Under The Hood

A Peek Inside the 'Black Box' of Machine Learning

Jack Fraser-Govil
The Wellcome Sanger Institute, Hinxton, UK

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Why bother?

In a world with dozens of pre-built ML tools....why bother studying the fundamentals?

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FOLKLORE

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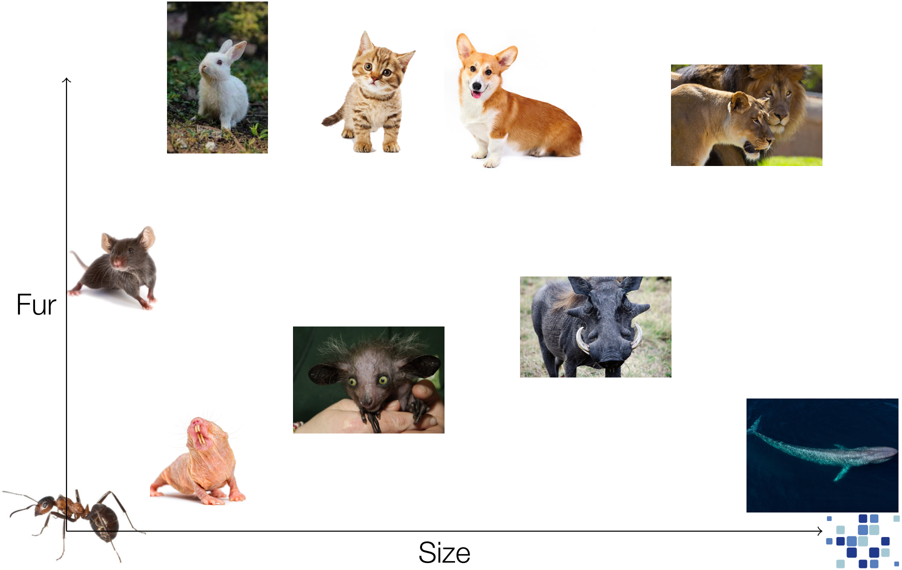
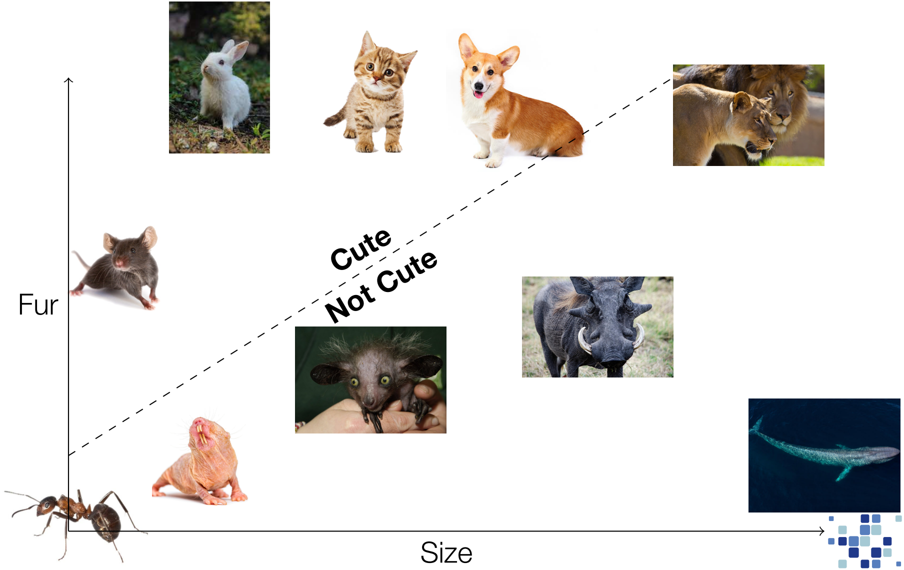
- Cross-Entropy vs Least Squares?
- Validation set magic numbers

Basic Decision Making: Defining Cuteness



Basic Decision Making: Defining Cuteness



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In maths...

Let $\vec{x}$ be the 'feature vector', $\vec{x} = \begin{pmatrix} 1 \\ \text{size} \\ \text{fur} \end{pmatrix}$, and $\vec{w} = \begin{pmatrix} w_0 \\ w_1 \\ w_2 \end{pmatrix}$ be our 'weights':

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The Perceptron algorithm is:

$$\mathcal{P}_{\vec{w}}(\vec{x}) = \begin{cases} 1 \text{ (cute)} & \text{when } \vec{w} \cdot \vec{x} > 0 \\ 0 \text{ (not cute)} & \text{else} \end{cases} \tag{1}$$

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Therefore $\vec{w}$ defines a *line* which divides our 2D space – Perceptron simply splits the region into two $\rightarrow$ though can pull some fancy tricks.

Training Perceptron

Training = finding the ***best*** $\vec{w}$

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Perceptron algorithm loops over a labelled 'training set', where the known cuteness of j is C_j

$$\vec{w} \rightarrow \vec{w} + r\left(C_j - \mathcal{P}_{\vec{w}}(\vec{x}_j)\right)\vec{x}_j \tag{2}$$

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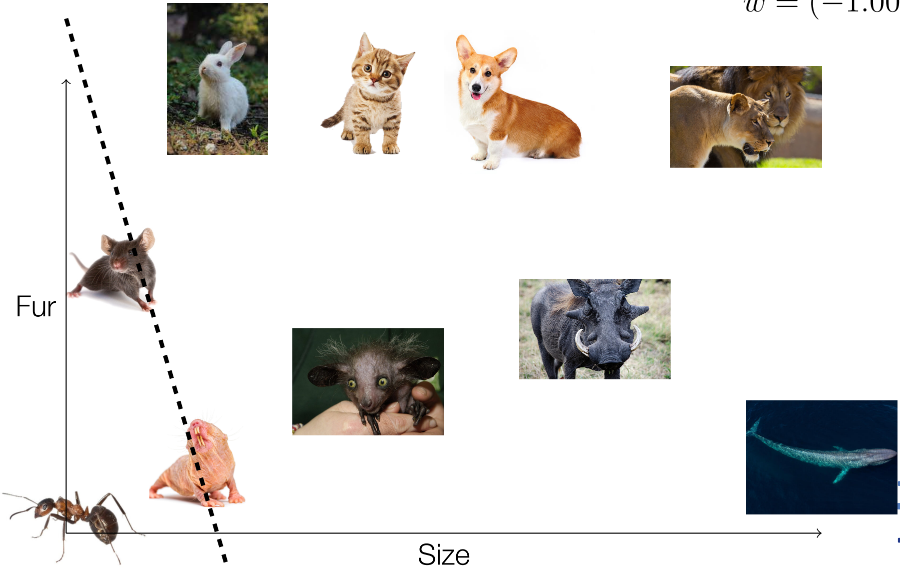
In words

For each element in the set, if I guess wrong ($C_j \neq \mathcal{P}_j$), move $\vec{w}$ by a small amount (r) to make me less wrong.

Training Perceptron

$$\vec{w} = (-1.00, 0.50, 0.15)$$



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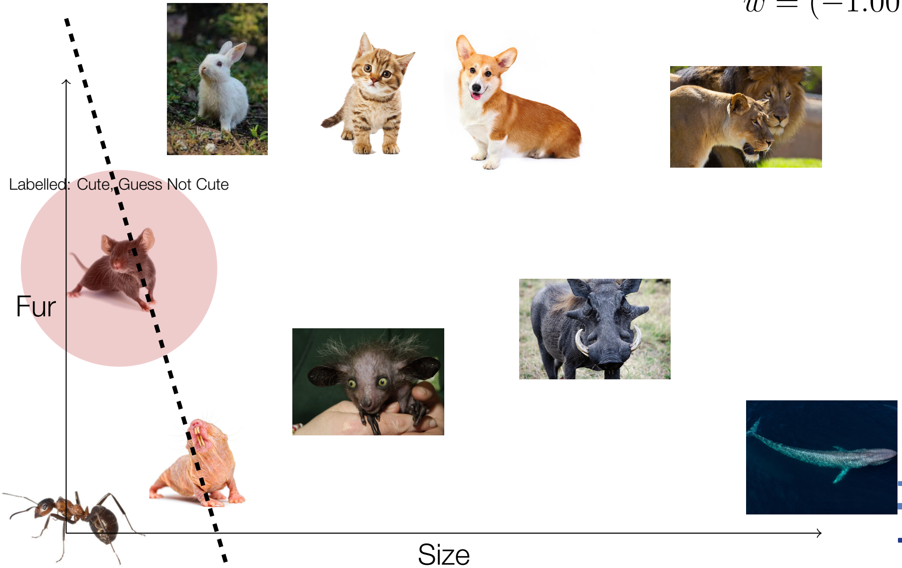
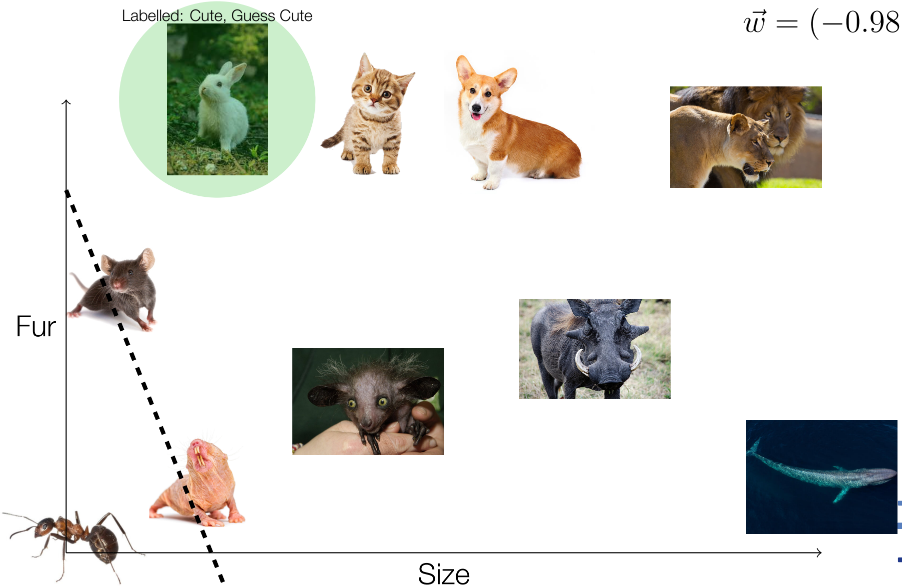


Training Perceptron

$$\vec{w} = (-0.98, 0.51, 0.20)$$



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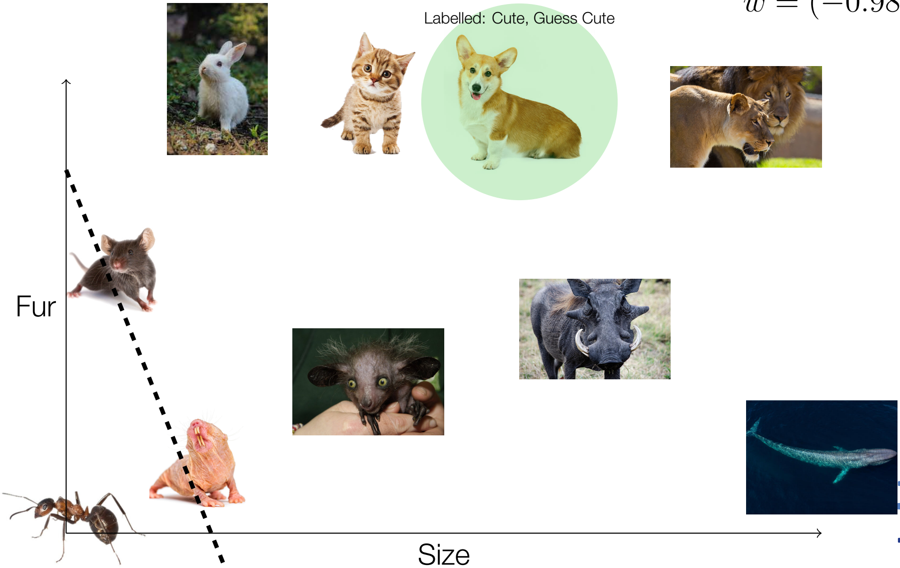

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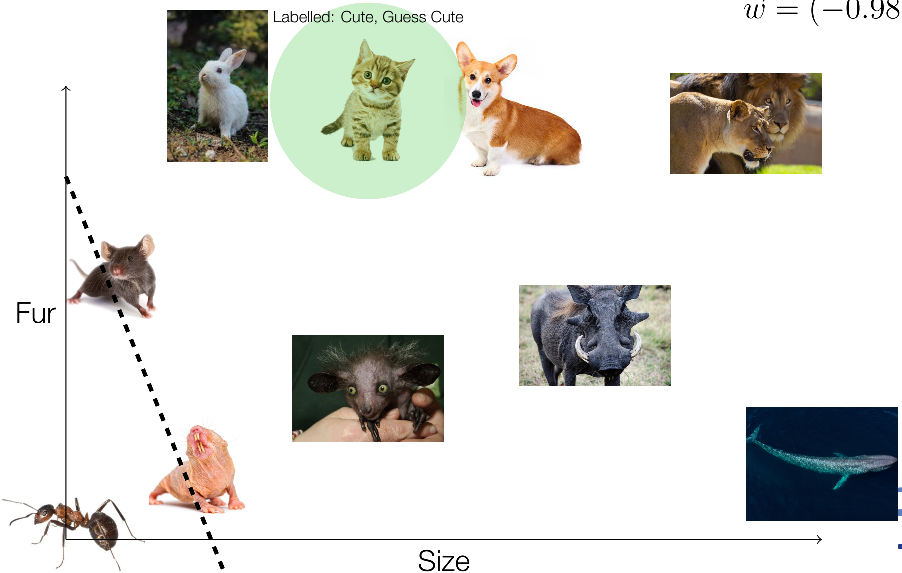

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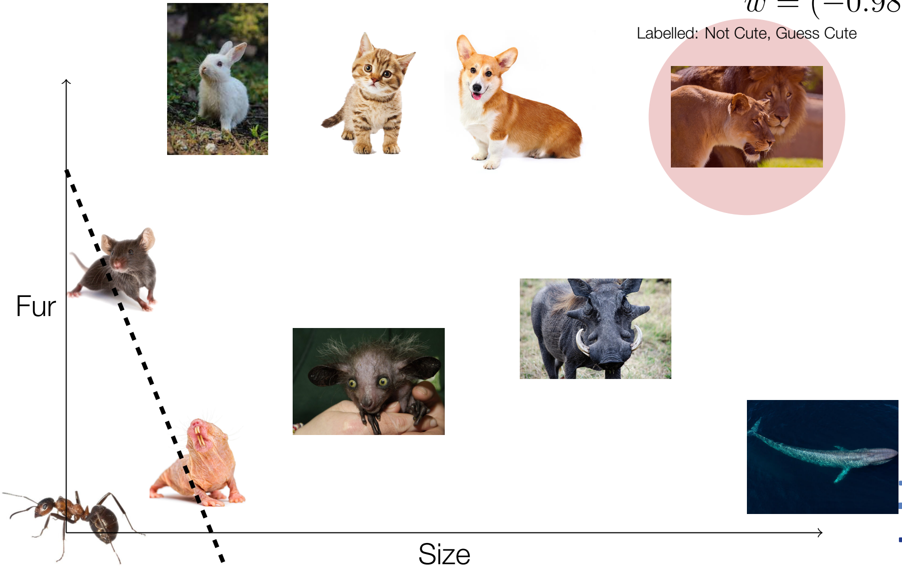
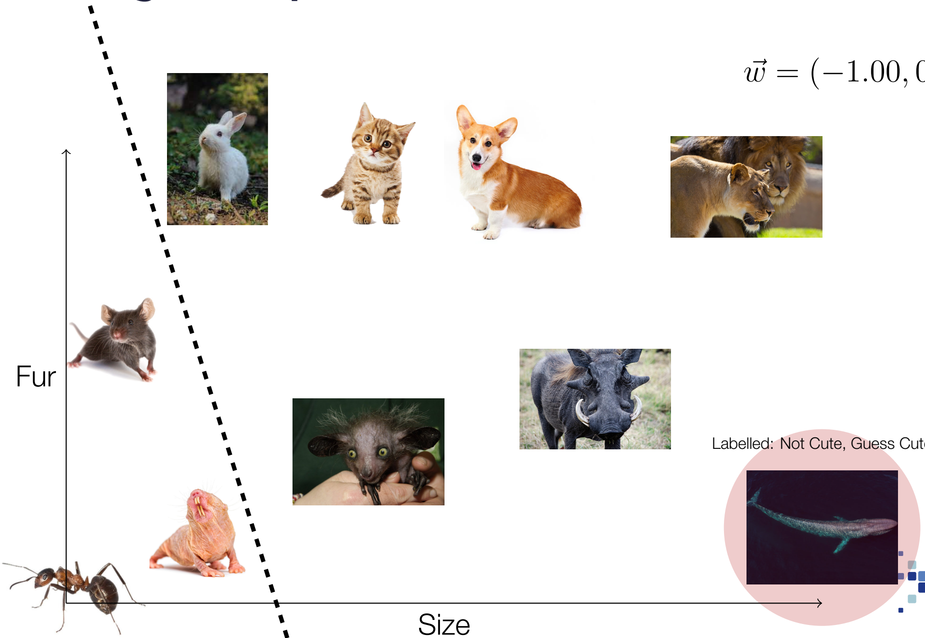


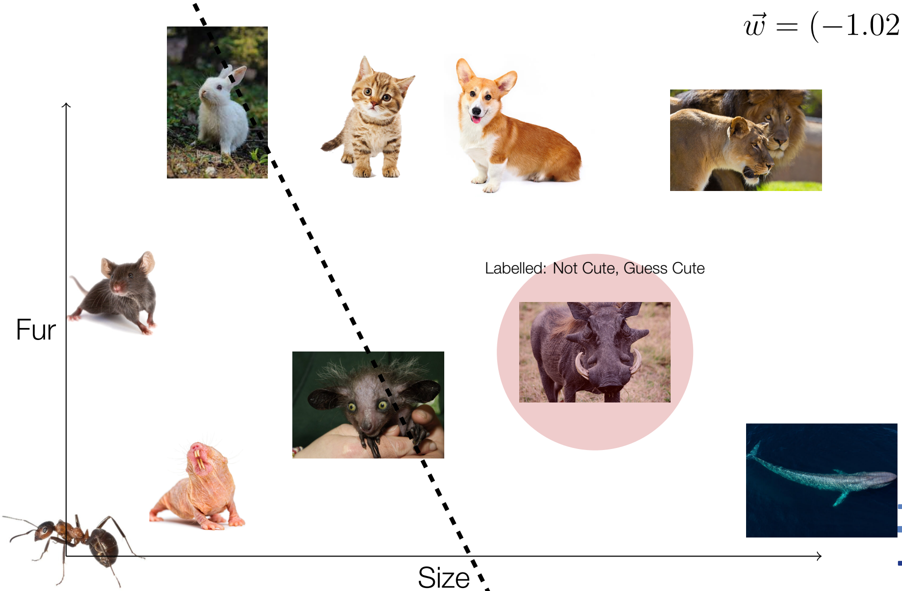
Training Perceptron

$$\vec{w} = (-1.00, 0.36, 0.11)$$



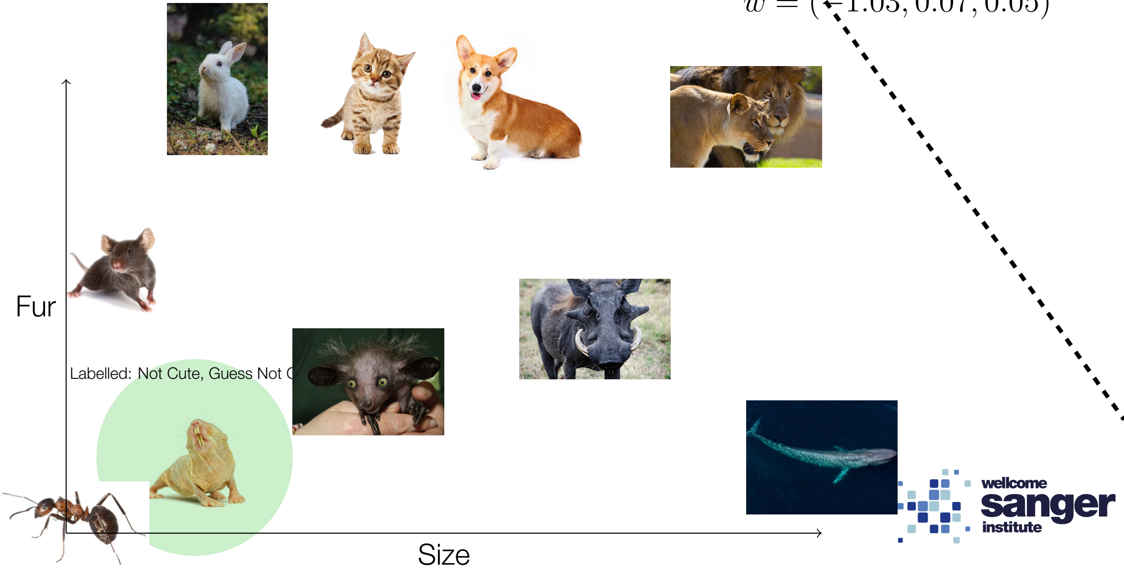
Training Perceptron

$$\vec{w} = (-1.02, 0.19, 0.09)$$



Training Perceptron

$$\vec{w} = (-1.03, 0.07, 0.05)$$



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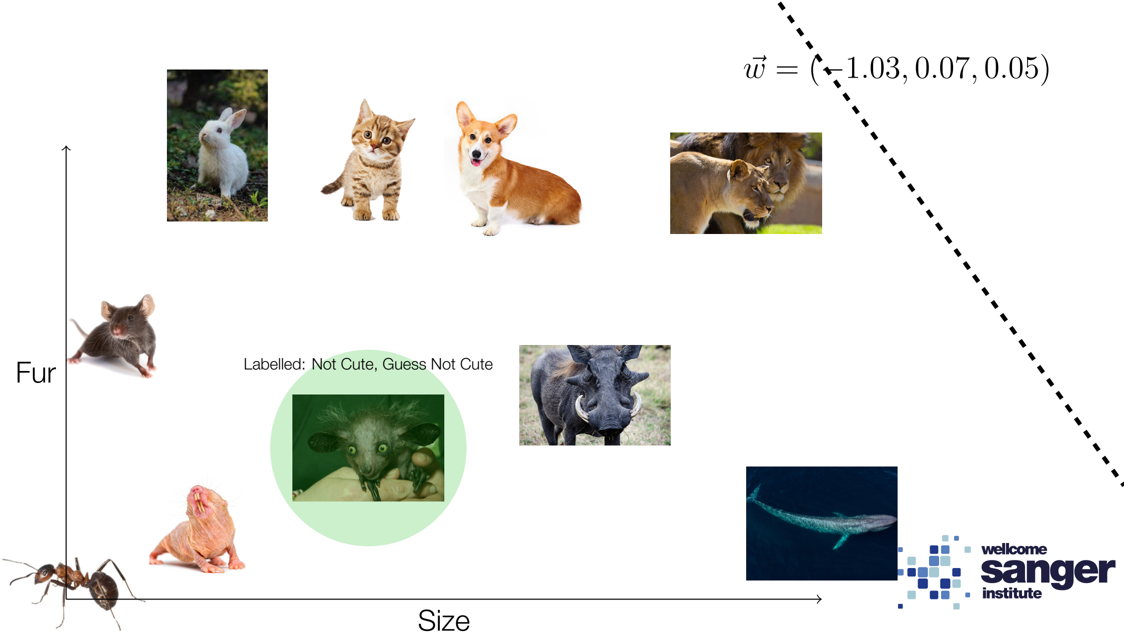

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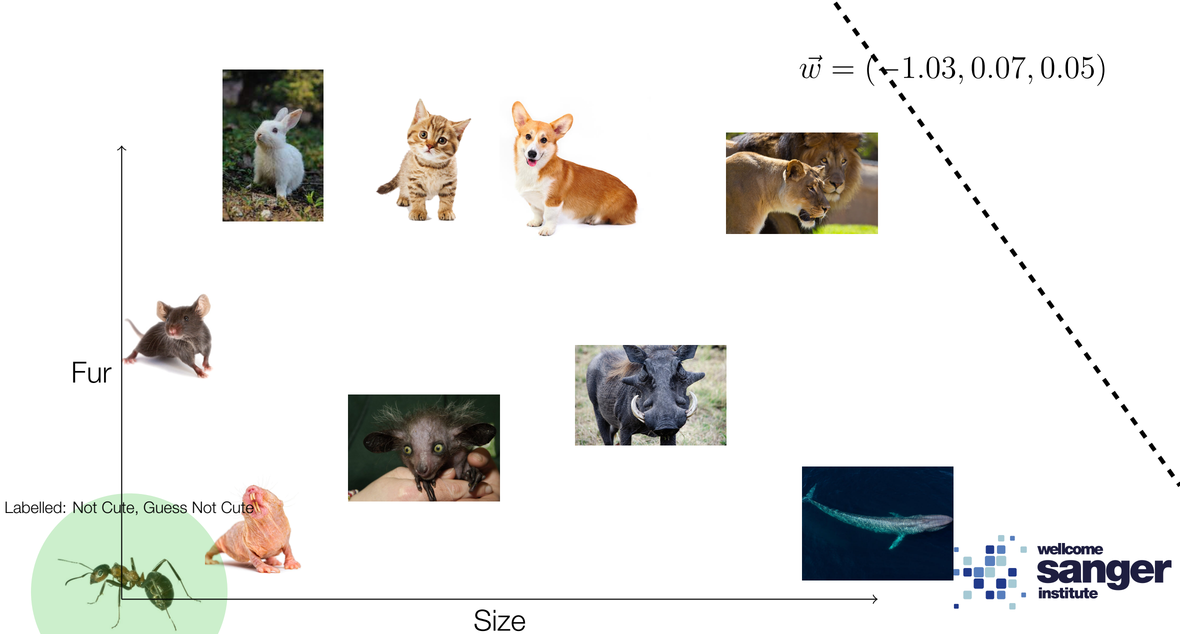

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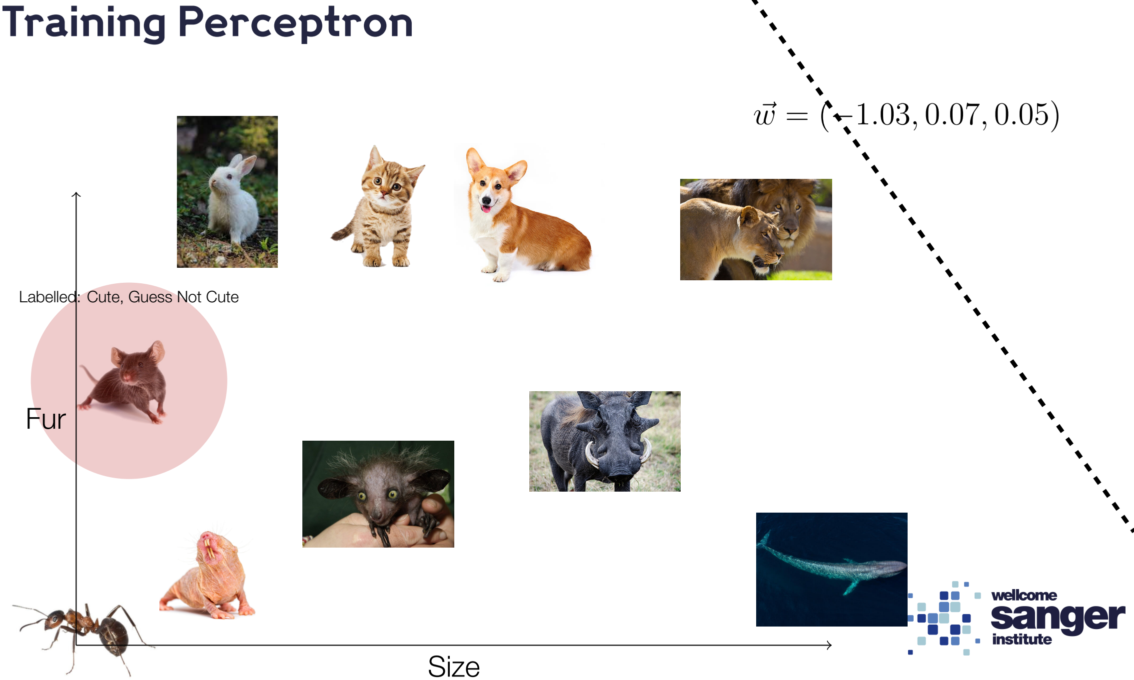

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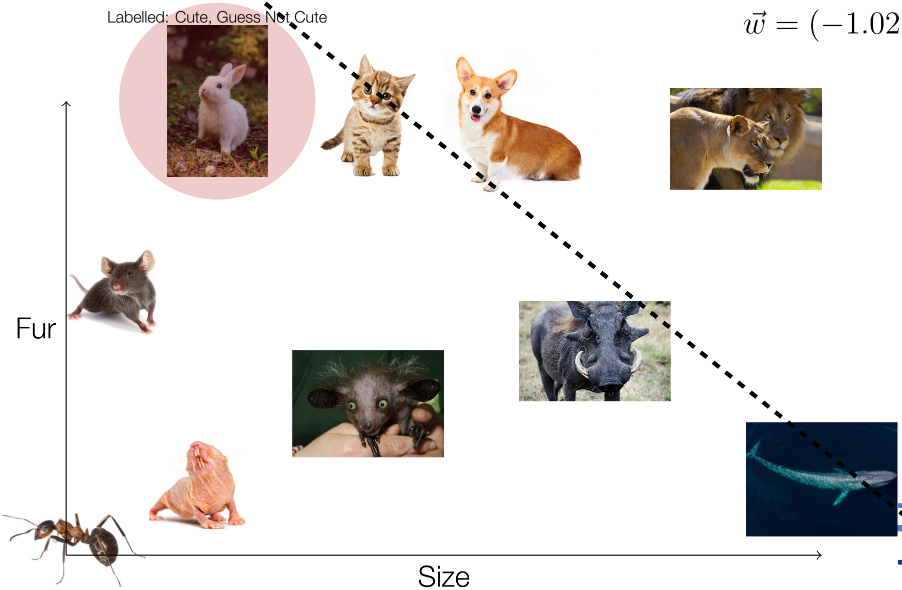
$$\vec{w} = (-1.02, 0.08, 0.11)$$



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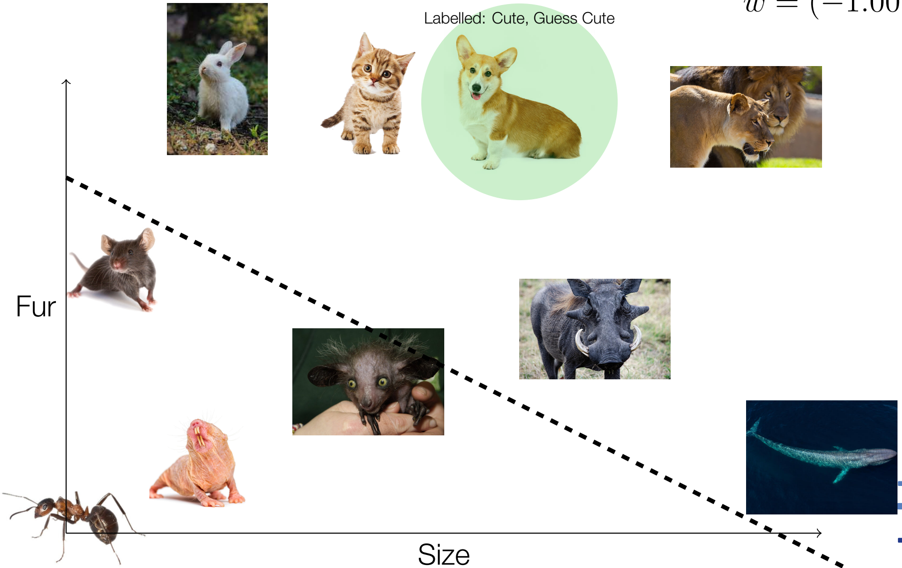
$$\vec{w} = (-1.00, 0.12, 0.21)$$



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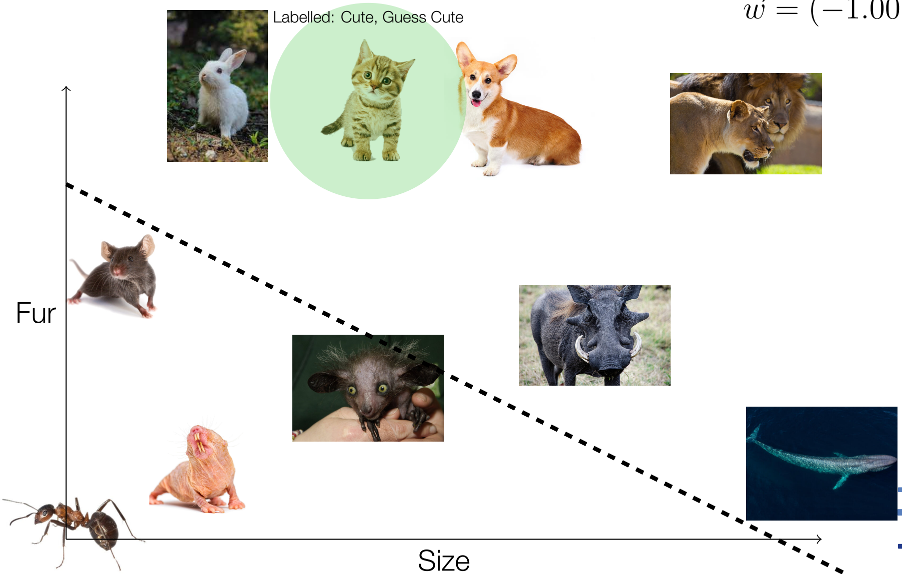

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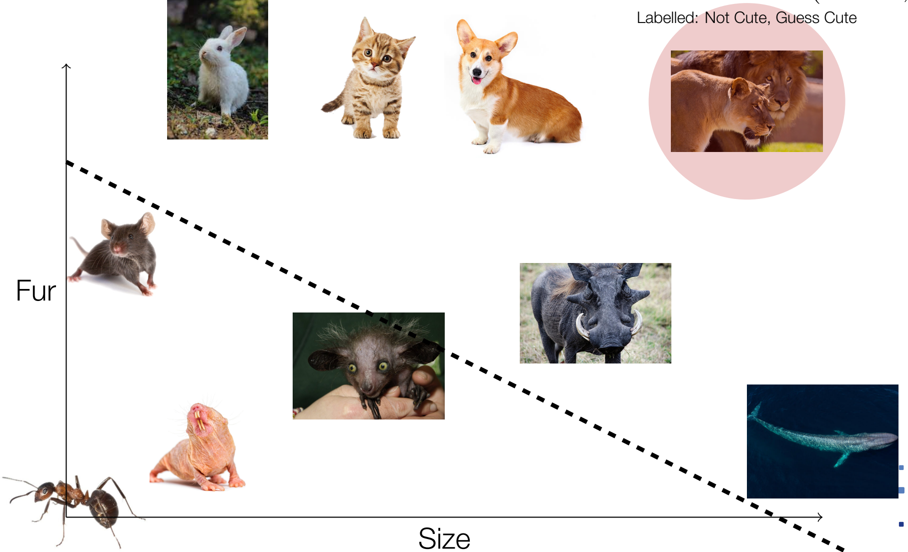

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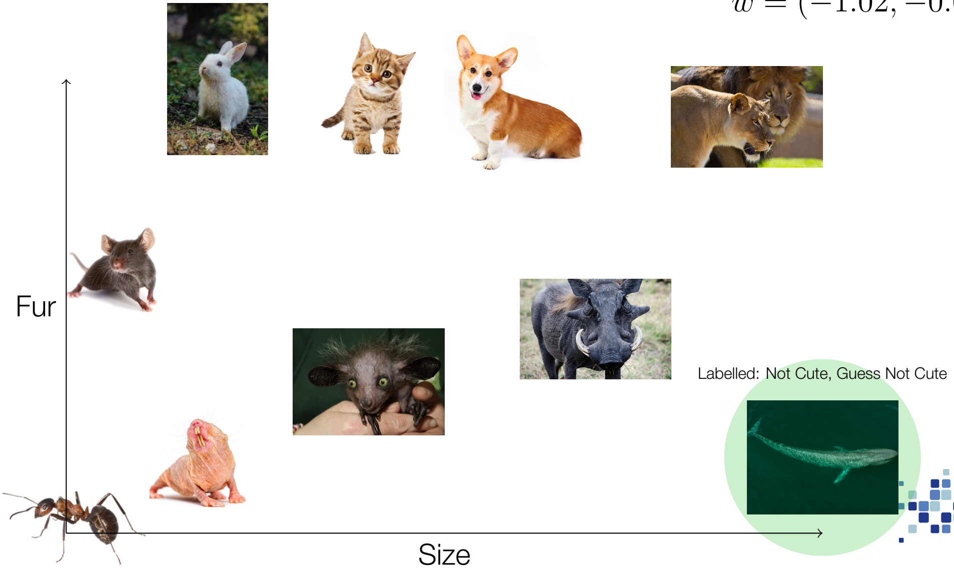
$$\vec{w} = (-1.02, -0.04, 0.12)$$



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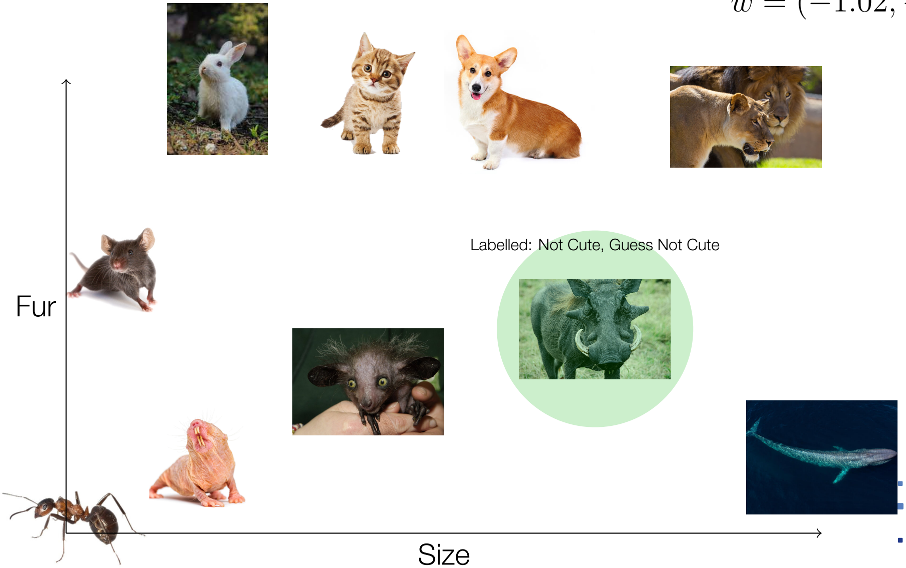

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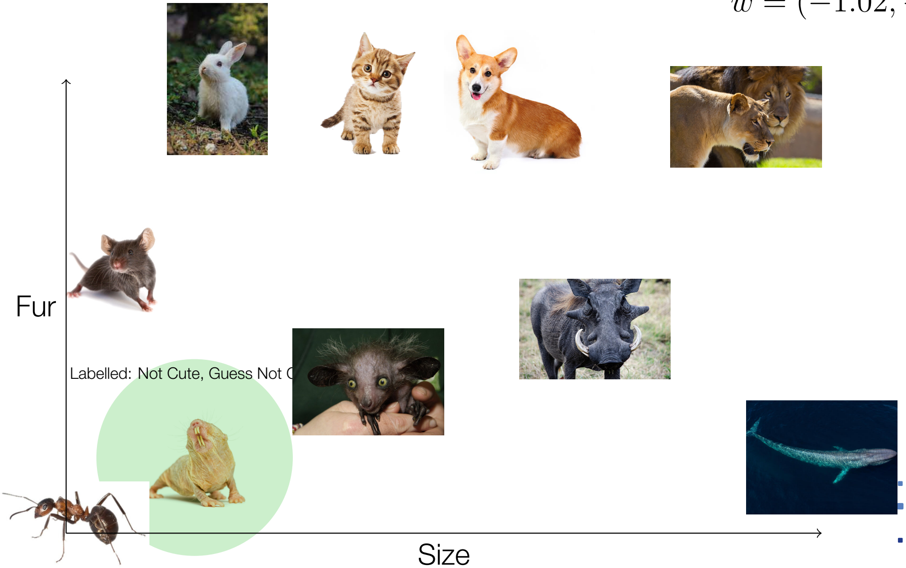

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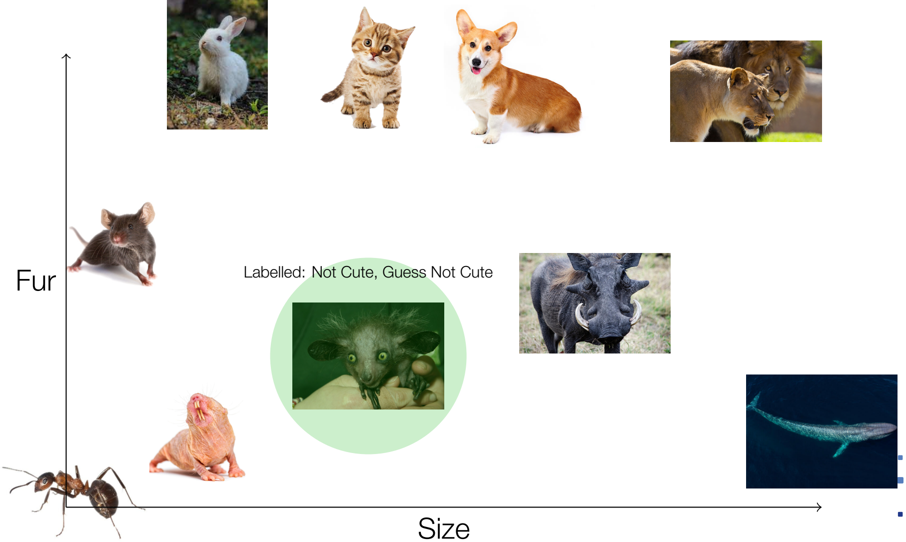

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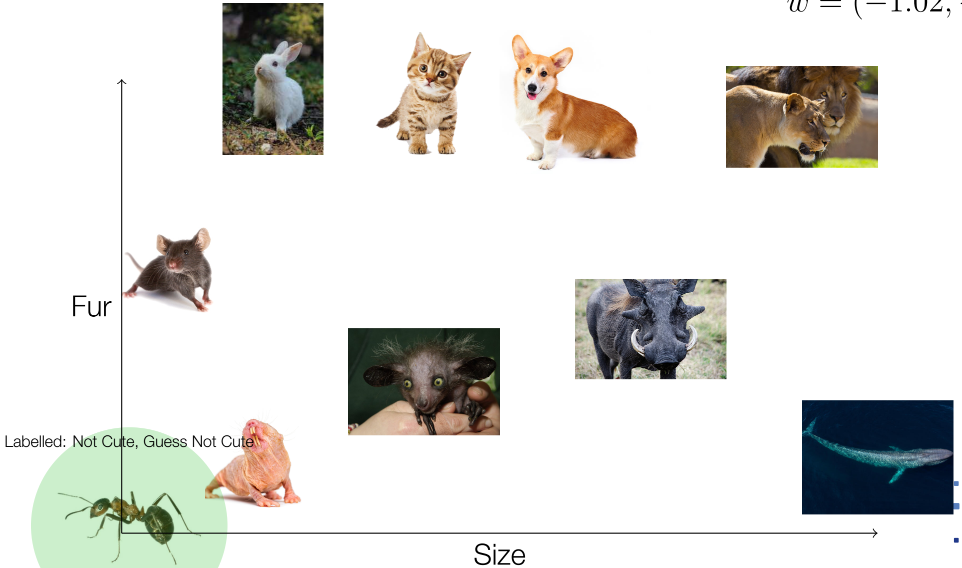

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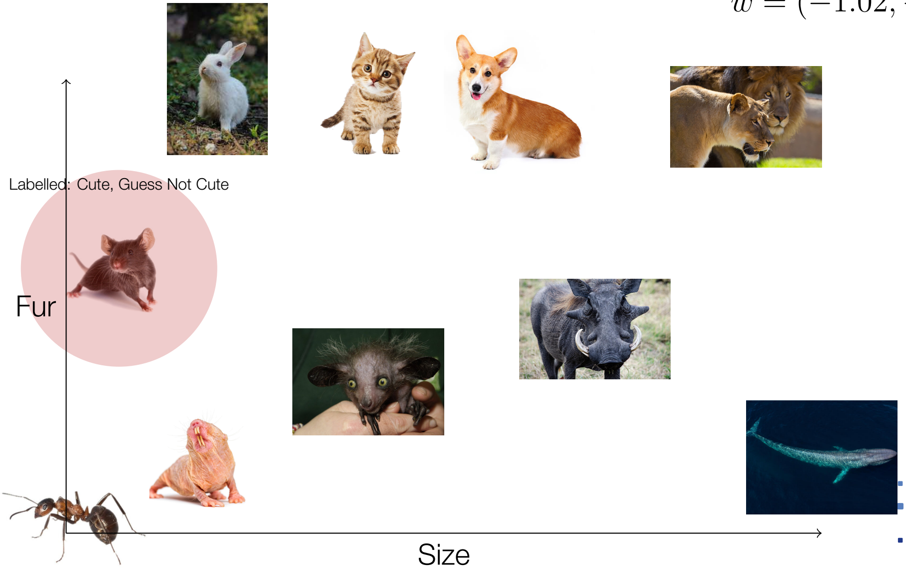

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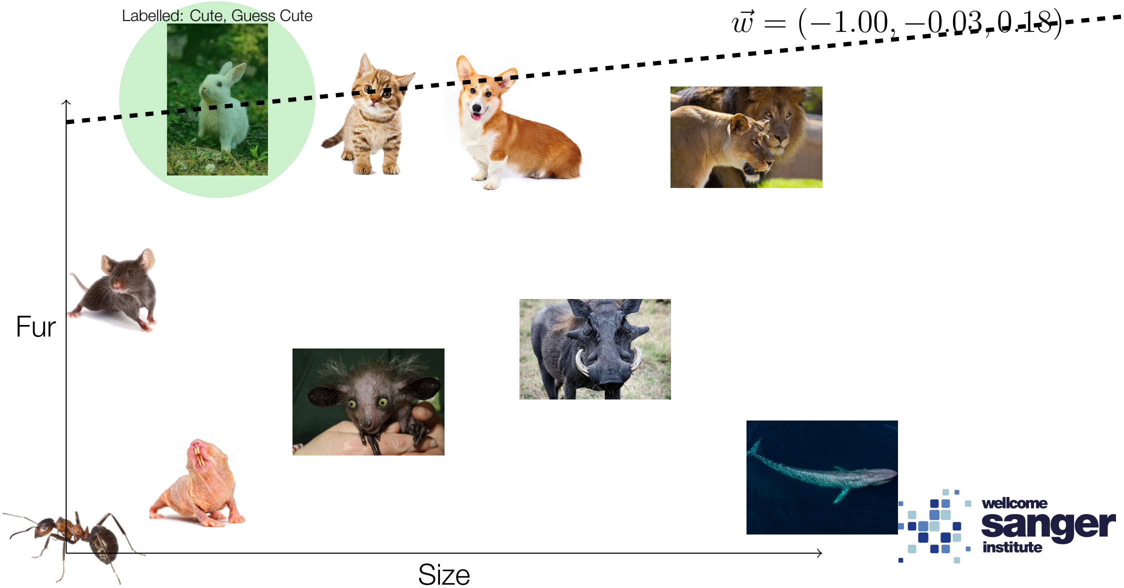

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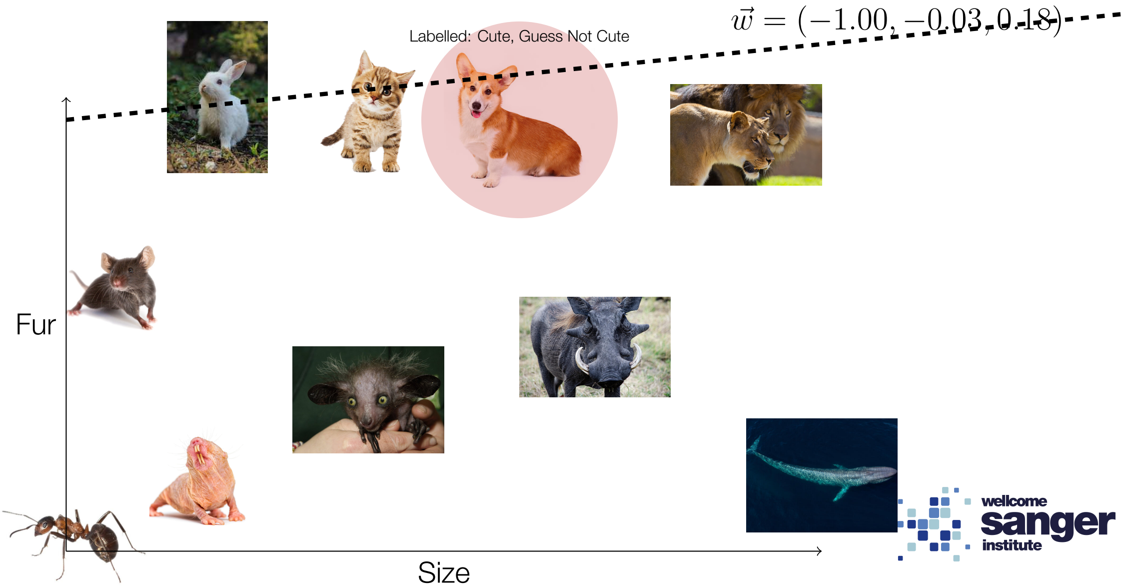

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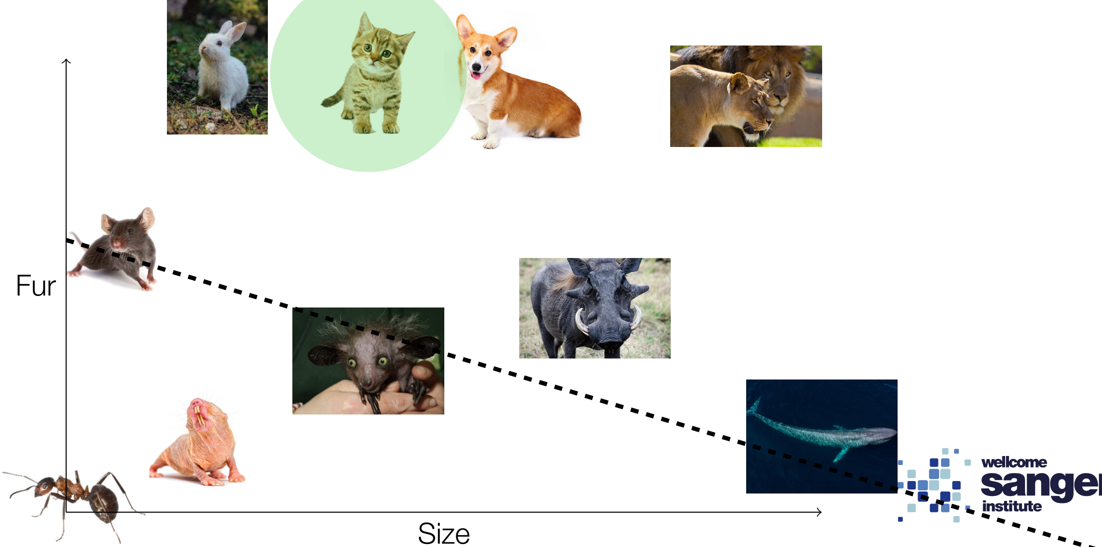

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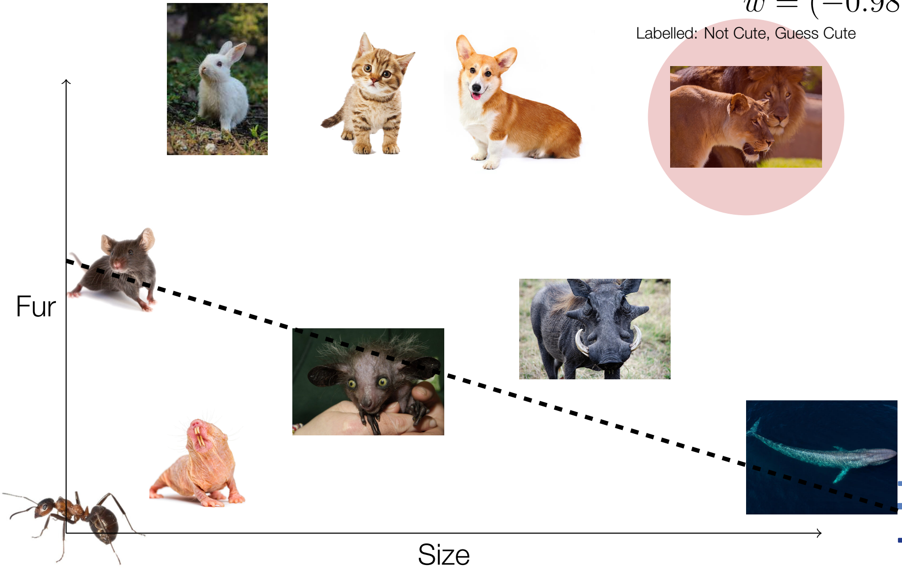

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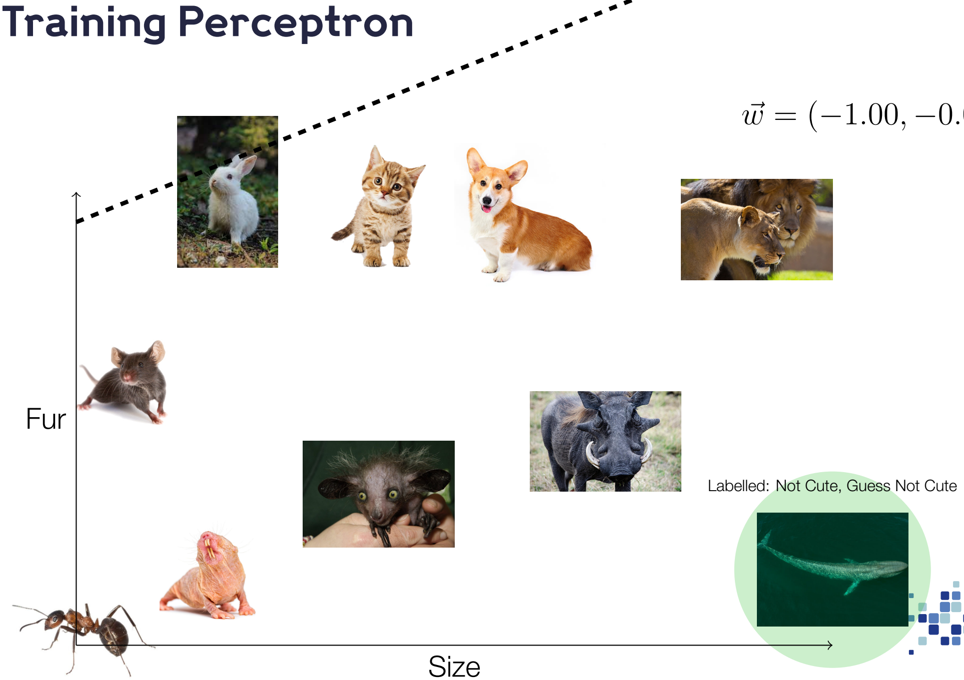

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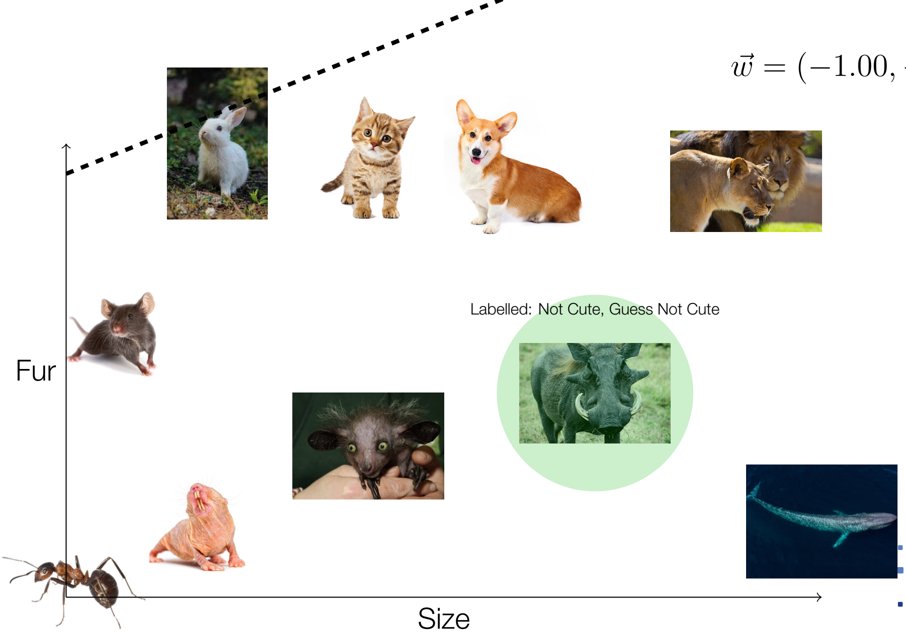

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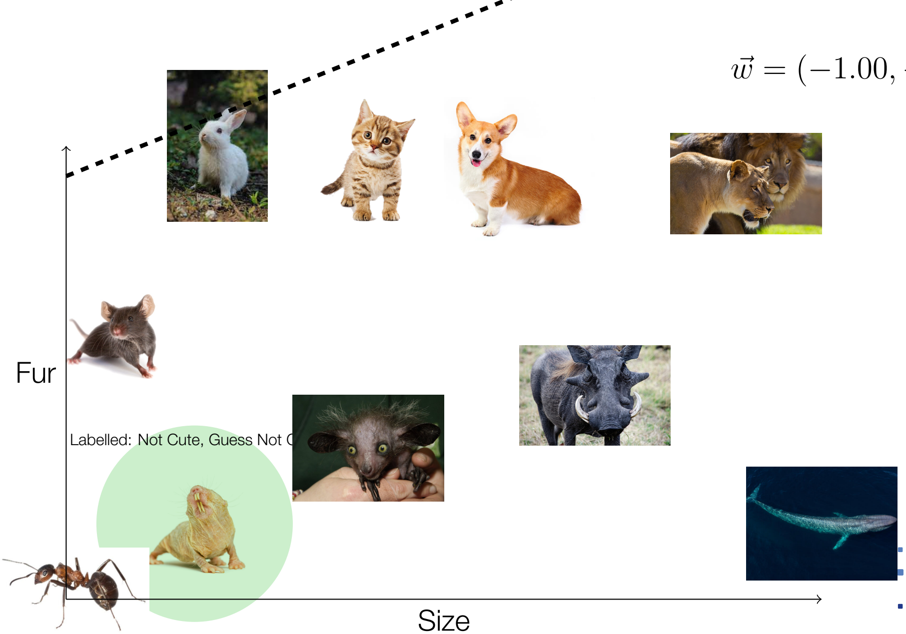

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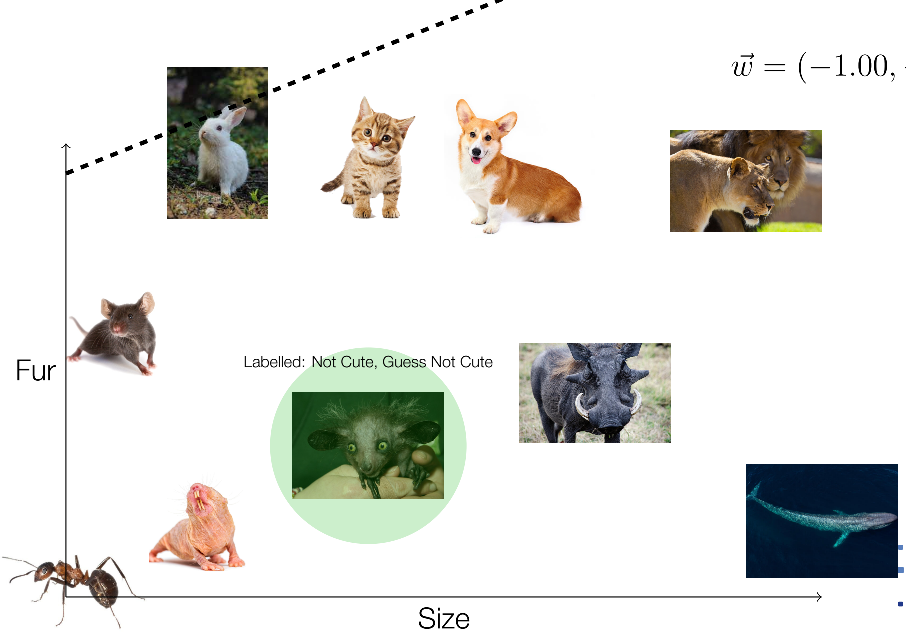

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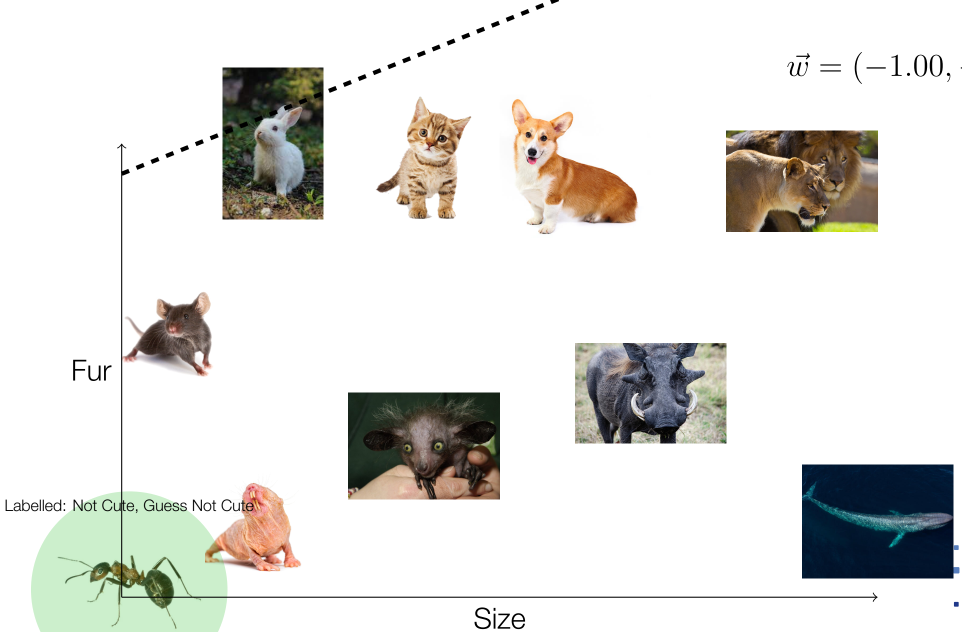

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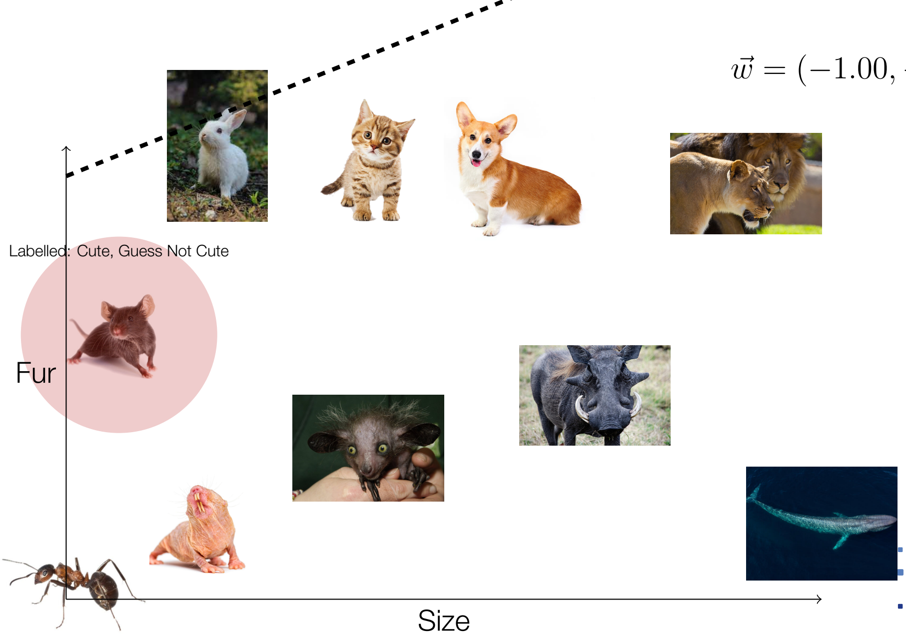

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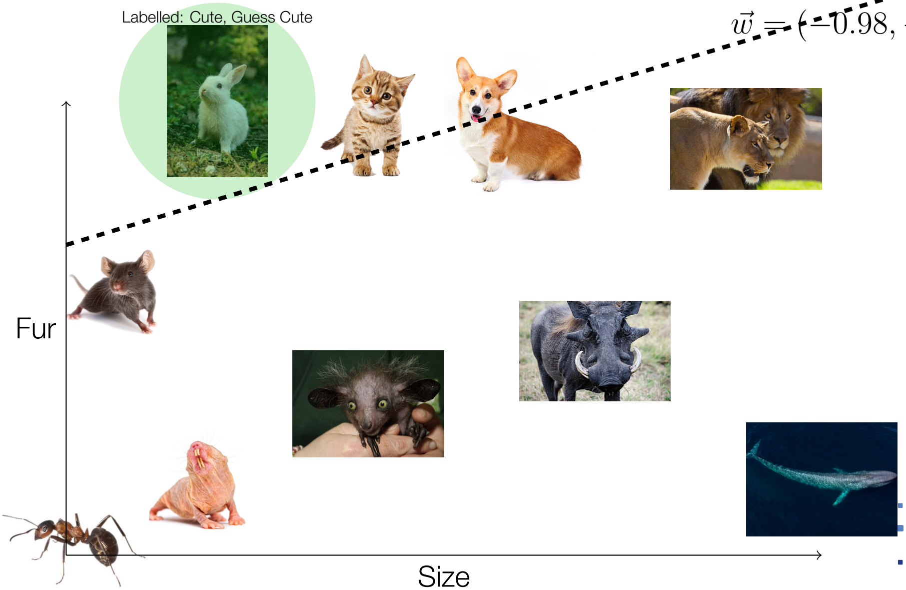
$\vec{w} = (-0.98, -0.06, 0.24)$



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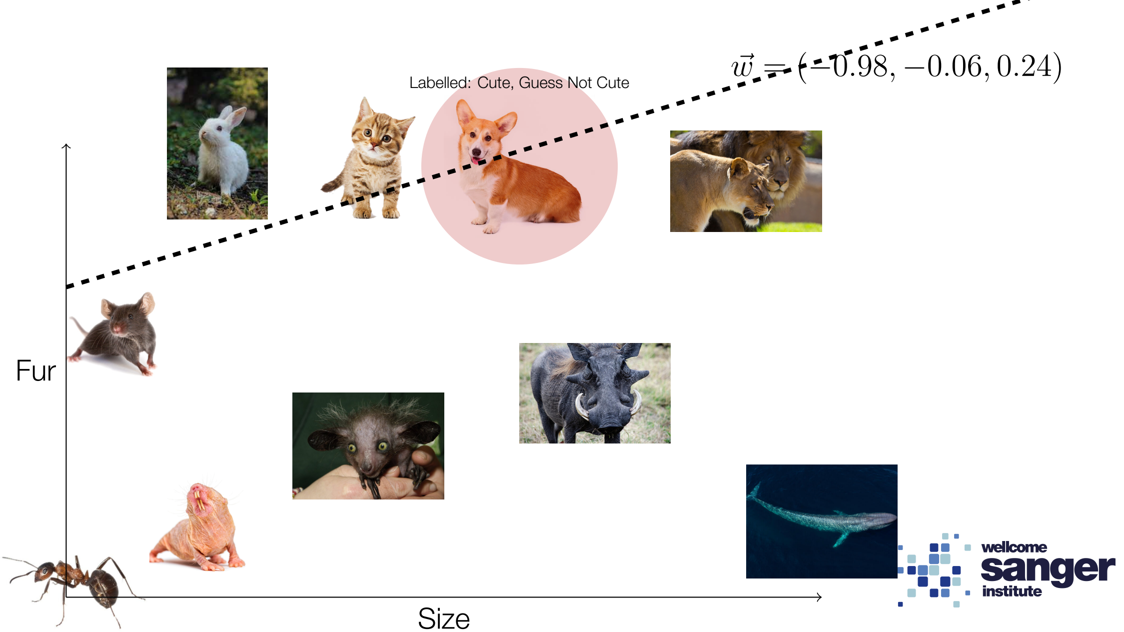

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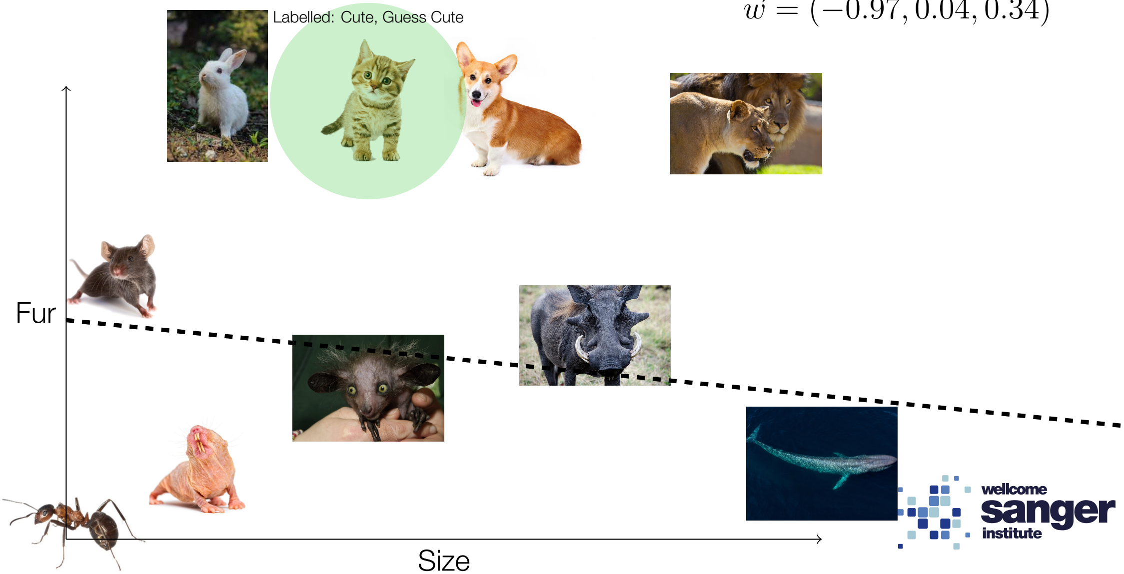

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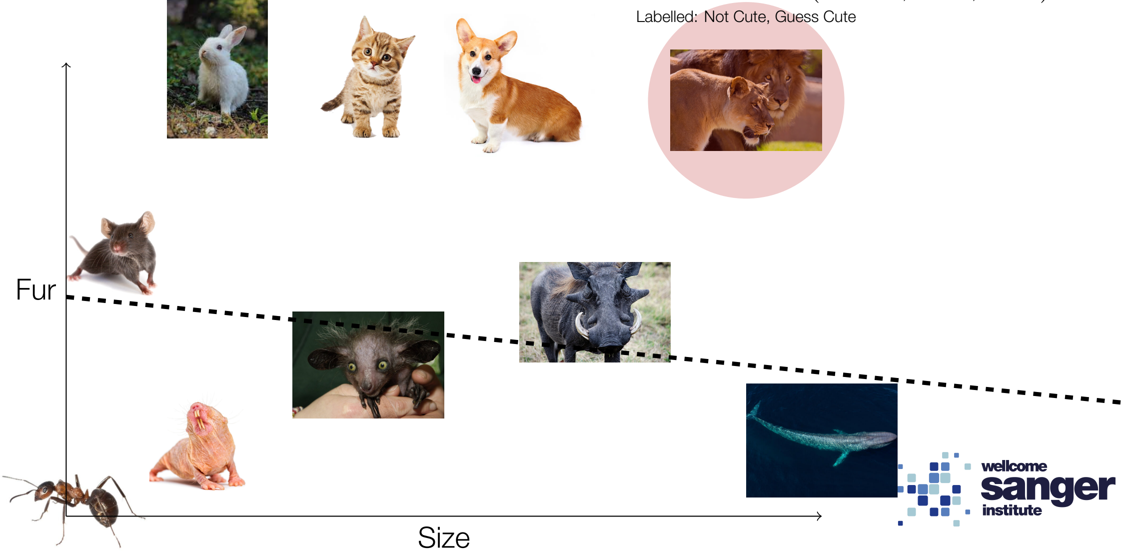

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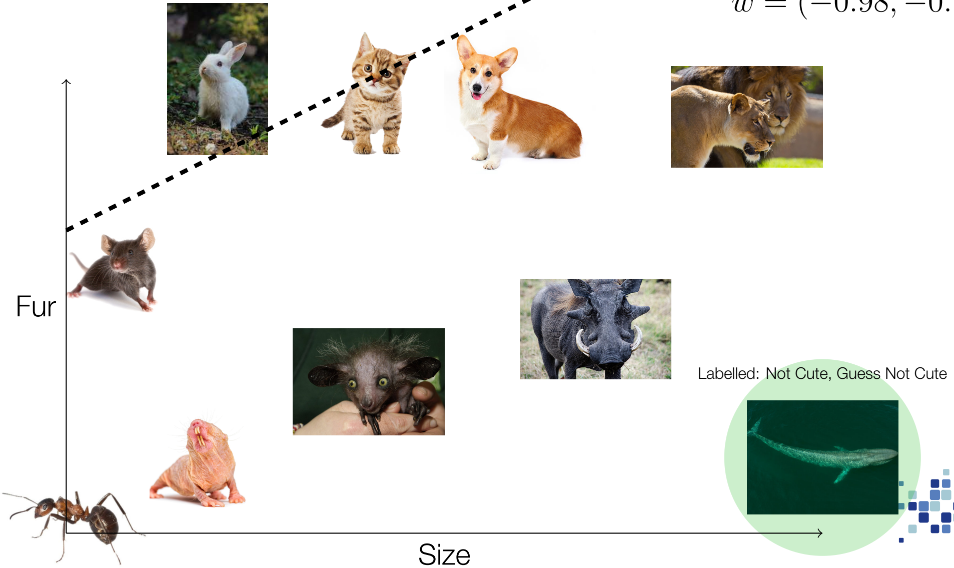

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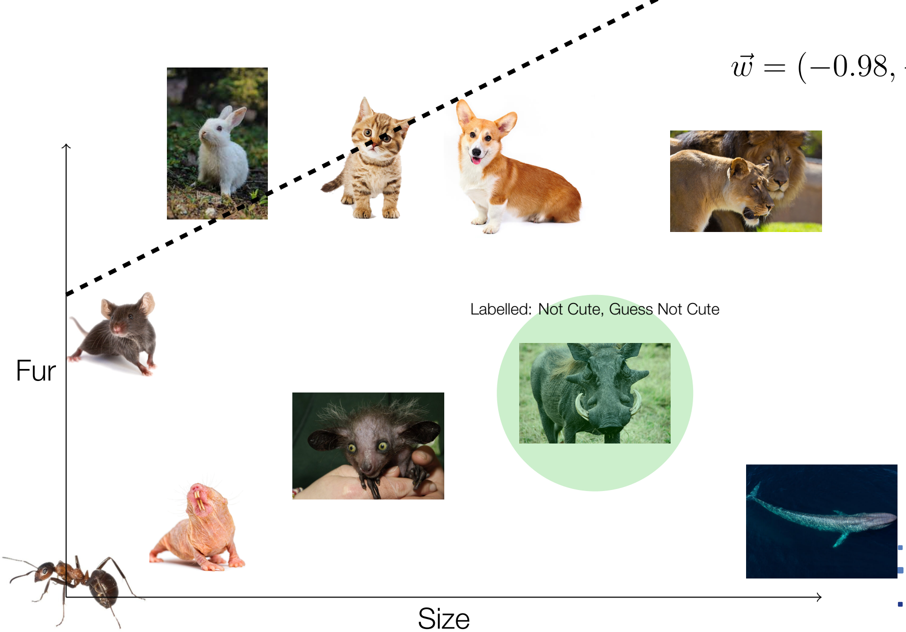

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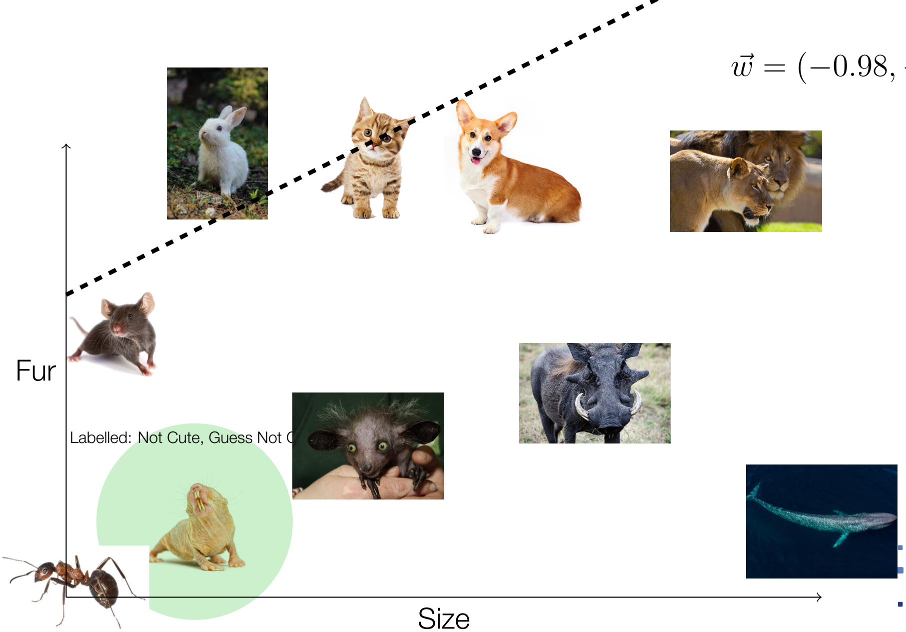

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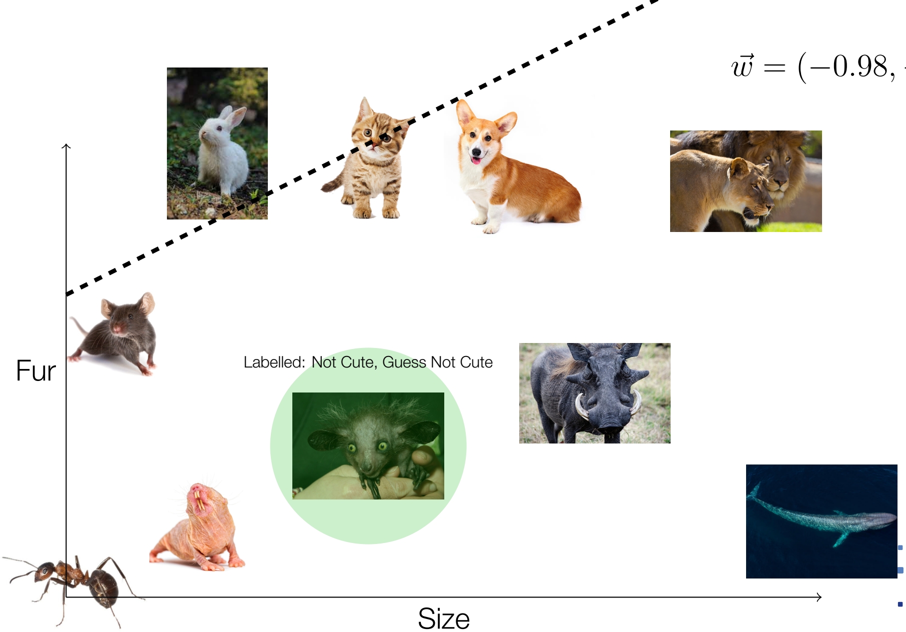

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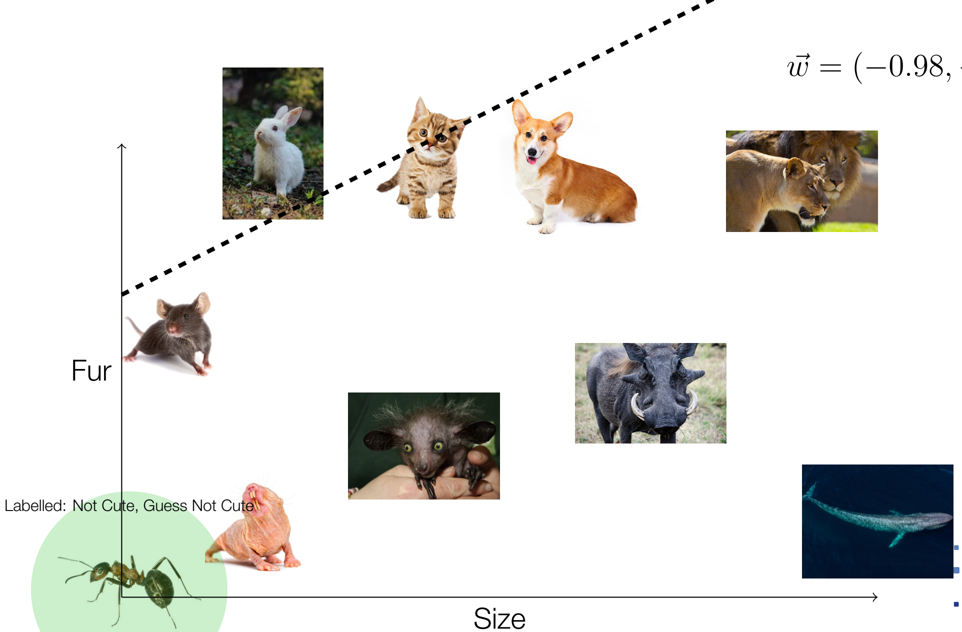

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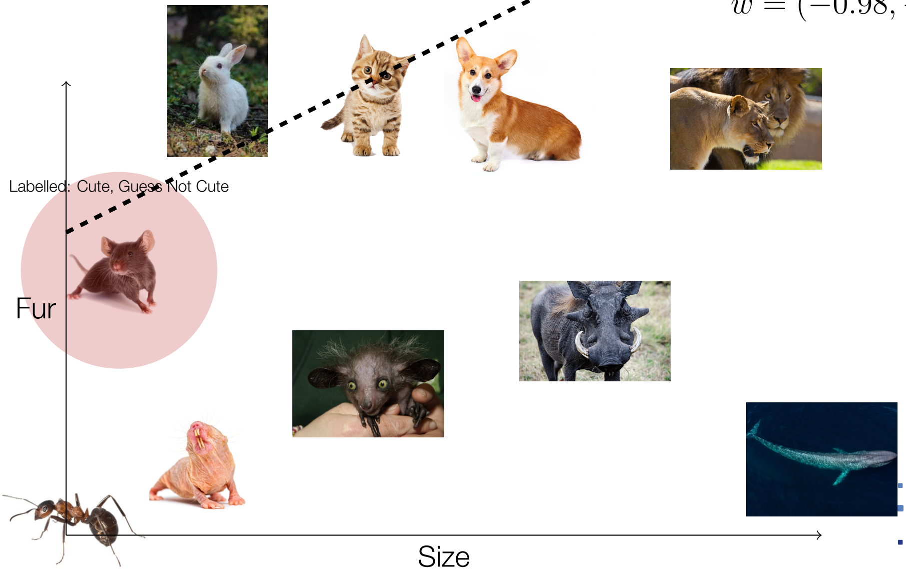

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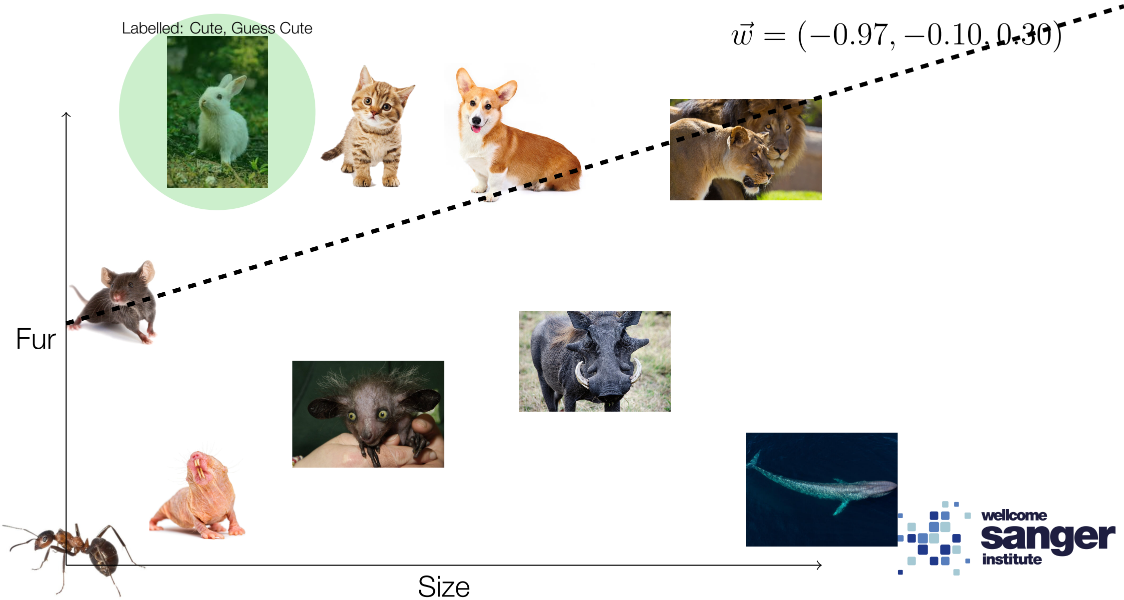

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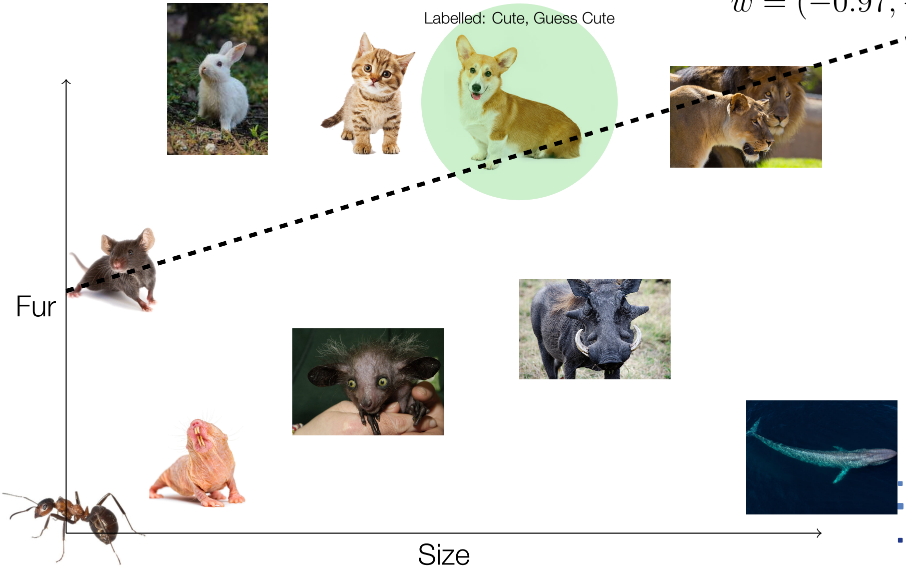

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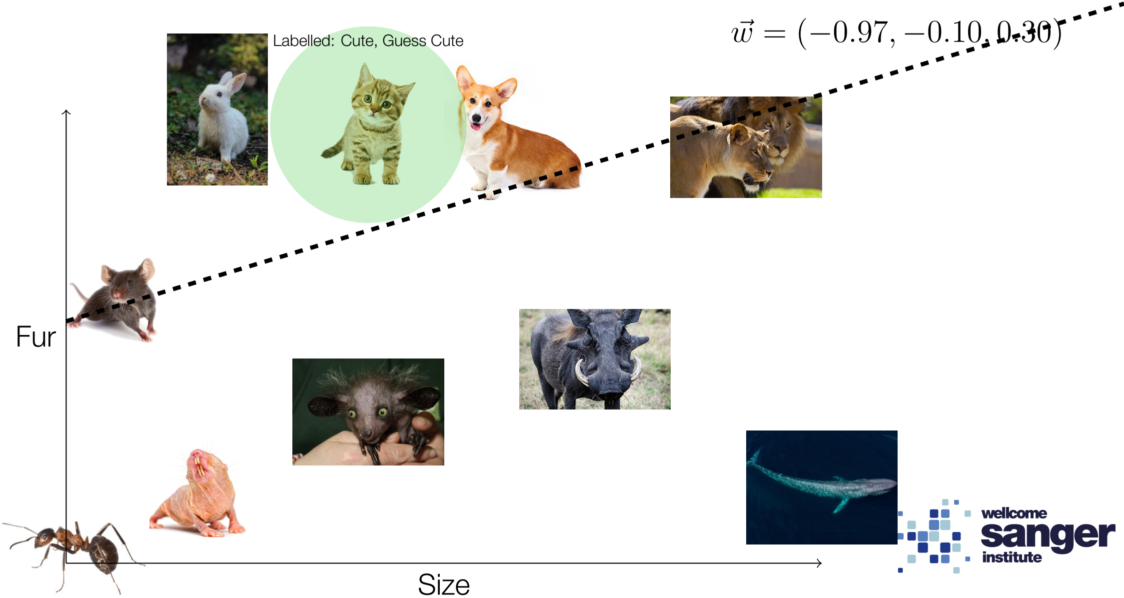

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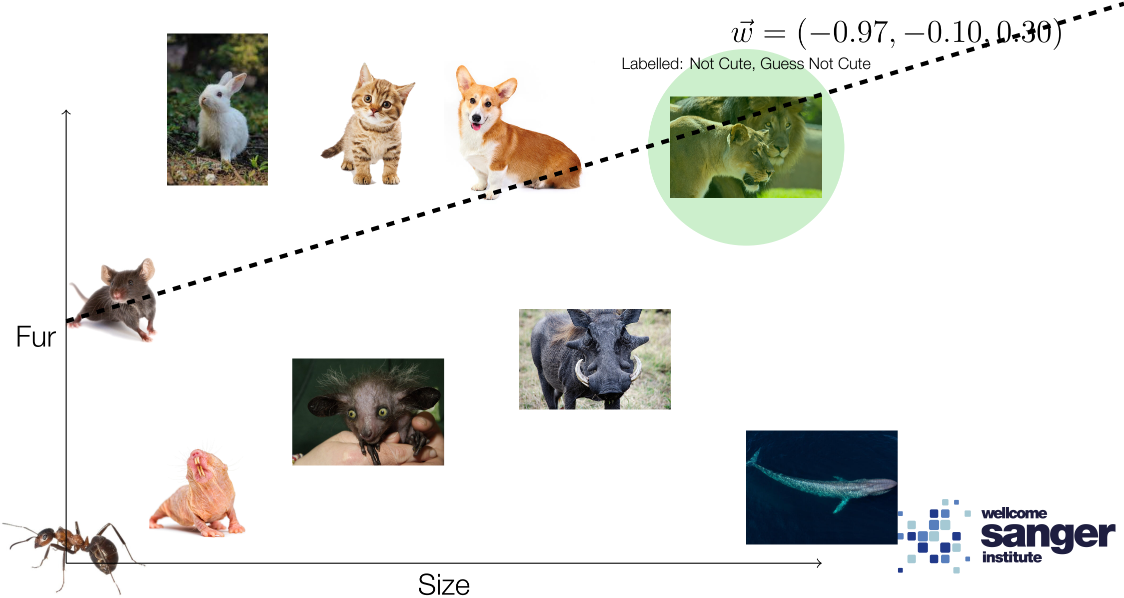

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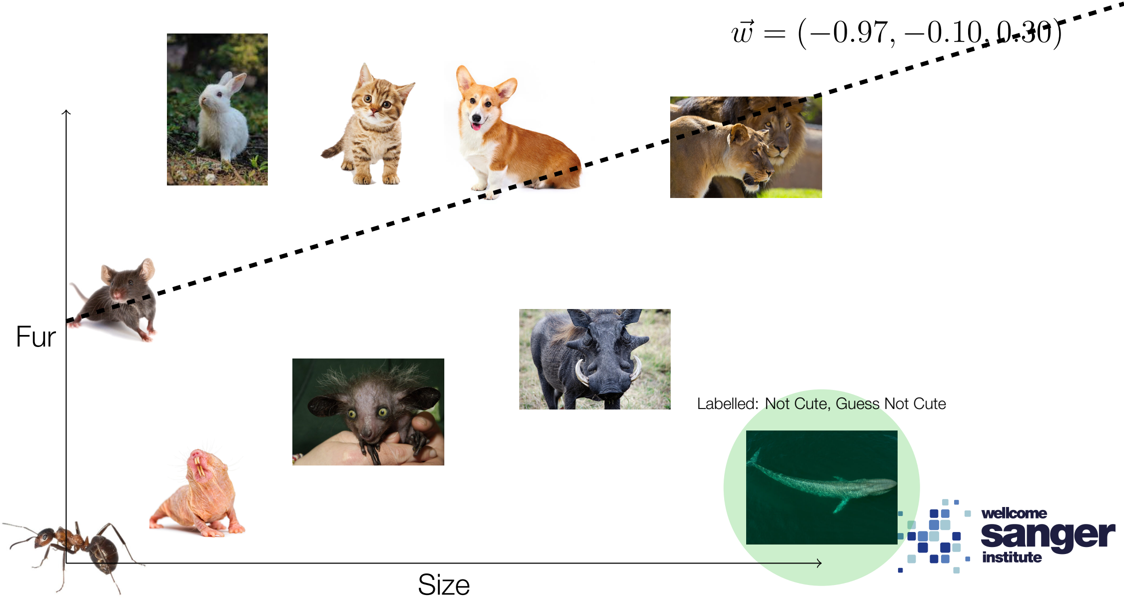

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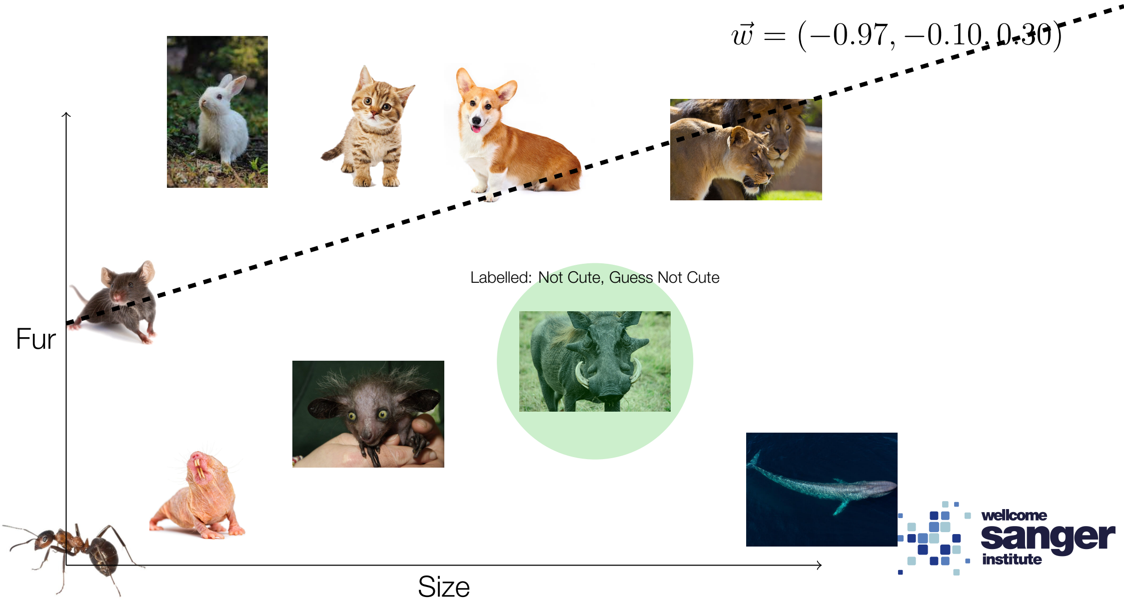

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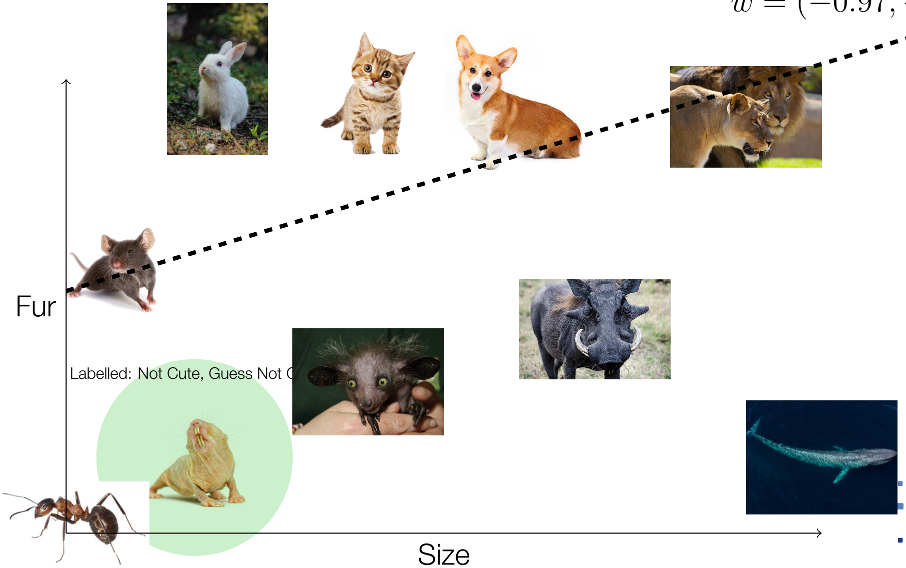

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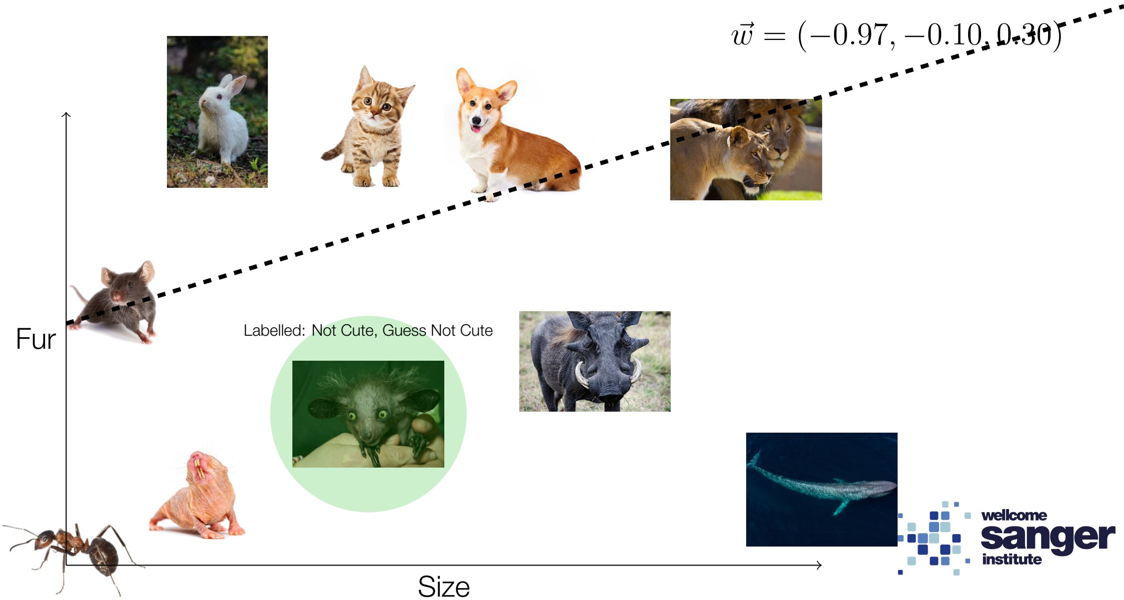

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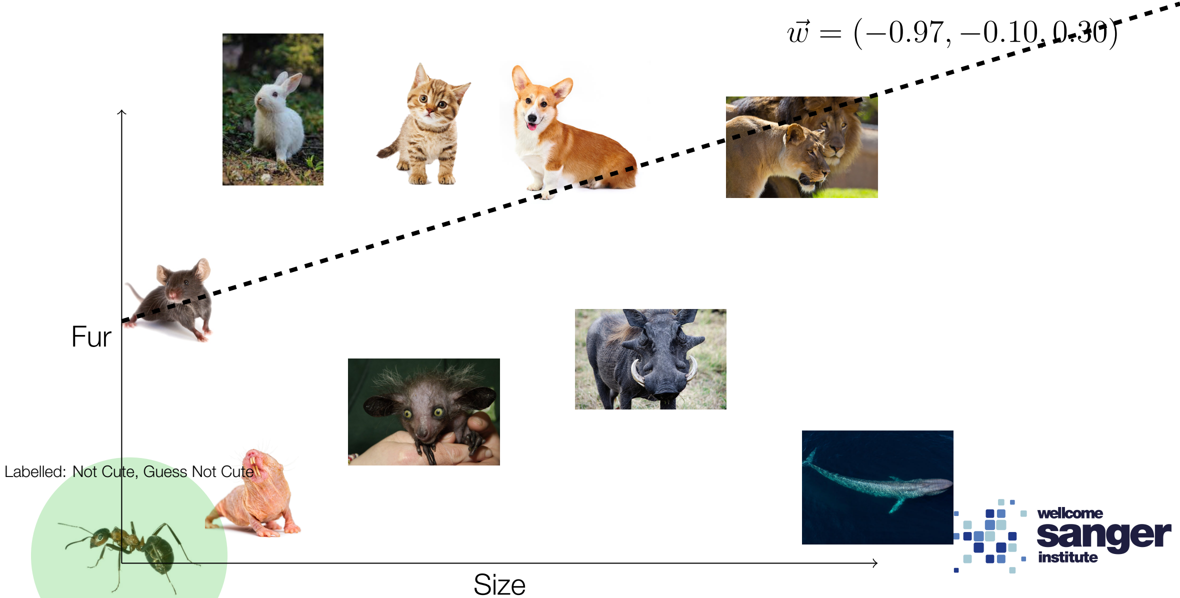

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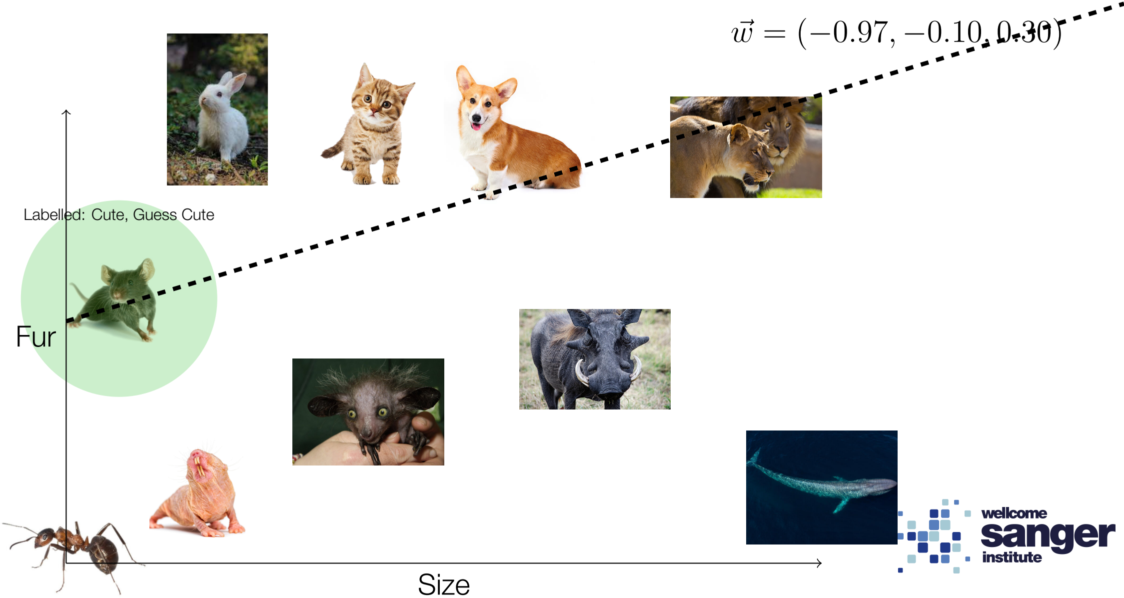

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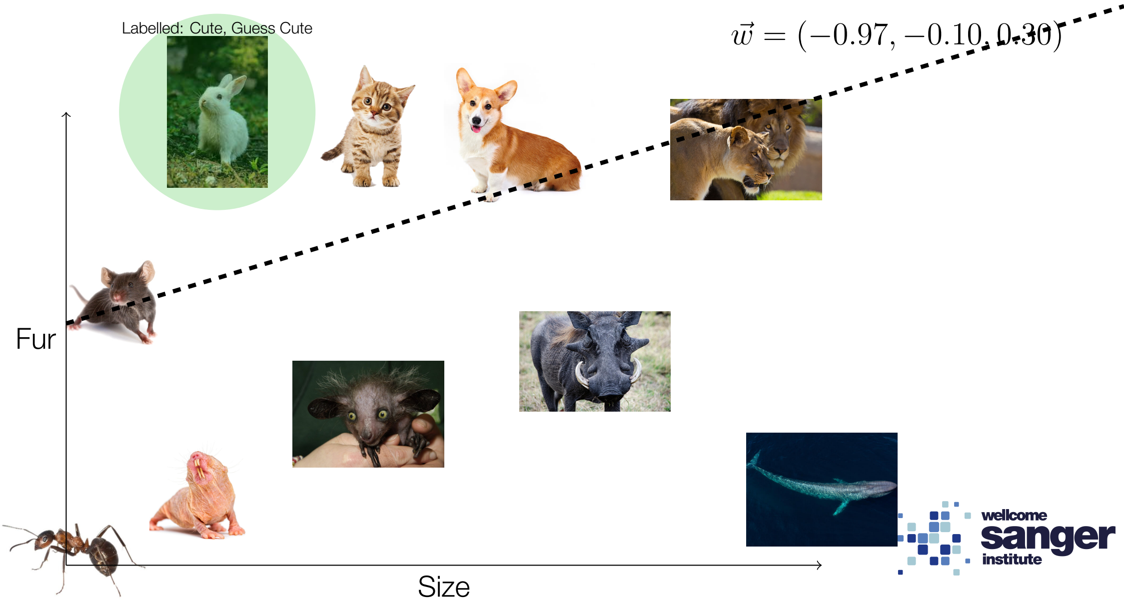

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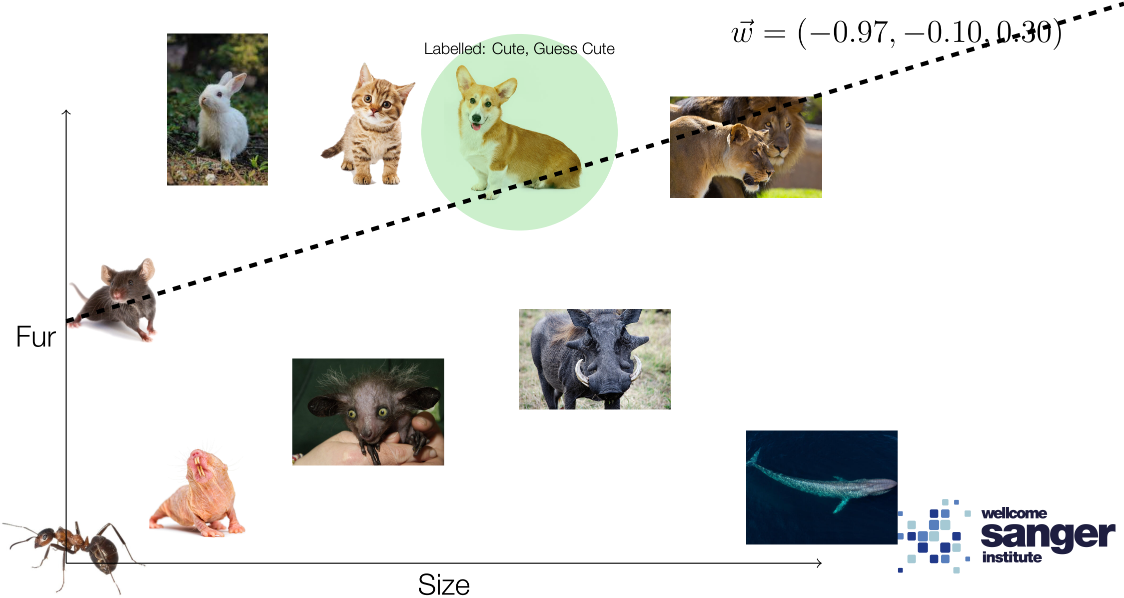

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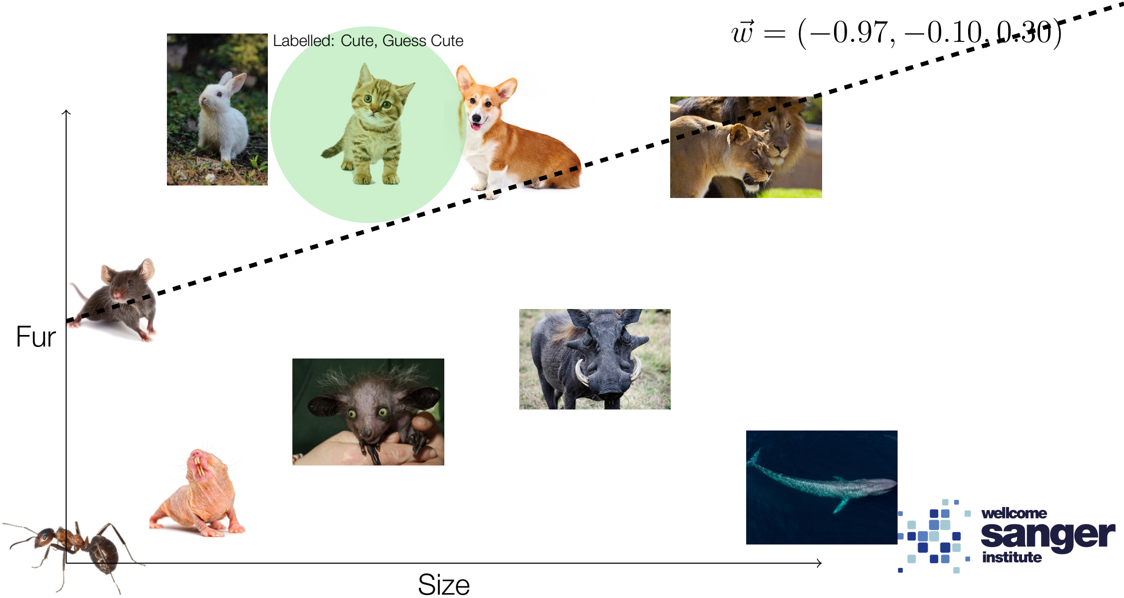

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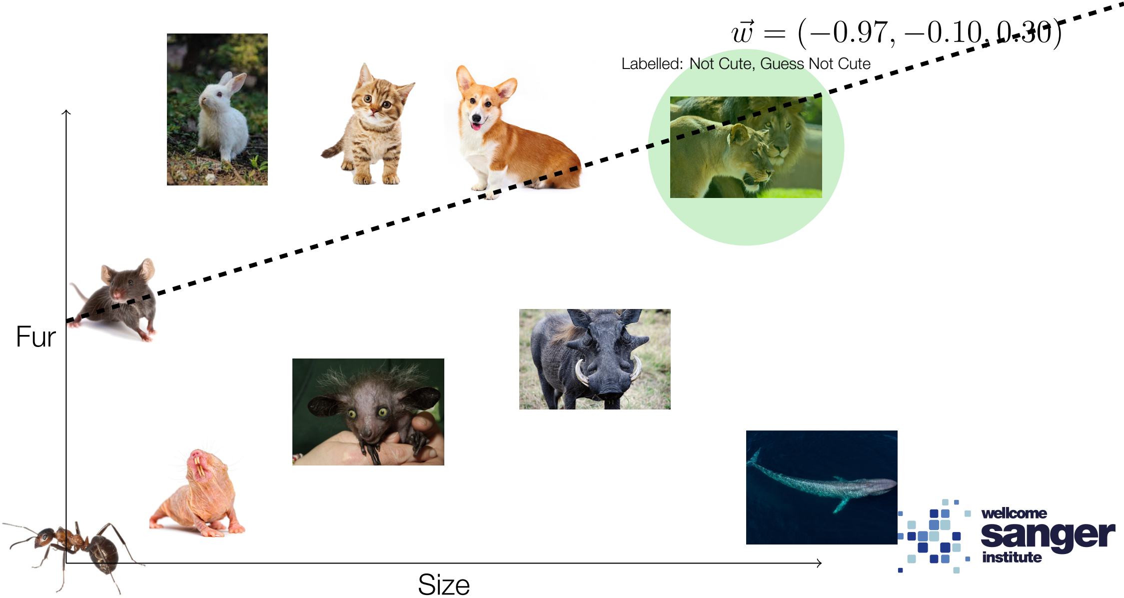
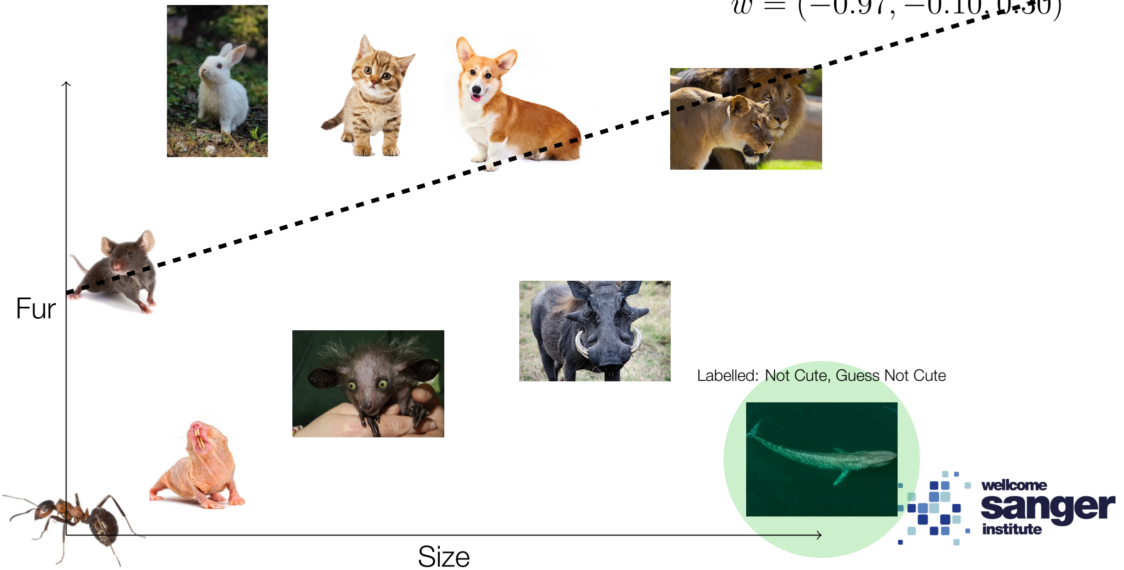


Training Perceptron

$$\vec{w} = (-0.97, -0.10, 0.30)$$



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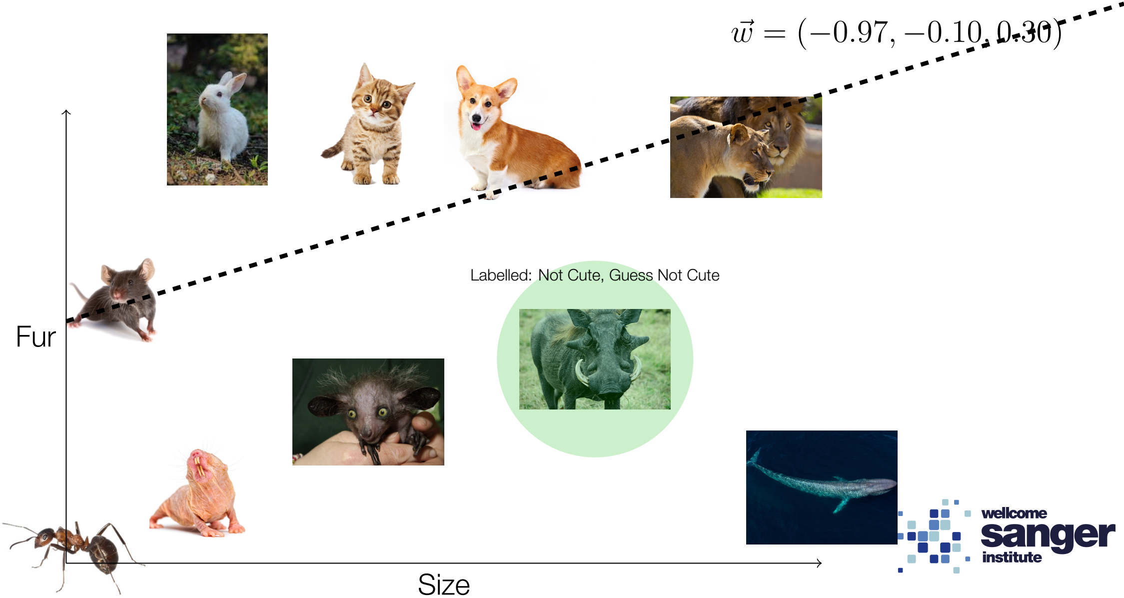

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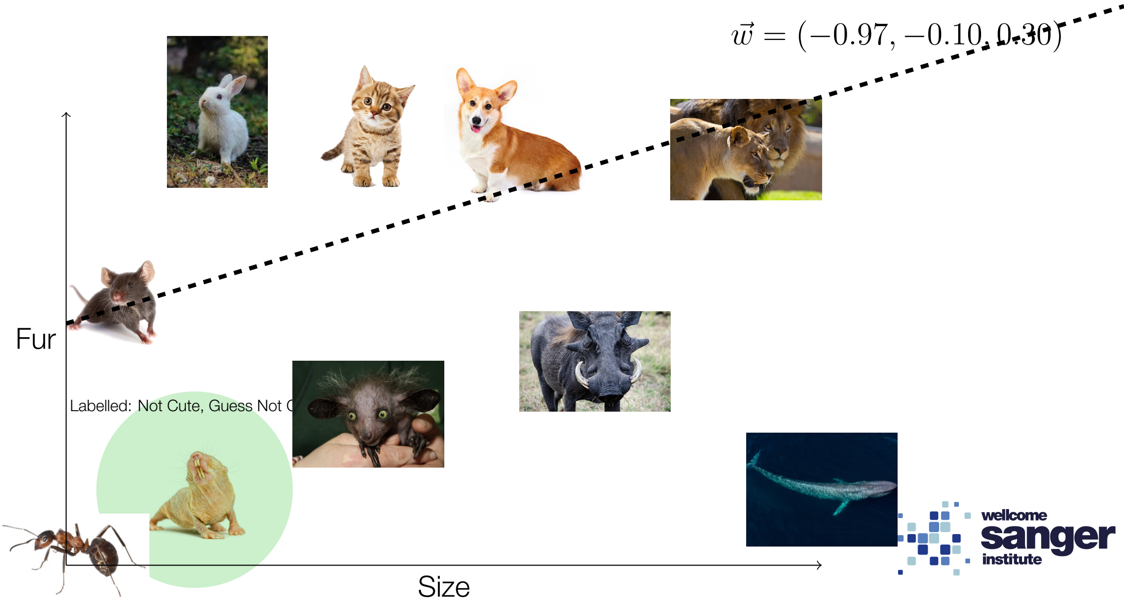

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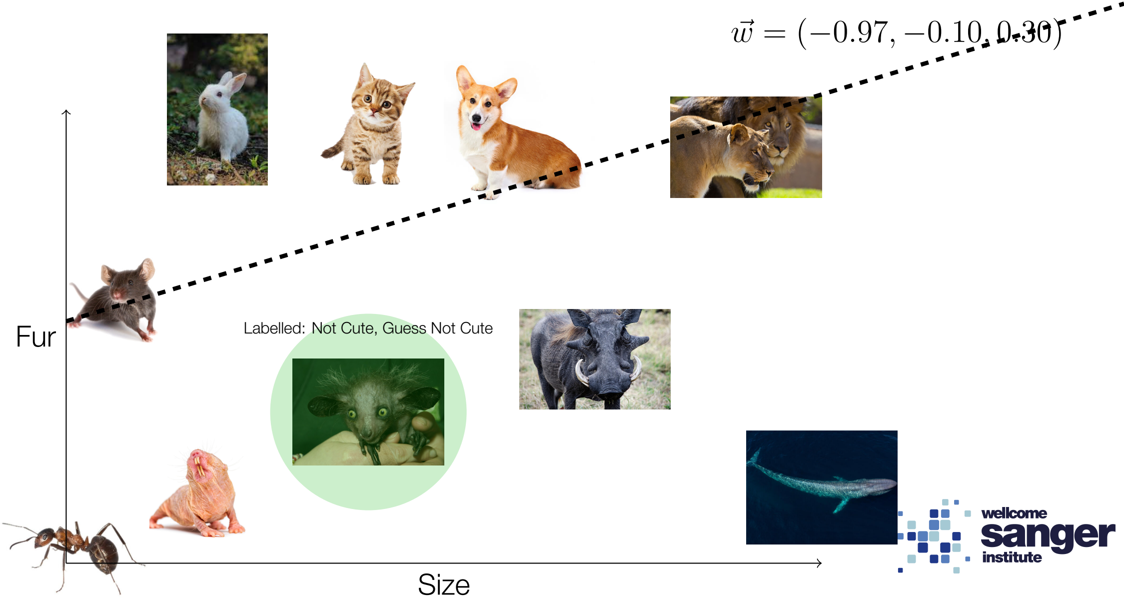

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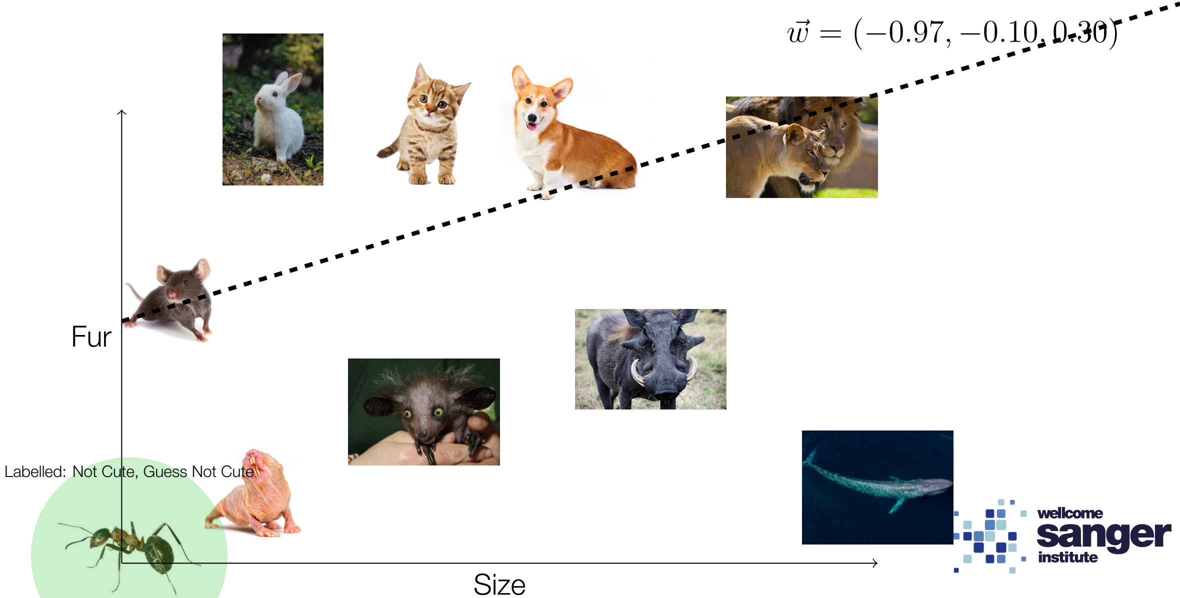

Getting clever....

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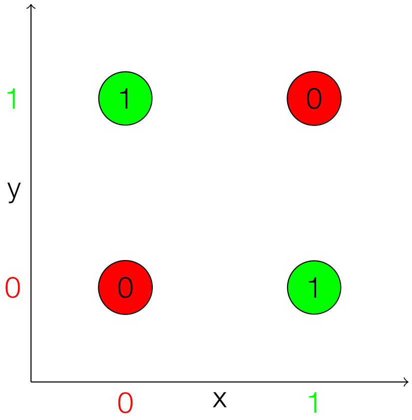
But needs pre-defined user input!

Major limitations....



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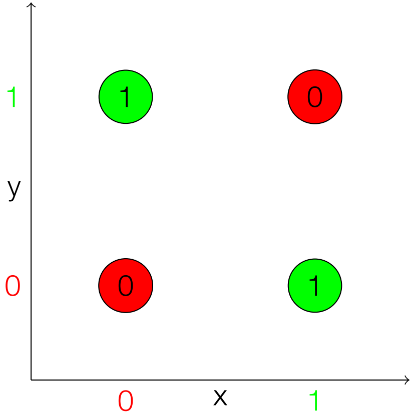

Can **never** be solved by perceptron

The Multilayered Perceptron

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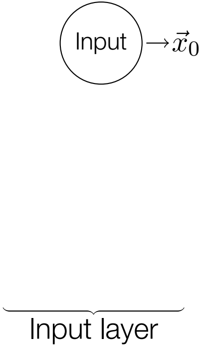

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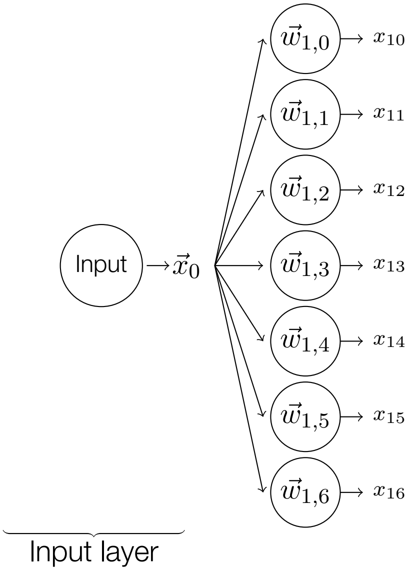

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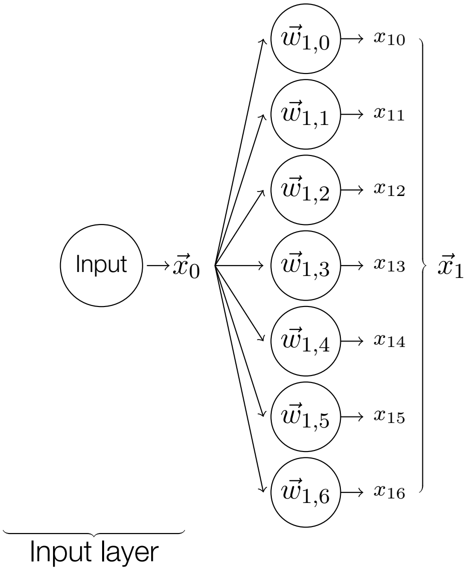

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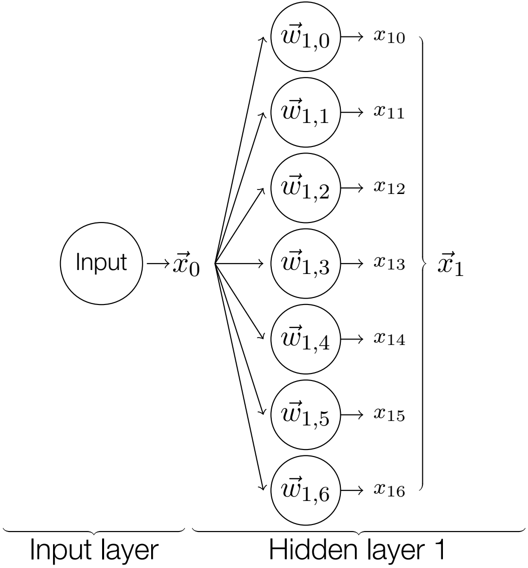

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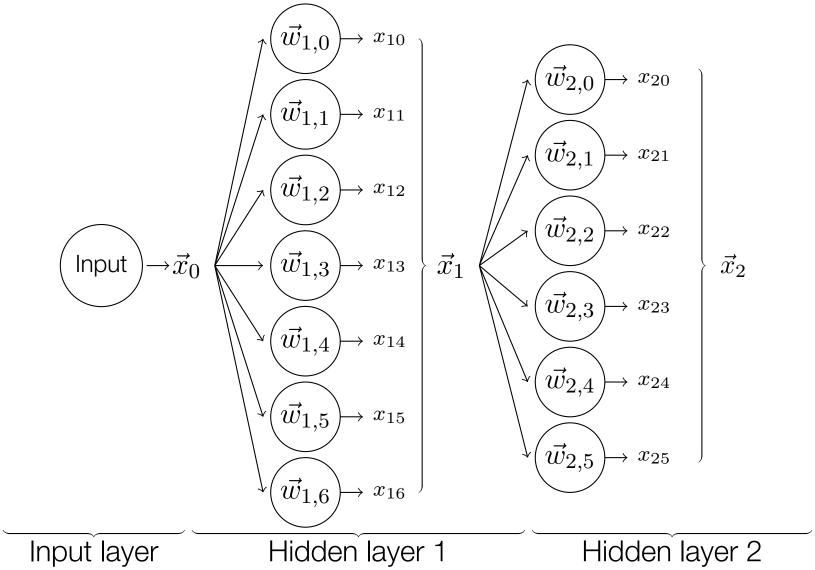

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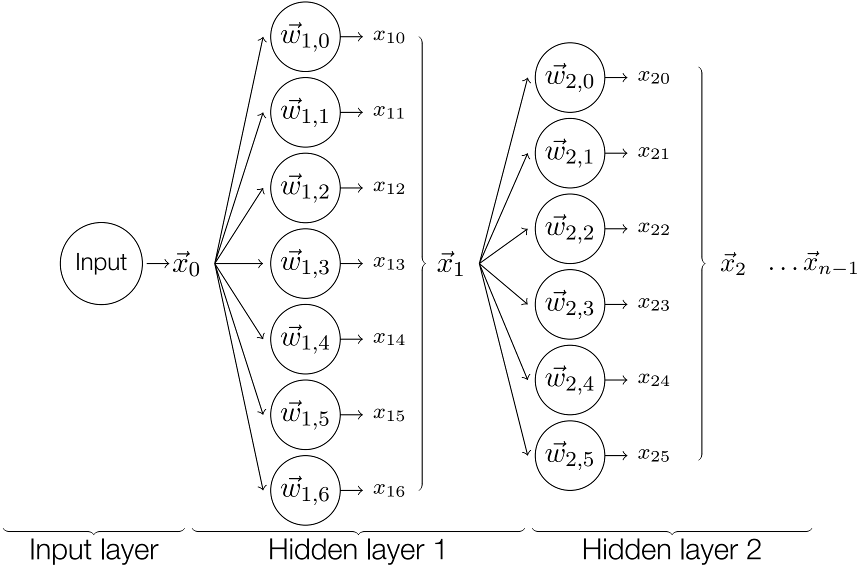

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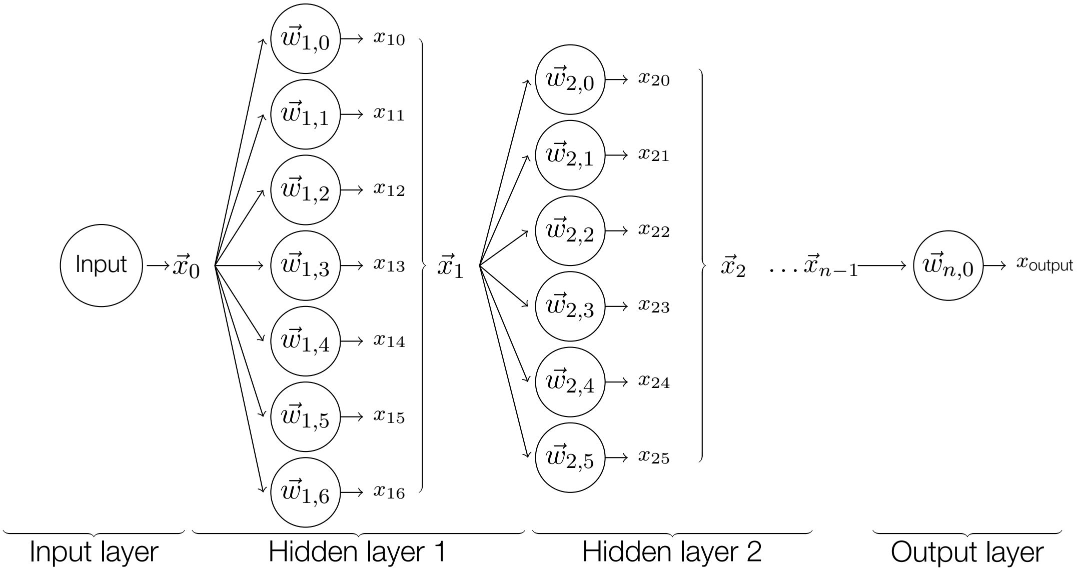

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For our ‘cute’ problem, even a 10,000 layer network with 5 million nodes will ultimately reduce into a single 2×1 matrix (i.e. a single dot product).

Breaking Linearity

Introduce the idea of ‘activation functions’:

$$x_{n,i} = \phi\left(\vec{w}_{n,i} \cdot \vec{x}_{n-1}\right) \tag{5}$$

ϕ has following properties:

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In practice, we like some other properties (analytical derivatives, easy to compute etc.)

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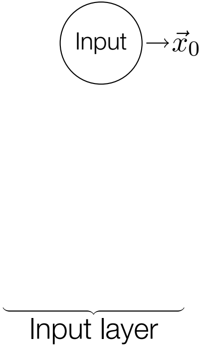

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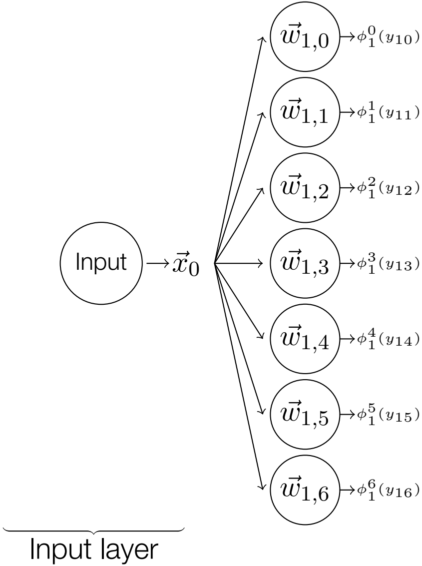

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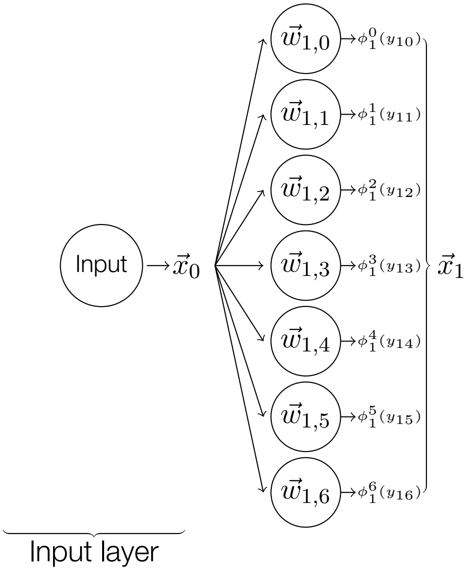

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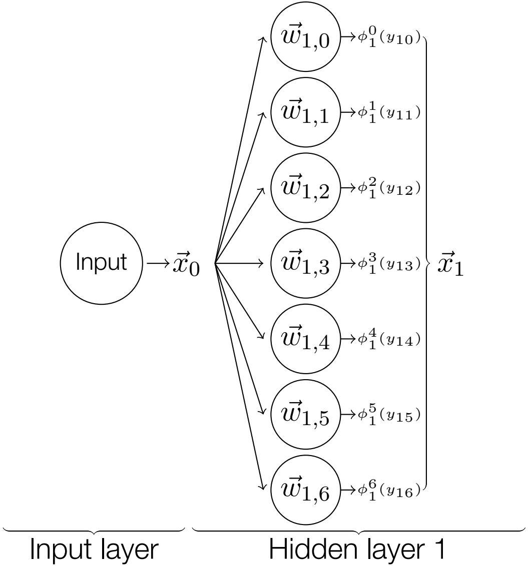

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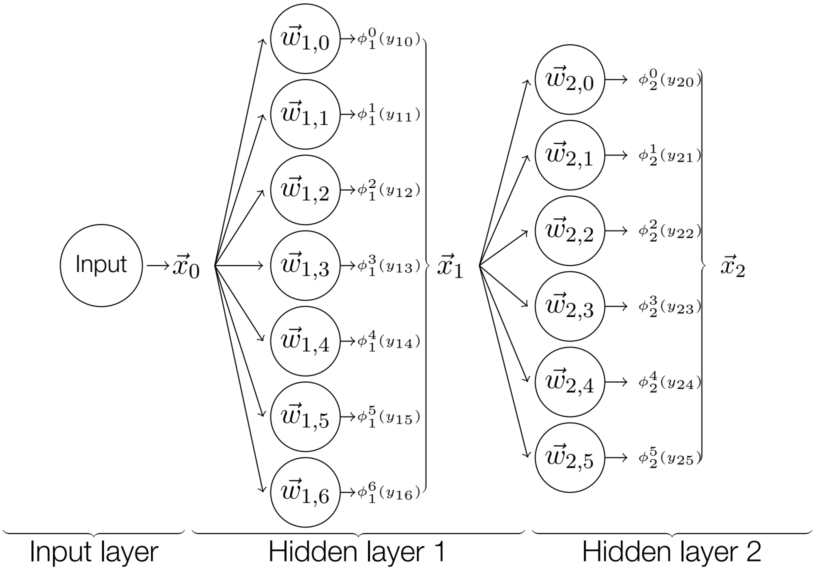

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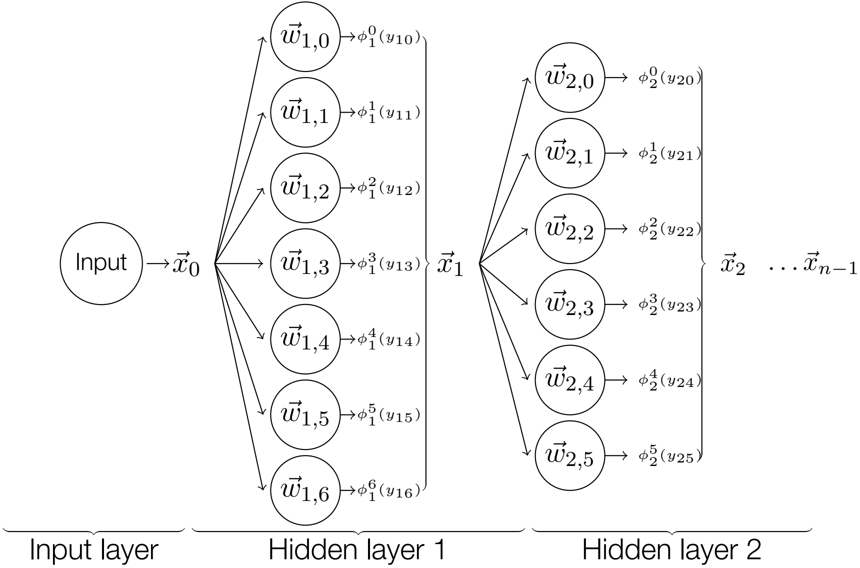

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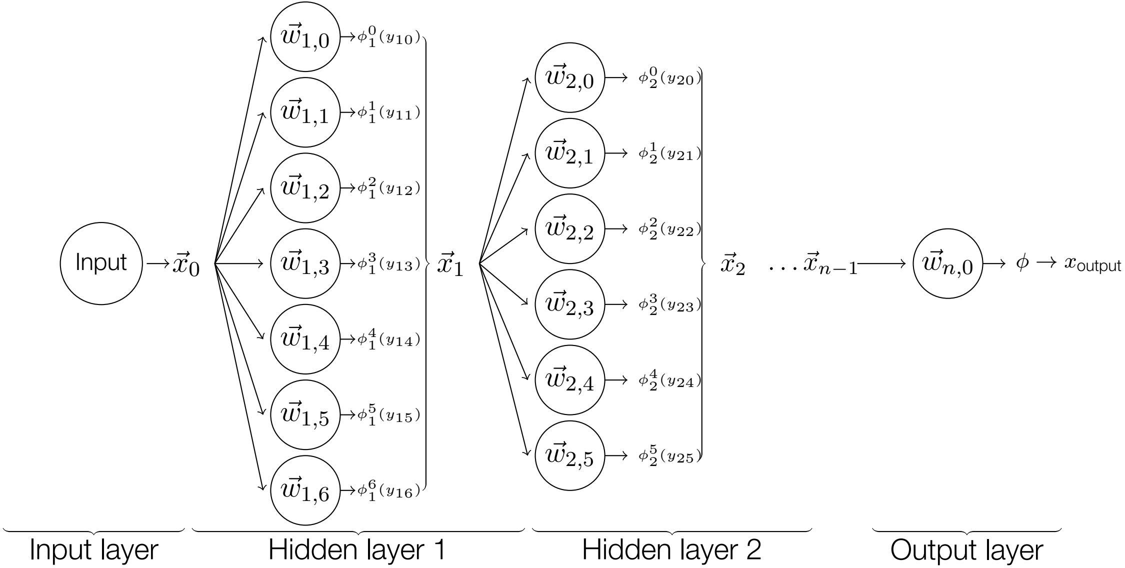

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Naive optimisation function (L_2 cost function):

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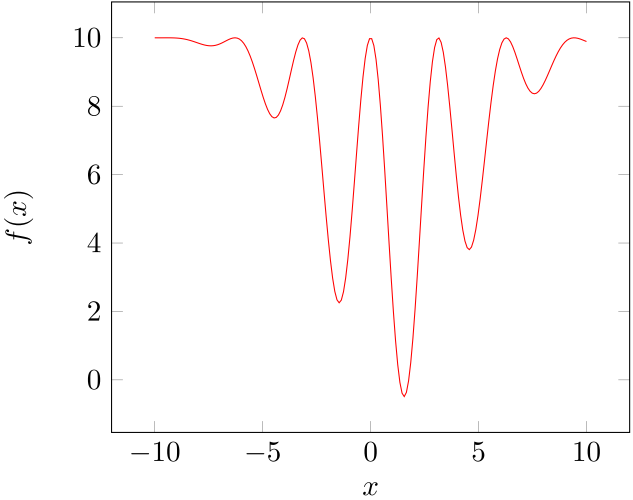
Big when $\mathcal{P} \neq L$, small when $\mathcal{P} = L$ $\rightarrow$ need to *minimise* this function

Optimisation



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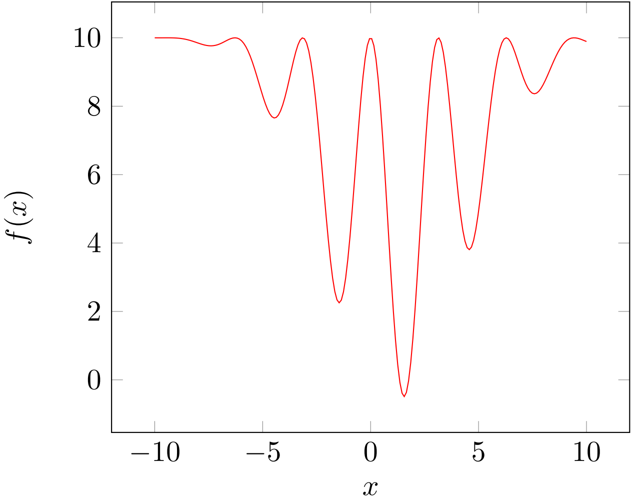

What value of x has lowest value of $f(x)$?

Optimisation

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- Theoretical solutions not **practical**

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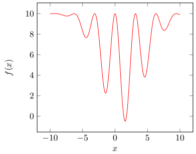

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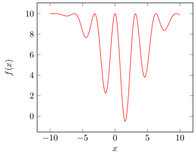

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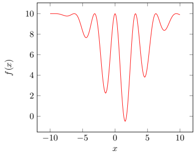

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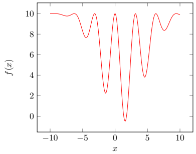

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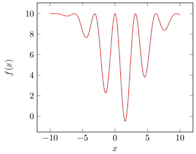

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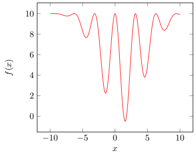

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Various modifications (adaptive learning, momentum etc.)

Derivatives of Networks

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Fundamentally need ***derivatives***: in which direction does changing $\{\vec{w}\}$ improve $\mathcal{L}$?

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But $\mathcal{L}$ is a *complicated* function of $\{\vec{w}\}$!

Chain Rule: Crash Course

If y is a function of x, and f is a function of y, then:

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \frac{\mathrm{d}f}{\mathrm{d}y}\frac{\mathrm{d}y}{\mathrm{d}x} \tag{8}$$

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In higher dimensions, have to sum over all possible combinations:

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Back to the optimisation problem

w_{ijk} is the k^{th} element of weight vector in the j^{th} node, in the i^{th} layer.

$$\frac{\partial \mathcal{L}}{\partial w_{ijk}} = \sum_{i \text{ in dataset}} \left(\mathcal{P}(\vec{x}_i | \{\vec{w}_{ij}\}) - L_i\right) \frac{\partial P}{\partial w_{ijk}} \tag{10}$$

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Have two cases: i is the final layer, or it is not. If in the final layer, this is trivial:

$$\mathcal{P} = x_{\text{final}} = \phi(\underbrace{\vec{w}_f \cdot \vec{x}_{i-1}}_{y_{ij}})$$

$$\frac{\partial P}{\partial \vec{w}_{ij}} = \left.\frac{\partial \phi}{\partial y}\right|_{y=y_{ij}} \vec{x}_{i-1} \tag{11}$$

$$= \phi'(y_{ij})\vec{x}_{n-1}$$

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Therefore:

$$\frac{\partial \mathcal{L}}{\partial w_{\text{final}k}} = \sum_{i \text{ in dataset}} \left(\mathcal{P}(\vec{x}_i | \{\vec{w}_{ij}\}) - L_i\right) \phi'(y_{\text{final}}) \left[\vec{x}_{i-1}\right]_k \tag{12}$$

What about non-final layers?

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$$\vec{x}_i = \begin{pmatrix} \phi(\vec{x}_i \cdot \vec{w}_{i,0}) \\ \phi(\vec{x}_{i-1} \cdot \vec{w}_{i,1}) \\ \vdots \\ \phi(\vec{x}_{i-1} \cdot \vec{w}_{i,j}) \end{pmatrix} = \begin{pmatrix} \phi(y_{i,0} \\ \phi(y_{i,1}) \\ \vdots \\ \phi(y_{i,j})) \end{pmatrix} \tag{13}$$

By the chain rule:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial w_{ijk}} &= \frac{\partial \mathcal{L}}{\partial y_{ij}} \frac{\partial y_{ij}}{\partial w_{ijk}} \\ &= \frac{\partial \mathcal{L}}{\partial y_{ij}} \left[\vec{x}_{i-1}\right]_k \end{aligned} \tag{14}$$

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$$\vec{x}_i = \begin{pmatrix} \phi(\vec{x}_i \cdot \vec{w}_{i,0}) \\ \phi(\vec{x}_{i-1} \cdot \vec{w}_{i,1}) \\ \vdots \\ \phi(\vec{x}_{i-1} \cdot \vec{w}_{i,j}) \end{pmatrix} = \begin{pmatrix} \phi(y_{i,0} \\ \phi(y_{i,1}) \\ \vdots \\ \phi(y_{i,j})) \end{pmatrix} \tag{13}$$

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By the chain rule:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial w_{ijk}} &= \frac{\partial \mathcal{L}}{\partial y_{ij}} \frac{\partial y_{ij}}{\partial w_{ijk}} \\ &= \frac{\partial \mathcal{L}}{\partial y_{ij}} \left[\vec{x}_{i-1}\right]_k \end{aligned} \tag{14}$$

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Almost there....

Finally, we note that $\frac{\partial \mathcal{L}}{\partial y_{i+1,j}}$ is simply a statement about how changing y (the dot product) alters L, but that via the chain rule again:

$$\frac{\partial \mathcal{L}}{\partial y_{ij}} = \sum_{p \text{ nodes in next layer}} \frac{\partial \mathcal{L}}{\partial y_{i+1,p}} \frac{\partial y_{i+1,p}}{\partial y_{ij}} \tag{15}$$

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The rate of change of L with respect to y_{ij} is equal to the sum of rates at which y_{ij} changes $y_{i+1,p}$ in the next layer, multiplied by how $y_{i+1,p}$ changes $\mathcal{L}$

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This is **backpropagation**: a fancy way of using the chain rule

And....you're done!

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Let’s see it in action!