Today's Resources

Access the Notebook:

- Local Clone (**Recommended**)
  `git clone https://github.com/wtsi-hpag/xAIWorkshop`
- Online Hosting (**Slow**) Visit
  `https://githubtocolab.com/wtsi-hpag/xAIWorkshop`

Interactive Questions
(Keep open in a browser tab!)

Join `menti.com` with code `2834 2684`

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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

Seem Familiar?

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```
>> import ml_toolbox
```

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>> data,labels = load_my_data()
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>> import ml_toolbox
>> data,labels = load_my_data()
>> model = ml_toolbox.make_model(layers=5,func=sigmoid)
>> model.Train(data,labels,epochs=1000)
```

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Epoch 0: 0%|                | [0/1000 10it/s, loss = 10.4]
```

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Epoch 100: 10%|xx              | [100/1000 10it/s, loss = 5.5]
```

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>> model.Train(data,labels,epochs=1000)

Epoch 200: 20%|xxxx            | [200/1000 12it/s, loss = 3.4]
```

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>> model.Train(data,labels,epochs=1000)

Epoch 300: 30%|xxxxxx          | [300/1000 9it/s, loss = 3.1]
```

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>> model.Train(data,labels,epochs=1000)

Epoch 400: 40%|xxxxxx          | [400/1000 16it/s, loss = 2.9]
```

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>> data,labels = load_my_data()
>> model = ml_toolbox.make_model(layers=5,func=sigmoid)
>> model.Train(data,labels,epochs=1000)

Epoch 500: 50%|xxxxxxxxx       | [500/1000 12it/s, loss = 1.4]
```

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>> data,labels = load_my_data()
>> model = ml_toolbox.make_model(layers=5,func=sigmoid)
>> model.Train(data,labels,epochs=1000)

Epoch 700: 70%|xxxxxxxxxxxx    | [700/1000 5it/s, loss = 1.39]
```

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```
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>> data,labels = load_my_data()
>> model = ml_toolbox.make_model(layers=5,func=sigmoid)
>> model.Train(data,labels,epochs=1000)

Epoch 900: 90%|xxxxxxxxxxxxxxx | [900/1000 8it/s, loss = 1.385]
```

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>> model = ml_toolbox.make_model(layers=5,func=sigmoid)
>> model.Train(data,labels,epochs=1000)

Epoch 1000: 100%|xxxxxxxxxxxxxxxx| [final loss = 1.382]
```

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Epoch 1000: 100%|xxxxxxxxxxxxxxxx| [final loss = 1.382]

>> model.Test()
```

Today's Agenda

The aim for today is:

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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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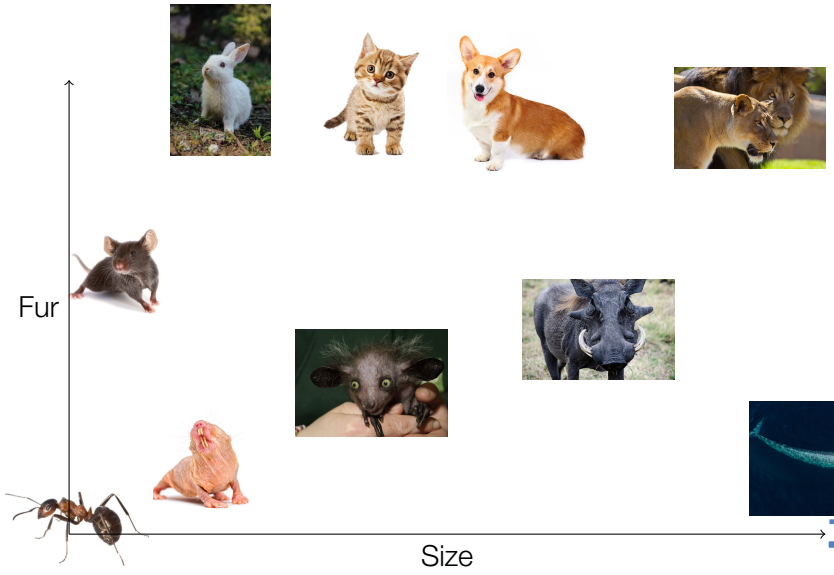
You will need to know what they mean!

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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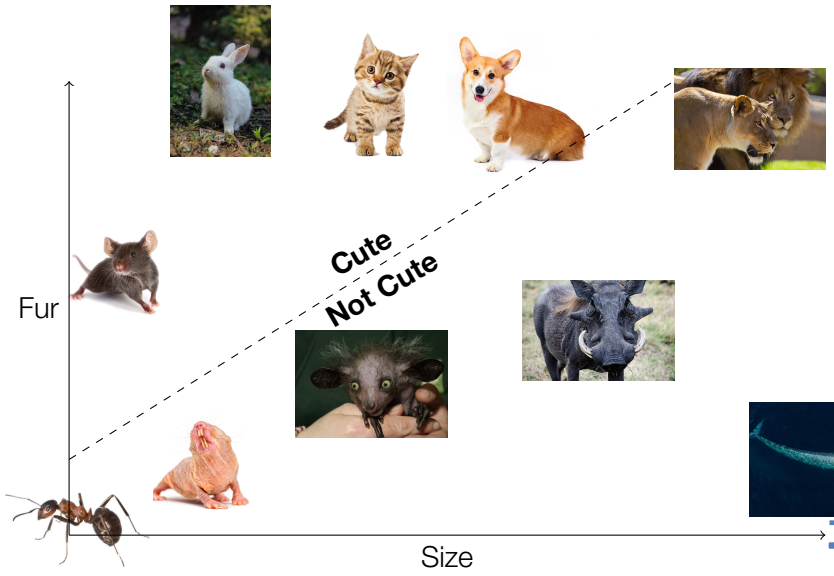
Basic Decision Making: Defining Cuteness



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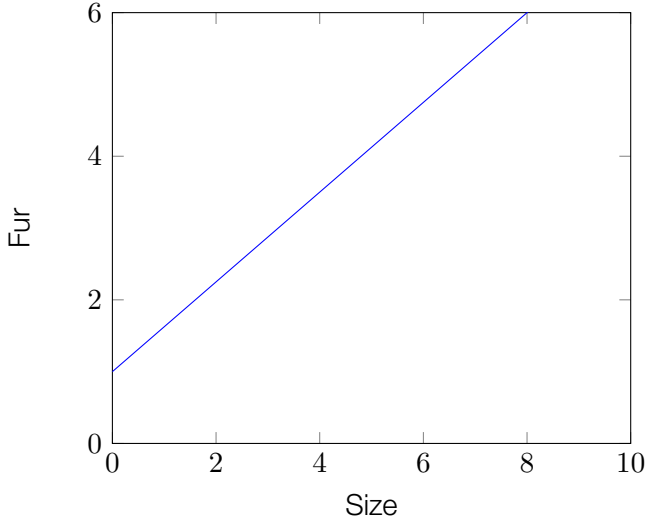
Splitting The Plane

In order to split the plane into two parts, we merely need to define a *line*.



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Question: If we have N dimensions ($N = 2$), how many parameters do we need to define a line?

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Answer: The answer is N - in 2 dimensions, this is friendly $y = mx + c \rightarrow (m, c)$

The Perceptron

The Perceptron classifier algorithm is:

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

[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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The Perceptron: Dimensions

Question: What is the dimensionality of the Perceptron? Does this conflict with our earlier statements?

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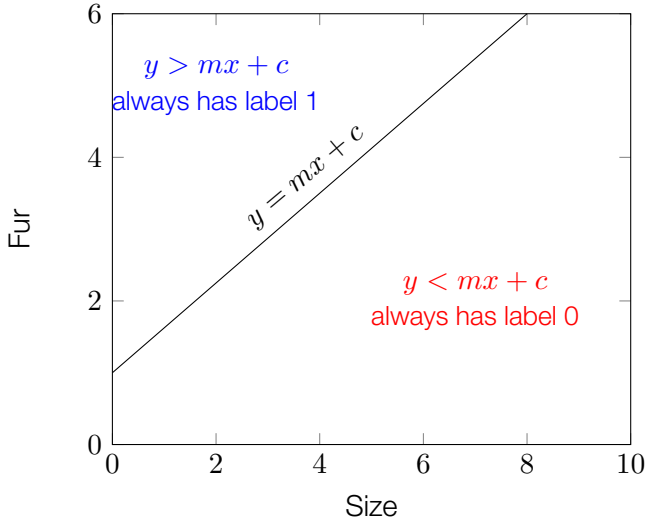
Hint: It has nothing to do with the 'bias'!

Answer: We need $N + 1$ dimensions. N dimensions define a line - but need an additional dimension to add *directionality*

The Perceptron: Dimensions



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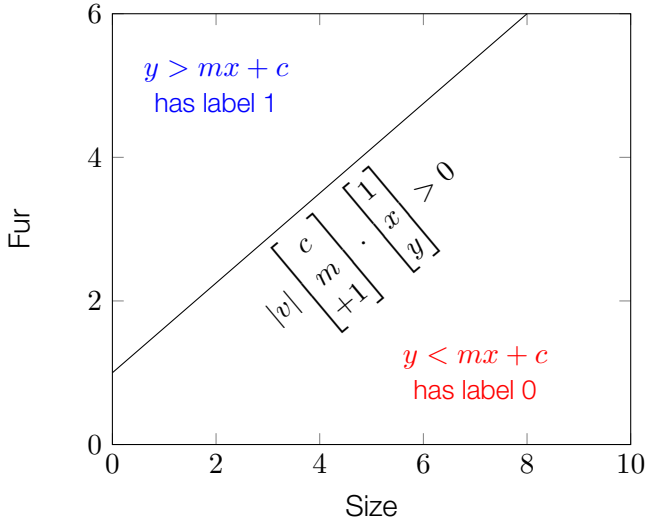

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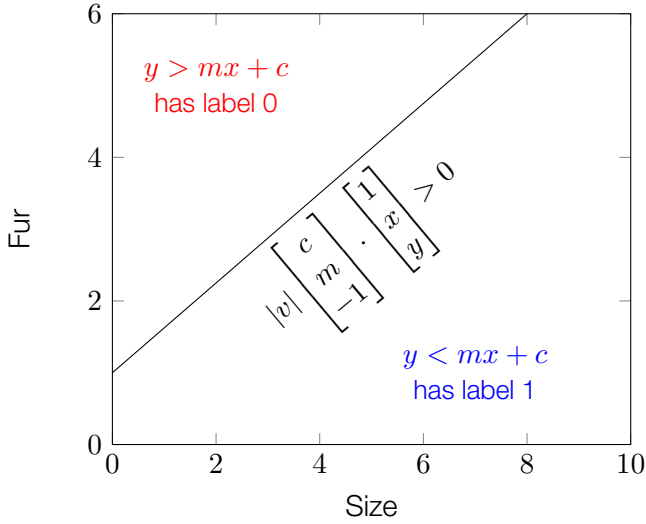

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Exercise 1: Perceptron Classifier

Task 1: Write a perceptron classifier for the data in `cuteness.dat`

Guidance: Class structure & predetermined weights are provided in the notebook. Ignore `Train()` for now

Question: 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

Task 2: Write the `Train()` method for your Perceptron, then apply to `cuteness` data.

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Give your answers on `menti.com` with code `2834 2684`

Exercise 3: The Limits of Linearity

Task 3: Apply your method to the data in `cuteness_augmented.dat`, which adds the Axolotl, Otter, Capybara, Quokka, Slug, Tasmanian Devil and Giant Panda.
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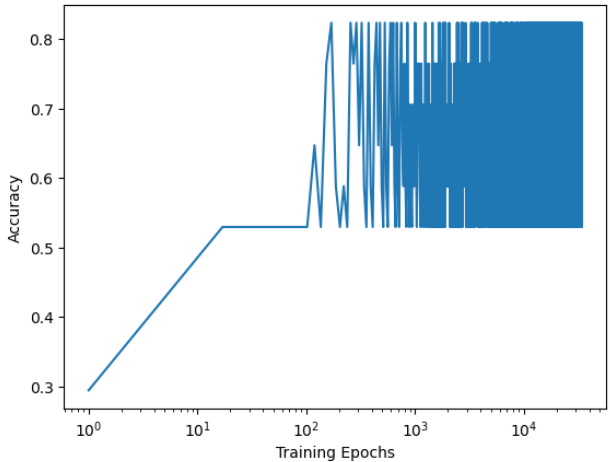

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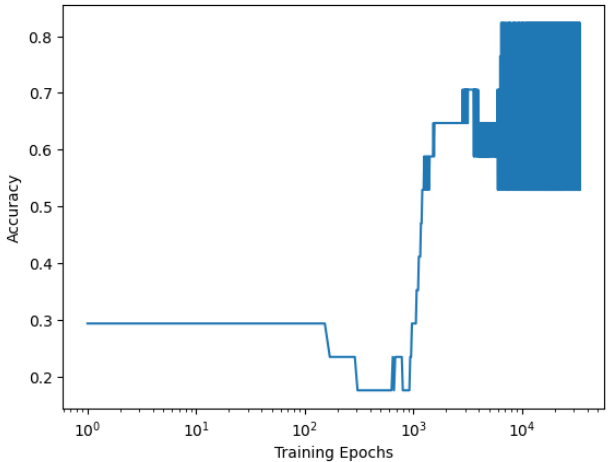

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The Nonlinear Perceptron

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:

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

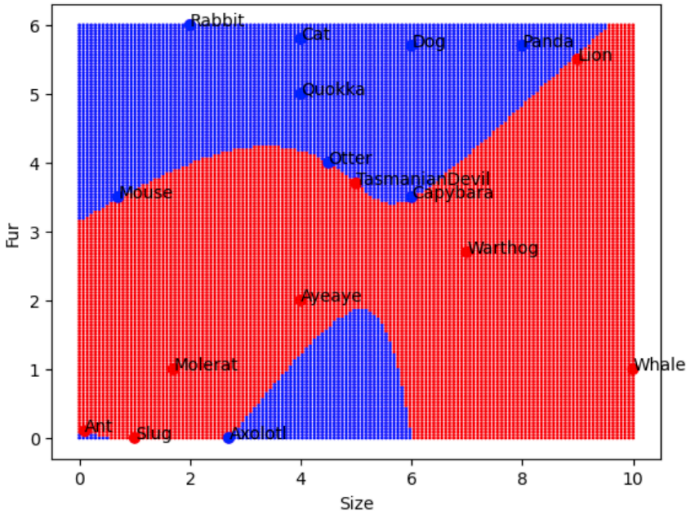
The Nonlinear Perceptron

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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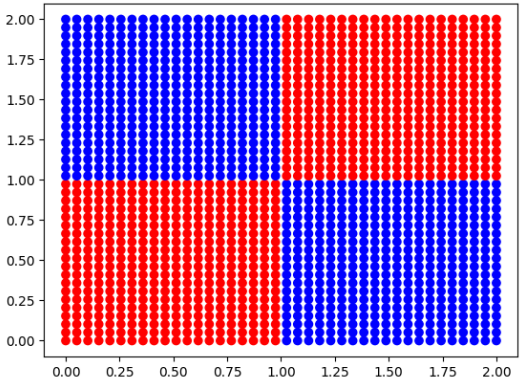
The Limits of NonLinearity

Target



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The Limits of NonLinearity

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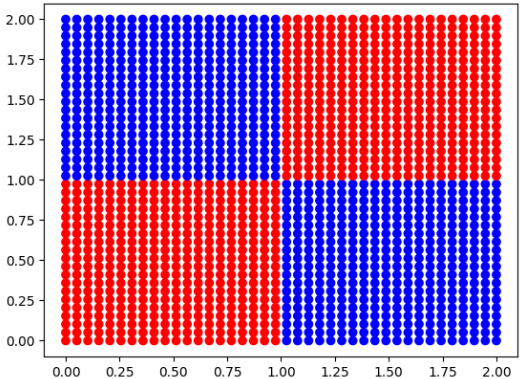
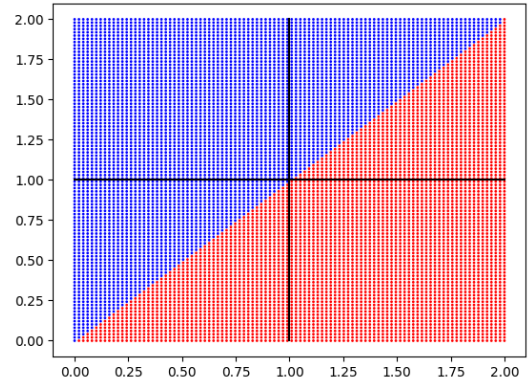


Reality (1st Order - 3 parameters)



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The Limits of NonLinearity

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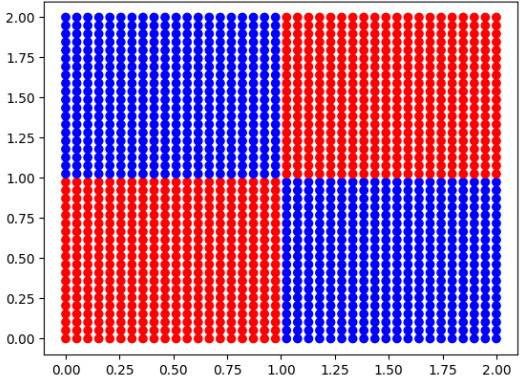
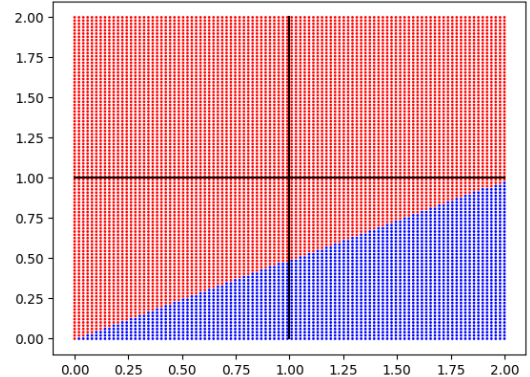


Reality (2nd Order - 6 parameters)



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The Limits of NonLinearity

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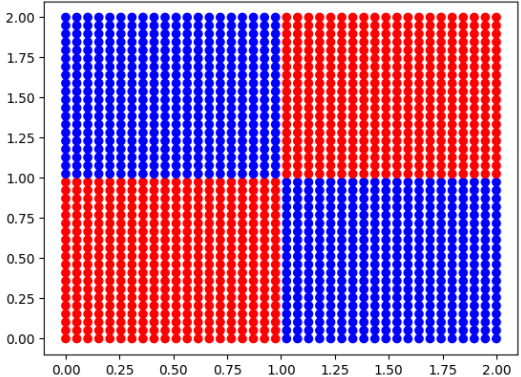
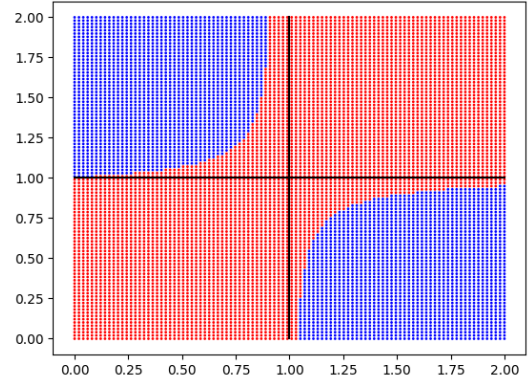


Reality (3rd Order - 10 parameters)



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The Limits of NonLinearity

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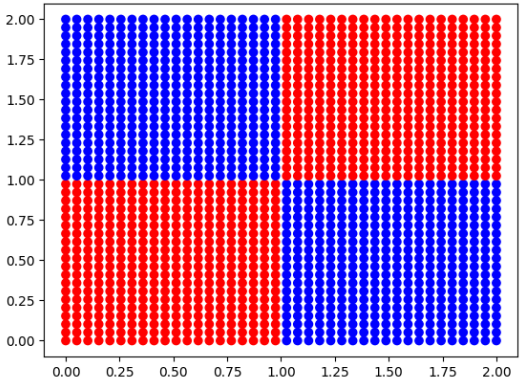
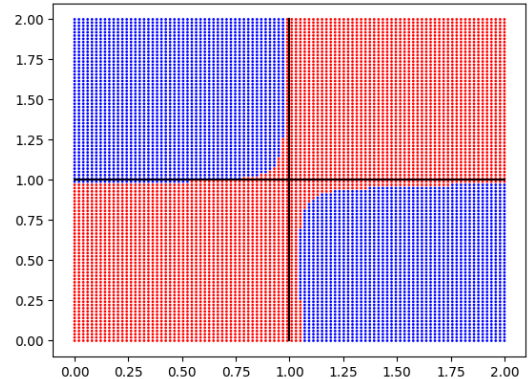


Reality (4th Order - 15 parameters)



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The Limits of NonLinearity

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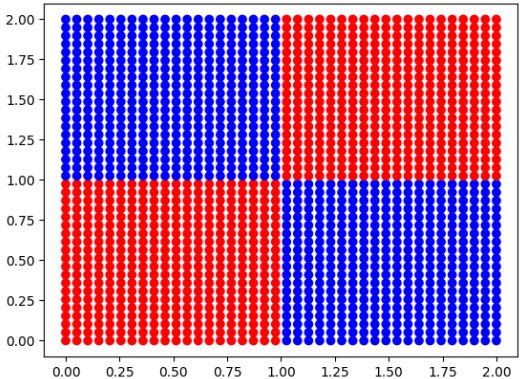
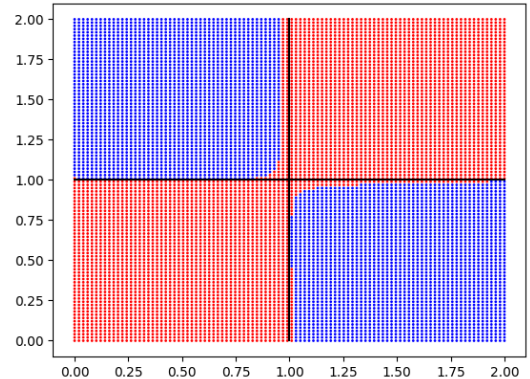


Reality (5th Order - 21 parameters)



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The Limits of NonLinearity

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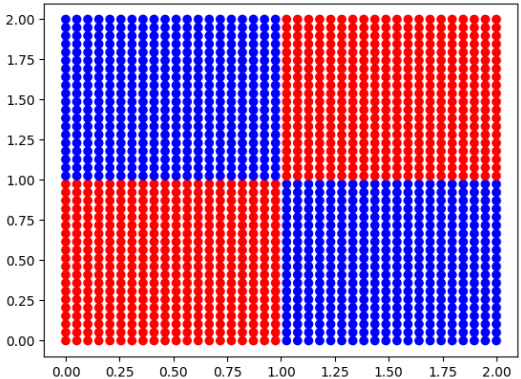

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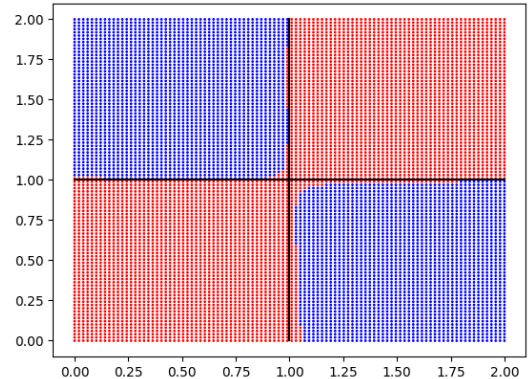

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The Limits of NonLinearity

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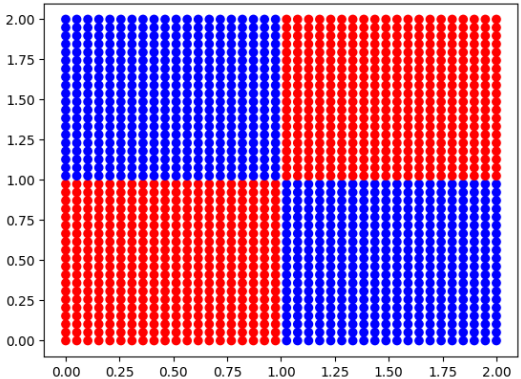
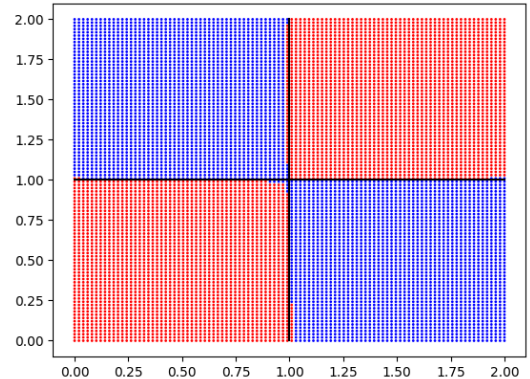


Reality (20th Order - 231 parameters)



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What do to?

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MORE!

The Multilayered Perceptron

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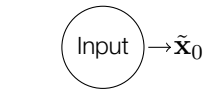
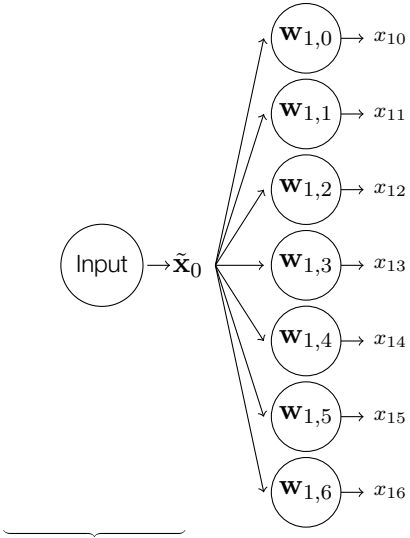


Input layer

The Multilayered Perceptron



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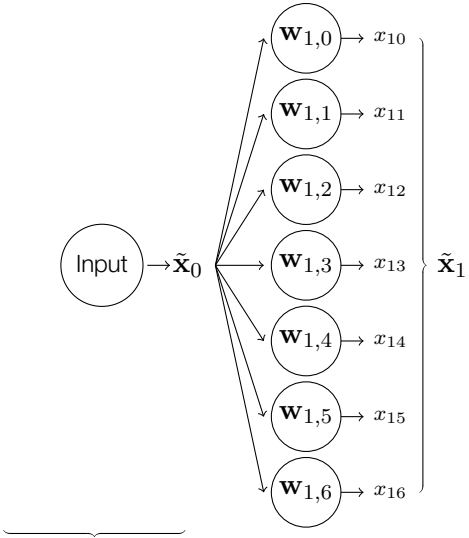

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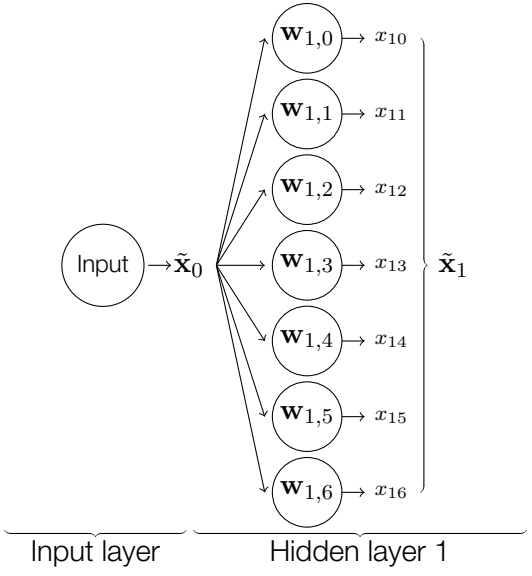

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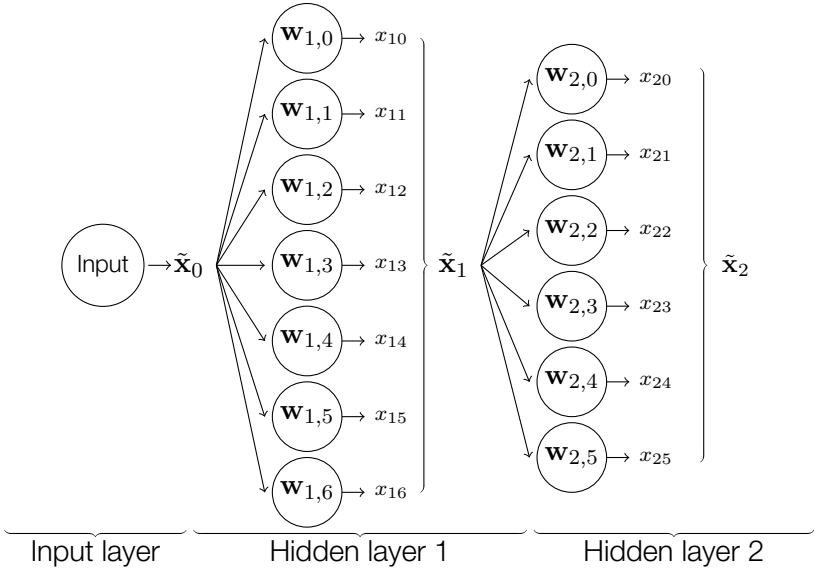

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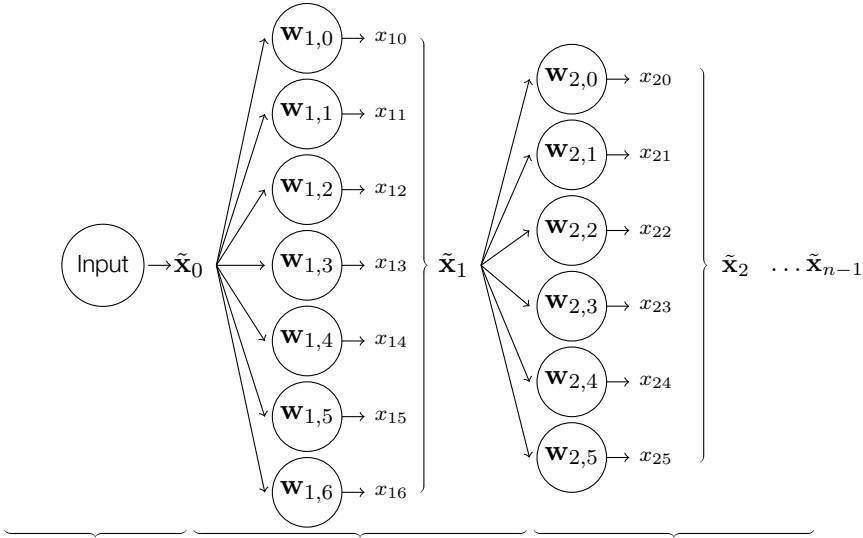
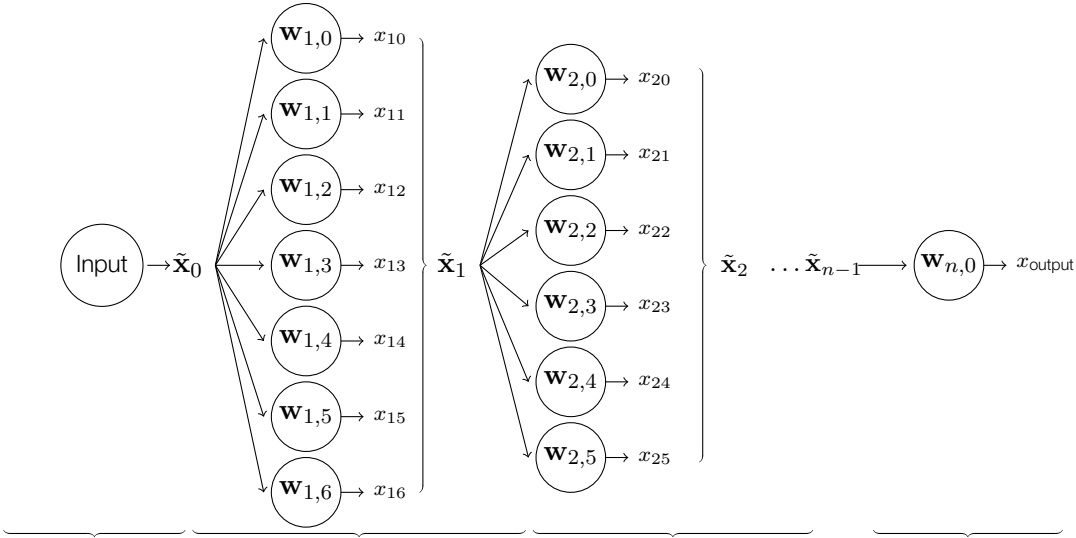


The Multilayered Perceptron



Exercise 4: The Multilayered Perceptron

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Question: Do you notice anything odd about how this predictor behaves?

All that for nothing?

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

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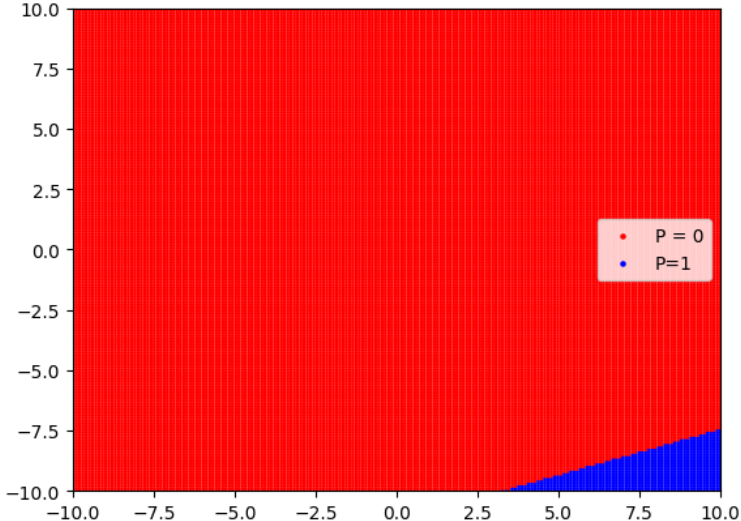

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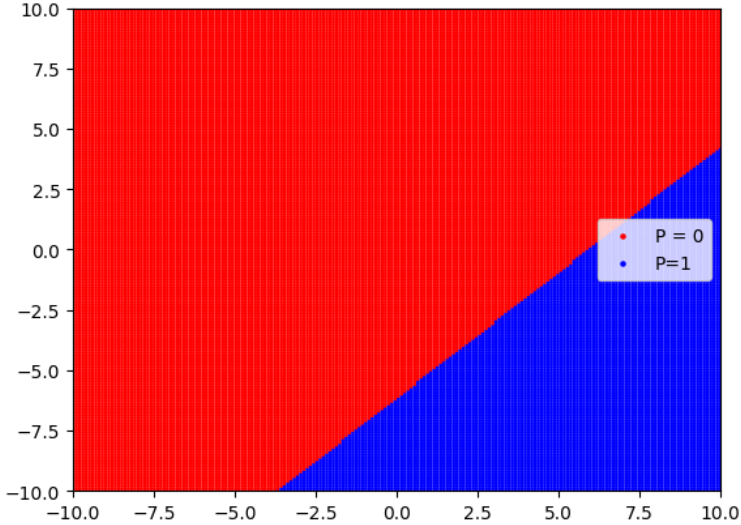

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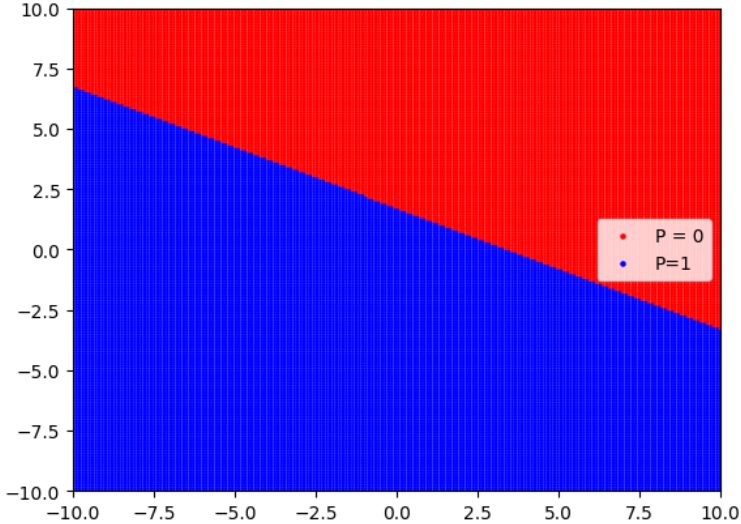

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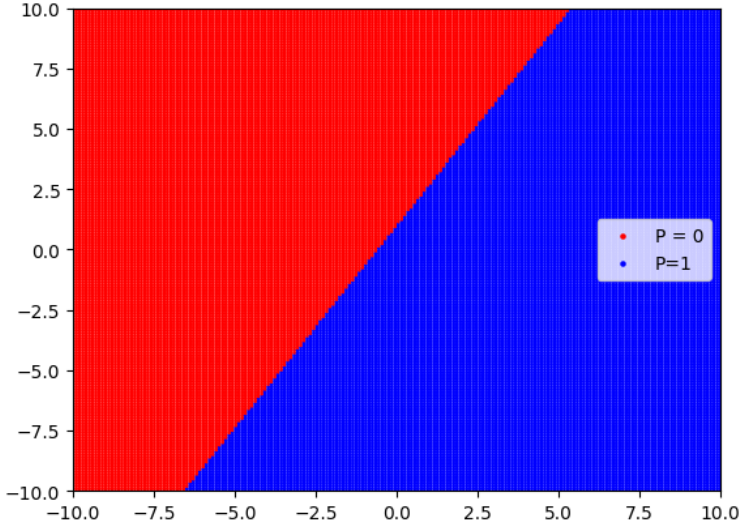

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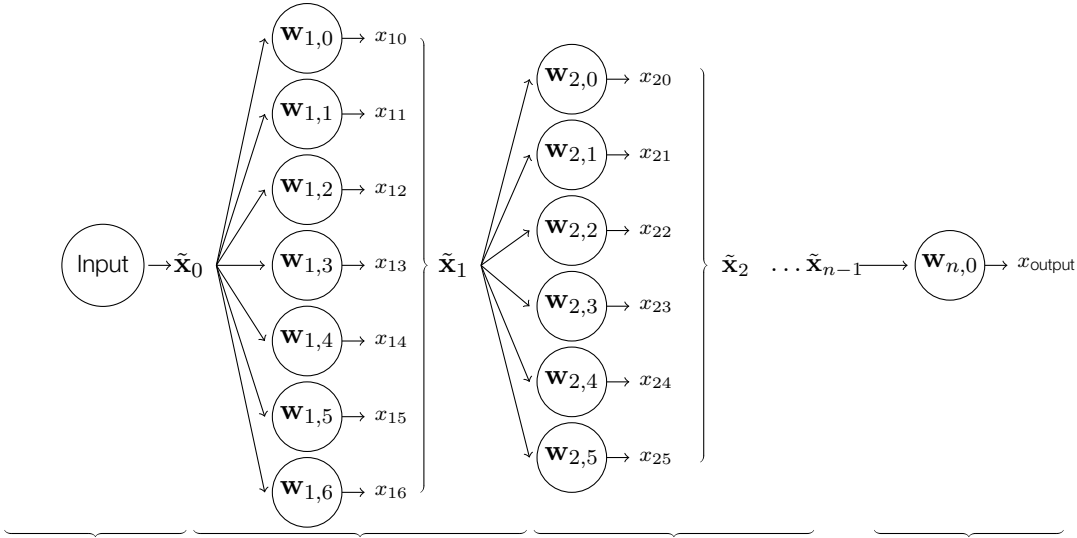
Affine Mess We Find Ourselves in



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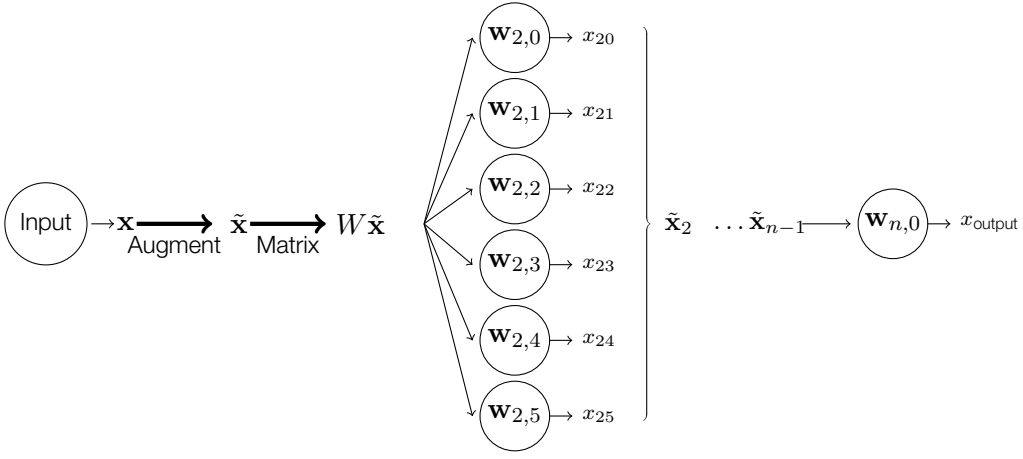

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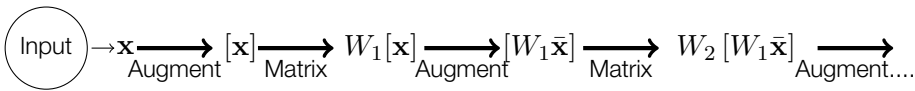

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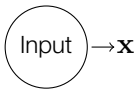
Or, in terms of **Affine Operators** (Chapter 3.4 in the notes):

$$\left(\text{Affine = Matrix multiplicaiton + translation} \implies \mathcal{W}\mathbf{v} = W\mathbf{v} + \mathbf{w}\right)$$



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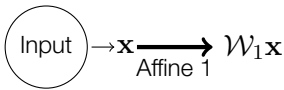

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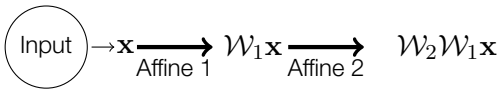

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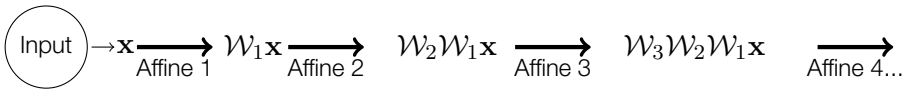

Affine Mess We Find Ourselves in

But...affine operators obey:

$$\hat{\mathcal{W}}_2\hat{\mathcal{W}}_1 = \hat{\mathcal{V}} \tag{5}$$

(Affine + Affine = Affine)
Which means:

$$\hat{\mathcal{W}}_N\hat{\mathcal{W}}_{N-1}\hat{\mathcal{W}}_{N-2}\ldots\hat{\mathcal{W}}_1\mathbf{x}_{\text{input}} = \hat{\mathcal{V}}\mathbf{x}_{\text{input}} \tag{6}$$

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$$\hat{\mathcal{V}}\mathbf{x} = \mathbf{v}\cdot\mathbf{x} + \mathbf{b} \tag{7}$$

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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**.

NonLinearity to the Rescue!

Let:

$$\mathbf{x}_n = \text{activate}\left(W\mathbf{x}_{n-1} + \mathbf{b}\right) \tag{8}$$

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One of the simples ways to break linearity is to add a ***elementwise function***:

$$\begin{aligned} \mathbf{v} &= W\mathbf{x}_{n-1} + \mathbf{b} \\ [\mathbf{x}_n]_i &= \sigma(v_i) \end{aligned} \tag{9}$$

Elementwise Activation Functions

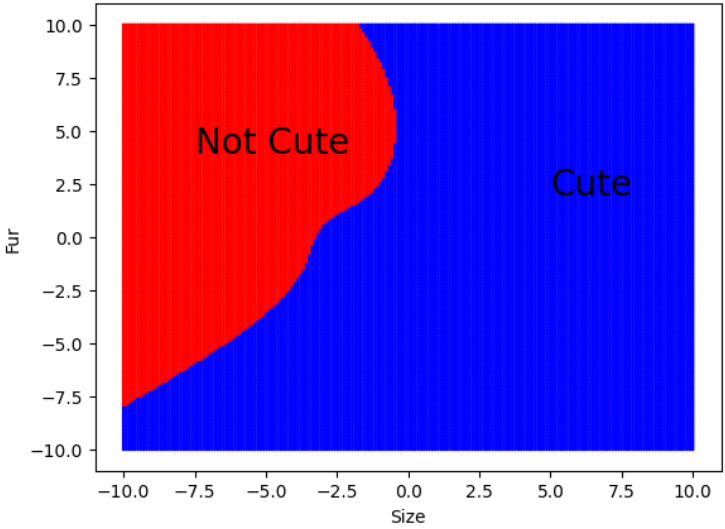
You can probably all name dozens of these functions in common use.

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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