\left(w_0 + w_1 x^{(0)} - y^{(0)}\right), 2x^{(0)}\left(w_0 + w_1 x^{(0)} - y^{(0)}\right)\right]$$

$$[w_0, w_1] = [w_0, w_1] - \eta \cdot \left[2\left(y^{(0)} - \hat{f}_w\left(x^{(i)}\right)\right), 2x^{(0)}\left(y^{(0)} - \hat{f}_w\left(x^{(i)}\right)\right)\right]$$

$$[w_0, w_1] = [w_0, w_1] - \eta \cdot \left[\left(y^{(0)} - \hat{f}_w\left(x^{(i)}\right)\right), x^{(0)}\left(y^{(0)} - \hat{f}_w\left(x^{(i)}\right)\right)\right]$$

Mini-batches

- We used only one example
- This is called "online learning"
- But it's common to use "mini-batches"
  - i.e., a number of samples togeather
- You would use every single sample
  - Often mini-batching much faster
  - Finding the right number of batches is tricky
  - Finding η is tricky

What if we had three weights and two features?

- Let's do the derivations

Some animations

http://imgur.com/a/Hqolp

http://imgur.com/SmDARzn

By Alec Reed

Creating higher order features

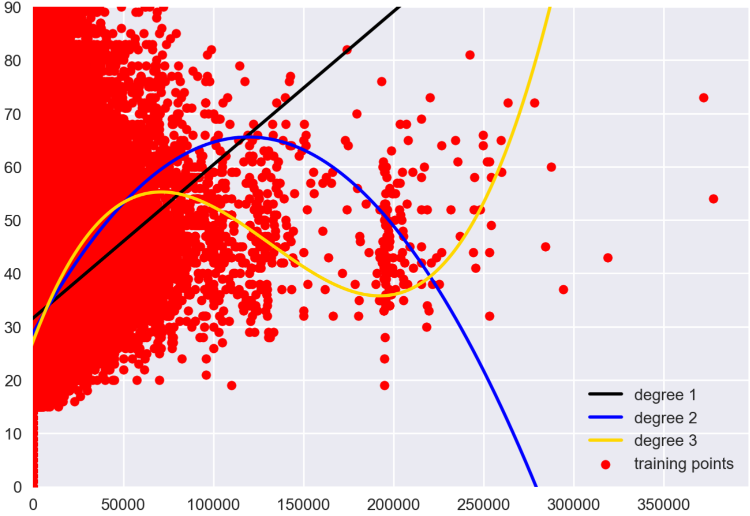
- What if the relationship between the features and the rewards is not linear?
- What if there is some other relationship?
- We can learn higher order features
- So for example, if we have x_0, x_1
  - Superscripts are rows, subscripts are columns!
- We can create new features $x_0^2, x_0 x_1, x_0^2$

Regression with higher order features

```
from sklearn.preprocessing import PolynomialFeatures

degree = 1
model = make_pipeline(PolynomialFeatures(degree),StandardScaler(), SGDRegressor())
model.fit(X, y)
y_hat = model.predict(X)
```

Plot


90
80
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50
40
30
20
10
0
0
50000
100000
150000
200000
250000
300000
350000
degree 1
degree 2
degree 3
training points

Adding any other kind of feature

- How about we add features in the form
  - $\max(0, x_0)$
  - $\max(0.3, x_0)$
  - $sin(x_0)$
  - $sin(\max(0, x_0))$
- The list is endless
- Or, even better, *discover* those features

Building abstractions

- You rarely operate directly on the input space
  - People seem to be building abstract features
- We go from shapes and colours to forms to objects
- From primitive sounds to music
- Hierarchies of features extractors

Learning features

- Let's revisit our example

$$\hat{f}_w(x) = w_1 x + w_0$$

- Let's add some depth using another function

$$\hat{f}_{w^{(0)}}(x) = w_1^{(0)} \hat{g_w}(x) + w_0^{(0)}$$

$$\hat{g}_{w^{(1)}}(x) = max\left(w_1^{(1)} x + w_0^{(1)}, 0.3\right)$$

- The neuron above (g) are known as a "leaky rectifier" neuron
  - But it's just a function - the neuron terminology comes from the original inspiration
  - Can you see why the name "deep learning" stuck?

Learning

- Use the same error function to find errors

$$J_w(x^{(0)}, y^{(0)}) = \left(y^{(0)} - \hat{f_w}\left(x^{(i)}\right)\right)^2$$

- Update each weight using the same method

$$w = w - \eta \cdot \nabla_w J_w(x, y)$$

$$\nabla_w J_w(x, y) \equiv \left[\frac{\partial J_w(x,y)}{\partial w_0}, \frac{\partial J_w(x,y)}{\partial w_1}, ..., \frac{\partial J_w(x,y)}{\partial w_n}\right]$$

- Use the chain rule to calculate partial derivatives

$$\frac{d}{dx}\left[f\left(g(x)\right)\right] = f'(g(x))g'(x)$$

Convexity

- We are going downhill
- What if the error surface is smooth, it's all good
- But what if the error surface is rugged mess with ups and downs?
- Local optima are not global optima
- Thus, NN training often somewhat unstable

Theano, Tensorflow

- As you understand doing all these calculations by hand is tedious
- Every new time of neuron or layer you invent would require a new gradient calculation
- Auto-differentiation
  - Theano
  - Tensorflow
- You just describe your network/graph
- The rest is done automatically by the machine

Building a network

- There are multiple packages for neural networks
- I think the most popular is Keras
- Though a massive number of people are using Lasagne

Keras API

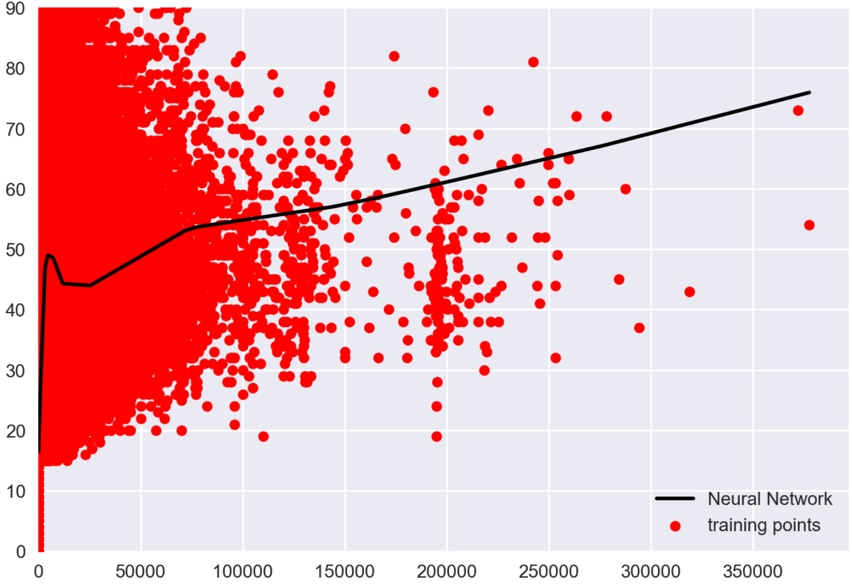
```
inputs = Input(shape=(1,))

x = Dense(64)(inputs)
x = PReLU()(x) # Non-linearity
x = Dense(64)(x)
x = PReLU()(x) # Non-linearity
predictions = Dense(1, activation='linear')(x)

model = Model(input=inputs, output=predictions)
model.compile(optimizer='adam',loss='mse')

model.fit(...)
```

Output plot


90
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50000
100000
150000
200000
250000
300000
350000
Neural Network
training points

Input Layer

```
inputs = Input(shape=(22,))
```

- The first layer
- Does not contain any neurons
  - Terminology changes between authors
- “Number of columns”
- “Number of features”

Hidden layers

```
x = PReLU()(x) # Non-linearity
x = Dense(64)(x)
x = PReLU()(x) # Non-linearity
```

- "Dense" layers specify the number of neurons
- You need to follow them up with a non-linear transformation
- Alternately you can pass this as parameter "activation"
- Non-linearity is often called the "activation function"

Output Layer

```
predictions = Dense(1, activation='linear')(x)
model = Model(input=inputs, output=predictions)
```

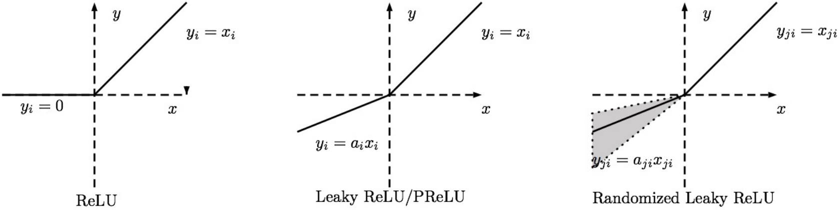
- The output layer
- A normal Dense layer
- “Number of outputs”
- You can predict multiple outputs at once

Cost (or objective) functions

- You can do both regression and classification with neural networks
- All it changes it the output layer and the objective function
- Categorical cross-entropy for classification
  - You need to convert your outputs to one-hot encoding
- Mean squared error for prediction

Neuron types

- Also called activation functions or non-linearities



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[2] http://lamda.nju.edu.cn/weixs/project/CNNTricks/imgs/relufamily.png

Learning Algorithms

- We have just seen SGD, which forms the basis of every modern learning algorithm for NNs
  - It will be dethroned eventually, but nobody knows from what
- SGD does not take into account specific information about individual weights
  - Not the curvature of the search space
- There are methods that auto-adapt the learning rate per individual weight
  - Adam
  - RMSProp
- Adam should be your default option

Regularisation

- Overfitting is a massive problem - with enough variables you can fit anything
- ℓ_1: Turn your weights down to zero
- ℓ_2: Make all your weights small
- You can define the regularisation strength
- Dropout:
    - Remove some of the weights during training uniform random
    - During testing/using put use everything, but toned down
    - Implemented as a distinct layer

(Batch) Normalisation

- Implemented as a different layer
- Covariate swift impact learning negatively
- Normalise the weights of each layer

$$\hat{w} = \frac{w - \mu}{\sigma}$$

$$y = \gamma \hat{w} + \beta$$

- γ and β are special types of parameters, to be learned as well
  - They scale and shift a bit
- Stops "internal covariate shift"
  - Accelerates learning

Weight sharing / multiple outputs

- You can create pathways for different things that share the same weights
- Thus imposing stronger regularisation
  - Use same features for different tasks
- Very effective method of generalising
- You can use different pathways within the same network

Metrics/ callbacks

- When should you stop training?
  - After i iterations over the whole dataset
  - After the validation error stops improving
- Save best validation model
  - … and use this for testing
- Reduce learning rates, log etc
- "Callbacks"

Creating custom layers

[3]

```
from keras import backend as K
from keras.engine.topology import Layer
import numpy as np

class MyLayer(Layer):
    def __init__(self, output_dim, **kwargs):
        self.output_dim = output_dim
        super(MyLayer, self).__init__(**kwargs)

    def build(self, input_shape):
        # Create a trainable weight variable for this layer.
        self.W = self.add_weight(shape=(input_shape[1], self.output_dim),
                                 initializer='random_uniform',
                                 trainable=True)
        super(MyLayer, self).build()  # Be sure to call this somewhere!

    def call(self, x, mask=None):
        return K.dot(x, self.W)

    def get_output_shape_for(self, input_shape):
        return (input_shape[0], self.output_dim)
```

[3] https://keras.io/layers/writing-your-own-keras-layers/

Conclusion

- We have touched upon neural networks
- It's a really hot topic right now
- Requires a bit of dedication
- New algorithms are coming out every day