Neural Networks and Statistical Models: A Java Implementation

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Introduction An Artificial Neural Network is a *computational model* composed of a set of simpler and conceptually atomic sub-models called neurons, which goal is to simulate a biological brain, in particular the ability of this to learn. From a statistical point of view, Artificial Neural Networks (from here on, NN) are a wide class of nonlinear regression models, data reduction models, and *non-linear* dynamical systems.
Neurons consist in interconnected computing elements (i.e. a neuron may compute a linear combination of some inputs) and they are often organized into *layers*. For these reasons, it is convenient to graphically represent a NN through a directed graph, keeping in mind that represent a NN model means to represent a model that nothing has to do with *Bayesian Networks*, always represented through a directed (acyclic) graph.
The alleged "intelligence" of a NN is a matter of dispute, since networks, like many statistical methods, are capable of processing vast amounts of data and making predictions, but this does not make them "intelligent" in the usual sense of the word. What engineers and computer scientists call "learning" is just what it is called "estimation" in the statistical jargon.
Most of the NN models are similar or identical to statistical techniques such as generalized linear models, polynomial regression, principal components and cluster analysis, etc, but there are also a few NN models that have no precise statistical equivalent but may be useful for data analysis.
Although many NN models are similar or identical to well-known statistical models, the terminology in the NN literature is quite different from that in statistics. Here it follows a brief table which explain such a difference.

Statistical Jargon	**NN Jargon**
Variables	Features
Independent Variable	Inputs
Predicted Values	Outputs
Dependent Variables	Targets
Residual	Errors
Estimation	Training, Learning
Estimation Criterion	Error Function
Observations	Patterns
Parameter Estimates	Synaptic Weights
Interactions	Higher-Order neurons
Transformations	Functional Links
Regression	Supervised Learning
Data reduction	Unsupervised Learning
Cluster Analysis	Competitive Learning
Interpolation and Extrapolation	Generalization

Terms like *sample* and *population* does not have NN equivalents, but data are often divided into a *training set* and *test set* for cross-validation.

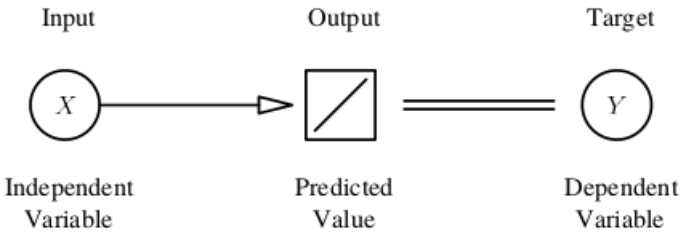
NN and Linear Regression Model Linear regression models are simple statistical models used to predict the expected value of a *dependent variable* $\mathbf{Y}$ given a set of *observed variables* $\mathbf{X}$. The model is the following:

$$\mathbf{Y}_i = \beta_0 + \beta_1 \mathbf{X}_i + \varepsilon_i$$

Where i variates between 1 to N where N is the number of observations, $\mathbf{Y}_i$ is the dependent variable, $\mathbf{X}_i$ is the independent variable, $\beta_0 + \beta_1 \mathbf{X}_i$ is the regression line and ε_i is the statistical error. Parameters β_0 and β_1 are called respectively the intercept and the angular coefficient of the regression line, and they must be estimated in order to have a reliable prediction of the $\mathbf{Y}$. To perform this task, it is often used the *ordinary least square* method. S is defined as:

$$S(\beta_0, \beta_1) = \sum_{i=1}^{N} (y_i - \beta_0 - \beta_1 \mathbf{X}_i)^2$$

S is a function from $\mathbb{R}^2 \to \mathbb{R}$ and parameters β_0, β_1 are estimated as the arguments of S on which the function evaluates to its minimum.
Consider the following NN:



Boxes represent values computed as a function of one or more arguments, the symbol inside the box indicate the type of the function (in this case, it is a linear combination of the input).
Arrows indicate that the source of the arrow is an argument of the function computed at the destination of the arrow, and usually each arrow has a corresponding *weight* (parameter in statistical jargon) to be estimated.
Two long parallel lines indicate that the values at each end are to be fitted by the ordinary least square method, or some other estimation criterion.
Such a NN represents the Linear Regression Model in the NN Jargon.

Logistic Regression: Perceptrons A perceptron is a very small NN, composed by more than one neuron, and it usually computes a linear combination of the inputs. A perceptron has $n > 0$ input. Each input has a specific *weight* β_i. The *weights* are the parameters to be estimated. More generally, the output of a perceptron is an evaluation of an *activation function* on the provided inputs. Activation functions are usually *bounded*. A bounded function maps any real input to a bounded range. Bounded activation functions are called *squashing functions*, for instance the logistic function:

$$\texttt{act}(x) = \frac{1}{1 + e^{-x}}$$

Maps any real argument to the range $(0, 1)$:

$$\lim_{x \to +\infty} \frac{1}{1 + e^{-x}} = \lim_{x \to +\infty} \frac{1}{1 + \frac{1}{e^x}} = \frac{1}{1 + 0} = 1$$

$$\lim_{x \to -\infty} \frac{1}{1 + e^{-x}} = \lim_{x \to +\infty} \frac{1}{1 + e^{x}} = \frac{1}{\infty} = 0$$

What a perceptron is supposed to do is, given $\mathbf{x}$ as an input, and assuming the logistic function as the activation function is to compute $\hat{x} = \sum_{i=1}^{N} \beta_i \mathbf{X}_i$ and return $\texttt{act}(\hat{x}) = \frac{1}{1 + e^{-(\beta_1 \mathbf{X}_1 + \cdots + \beta_n \mathbf{X}_n)}}$.
Notice that

$$\frac{1}{1 + e^{-(\beta_i \mathbf{X}_i + \cdots + \beta_n \mathbf{X}_n)}} = \frac{e^{(\beta_i \mathbf{X}_i + \cdots + \beta_n \mathbf{X}_n)}}{1 + e^{(\beta_i \mathbf{X}_i + \cdots + \beta_n \mathbf{X}_n)}}$$

The *logisitc regression model* is a *non-linear* regression model used when the dependent variable is dichotomic. The model formula is the following:

$$\mathbb{E}(\mathbf{Y}|\mathbf{X}) = \frac{e^{\beta_0+\beta_1 x_1+\cdots+\beta_n x_n}}{1+e^{\beta_0+\beta_1 x_1+\cdots+\beta_n x_n}}$$

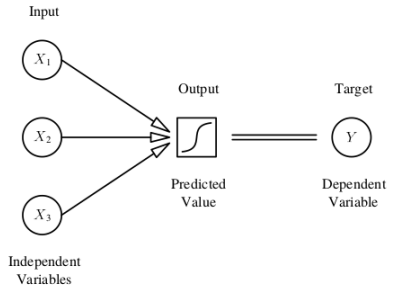
That is, exactly, what a perceptron with a logistic activation function computes. In order to estimate the β_i parameters we have two options:

- Maximum likelihood method
- Gradient descent method

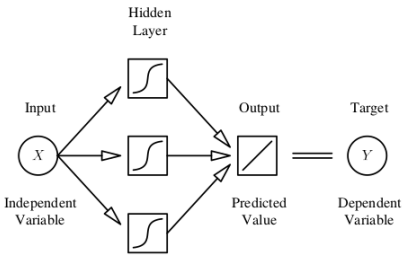
The gradient descent method is an optimization algorithm which aims to estimate parameters given a set of pairs `input - expected output` (the training set). The goal here is to minimize

$$\sum\sum r_j^2$$

Where the r_j is the difference between the expected output and the predicted value.
The following perceptron with a logistic activation function is a logistic regression model:



Nonlinear Regression: Multilayer Perceptrons In the introduction section, it is exposed that neurons are often organized into *layers*. NN seen before are simple perceptrons composed of two layers: the input layer and the output layer. If it is introduced another *hidden* layer between input and output, you obtain a multi-layer perceptron (MLP).
If the model includes estimated weights between the inputs and the hidden layer, and the hidden layer uses nonlinear activation functions such as the logistic function, the model becomes nonlinear.



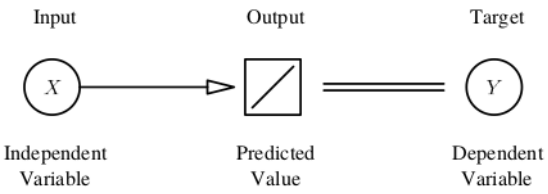
This is a simple MLP implementing a non linear regression model:

$$\mathbf{Y} = f(\mathbf{X}) + \mathbf{b}$$

MLP are general-purpose, flexible, nonlinear models that can approximate virtually any function to any desired degree of accuracy. MLP are called *universal approximators* and they can be used when you have little knowledge about the relationship between the independent and dependent variables.

Java Implementation Start from the linear regression model:

$$\mathbf{Y}_i = \beta_0 + \beta_1 \mathbf{X}_i + \varepsilon_i$$



Suppose it is $\varepsilon_i = 0$. Consider the following class:

```
public class Neuron {
private double b0,b1;

public double predict(double x) {
    return b0 + b1*x;
}
public static void main(String[] args) {
    Neuron y = new Neuron();
    System.out.println(y.predict(7));
}
}

```

It is clear that the output provided by the execution of this code it is `0.0`, and it is due to the fact that the β_0, β_1 parameters are not yet estimated. It is known that β_0, β_i are estimated as the minima of the function

$$S(\beta_0, \beta_1) = \sum_{i=1}^{N} (y_i - \beta_0 - \beta_1 x_i)^2$$

As it is known in the mathematical analysis theory, it is possible to find the minima setting the partial derivatives equal to zero:

$$\frac{\vartheta S}{\vartheta \beta_0} = -2 \sum_{i=1}^{N} (y_i - \beta_0 - \beta_1 x_i) = 0, \quad \frac{\vartheta S}{\vartheta \beta_1} = -2 \sum_{i=1}^{N} (y_i - \beta_0 - \beta_1 x_i) x_i = 0$$

From which the following solutions are derived:

$$\beta_1 = \frac{\sigma(x,y)}{\sigma^2(x)}, \quad \beta_0 = \overline{y} - \beta_1 \overline{x}$$

Where x_i is the $i-th$ observation for which it is known a-priori the dependant variable value y_i;
$\sigma(x,y)$ is the covariance between variables $\mathbf{X}, \mathbf{Y}$;
$\sigma^2(x)$ is the observed variance of the variable $\mathbf{X}$;
$\overline{x}, \overline{y}$ are respectively the observed mean of the variable $\mathbf{X}$ and the observed mean of the variable $\mathbf{Y}$.
It is needed to extend the code adding the following piece of code:

```
public void estimateParameters(double[] xi, double[] yi) {
    b1 = var(xi,yi) / var(xi,xi);
    b0 = mean(yi) - b1*mean(xi);
}
private double mean(double[] v) {
    double m = 0;
    for(int i=0; i<v.length;i++) {
        m+=v[i];
    }
    return m/v.length;
}
```

```
private double var(double[] x, double[] y) {
    double var = 0;
    double mx = mean(x);
    double my = mean(y);
    for(int i=0; i<x.length;i++) {
        var+= (x[i]-mx)*(y[i]-my);
    }
    return var/x.length;
}
```

Suppose it exists a sample $\mathbf{X}$ for which it is known that all the values of the dependent variable $\mathbf{Y}$ are on the bisector of the second quadrant of the Cartesian plane:

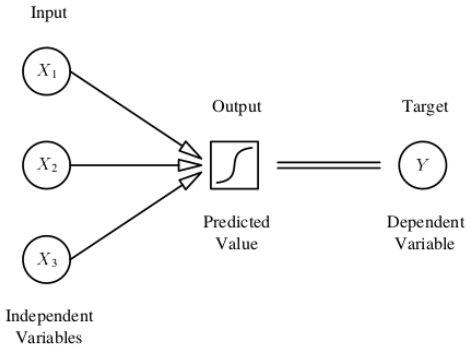
$$\mathbf{X} = \{X_i\} = \{1,2,3,4,5\} \quad \mathbf{Y} = \{Y_i\} = \{1,2,3,4,5\}$$

```
Neuron y = new Neuron();
y.estimateParameters(new double[]{1,2,3,4,5}, new double[]{1,2,3,4,5});
System.out.println(y.predict(7));
System.out.println("Y=" + y.b0 + "+" + y.b1+"X");
```

As it is expected, even if in the *training set* does not appear the expected output for value 7, our linear regression model is able to predict the output for such a value: `7.0`. In fact the regression line is exactly the requested identity function:

```
Y = 0.0 + 1.0X
```

Consider now the logistic regression perceptron model:



The code must be modified in order to implement a logistic regression model:

```
public class Neuron {
    private double[] weights;
    public Neuron(int n_inputs) {
        weights = new double[n_inputs];
    }
    private double logistic(double x) {
        return 1 / (1 + Math.exp(-x));
    }
    public double predict(double[] inputs) {
        double sum = 0;
        for (int i = 0; i < inputs.length; i++) {
            sum += weights[i] * inputs[i];
        } return logistic(sum); } }
```

Now there is an array of weights to be approximated, and the prediction is performed by applying the logistic function to the linear combination of the given inputs. Since weights are all zero by default, every invocation on the `predict()` method evaulates to `0.5` because

$$\frac{1}{1+e^0} = \frac{1}{2} = 0.5$$

Now the job is to modify the `estimateParameter()` method seen before in order to estimate weights using the gradient descent method:

```
public void estimateParameters(double[][] xi, double[] yi) {
    double[] gradient = new double[weights.length];
        for (int i = 0; i < xi.length; i++) {
            for (int j = 0; j < xi[0].length; j++) {
                gradient[j] += (double) xi[i][j] *
                 (yi[i] - predict(xi[i]));
            }
        }
    for (int j = 0; j < weights.length; j++)
        weights[j] += gradient[j];
}
```

Note that the logistic function has a "friendly" derivative that permit us to compute its gradient in such an easy way. Consider this piece of python code:

```
import math
b0 = -1
b1 = -2
squash = lambda x: math.exp((b0*x[0]+b1*x[1]))/(1+math.exp((b0*x[0]+b1*x[1])))
print squash([1,0])
print squash([0,1])
print squash([0,0])
print squash([1,1])
```

Executing it, it is possible to generate data from the logistic function:

$$f(\mathbf{x}) = \frac{e^{-x_1-2x_2}}{1+e^{-x_1-2x_2}},$$

Obtaining:

$f(1,0) \approx 0.2689414213699951, f(0,1) \approx 0.11920292202211755, f(0,0) = 0.5, f(1,1) \approx 0.04742587317756679$

It is possible now to train this simple network with such data:

```
Neuron n = new Neuron(2);
double[][] in = {{1,0},{0,1},{0,0},{1,1}};
double[] out = {0.2689414213699951,0.11920292202211755,0.5,0.04742587317756679};
for(int i=0; i<10000;i++)
    n.estimateParameters(in, out);
System.out.println(Arrays.toString(n.weights));
```

Obtaining the following coefficients:

```
[-1.0000000000000004, -1.9999999999999993]
```

Which are approximately the β_0, β_1 used to generate data. Here it follows a simple trial:

```
public static void main(String[] args){
    Neuron n = new Neuron(2);
    //estimate parameters as above
    System.out.println(n.predict(new double[] {17,21}));
}
```

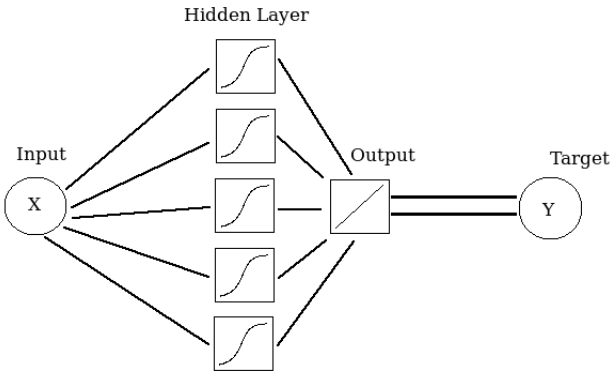
```
2.3802664086944176E-26
```

And the python output which computes the exact function we are approximating is:

```
print squash([17,21])
2.3802664086944176E-26
```

As expected, the two outputs are the same.
Consider the following *truth table*:

x_1	x_2	$x_1 \oplus x_2$
0	0	0
0	1	1
1	0	1
1	1	0



This is known as the logical operator *xor*. A Neural Network is capable to learn the *xor* computation of two logical variables.
Consider the NN model shown above. This is a MLP, or *universal approximator*. The aim is to modify the provided code in order to implement such a MLP which is able to learn to compute the *xor*.
Start from the Neuron class[1]:

```
public class Neuron {
    public double[] weights;
    public double[] inputs;
    public double output;
    public Neuron(int n_inputs) {
        weights = new double[n_inputs];
        for(int i = 0; i < n_inputs; i++)
            weights[i] = Math.random();
    }
    private double logistic(double x) {
        return 1/(1+Math.exp(-x));
    }
    public double predict(double[] inputs) {
        this.inputs = inputs;
        double sum = 0;
        for(int i=0; i<inputs.length;i++) {
            sum += inputs[i] * weights[i];
        }
        this.output = logistic(sum);
    return output;
    }
}
```

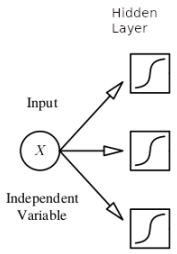
The main modification is that the `estimateParameters()` method will be moved in another class. Now a Neuron does also keep track of the provided inputs, this will be useful when it will be implemented the *back-propagation algorithm*, an algorithm which estimate weights aiming to minimize the error between the predicted output and the desired output using the *descent gradient* principle.
Since MLPs have more than one layer, it is needed to define, from a programming point of view, what a layer is: a collection of Neurons.

```
public class NeuronLayer {
    public Neuron[] neurons;
    public NeuronLayer(int n, int inputsPerNeuron) {
        this.neurons = new Neuron[n];
        for (int i = 0; i < n; i++) {
            this.neurons[i] = (new Neuron(inputsPerNeuron));
        }
    }
    public double[] feedForward(double[] inputs) {
        double[] outputs = new double[neurons.length];
        for (int i = 0; i < neurons.length; i++) {
```

[1]The information hiding principle has been completely ignored, in order to simplify the code

```
            outputs[i] = (neurons[i].predict(inputs));
        }
        return outputs;
    }
    public double[] getOutputs() {
        double[] outputs = new double[neurons.length];
        for (int i = 0; i < neurons.length; i++) {
            outputs[i] = neurons[i].output;
        }
        return outputs;
    }
}
```

In this class it is defined the number of neurons the layer is composed of, the inputs that each neuron will handle (equivalently, the length of the vector of weights to estimate for each neuron) and two methods: the `feedForward()` which is a generalization of the `predict()` method defined for each neuron, and it returns a collection of prediction computed by each neuron; and the `getOutputs()` which simply collects each neuron's output without providing them of any input. The scope here is clear, we have implemented the MLP's hidden layer with a variable amount of hidden neurons:



Putting layers together means to construct a MLP Neural Network.

```
public class NeuralNetwork {
    private int n_in,n_hid,n_out;
    private NeuronLayer hidden,output;
    public NeuralNetwork(int inputNeurons,int hiddenNeurons,int numberOfOutputs){
        n_in = inputNeurons;
        n_hid = hiddenNeurons;
        n_out = numberOfOutputs;
        hidden = new NeuronLayer(n_hid, n_in);
        output = new NeuronLayer(n_out, n_hid);
    }
}
```

The MLP must be capable of performing prediction:

```
public double[] feedForward(double[] inputs) {
    double[] hidden_outputs = hidden.feedForward(inputs);
    return output.feedForward(hidden_outputs);
}
```

Last, the MLP must be capable of being trained in order to estimate neurons weights:

```
    public void train(double[] training_in, double[] training_out) {
    feedForward(training_in);
    double[] deltaWrtOut = new double[n_out];
    for (int i = 0; i < n_out; i++) {
        double target_output = training_out[i];
        double actual_output = output.neurons[i].output;
        double deltaWrtInput = -(target_output - actual_output) * actual_output *
    (1 - actual_output);
        deltaWrtOut[i] = deltaWrtInput;
    }
    double[] deltaWrtHid = new double[n_hid];
    for(int i=0; i<n_hid;i++) {
        double deltaWrtHiddenOut = 0;
        for(int j=0; j<n_out;j++) {
```

```
            deltaWrtHiddenOut+=deltaWrtOut[j] * output.neurons[j].weights[i];
        }
        double actual_output = hidden.neurons[i].output;
        double deltaWrtIn = actual_output * (1 - actual_output);
        deltaWrtHid[i] = deltaWrtHiddenOut * deltaWrtIn;
    }
    for (int i = 0; i < n_out; i++) {
        for (int j = 0; j < n_hid; j++) {
            double act_input = output.neurons[i].inputs[j];
            double deltaWrtWeight = deltaWrtOut[i] * act_input;
            output.neurons[i].weights[j] -= deltaWrtWeight;
        }
    }
    for (int i = 0; i < n_hid; i++) {
        for (int j = 0; j < n_in; j++) {
            double act_input = hidden.neurons[i].inputs[j];
            double deltaWrtWeight = deltaWrtHid[i] * act_input;
            hidden.neurons[i].weights[j] -= deltaWrtWeight;
        } } }
```

The logic of the method shown above is the logic of the *back-propagation algorithm*. Another method is added in order to compute the total network error with respect to a training set:

```
public double totalError(double[][][] training_sets) {
    double err = 0;
    for (int i = 0; i < training_sets.length; i++) {
        double[] t_in = training_sets[i][0];
        double[] t_out = training_sets[i][1];
        double[] act_out = feedForward(t_in);
        for (int j = 0; j < act_out.length; j++) {
            double target_output = t_out[j];
            double actual_output = output.neurons[j].output;
            double squareError = 0.5 * Math.pow(target_output - actual_output, 2);
            err += squareError;
        }
    }
    return err;
}
```

Now the model is ready to being trained and used. Start from constructing the model shown at the top of this section. It has 2 inputs, 5 hidden neurons, 1 output:

```
NeuralNetwork nn = new NeuralNetwork(2, 5, 1);
```

Define the training sets as defined in the *xor* table of truth:

```
double[][][] training_sets = {
{{0, 0}, {0}},
{{0, 1}, {1}},
{{1, 0}, {1}},
{{1, 1}, {0}}
};
```

Train the network:

```
System.out.println("Error before training: "+nn.totalError(training_sets));
for (int i = 0; i < 20000; i++) {
    int randIndex = (int) (Math.random() * training_sets.length);
    double[] t_in = training_sets[randIndex][0];
    double[] t_out = training_sets[randIndex][1];
    nn.train(t_in, t_out);
}
System.out.println("Error after training: "+nn.totalError(training_sets));
```

And this is the output:

```
Error before training: 0.7825167086789118
Error after training: 0.0019131802708672071
```

What it is implemented is a MLP which performs a *xor* approximation using the statistical model *non-linear regression*. If you try to train the MLP with other datasets which arise from

considering other functions than the *xor*, such as the *and*, *nand*, etc, the MLP will approximate them with the same degree of accuracy. Here it follows a `main()` example. [2]

```
public static void main(String[] args) {
    double[][][] training_sets = {
    {{0, 0}, {0}},
    {{0, 1}, {1}},
    {{1, 0}, {1}},
    {{1, 1}, {0}}
    };
    NeuralNetwork nn = new NeuralNetwork(2, 5, 1);
    System.out.println("Before training");
    makePredictions(nn);
    //perform training as before
    System.out.println("After training");
    makePredictions(nn);
}
private static void makePredictions(NeuralNetwork nn) {
    double[] prediction = nn.feedForward(new double[] {0,0});
    System.out.println("0 xor 0 = " + Arrays.toString(prediction));
    prediction = nn.feedForward(new double[] {0,1});
    //... and so on
}
```

```
Before training
0 xor 0 = [0.8259446970943887]
0 xor 1 = [0.8743300669508968]
1 xor 0 = [0.8715849495984895]
1 xor 1 = [0.9057890050448435]

After training
0 xor 0 = [0.03292275347937093]
0 xor 1 = [0.9742047963078706]
1 xor 0 = [0.9755612350006293]
1 xor 1 = [0.020623955109387932]
```

Conclusions In this study, based on the paper "Neural Networks and Statistical Model" by Warren S. Sarle, I illustrated the similarities between models of artificial neural networks and some known statistical regression models. Artificial neural networks are nothing more than a technical implementation of these theoretical models of estimation. The purpose of a regression model is to infer a function that is as close as possible to the real function that generated a certain set of data, always assuming that this function exists. Therefore, what is called "intelligence" of a Neural Network, is the degree of accuracy with which a certain regression model can approximate a distribution from which the data is assumed to be observed. My opinion is that the assumption underlying these models is very heavy, and we are still far away from a true reproduction of human intelligence. Moreover, when any artificial intelligence system is used, the questions we have to ask are:

- Does a precise distribution for the data we have observed really exist?
- How was the sample formed?

These questions impose some important ethical consideration, since artificial intelligence systems are often used to profile human beings, as for example in the USA when the COMPAS software has been used by the Florida Supreme Court, to decide whether, after an interview to the suspect, it had to be kept in custody, and what the ransom was supposed to be.
Last, starting from the simple linear regression model, I implemented step by step a small Neural Network able to compute the xor of two Boolean variables, in Java language.

[2] The entire code is available at:
https://github.com/alexfoglia1/MASL/tree/master/exam/JavaNN/src