First Principles of ML

A Peek Inside the 'Black Box' of Machine Learning

Jack Fraser-Govil
The Wellcome Sanger Institute, Hinxton, UK
15th October 2024

Why bother?

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FOLKLORE

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- (Explainability!)

Today's Agenda

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- Classic Perceptron

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As we progress you will slowly build up your own ML toolkit, built entirely from scratch!

A Warning

There will be equations.

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You will need to know what they mean!

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Please, please, please, ask if you want clarification on the underlying mathematics and theory! That's why you're here today!

Part 1
The Perceptron

Basic Decision Making: Defining Cuteness

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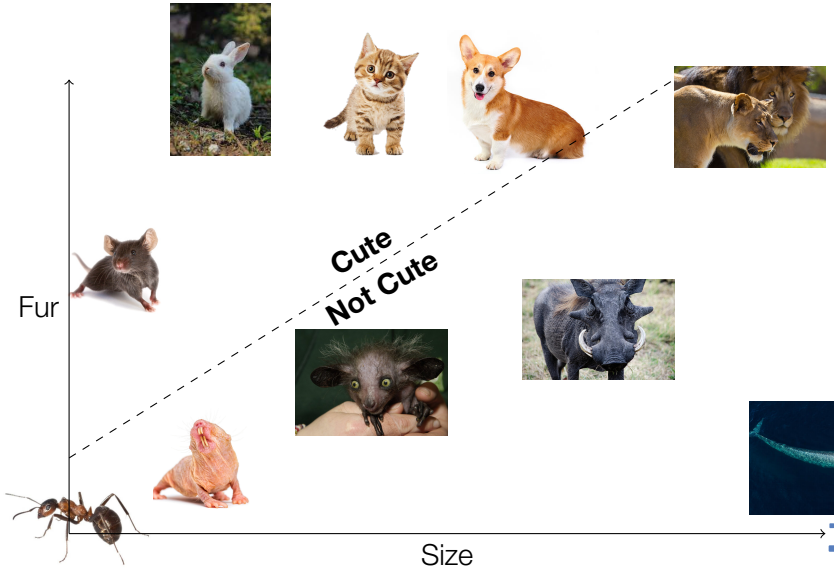

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Question: Why then do we need $N + 1$ dimensions?

The Perceptron

We need 3 parameters to define a **directional line**. The Perceptron classifier algorithm is:

$$P(\mathbf{x}) = \begin{cases} 1 & \text{if } \tilde{\mathbf{x}} \cdot \mathbf{w}^1 > 0 \\ 0 & \text{else} \end{cases} \tag{1}$$

[1] The dot/inner product is covered in Section 3.1 in the notes

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$\mathbf{w}$ are the **weights**.

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Exercise 1: Perceptron Classifier

Using the provided class structure & weights, write a perceptron classifier for the cuteness data.
The provided weights classify only one animal correctly. Which is it?

Training A Perceptron

Training a perceptron is easy. Loop over the data, make a prediction (P), compare it to the truth (T) and if it is wrong:

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$$\mathbf{w} \rightarrow \mathbf{w} + r \times (T - P)\, \tilde{\mathbf{x}} \tag{2}$$

This works because it always makes $\mathbf{w} \cdot \tilde{\mathbf{x}}$ move closer towards zero (and hence to the tipping point of altering its decision).

Exercise 2: Train Your Perceptron

Write the Train() method of your Perceptron. Run it on the cuteness data.

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Write the Train() method of your Perceptron. Run it on the cuteness data.
How long does it take to train to 100% accuracy?

Exercise 3: The Limits of Linearity

Add in more data – what goes wrong?

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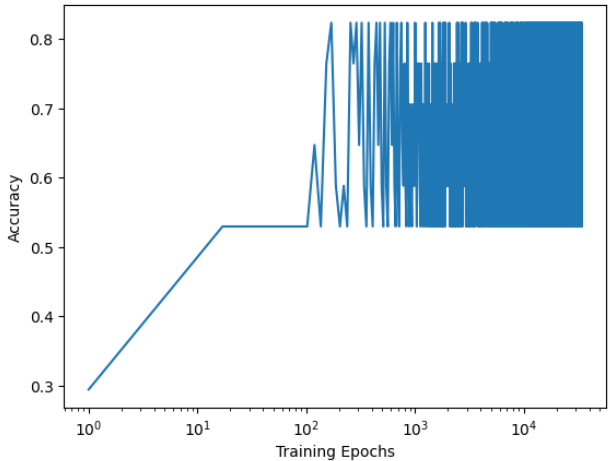

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Exercise 3: The Limits of Linearity

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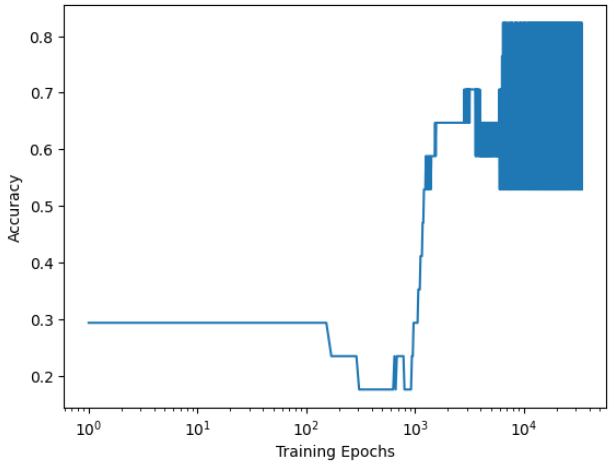

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The Nonlinear Perceptron

Eminently possible to have a non-linear perceptron.

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Eminently possible to have a non-linear perceptron.
Pass $\mathbf{x}$ through a non-linear transform to make it:

$$\mathbf{x}' = \begin{pmatrix} 1 \\ x \\ y \\ x^2 \\ \sin(x) \\ x^2 \exp(y) \\ \cos(\sin(\exp(\sin(\log(x^2 + 9xy))))) \\ \vdots \end{pmatrix} \tag{3}$$

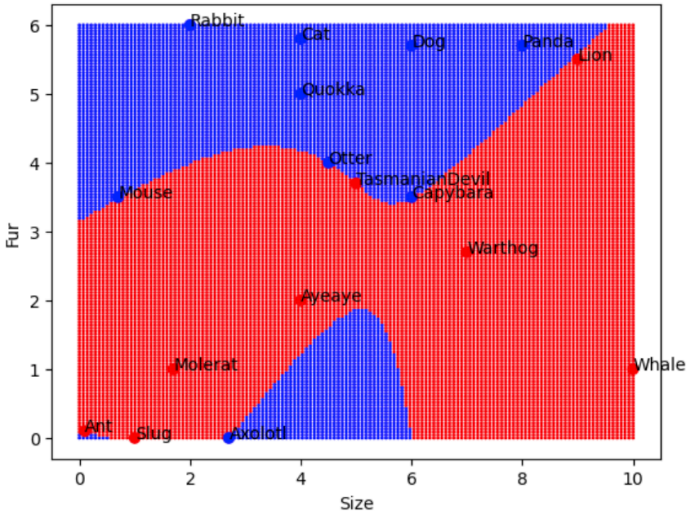
The Nonlinear Perceptron

Here is the results of a perceptron where:

$$\mathbf{x}'(x,y) = \begin{pmatrix} 1 & x & y & x^2 & xy & y^2 & x^3 & x^2y & xy^2 & y^3 & x^4 & x^3y & x^2y^2 & xy^3 & y^4 \end{pmatrix}^\intercal \tag{4}$$

Bonus Question: Why did I choose this?

The Nonlinear Perceptron



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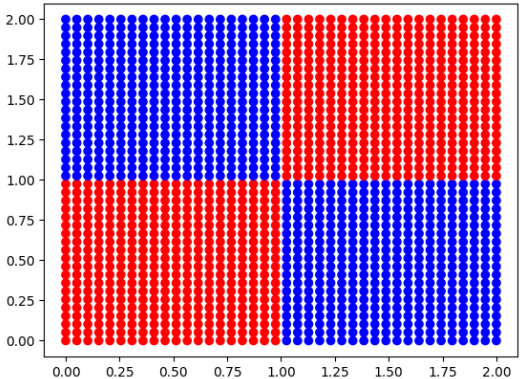
The Limits of NonLinearity

Target



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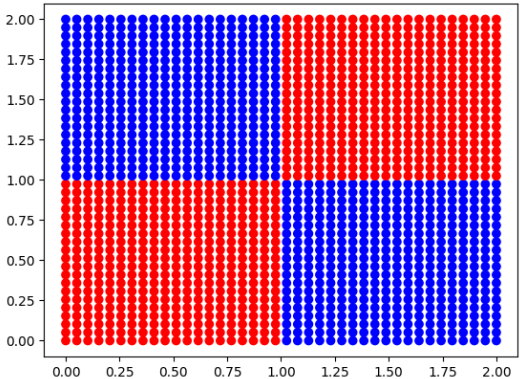
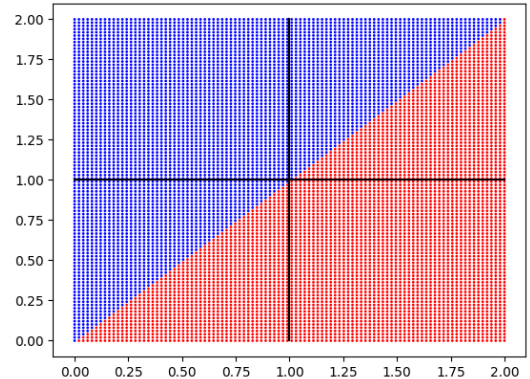


Reality (1st Order - 3 parameters)



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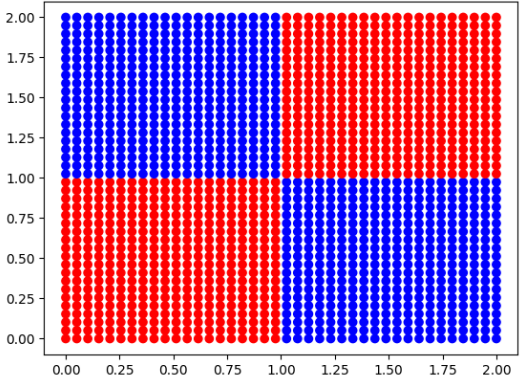
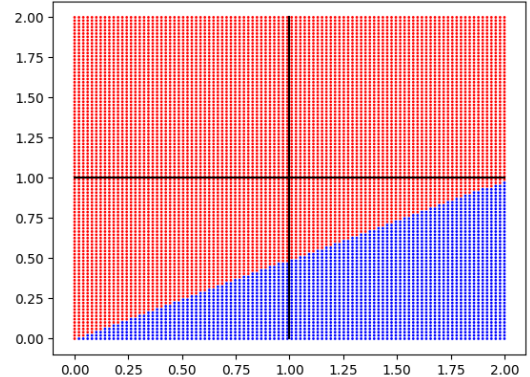


Reality (2nd Order - 6 parameters)



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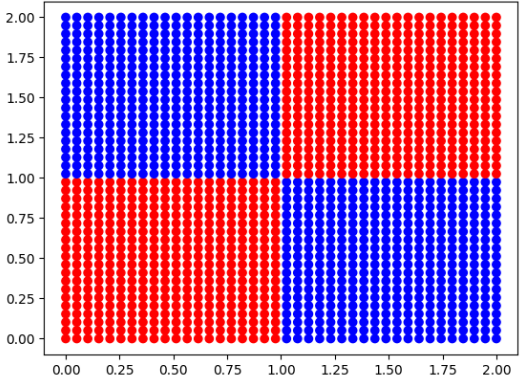
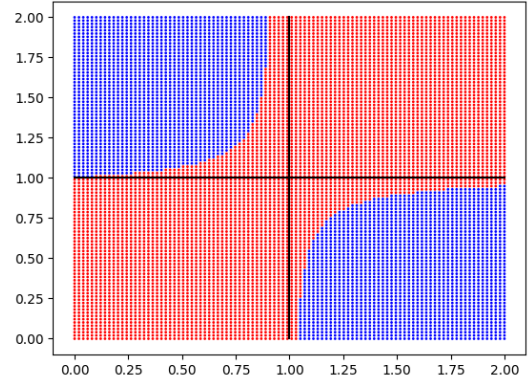


Reality (3rd Order - 10 parameters)



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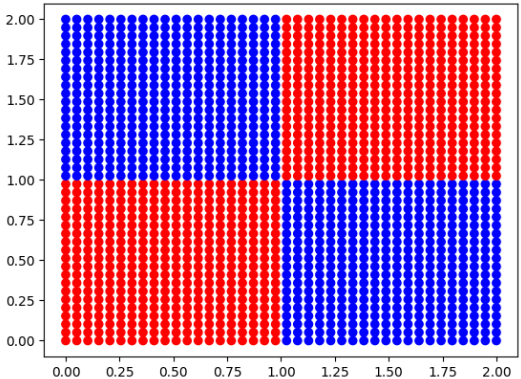
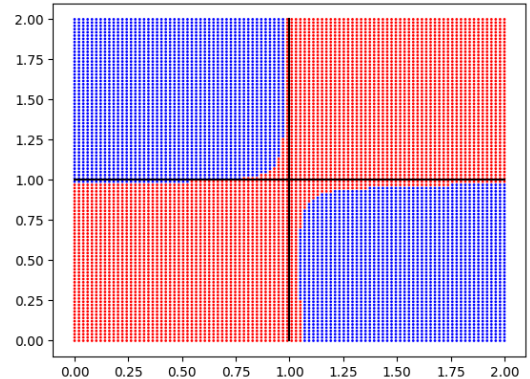


Reality (4th Order - 15 parameters)



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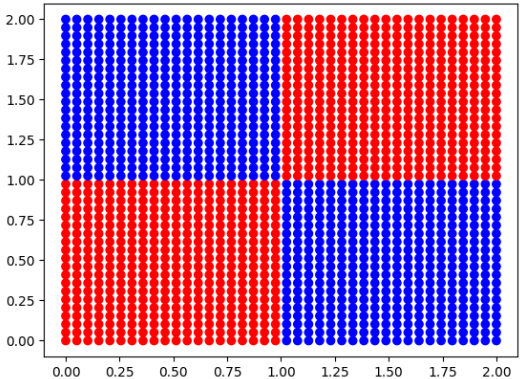
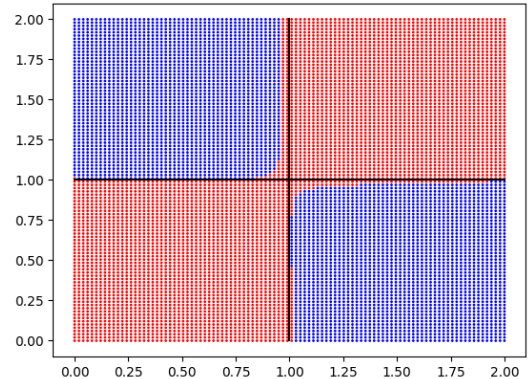


Reality (5th Order - 21 parameters)



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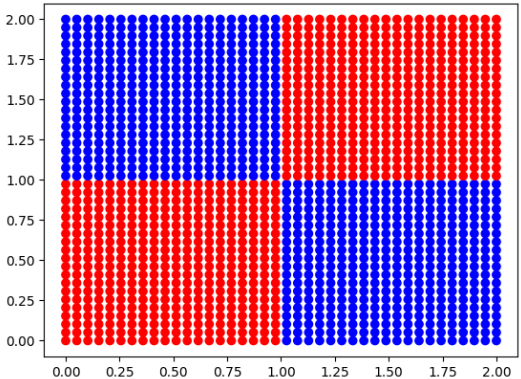

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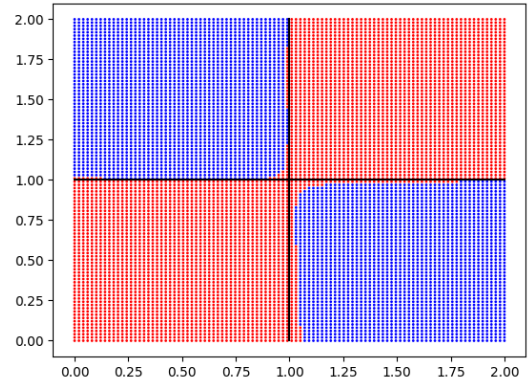

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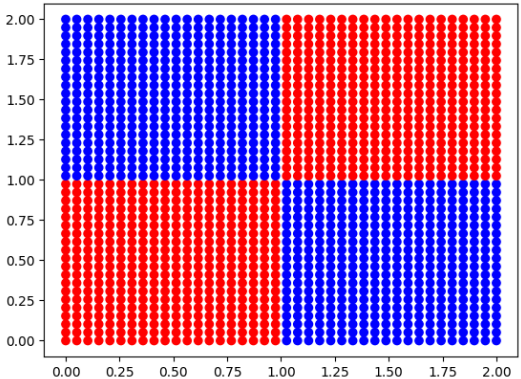
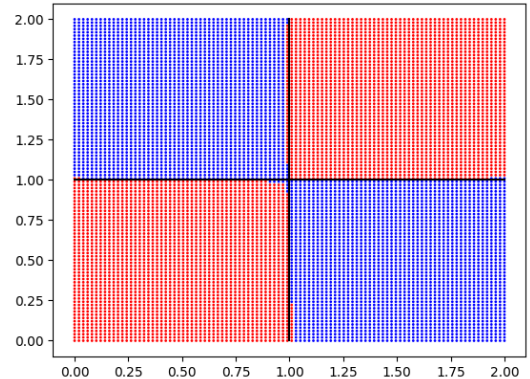


Reality (20th Order - 231 parameters)



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What do to?

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MORE!

The Multilayered Perceptron

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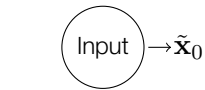
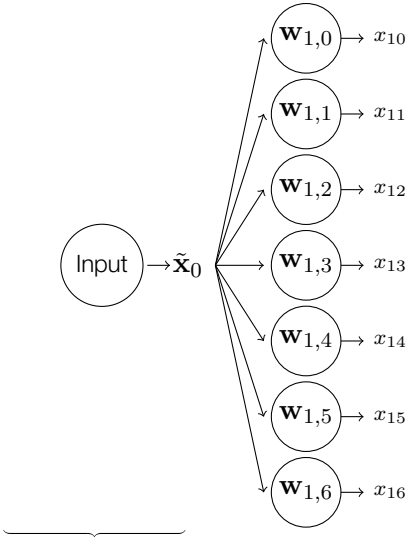


Input layer

The Multilayered Perceptron



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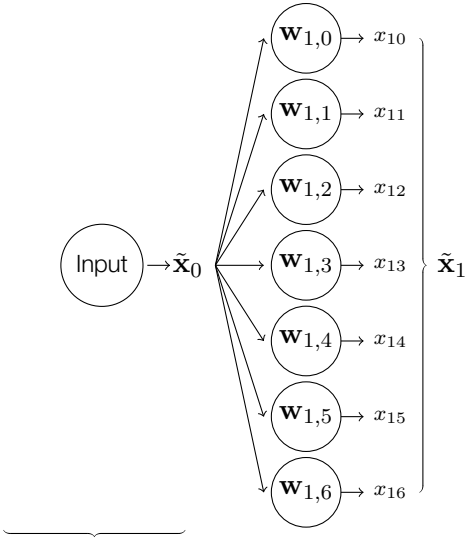

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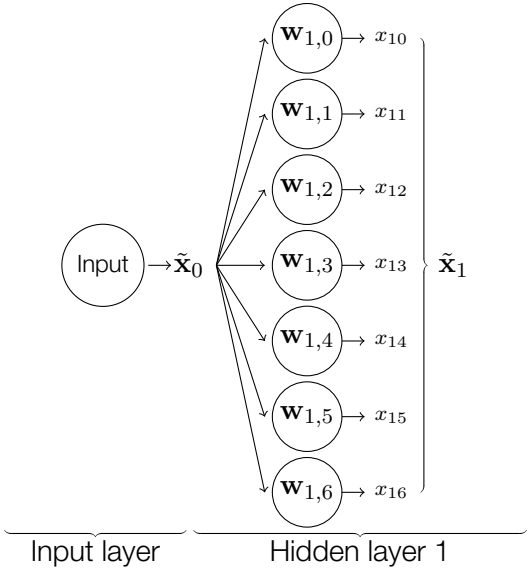
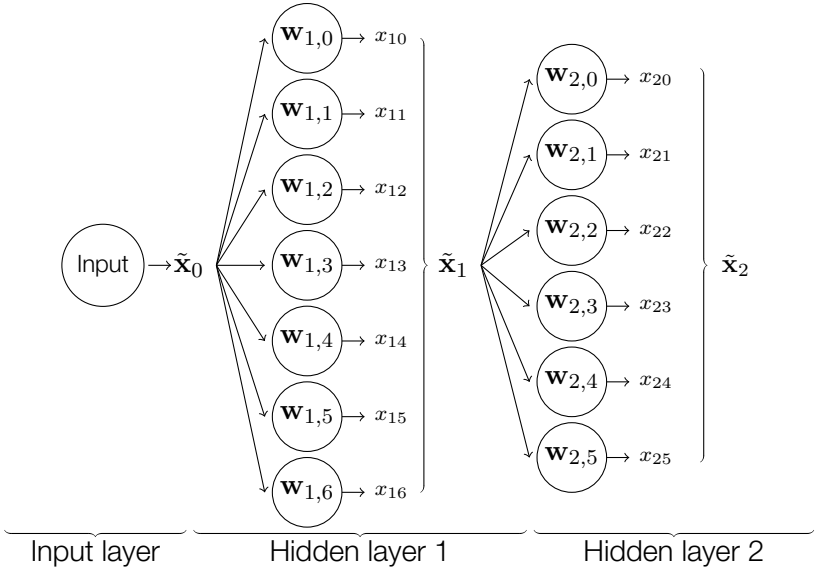


The Multilayered Perceptron



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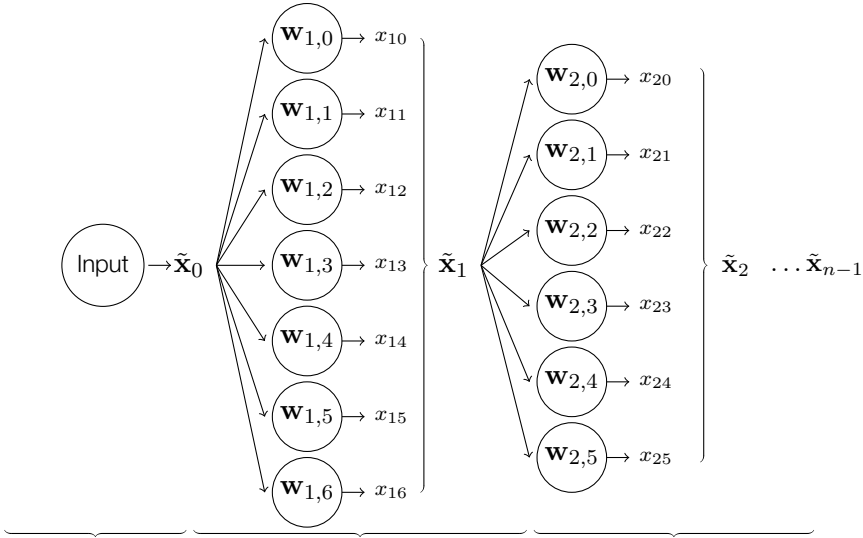

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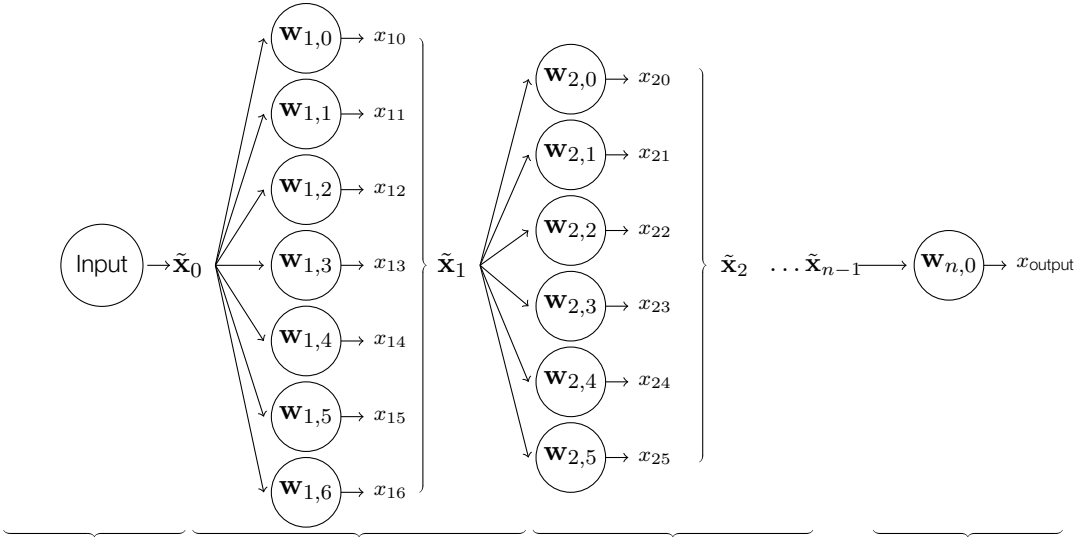

Exercise 4: The Multilayered Perceptron

I have provided the skeleton of a Node, Layer and Network class.

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I have provided the skeleton of a Node, Layer and Network class.

Fill them in so that you can construct and operate a network.

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Do you notice anything odd about how this predictor behaves?

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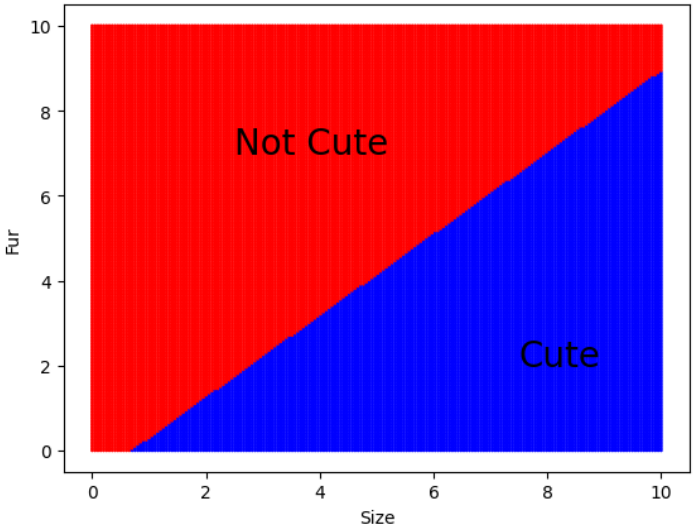
Fill them in so that you can construct and operate a network.

Do you notice anything odd about how this predictor behaves?

(For now: randomly initialise your weights)

All that for nothing?

If everything went well, you should see something like this:



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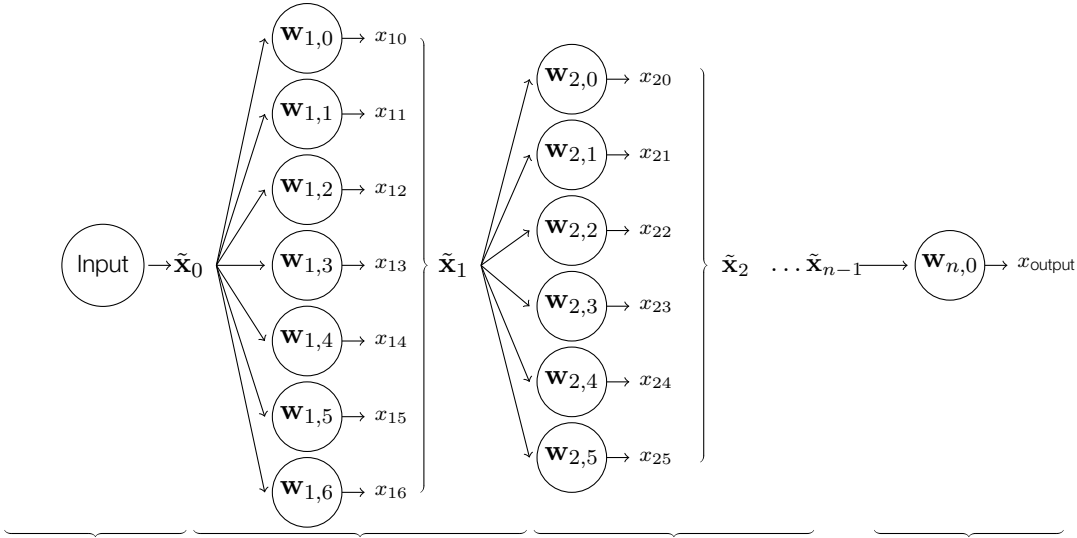
Affine Mess We Find Ourselves in



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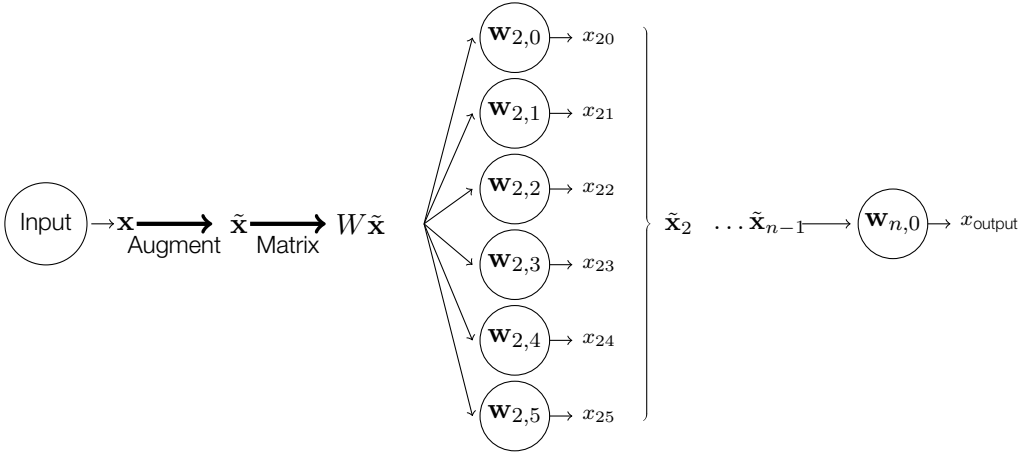

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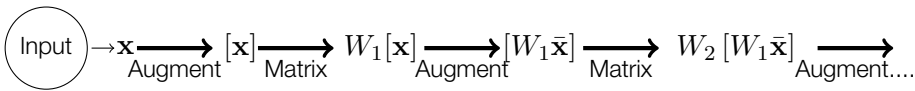

Affine Mess We Find Ourselves in

Or, in terms of **Affine Operators** (Chapter 3.4 in the notes):

$$
\begin{aligned}
\mathbf{x}_1 &= \hat{\mathcal{W}}_1 \mathbf{x}_{\text{input}} \\
\mathbf{x}_2 &= \hat{\mathcal{W}}_2 \mathbf{x}_1 = \hat{\mathcal{W}}_2 \hat{\mathcal{W}}_1 \mathbf{x}_{\text{input}} \\
\mathbf{x}_3 &= \hat{\mathcal{W}}_3 \mathbf{x}_2 = \hat{\mathcal{W}}_3 \hat{\mathcal{W}}_2 \hat{\mathcal{W}}_1 \mathbf{x}_{\text{input}} \\
&\vdots \\
x_{\text{output}} &= \begin{cases} 1 & \hat{\mathcal{W}}_N \mathbf{x}_{N-1} > 0 \\ 0 & \text{else} \end{cases}
\end{aligned}
\tag{5}
$$

Affine Mess We Find Ourselves in

But...affine operators obey:

$$\hat{\mathcal{W}}_2\hat{\mathcal{W}}_1 = \hat{\mathcal{V}} \tag{6}$$

(Affine + Affine = Affine)
Which means:

$$\hat{\mathcal{W}}_N\hat{\mathcal{W}}_{N-1}\hat{\mathcal{W}}_{N-2}\ldots\hat{\mathcal{W}}_1\mathbf{x}_{\text{input}} = \hat{\mathcal{V}}\mathbf{x}_{\text{input}} \tag{7}$$

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If you do the maths:

$$\hat{\mathcal{V}}\mathbf{x} = \mathbf{v}\cdot\mathbf{x} + \mathbf{b} \tag{8}$$

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Which is just....a single perceptron layer

Affine Mess We Find Ourselves in

If all you do is multiply by matrices & add vectors, you will *never* be doing anything other than an (extremely wasteful) perceptron algorithm

NonLinearity to the Rescue!

Need to break this affine relationship: enter **activation functions**.
Let:

$$\mathbf{x}_n = \text{activate}\left(W\mathbf{x}_{n-1} + \mathbf{b}\right) \tag{9}$$

Where activate (x) is a non-linear function, the activation function.
One of the simples ways to break linearity is to add a *elementwise function*:

$$\begin{aligned} \mathbf{v} &= W\mathbf{x}_{n-1} + \mathbf{b} \\ [\mathbf{x}_n]_i &= \sigma(v_i) \end{aligned} \tag{10}$$

Elementwise operations on vectors are – except for very specific cases – great for making vectors forget that they're vectors.

Elementwise Activation Functions

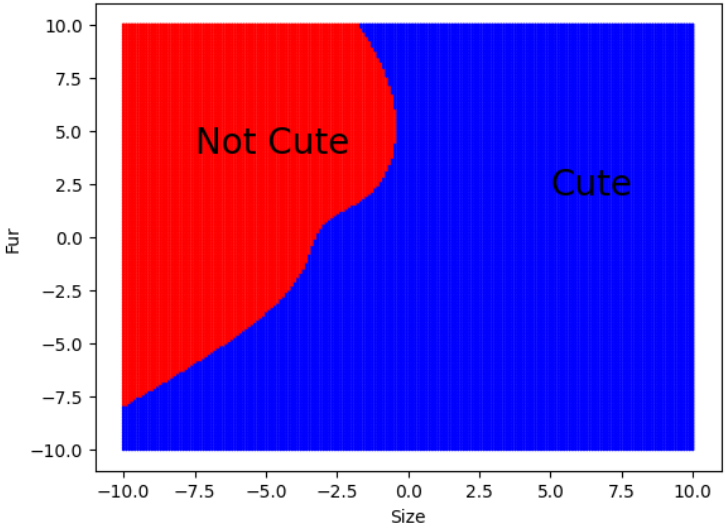
You can probably all name dozens of these functions in common use.

Sigmoid /Logit	$\sigma(x)$	$= \frac{1}{1+\exp(-x)}$
Rectified Linear Unit (ReLU)	$\text{Relu}(x)$	$= \begin{cases} x & x > 0 \\ 0 & \text{else} \end{cases}$
Leaky ReLU	$\text{Lelu}(x)$	$= \begin{cases} x & x > 0 \\ 0.01x & \text{else} \end{cases}$
tanh	$\tanh(x)$	$= \frac{\exp(x)-\exp(-x)}{\exp(x)+\exp(-x)}$
Softplus	$\text{sft}(x)$	$= \log\left(1+\exp(-x)\right)$

*(Bonus Question: Can you name any commonly used functions which **don't** follow this pattern?)*

NonLinearity Ahoy!

By replacing my (randomly initialised) hidden layers with Sigmoid nodes, I get:



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