# Data Analysis, Neural Networks and the use of Keras

### Cecilia Jarne

# cecilia.jarne@unq.edu.ar







Twitter: @ceciliajarne





Cecilia Jarne

Neural Networks and Keras

cecilia.jarne@unq.edu.ar

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- What is Machine Learning, Neural Networks, and Deep Learning?
- Neural Networks concepts and topologies.
- A brief review of the use of python ML libraries.



We are interested in:

- Data Visualization.
- Data Analysis (Identify features from the data).
- Data Classification.
- Implementation of different algorithms as intelligent as we can get.

# Which are the available algorithms?



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# Which are the available algorithms?



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# What about machine learning?



### ARTIFICIAL INTELLIGENCE

A technique which enables machines to mimic human behaviour

### MACHINE LEARNING

Subset of AI technique which use statistical methods to enable machines to improve with experience

### **DEEP LEARNING**

Subset of ML which make the computation of multi-layer neural network feasible

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- Data driven approach.
- Can we learn the underlying features directly from data?

Low Level Features



Lines & Edges

**Mid Level Features** 



Eyes & Nose & Ears

High Level Features



Facial Structure



Neural Networks date back decades, so why the resurgence?

### I. Big Data

- Larger Datasets
- Easier Collection
   & Storage

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### 2. Hardware

- Graphics Processing Units (GPUs)
- Massively Parallelizable



### 3. Software

- Improved Techniques
- New Models
- Toolboxes





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- Training set: The data where the model is trained on. We train our model, by pairing the input with the expected output.
- Validation set: Data the model has not been trained on and is used to tune hyperparameters. Here we estimate how well your model has been trained.
- Test set: Same like the validation set.. just used at the final end. This is an Application phase: we apply our developed model to the real-world data and get the results. This fase is split into two parts:
  - First you look at your models and select the best performing approach using the validation data (=validation).
  - Then you estimate the accuracy of the selected approach (=test).

# Neural Networks:







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The structural building block of Deep Learning



The structural building block of Deep Learning:



The structural building block of Deep Learning:



The structural building block of Deep Learning:





### **Activation Functions**

$$\hat{y} = \frac{g}{g} \left( w_0 + X^T W \right)$$

· Example: sigmoid function

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



# The purpose of Activation functions is to introduce non linearities into the network $% \left( {{{\bf{n}}_{\rm{c}}}} \right)$



# Neural Networks: Activation Functions

Nanc	Plot	Equation	Derivative
Identity	_/	f(x) = x	f'(x) = 1
Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0\\ 1 & \text{for } x \ge 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ ? & \text{for } x = 0 \end{cases}$
Logistic (a.k.a Soft step)		$f(x) = \frac{1}{1 + e^{-x}}$	f'(x) = f(x)(1 - f(x))
Tanfi	$\square$	$f(x)=\tanh(x)=\frac{2}{1+e^{-2x}}-1$	$f'(x) = 1 - f(x)^2$
ArcTan	/	$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2 + 1}$
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for } x < 0\\ x & \text{for } x \ge 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x < 0\\ 1 & \text{for } x \ge 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU) <sup>(2)</sup>	/	$f(x) = \begin{cases} \alpha x & \text{for } x < 0 \\ x & \text{for } x \ge 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for } x < 0\\ 1 & \text{for } x \ge 0 \end{cases}$
Exponential Linear Unit (ELU) <sup>[3]</sup>	/	$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for } x < 0\\ x & \text{for } x \ge 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{for } x < 0\\ 1 & \text{for } x \ge 0 \end{cases}$
SoftPlus	/	$f(x) = \log_e(1 + e^x)$	$f'(x) = \frac{1}{1+e^{-x}}$

# Neural Networks: Non linear decision



Linear activation functions produce linear decisions no matter the network size



Non-linearities allow us to approximate arbitrarily complex functions

# Building Neural Networks with Perceptrons

A simplified perceptron:



$$z = w_0 + \sum_{j=1}^m x_j w_j$$

Because all inputs are connected to all outputs these are called Dense layers:



$$z_{\underline{i}} = w_{0,\underline{i}} + \sum_{j=1}^{m} x_j w_{j,\underline{i}}$$

# Single Layer Neural Network



$$z_i = w_{0,i}^{(1)} + \sum_{j=1}^m x_j w_{j,i}^{(1)} \quad \hat{y}_i = g\left(w_{0,i}^{(2)} + \sum_{j=1}^{d_1} g(z_j) w_{j,i}^{(2)}\right)$$

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# Single Layer Neural Network



$$z_{2} = w_{0,2}^{(1)} + \sum_{j=1}^{m} x_{j} w_{j,2}^{(1)}$$
  
=  $w_{0,2}^{(1)} + x_{1} w_{1,2}^{(1)} + x_{2} w_{2,2}^{(1)} + x_{m} w_{m,2}^{(1)}$ 

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# A deep neural network structure



$$z_{k,i} = w_{0,i}^{(k)} + \sum_{j=1}^{n_{k-1}} g(z_{k-1,j}) w_{j,i}^{(k)}$$

# (... or Cost Function or Objective Function)

Depends on the kind of problem.

- Regression  $\rightarrow$  Mean square error
- Classification  $\rightarrow$  Cross entropy, binary cross entropy.

$\operatorname{symbol}$	name	equation
$\mathcal{L}_1$	$L_1$ loss	$\ y - o\ _1$
$\mathcal{L}_2$	$L_2$ loss	$\ y - o\ _2^2$
$\mathcal{L}_1 \circ \sigma$	expectation loss	$\ \mathbf{y} - \sigma(\mathbf{o})\ _1$
$\mathcal{L}_2 \circ \sigma$	regularised expectation loss <sup>1</sup>	$\ y - \sigma(o)\ _{2}^{2}$
$\mathcal{L}_{\infty} \circ \sigma$	Chebyshev loss	$\max_{j}  \sigma(\mathbf{o})^{(j)} - \mathbf{y}^{(j)} $
hinge	hinge 13 (margin) loss	$\sum_{j} \max(0, \frac{1}{2} - \hat{\mathbf{y}}^{(j)} \mathbf{o}^{(j)})$
$hinge^2$	squared hinge (margin) loss	$\sum_{j}^{j} \max(0, \frac{1}{2} - \hat{\mathbf{y}}^{(j)} \mathbf{o}^{(j)})^2$
$hinge^{3}$	cubed hinge (margin) loss	$\sum_{j}^{j} \max(0, \frac{1}{2} - \hat{\mathbf{y}}^{(j)} \mathbf{o}^{(j)})^3$
log	log (cross entropy) loss	$-\sum_{i} \mathbf{y}^{(j)} \log \sigma(\mathbf{o})^{(j)}$
$\log^2$	squared log loss	$-\sum_{j}^{j} [\mathbf{y}^{(j)} \log \sigma(\mathbf{o})^{(j)}]^2$
$\tan$	Tanimoto loss	$\frac{-\sum_{j}\sigma(\mathbf{o})^{(j)}\mathbf{y}^{(j)}}{\ \sigma(\mathbf{o})\ _{2}^{2}+\ \mathbf{y}\ _{2}^{2}-\sum_{j}\sigma(\mathbf{o})^{(j)}\mathbf{y}^{(j)}}$
$\mathbf{D}_{\mathbf{CS}}$	Cauchy-Schwarz Divergence 3	$-\log \frac{\sum_{j} \sigma(\mathbf{o})^{(j)} \mathbf{y}^{(j)}}{\ \sigma(\mathbf{o})\ _2 \ \mathbf{y}\ _2}$

See: https://arxiv.org/pdf/1702.05659.pdfs

### Cross entropy loss can be used with models that output a probability between 0 and 1



Mean squared error loss can be used with regression models that output continuous real numbers



$$\begin{split} \boldsymbol{W}^* &= \operatorname*{argmin}_{\boldsymbol{W}} \frac{1}{n} \sum_{i=1}^n \mathcal{L} \big( f \big( \boldsymbol{x}^{(i)}; \boldsymbol{W} \big), \boldsymbol{y}^{(i)} \big) \\ \boldsymbol{W}^* &= \operatorname*{argmin}_{\boldsymbol{W}} J (\boldsymbol{W}) \end{split}$$







### We want to find the network weights that achieve the lowest loss



Take small step in opposite direction of gradient



# Algorithm

- 1. Initialize weights randomly  $\sim \mathcal{N}(0, \sigma^2)$
- 2. Loop until convergence:

3. Compute gradient, 
$$\frac{\partial J(W)}{\partial W}$$

4. Update weights, 
$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$$

5. Return weights

### How a small change in one weight affect the loss



# We apply chain rule



Repeat this for every weight in the network using gradients from later layers

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# Optimization through gradient descent

$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \, \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$$

# Optimization through gradient descent

$$W \leftarrow W - \eta \frac{\partial J(W)}{\partial W}$$
  
How can we set the learning rate?

# Gradient Descent Algorithms

### Algorithm

- SGD
- Adam
- Adadelta
- Adagrad
- RMSProp
- TF Implementation

  tf.keras.optimizers.SGD

  tf.keras.optimizers.Adam

  tf.keras.optimizers.Adadelta

  tf.keras.optimizers.Adadelta

  tf.keras.optimizers.RdSProo

### Reference

Kiefer & Wolfowitz. "Stochastic Estimation of the Maximum of a Regression Function." 1952.

Kingma et al."Adam: A Method for Stochastic Optimization." 2014.

Zeiler et al."ADADELTA: An Adaptive Learning Rate Method." 2012.

Duchi et al. "Adaptive Subgradient Methods for Online Learning and Stochastic Optimization." 2011.

# The problem of Overfitting



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- A technique that constraint the optimization problem to avoid complex models.
- We use it to improve the generalization on our model to unseen data.
- There are different kind of methods.

# During training randomly set some activations to 0.



During training randomly set some activations to 0.



To stop before having the opportunity to overfit by monitoring testing and training data.



### The Perceptron

- Structural building blocks
- Nonlinear activation functions

### Neural Networks

- Stacking Perceptrons to form neural networks
- Optimization through backpropagation

### Training in Practice

- · Adaptive learning
- Batching
- Regularization







# Neural Networks: The Zoo of topologies



# Neural Networks: The Zoo of topologies



- Feed Foward networks (alredy seen).
- Recurrent neural networks simple, LSTM, and GRU.
- Convolutional neural networks

# Topologies: Recurrent neural networks



# Topologies: Recurrent neural networks



- Recurrent neural networks are a class of neural networks that exploit the sequential nature of their input.
- Inputs could be: a text, a speech, time series, and anything else where the occurrence of an element in the sequence is dependent on the elements that appeared before it.

- ConvNets are a class of neural networks using convolutional and pooling operations for progressively learning rather sophisticated models based on progressive levels of abstraction.
- This learning via progressive abstraction resembles vision models that have evolved over millions of years inside the human brain.
- People called it deep with 3-5 layers a few years ago, and now it has gone up to 100-200.

# Convolutional Neural Networks.



### End to end to mapping from EBSD patterns to crystallographic orientations

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Where can we work?

Locally in Virtual env:

Main purpose of Python virtual env is to create an isolated environment for Python projects. Each project can have its own dependencies, regardless of what dependencies every other project has. https:

//realpython.com/python-virtual-environments-a-primer/

Google Cloud ML.

https://cloud.google.com/ai-platform/docs/
getting-started-keras

other Services

# About installation Local: What is Anaconda for?



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# We can use Scikit learn also...



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- From zero with math libraries and python.
- Using dedicated open source frameworks:
  - Tensorflow.
  - Keras.

# TensorFlow

Tensorflow is an end-to-end open source platform for machine learning. It has a comprehensive, flexible ecosystem of tools, libraries and community resources that lets researchers push the state-of-the-art in ML and developers easily build and deploy ML powered applications.

# K Keras

Keras: A high-level neural networks API, written in Python and capable of running on top of TensorFlow, CNTK, or Theano. It was developed with a focus on enabling fast experimentation. Being able to go from idea to result with the least possible delay is key to doing good research.

# Keras is now embedded in Tensorfow



### https://www.tensorflow.org/guide/keras/functional

- Modularity: A model is either a sequence or a graph of standalone modules that can be combined together like LEGO blocks for building neural networks
- The libraries predefines a large number of modules implementing different types of neural layers, cost functions, optimizers, initialization schemes, activation functions, and regularization schemes.
- Minimalism: The library is implemented in Python and each module is kept short and self-describing.
- Easy extensibility: The library can be extended with new functionalities.

# Keras Basics:

### Python For Data Science Cheat Sheet

Keras

Learn Python for data science Interactively at www.DataCamp.com

### Keras

Keras is a powerful and easy-to-use deep learning library for Theano and TensorFlow that provides a high-level neural networks API to develop and evaluate deep learning models.

### A Basic Example

A current computer (\* current computer \*\* from trans.layers import Beese \*\* from trans.tran

Your data needs to be stored as NumPy arrays or as a list of NumPy arrays. Ideally, you split the data in training and test sets, for which you can also resort to the train test split module of stearn.cross validation.

### Keras Data Sets

>>> (x train2,y train2), (x test2,y test2) = koston housing.load\_data()
>>> (x train3,y train3), (x test3,y test3) = cifarl0.load\_data()
>>> (x train4,y train4), (x bist4,y test4) = imb.load\_data(num\_sords=2010)
>>> num\_classes = 10

### Other

>>> fors urlib.request import urlopen >>> dats = mp.loadtxt(urlopen("http://archive.ics.uci.edu ml/machine-learning-databases/pina-indiana-diabetes/ pina-indiana-diabetes(dat"),delimiter=",") >>> x = data(:,0:8) >>> x = data(:,0:8)

### Preprocessing

### Sequence Padding

>>> from keras.preprocessing import sequence >>> x\_train4 = sequence.pad sequences(x\_train4,maxlen=80) >>> x\_test4 = sequence.pad sequences(x\_test4,maxlen=80)

### One-Hot Encoding

- >>> from keras.utils import to\_categorical
- >> Y\_train = to categorical(y\_train, num\_classes)
- >>> Y train3 = to categorically train3, num classes
- >>> Y\_test3 = to\_categorical(y\_test3, num\_classes)

### Model Architecture

### Sequential Model

>>> from keras.models import Sequential
>>> model = Sequential()
>>> model2 = Sequential()
>>> model3 = Sequential()

### (Multilayer Perceptron (MLP)

### Binary Classification

>>> model.add(Dense(6,kernel initializer='uniform',activation='relu')
>>> model.add(Dense(1,kernel\_initializer='uniform',activation='sigmoid'))

### multi-class classification

- >>> room kerss:sayers import propout >>> model.add(Oense(512,activation='relu',input\_shape=(784,))) >>> model.add(Dropout(0,2)) >>> model.add(Dropout(0,2)) >>> model.add(Oromout(0,2))
- >>> model.add(Dense(10,activation='softmax'))

### Regression

> model.add(Dense(64,activation='relu',input\_dim=train\_data.shape(1)))
> model.add(Dense(1))

### Convolutional Neural Network (CNN)

- >>>> from keras.layers import Activation,Conv2D,NaxPooling2D,Flatten >>> model2.add(Conv2D(32, (3, 3),padding='same',imput shape=x train.shape[1:1))
- >>> mode12.add(Conv2D(32, (3, 3), padding="
- bid model2.add(Activation(\*relu
- >>> model2.add(Conv2D(32,(3,3)))
  >>> model2 add(Activation('relu'))
- >>> model2,add(MaxPooling2D(pool size=(2,
- >>> model2.add(Dropout(0.251)
- >>> model2.add(Conv2D(64,(3,3), padding='same'))
- >>> model2.add(Activation('relu'))
- >>> mode12.add(Conv2D(64,(3, 3)))
- >>> model2.add(Activation('relu'))
- >>> model2.add(MaxPooling2D(pool\_size=(2,2))
  >>> model2.add(Dropout(0,25))
- >>> model2 add/Flatten())
- >>> mode12.add(Dense(512))
- >>> model2.add(Activation('relu
- >>> model2.add(Dropout(0.5))
- >>> model2.add(Dense(num\_classes)) >>> model2.add(Activation('softmaw'))

### Recurrent Neural Network (RNN)

- >>> from keras.klayers import Embedding,LSTM
  >>> model3.add(Embedding(20000,128))
  >>> model3.add(LSTM(128,dropout=0.2,recurrent\_dropou
  - model3.add(Dense(1,activation="sigmoid"))

### Also see NumPy & Scikit-Lear

### Train and Test Sets

- >>> from sklearn.model\_selection import train\_test\_split
  - x\_train5,x\_test5,y\_train5,y\_best5 = train\_test\_split(X, y)

test size+0.33, random states42

### Standardization/Normalization

>>> from sklearn.preprocessing import StandardScaler >>> scaler = StandardScaler().fit(x train2) >>> standardized X = scaler.transform(x train2) >>> standardized X test = scaler.transform(x test2)

### Inspect Model

>>> model.output\_shape
>>> model.summary()
>>> model.get\_config()
>>> model.get\_weights()

Model output shape Model summary representation Model configuration List all weight tensors in the model

### **Compile Model**

MLP: Binary Classification

MLP: Multi-Class Classification >>> model.compile(optimizer='rmsprop', loss='categorical\_crossentropy', metrics=''accuracy'l)

MLP: Regression >>> model.compile(optimizer='rmsprop',

loss='mse', metrics=['mse'])

### urrent Neural Network

### Model Training

odel3.fit(x\_train4, y\_train4, batch\_size=32

- epochs=15,
- erbose=1,

### **Evaluate Your Model's Performance**

>> score = model3.evaluate(x\_test, v\_test.

batch size=32

### Prediction

>> model3.predict[x\_test4, batch\_size=32)
>> model3.predict\_classes(x\_test4,batch\_size=32)

### Save/ Reload Models

>>> from keras.models import load\_model

>>> model3.save('model file.h5')
>>> mv model = load model('mv model.h'

### Model Fine-tuning

### Optimization Parameters

### Early Stopping

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cecilia.jarne@unq.edu.ar

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You can create a Sequential model by passing a list of layer instances to the constructor:

```
1
2 from keras.models import Sequential
3 from keras.layers import Dense,
        Activation
4
5 model = Sequential([
6      Dense(32, input_shape=(784,)),
7      Activation('relu'),
8      Dense(10),
9      Activation('softmax'),
10 ])
1
```

You can also simply add layers via the .*add*() method:

```
1 model = Sequential()
2 model.add(Dense(32, input_dim=784))
3 model.add(Activation('relu'))
```

https://github.com/katejarne/Keras\_tensorflow\_course Classes and material will be at: http://ceciliajarne.web.unq.edu.ar/cns-2020-tutorial/

- Deep Learning (The MIT Press Essential Knowledge series)
- http://introtodeeplearning.com/ MIT course.
- https://www.tensorflow.org/
- https://keras.io/ Francois Chollet et al. Keras. 2015.
- Martín Abadi, et al. TensorFlow: Large-scale machine learning on heterogeneous systems, 2015.