

# 6.036/6.862: Introduction to Machine Learning

**Lecture:** starts Tuesdays 9:35am (Boston time zone)

**Course website:** [introml.odl.mit.edu](http://introml.odl.mit.edu)

**Who's talking?** Prof. Tamara Broderick

**Questions?** [discourse.odl.mit.edu](http://discourse.odl.mit.edu) (“Lecture 4” category)

**Materials:** Will all be available at course website

## Last Time(s)

- I. Linear classifiers
- II. Perceptron algorithm
- III. A more-complete ML analysis

## Today's Plan

- I. Linear logistic classification/logistic regression
- II. Gradient descent

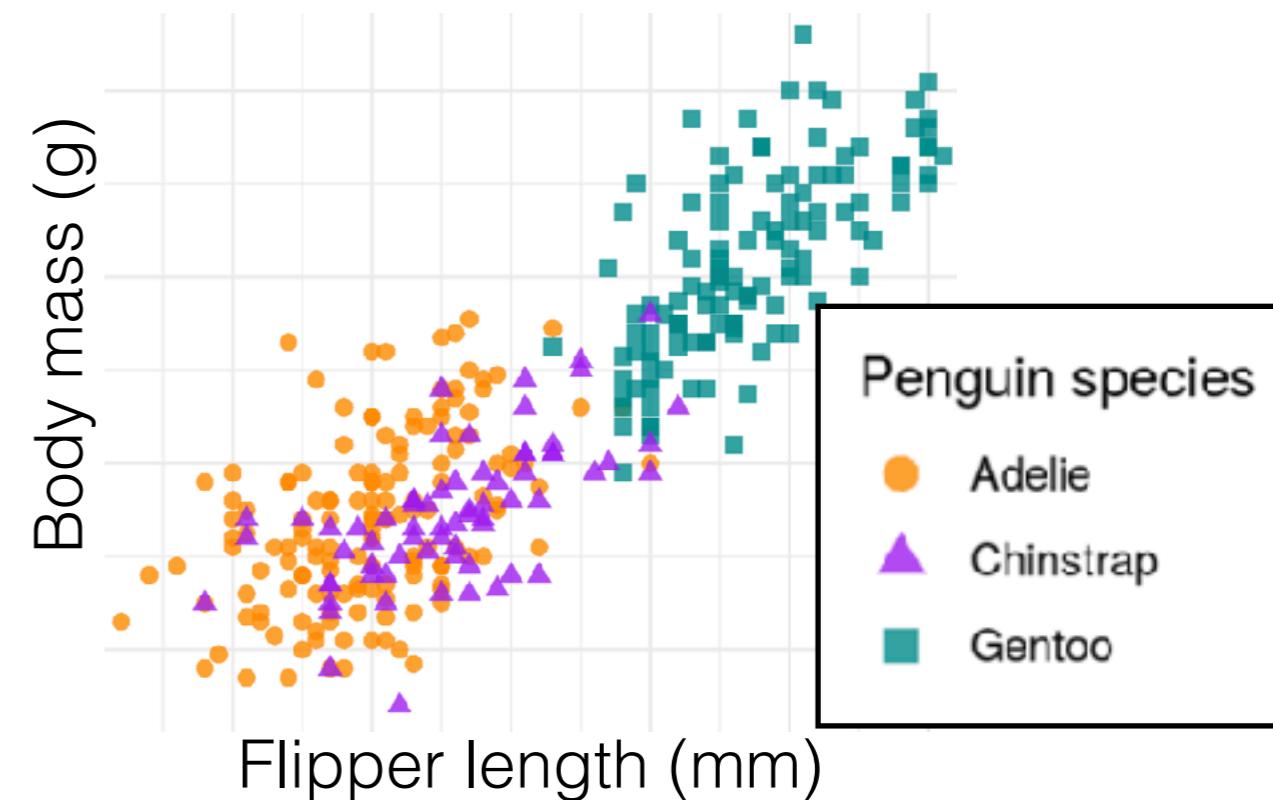
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- Perceptron struggles with data that's not linearly separable

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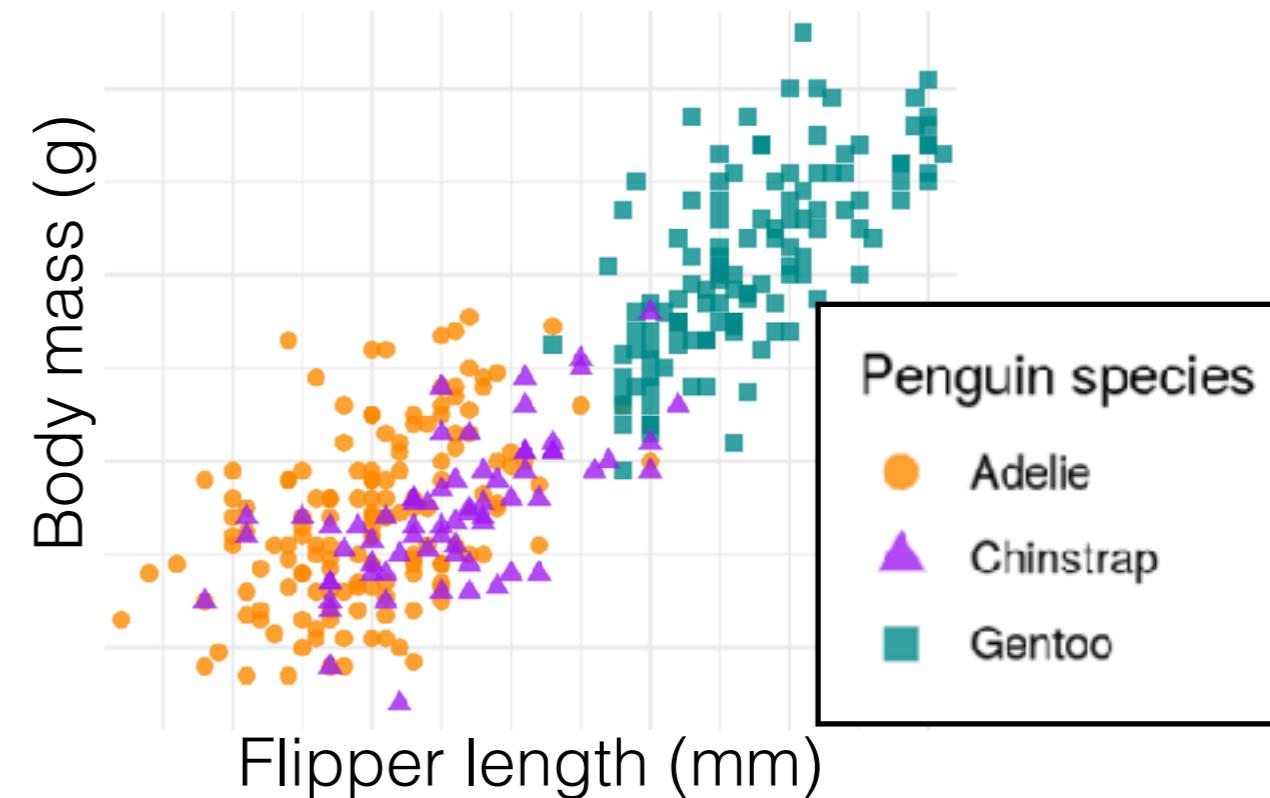


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- Perceptron doesn't have a notion of uncertainty (how well do we know what we know?)

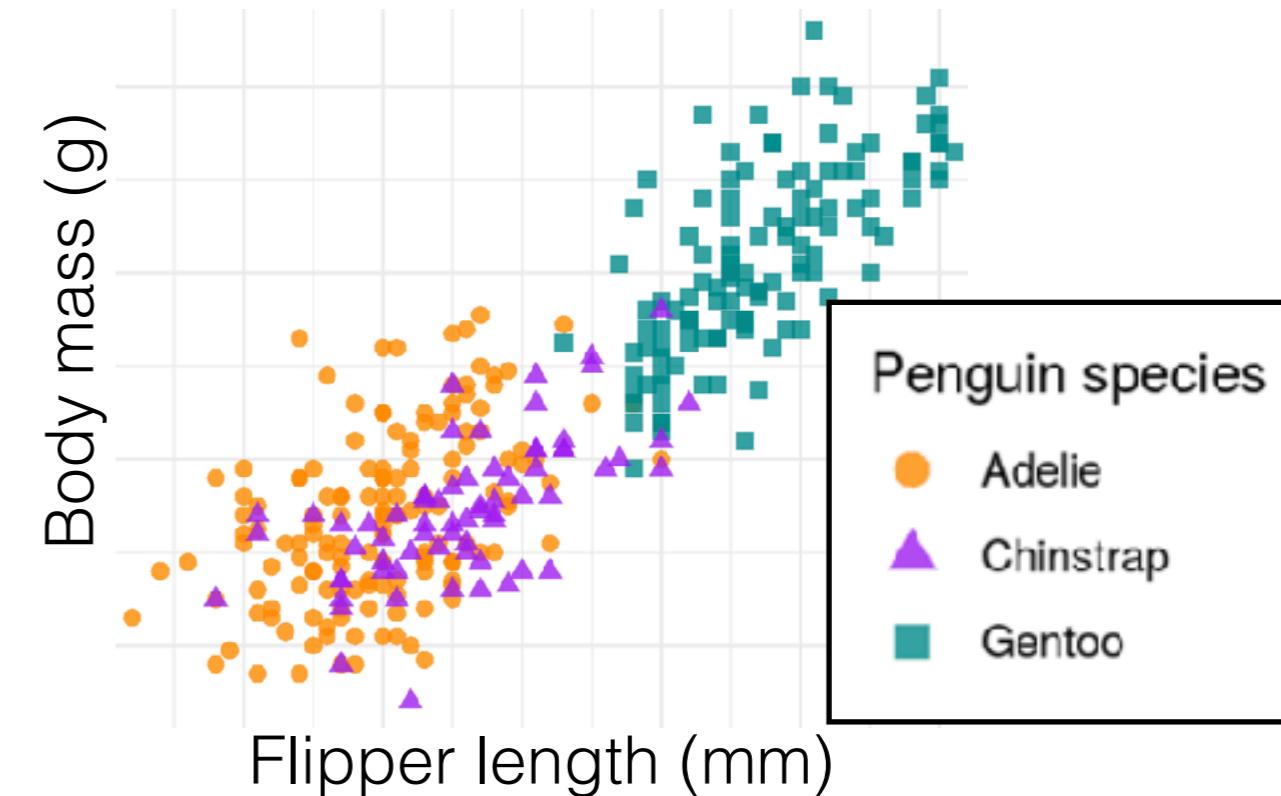
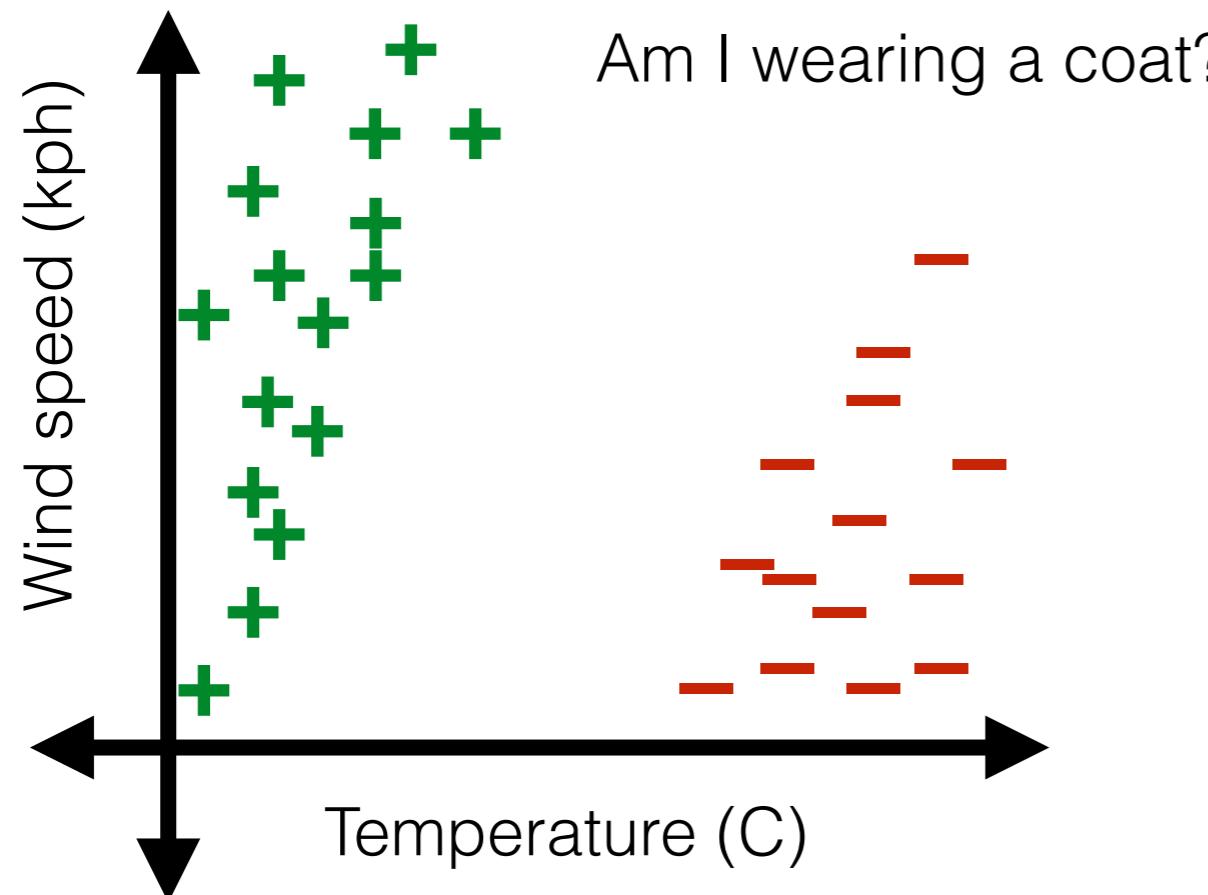


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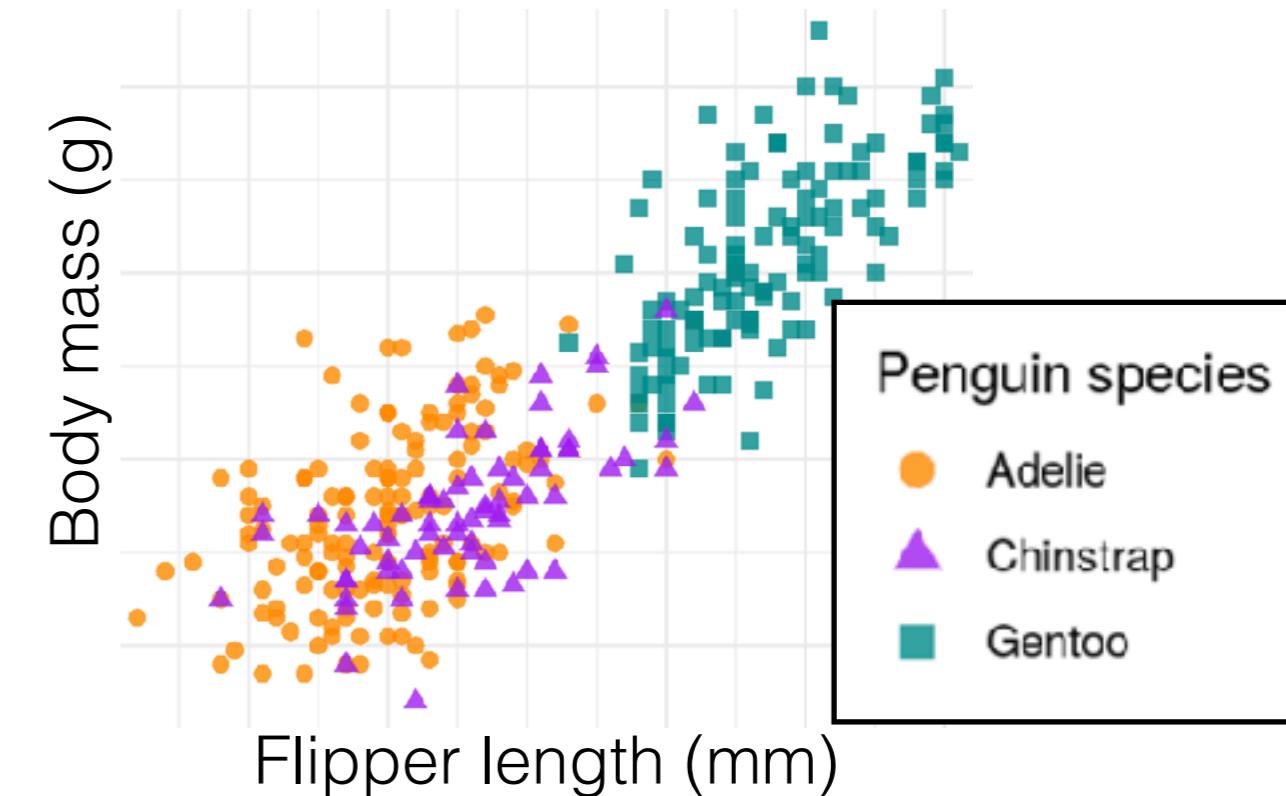
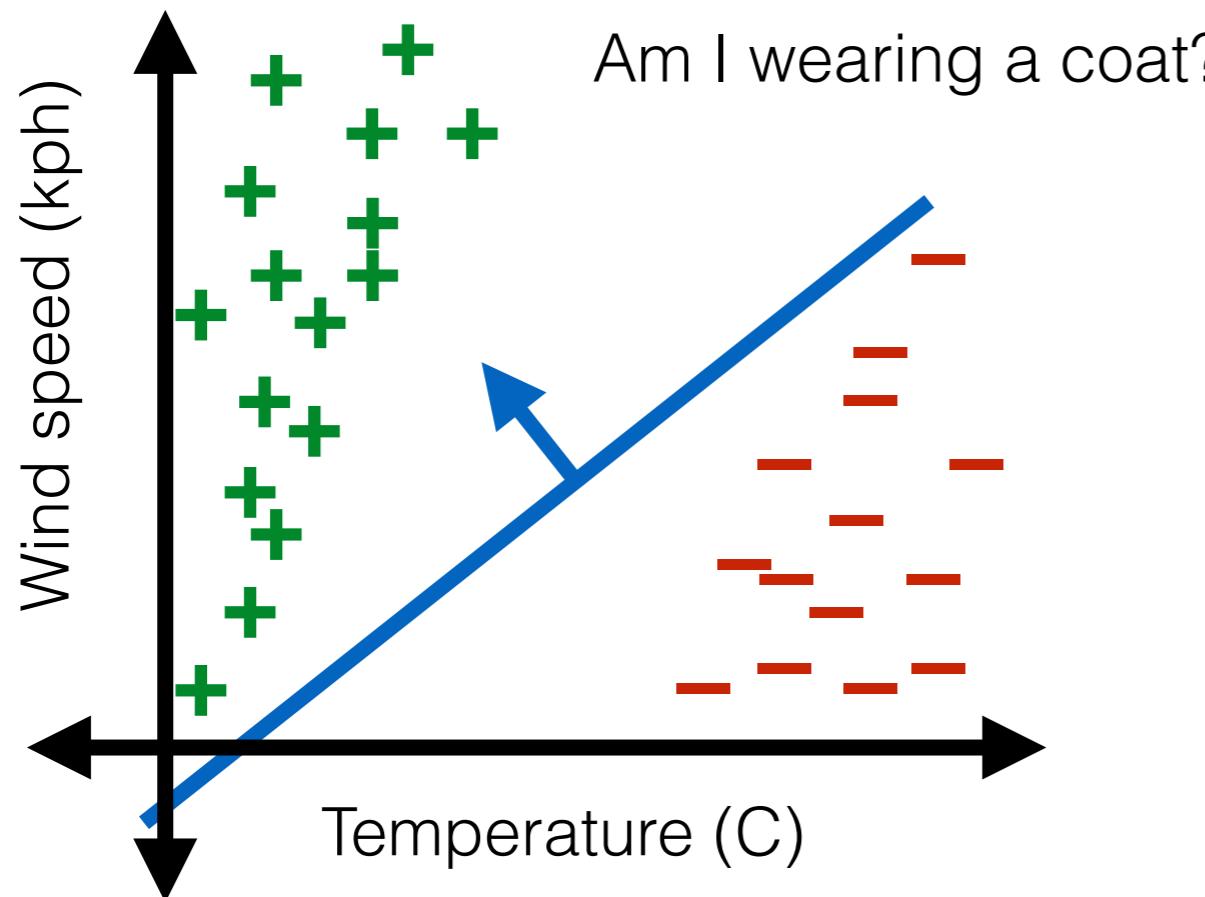


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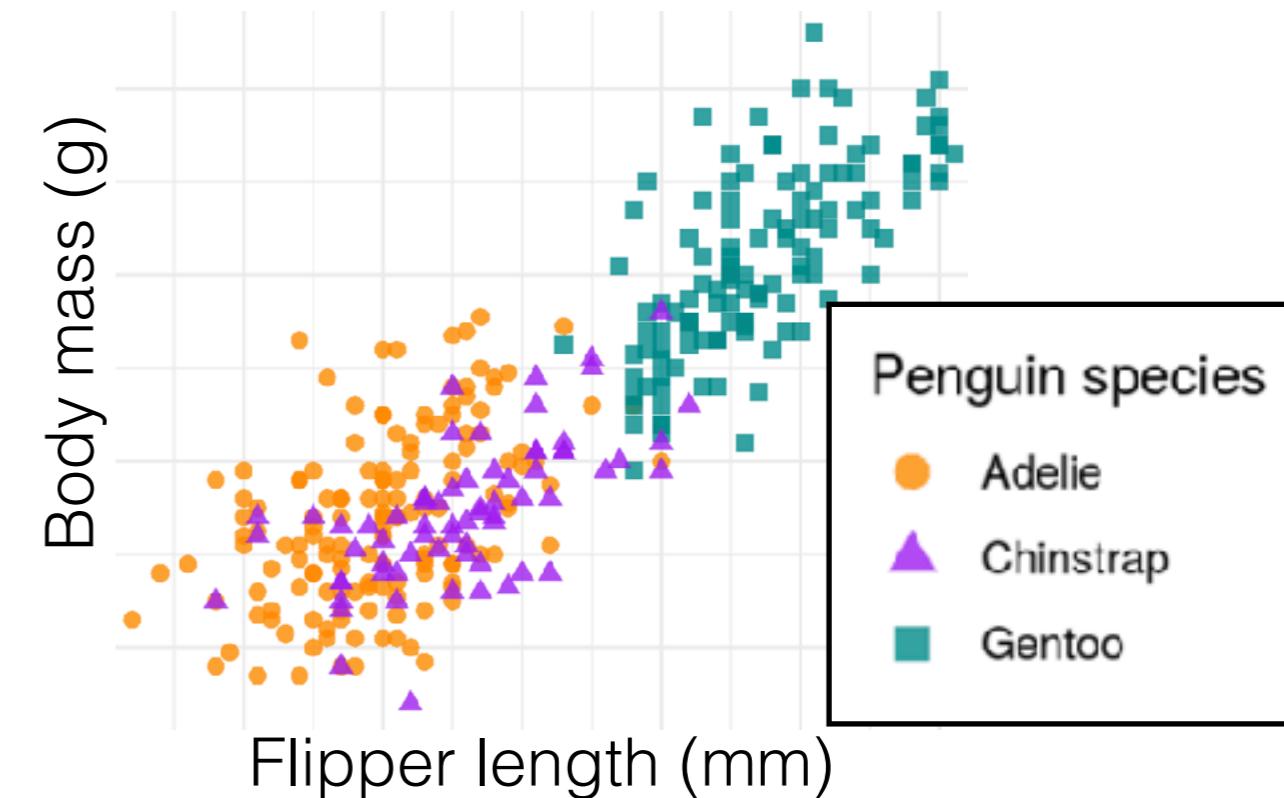
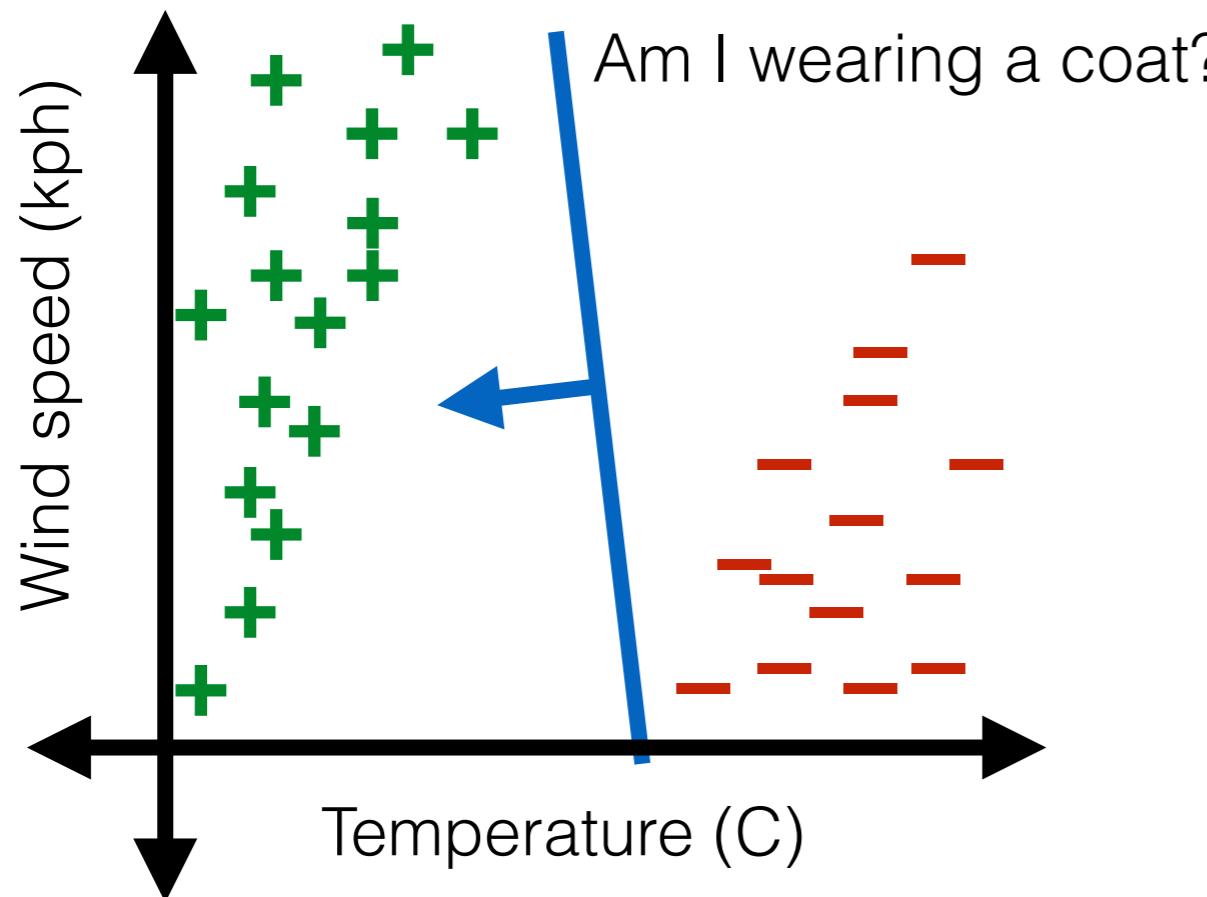


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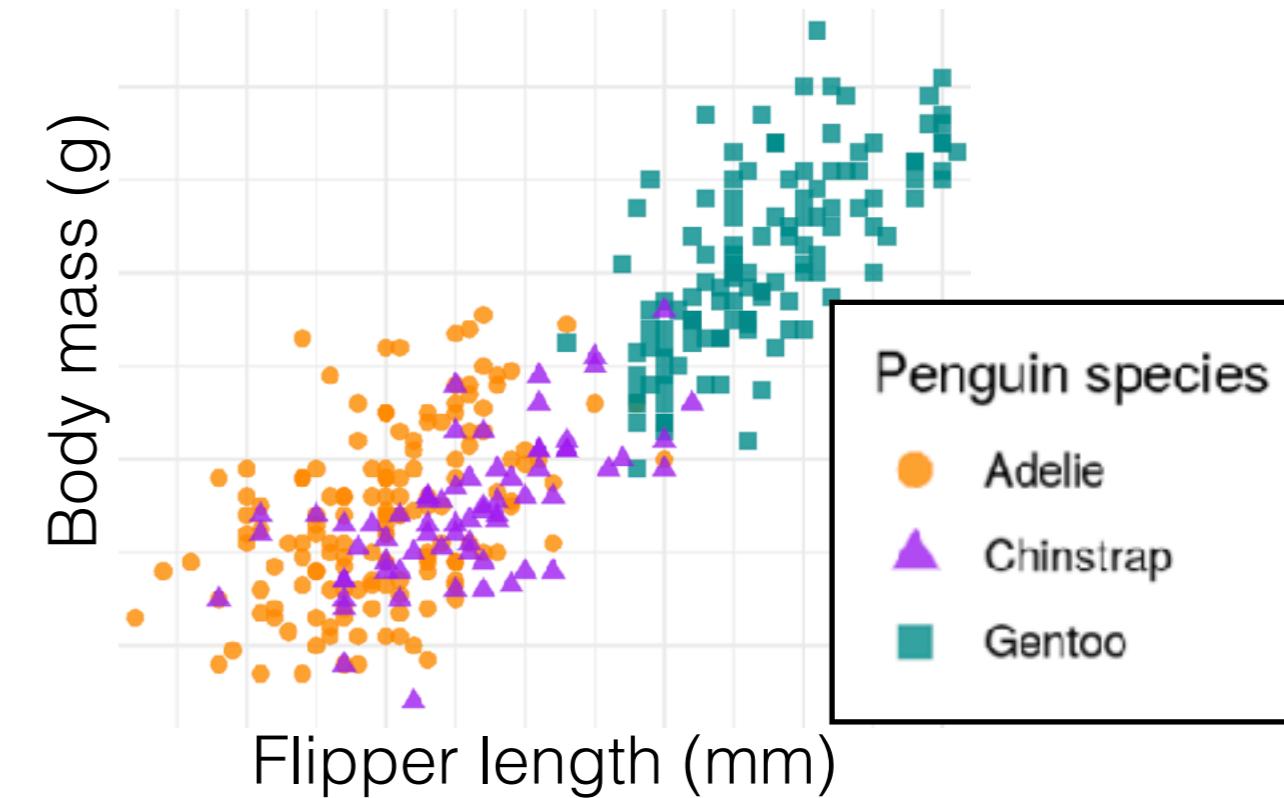
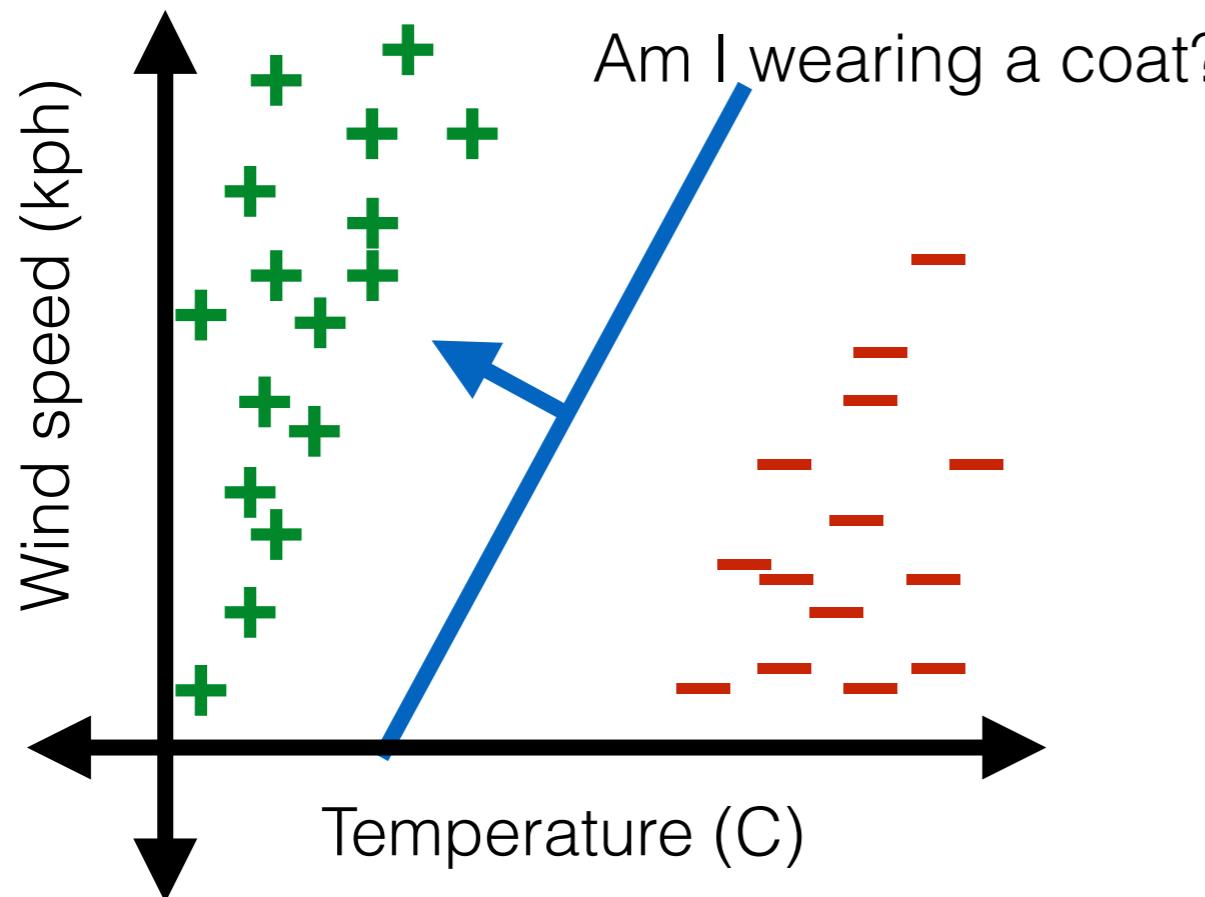


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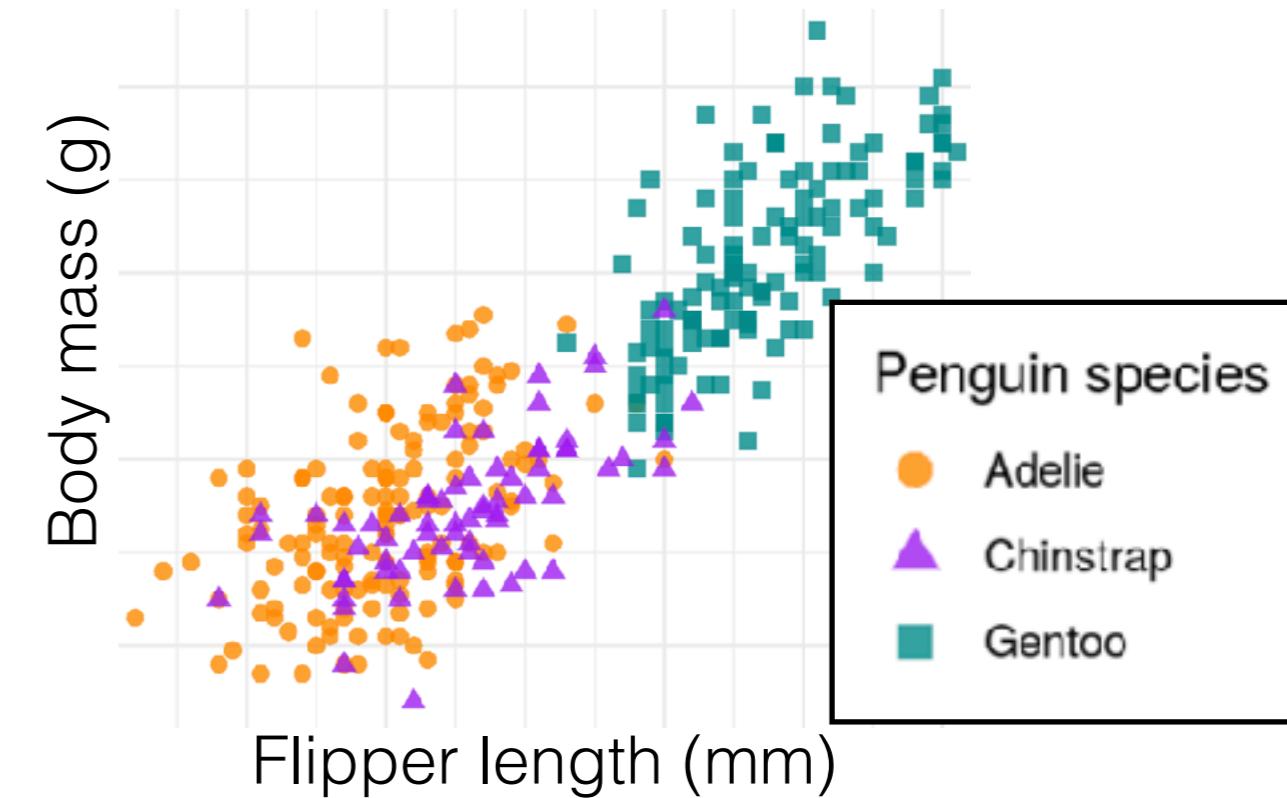
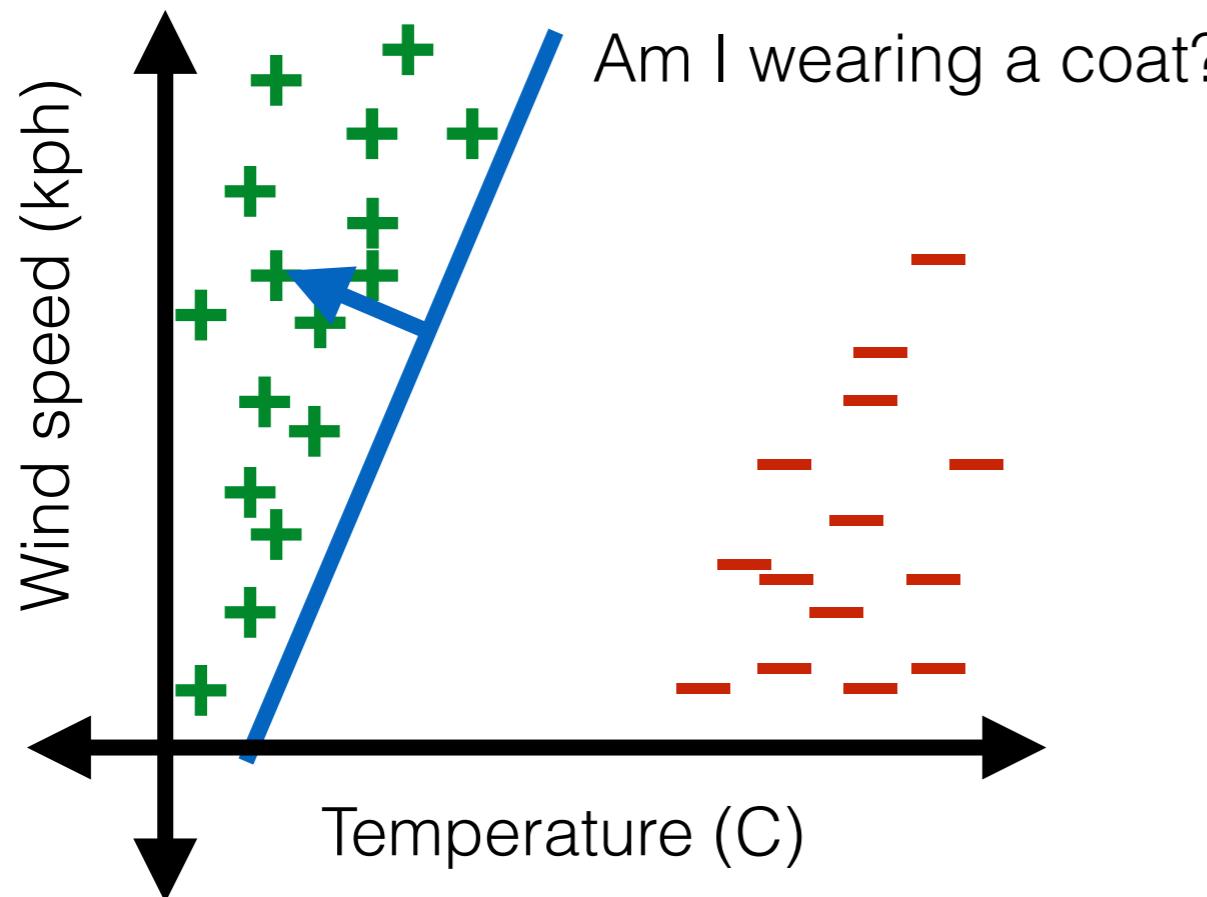


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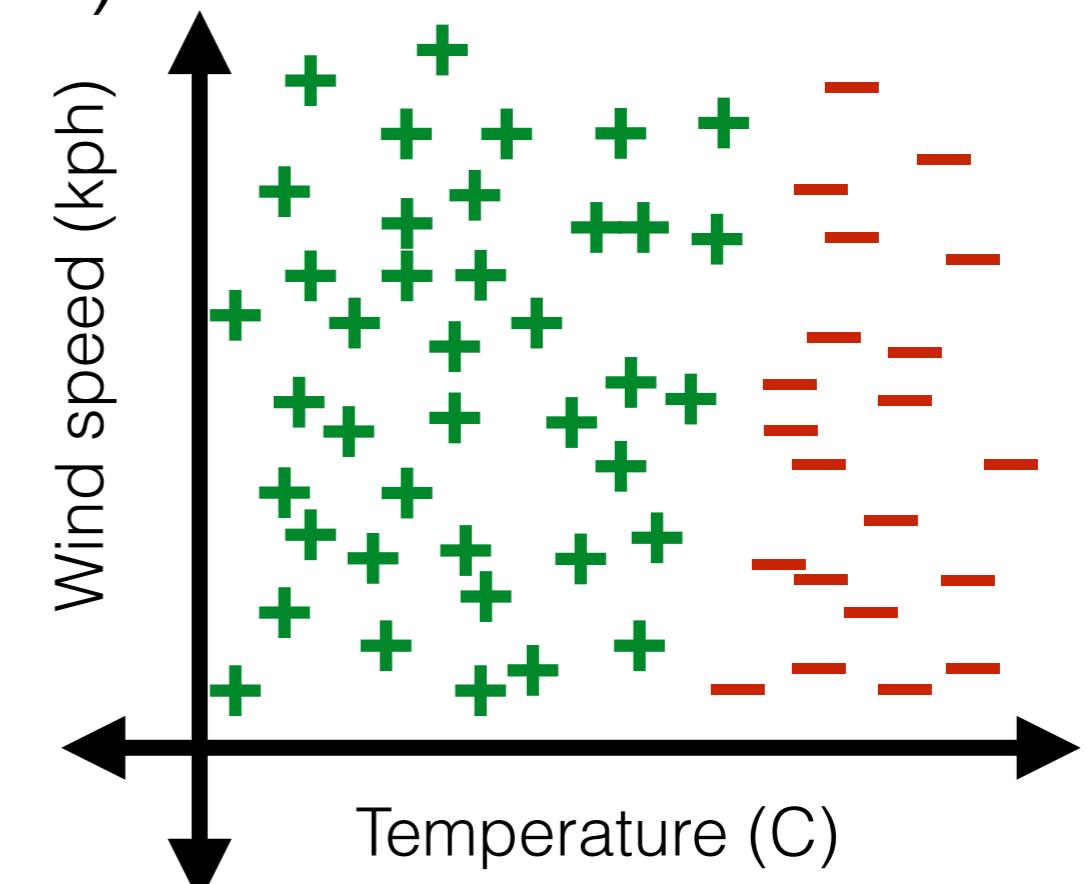
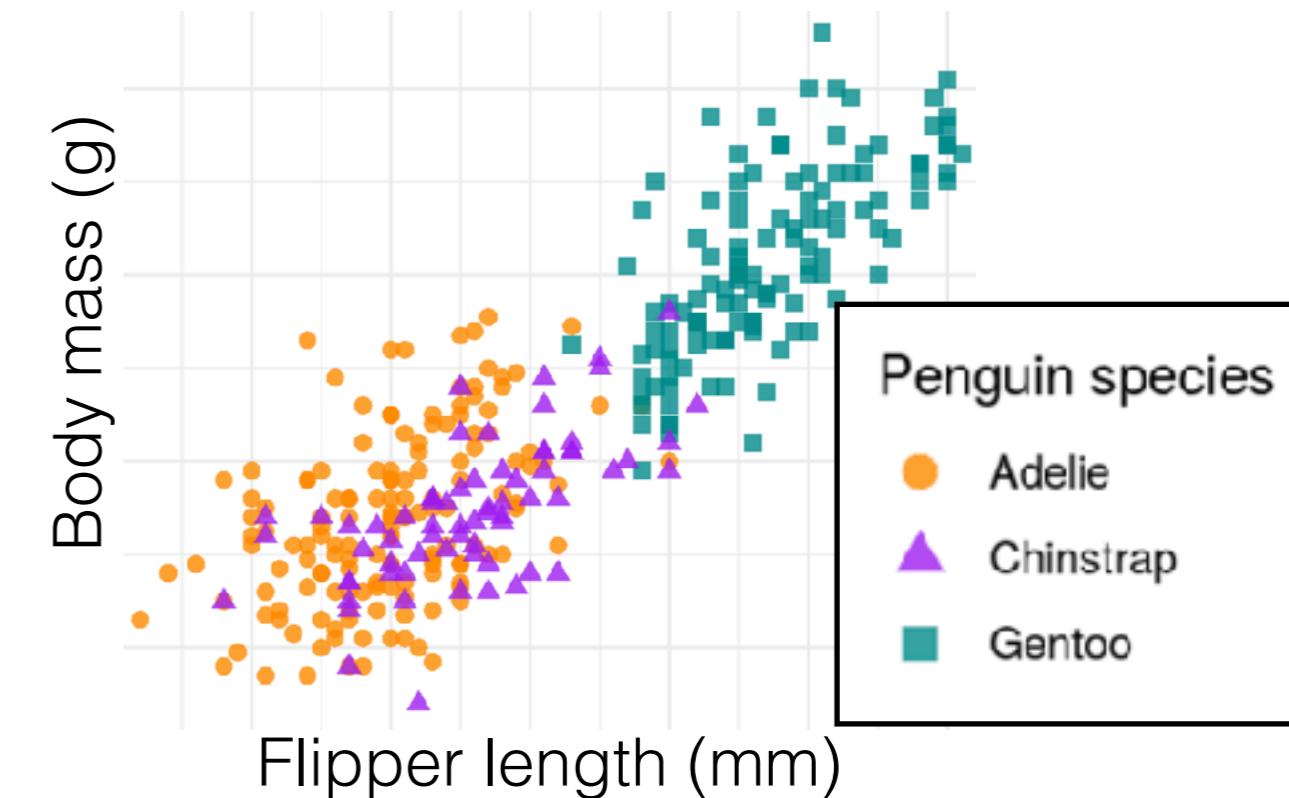
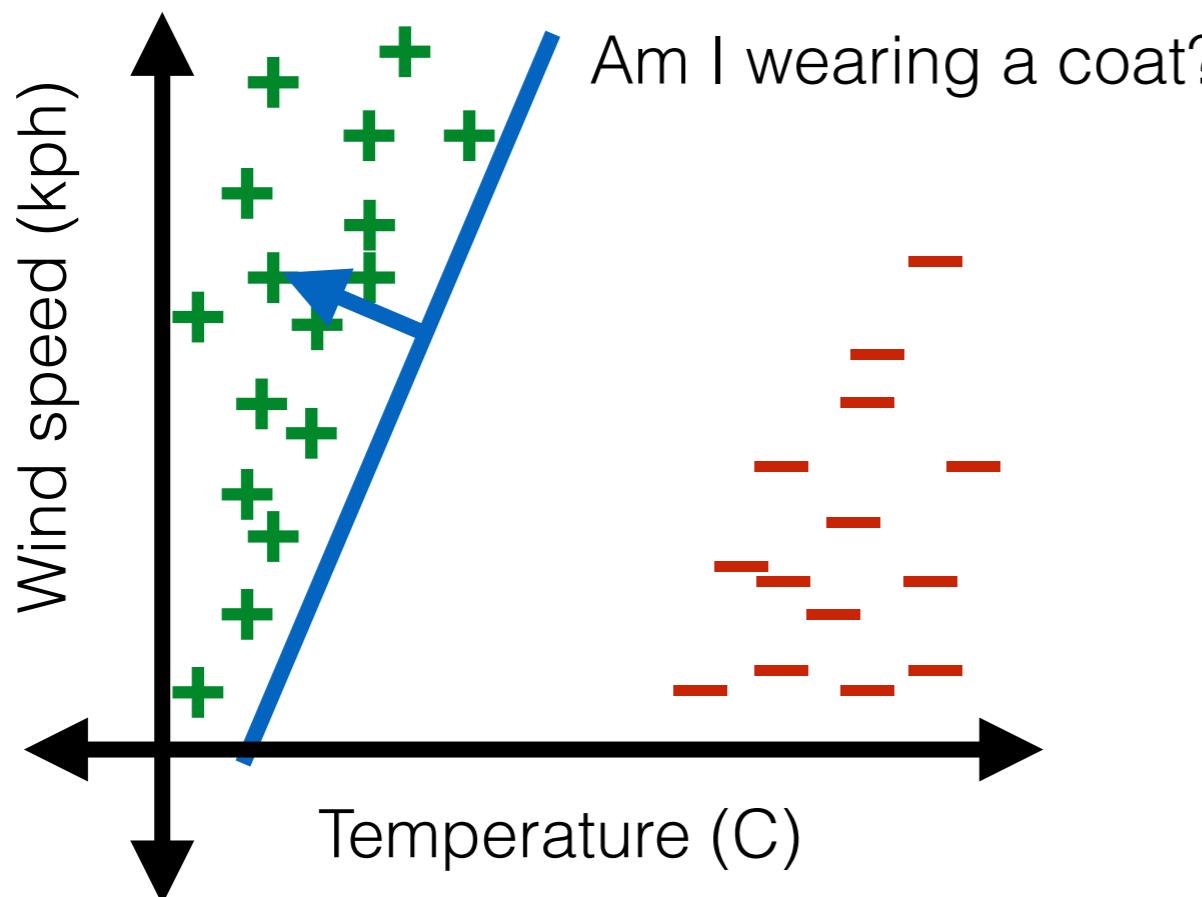


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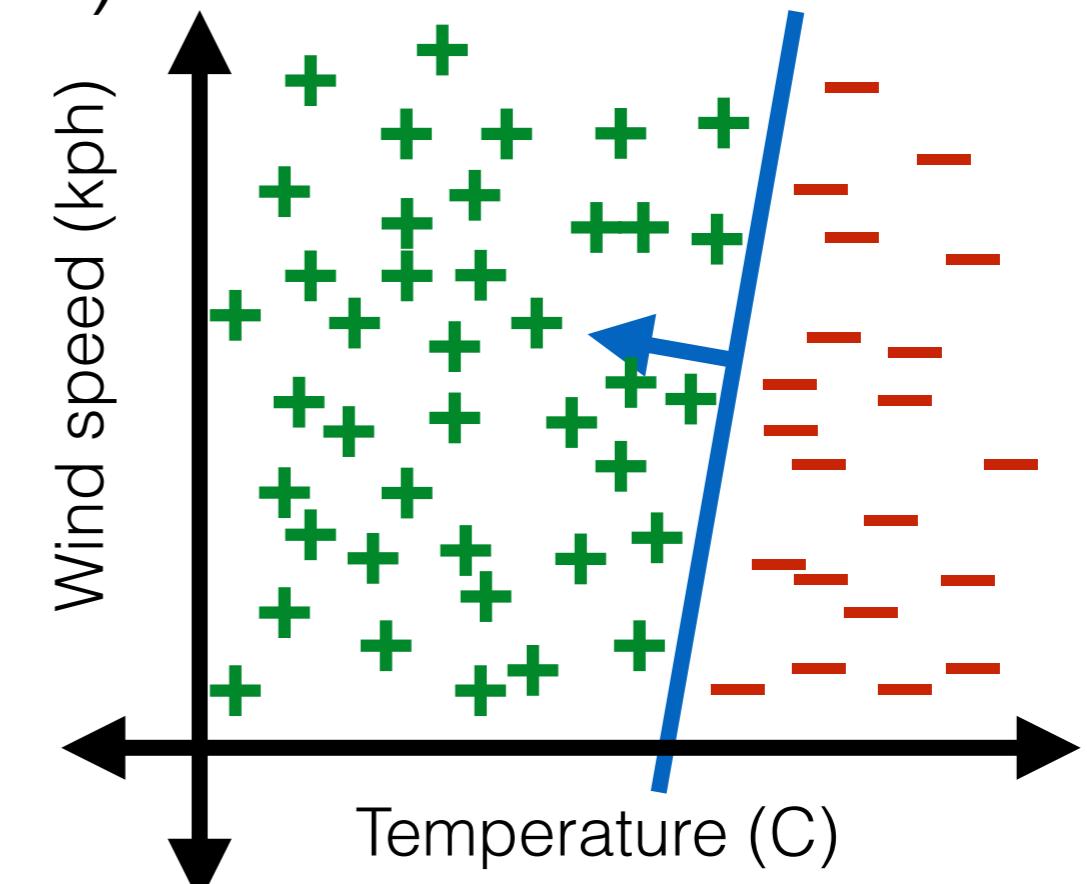
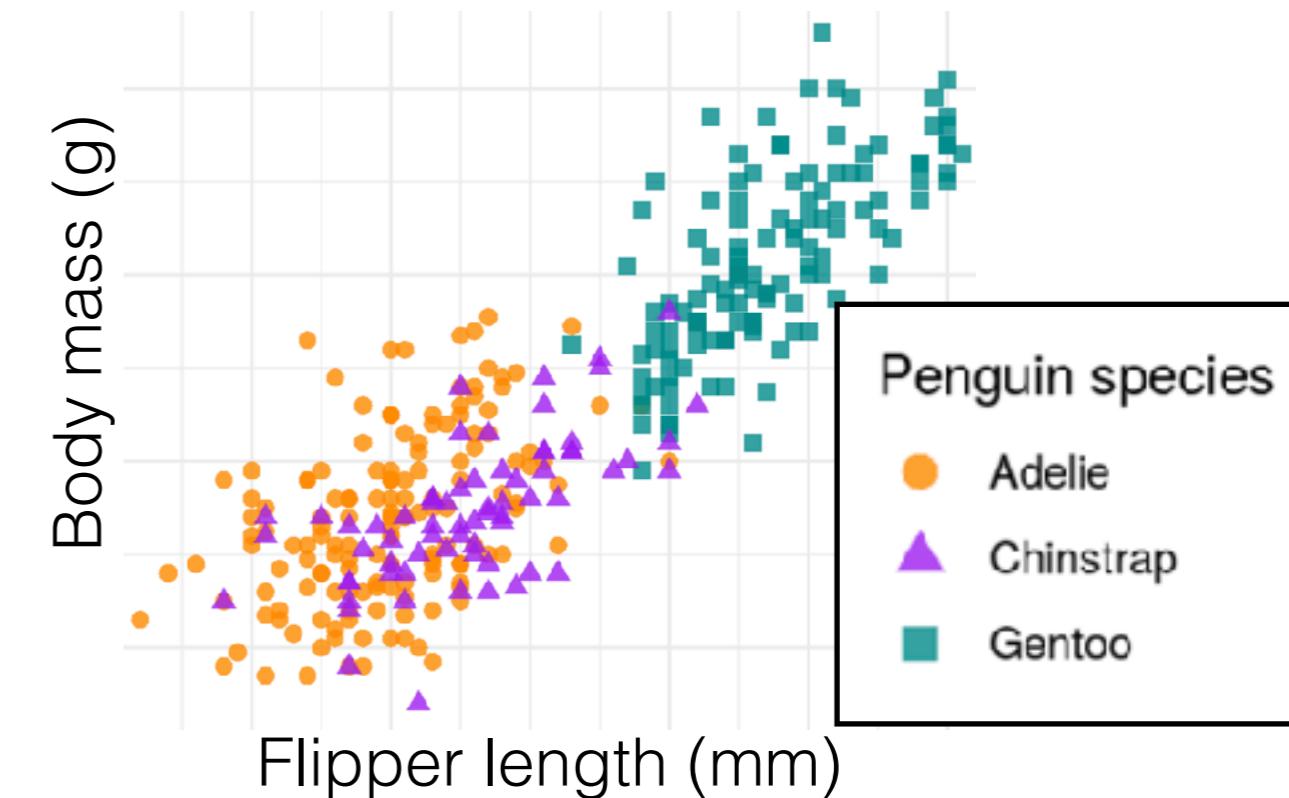
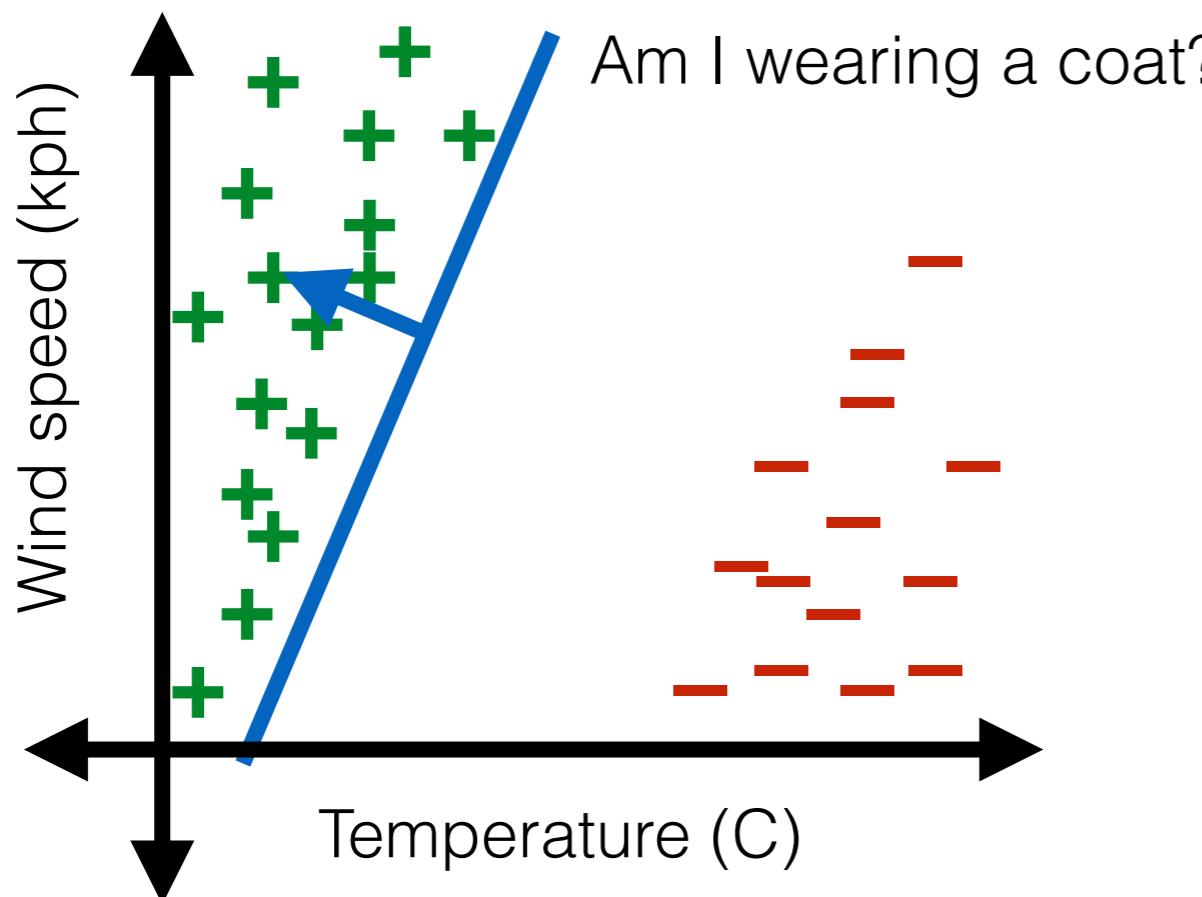


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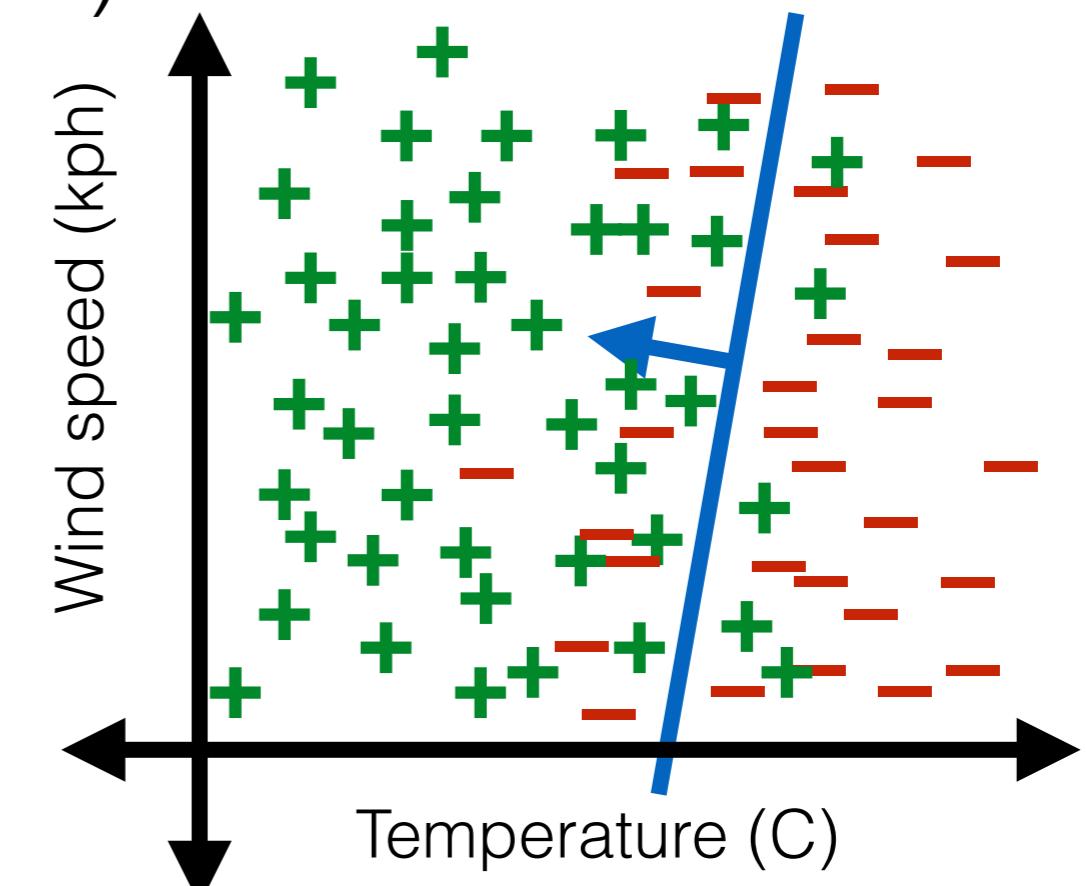
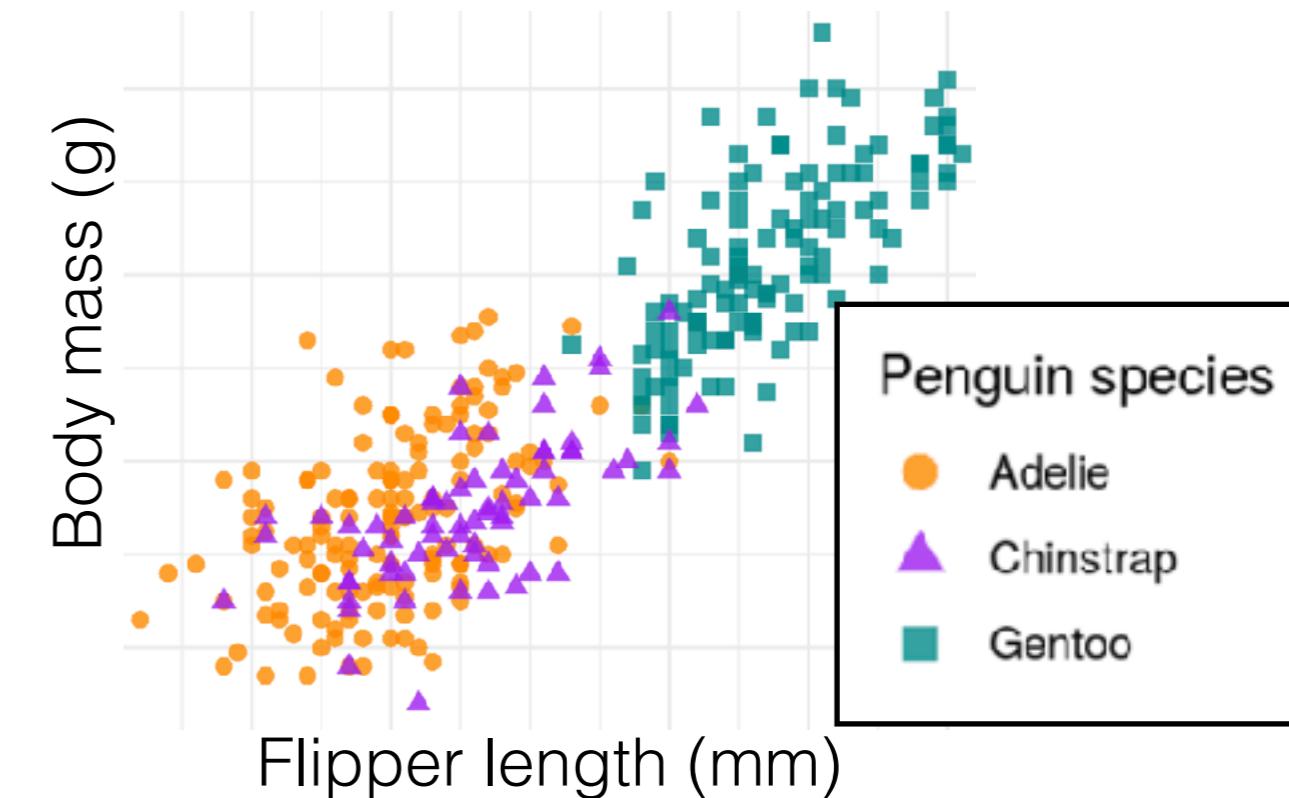
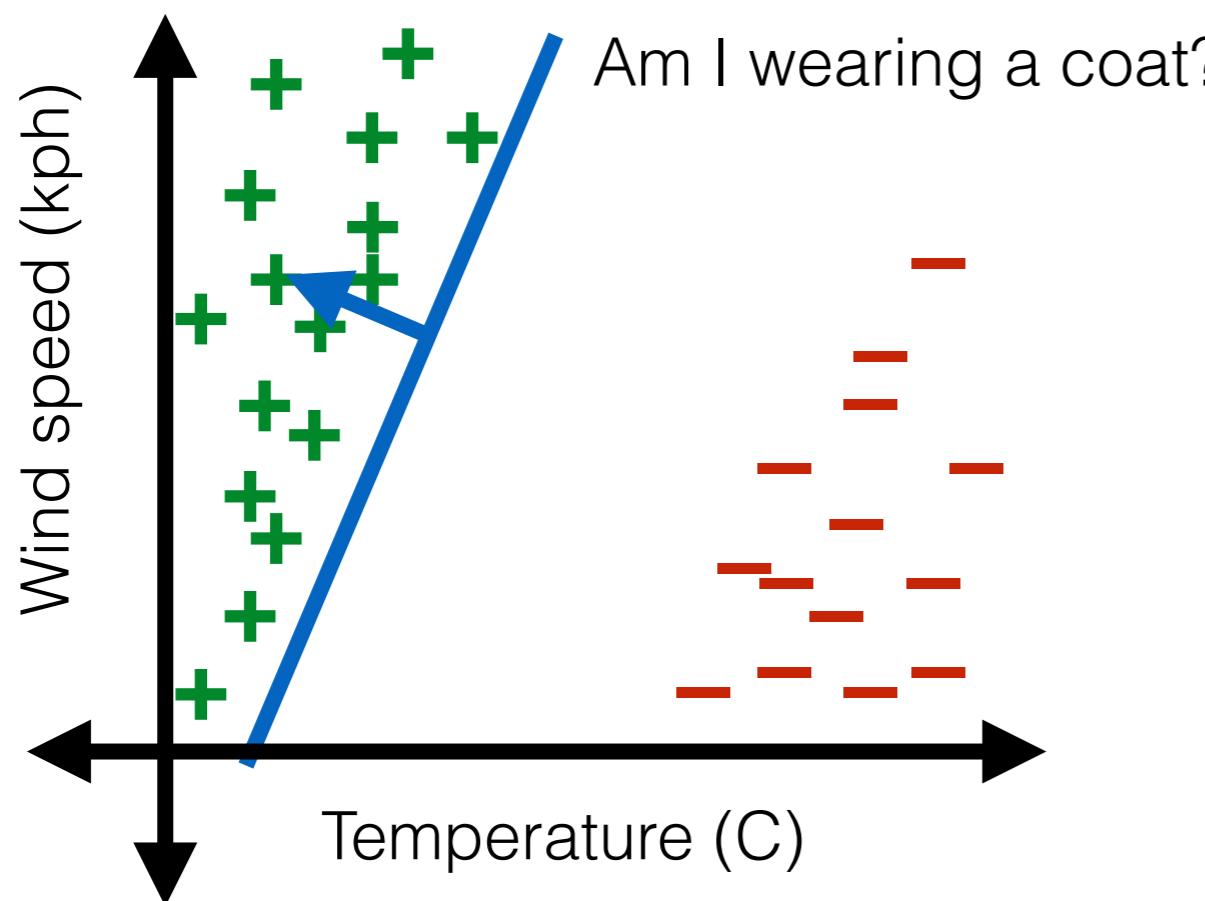


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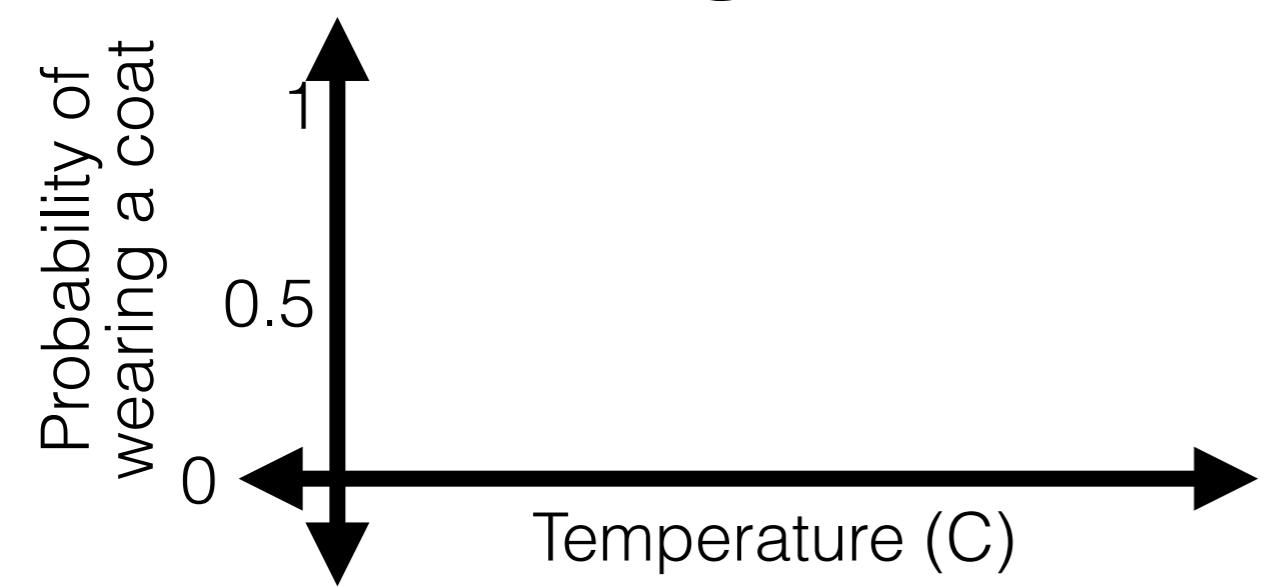
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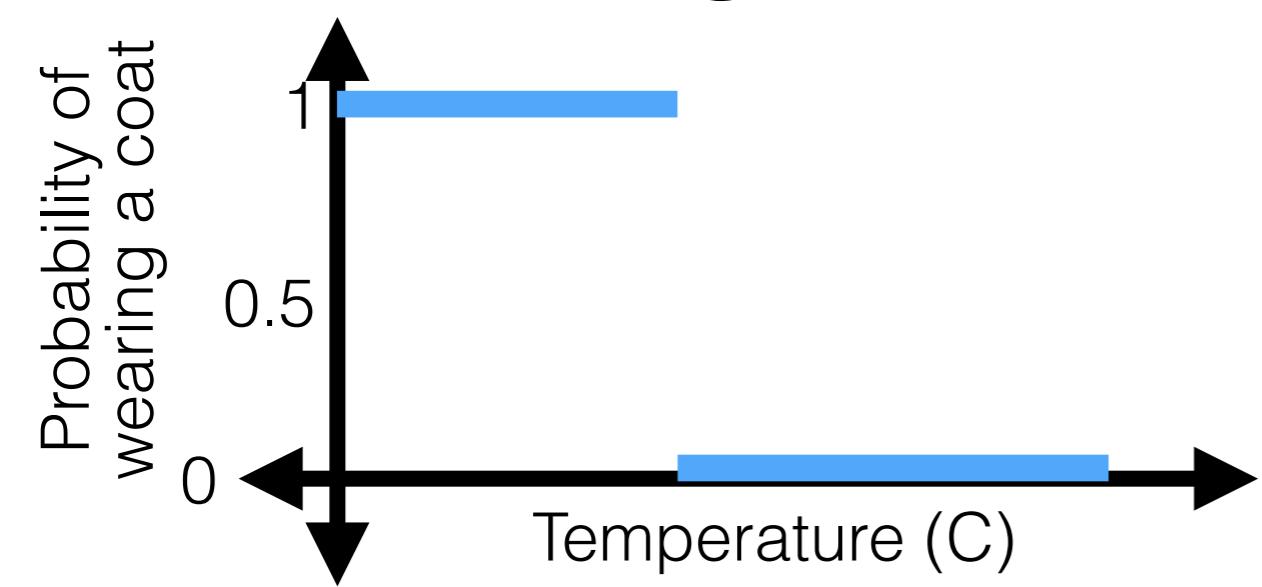


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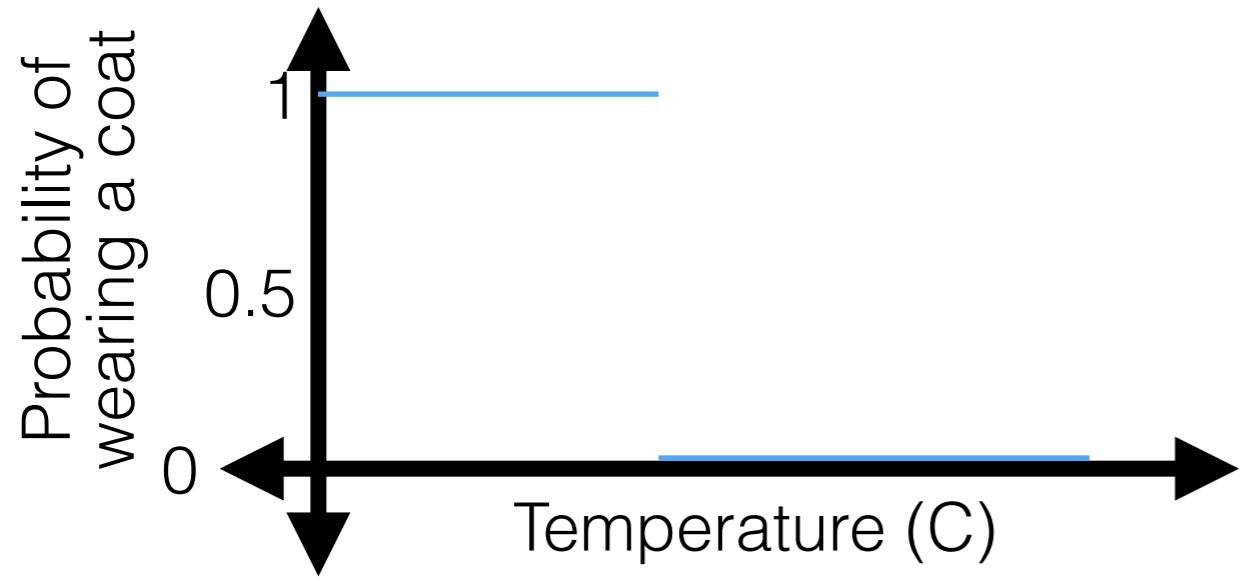
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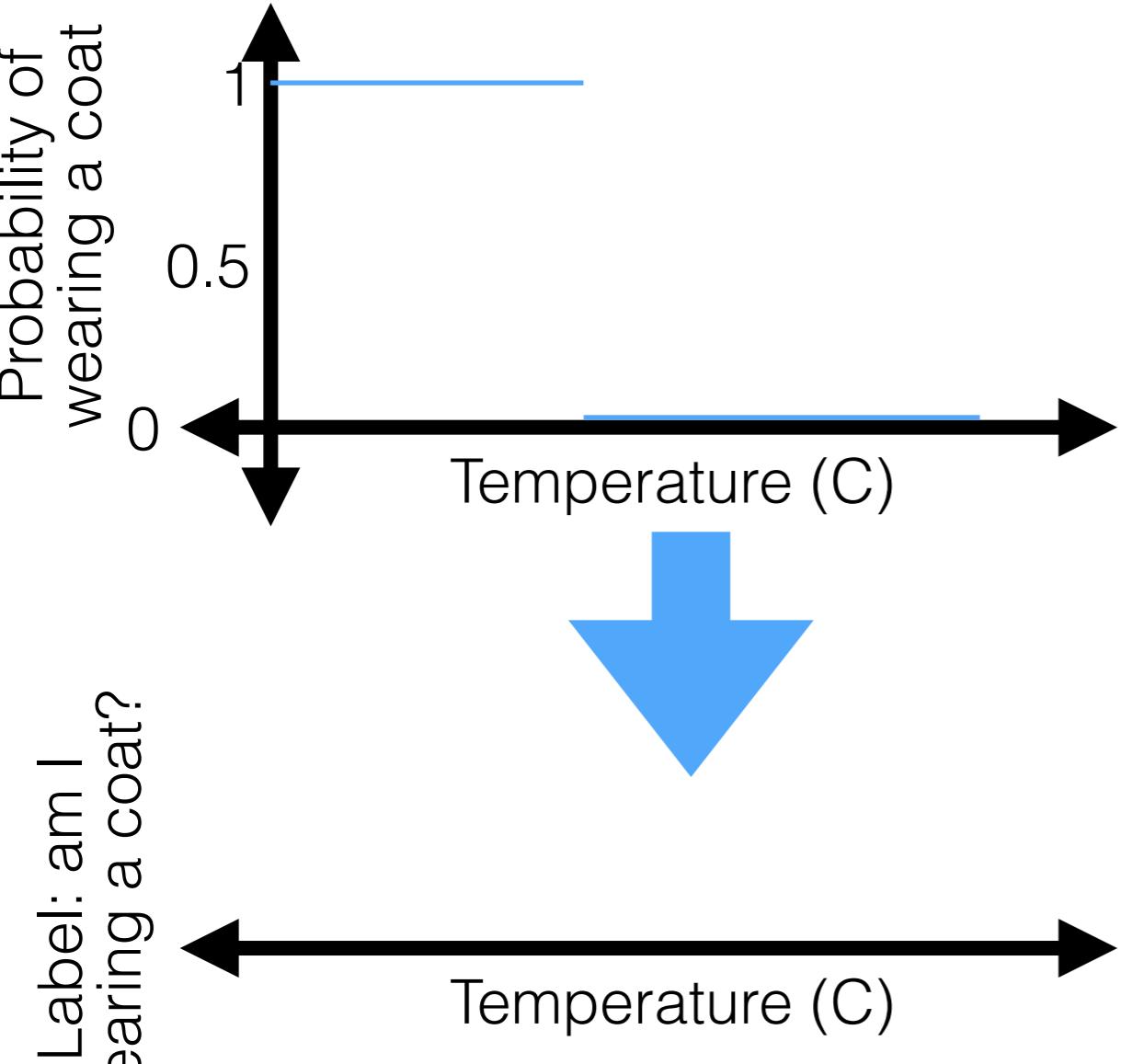
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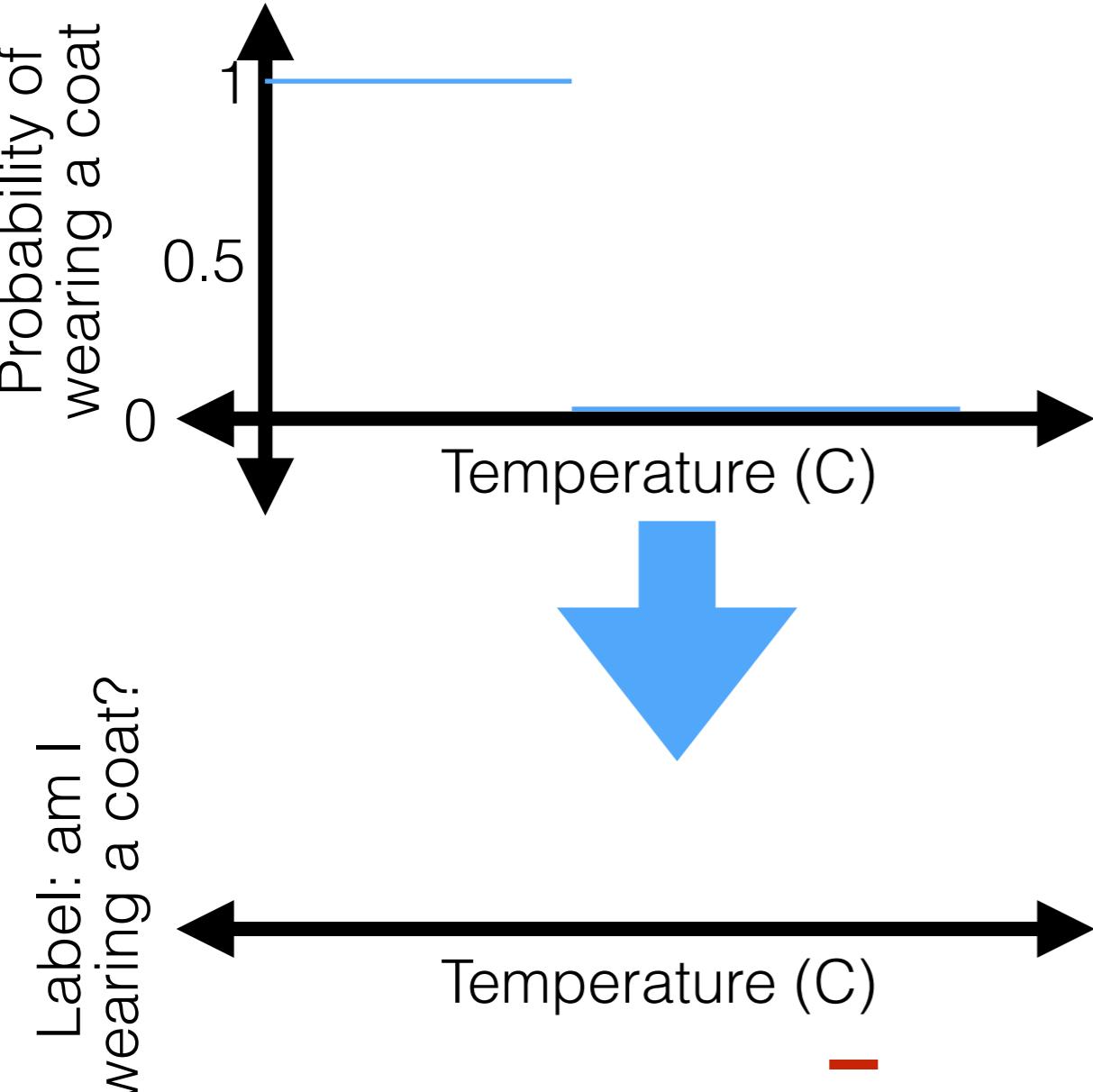
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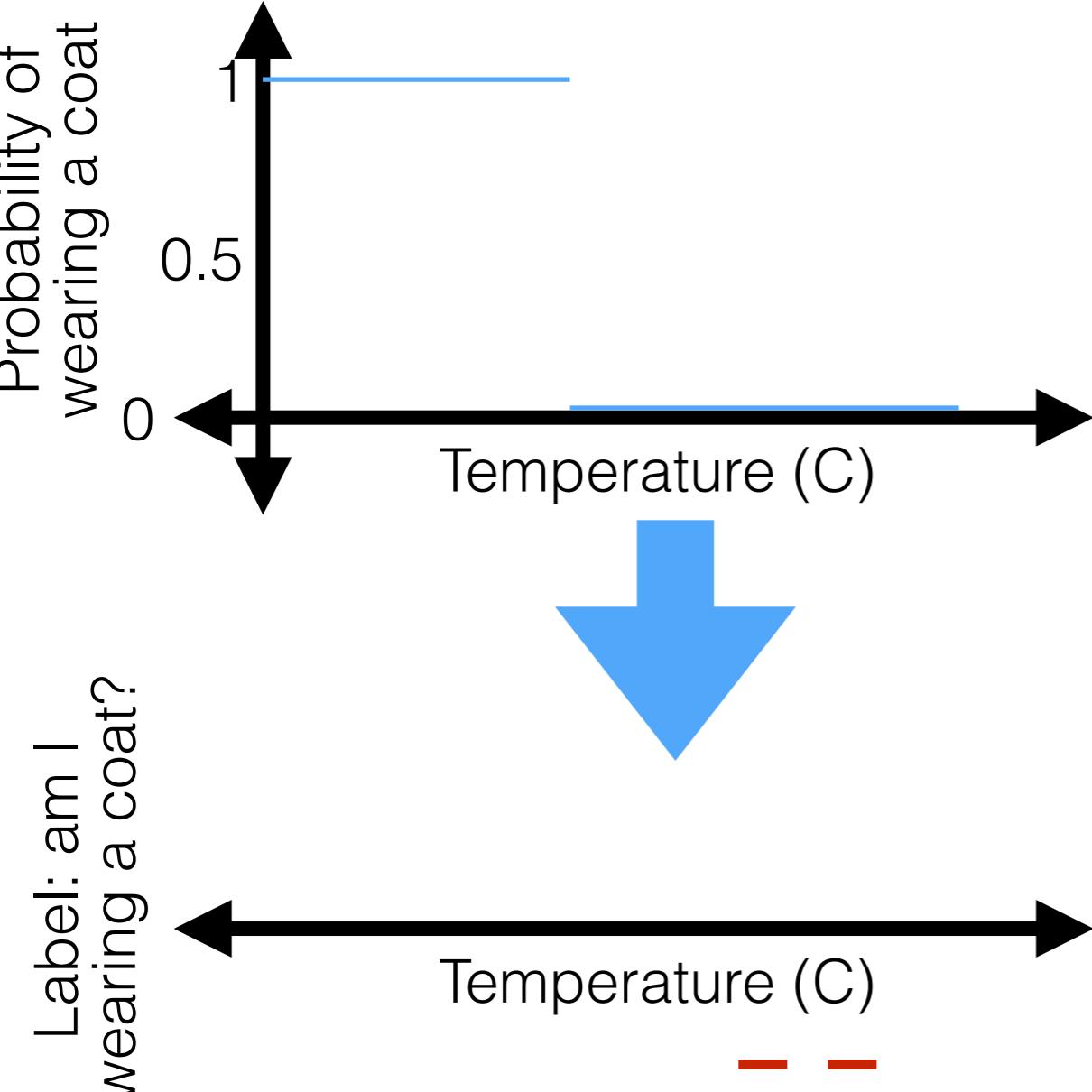
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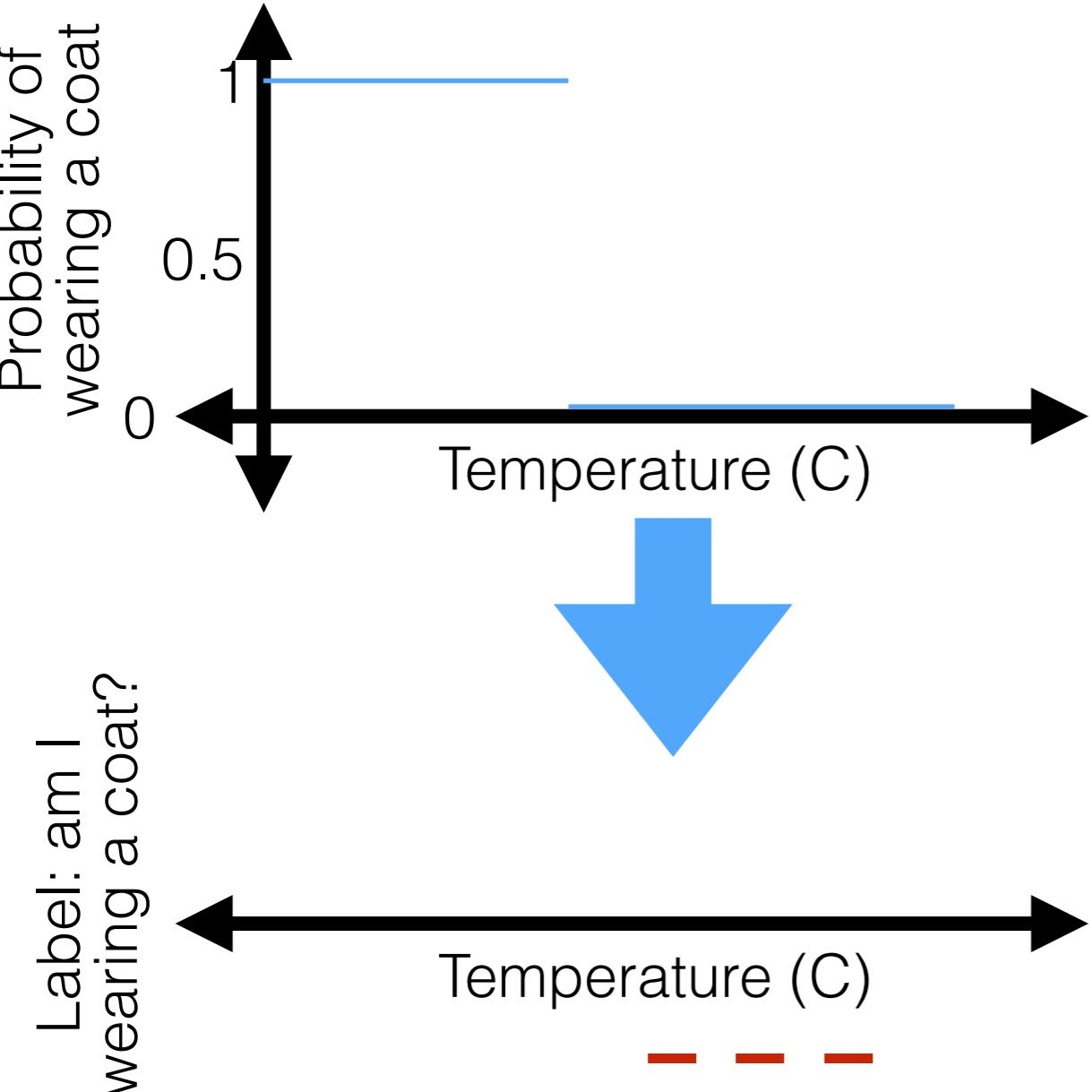
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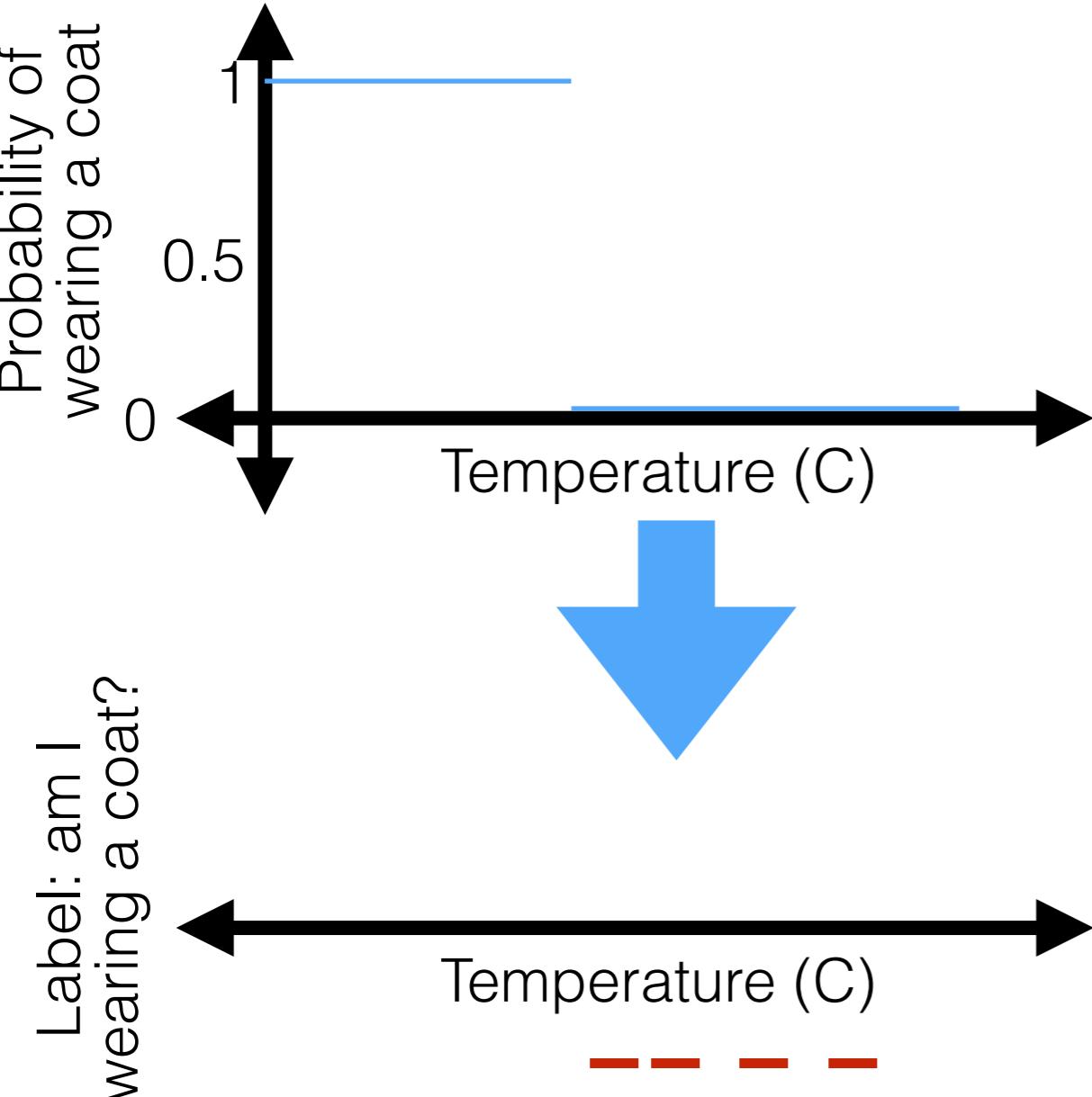
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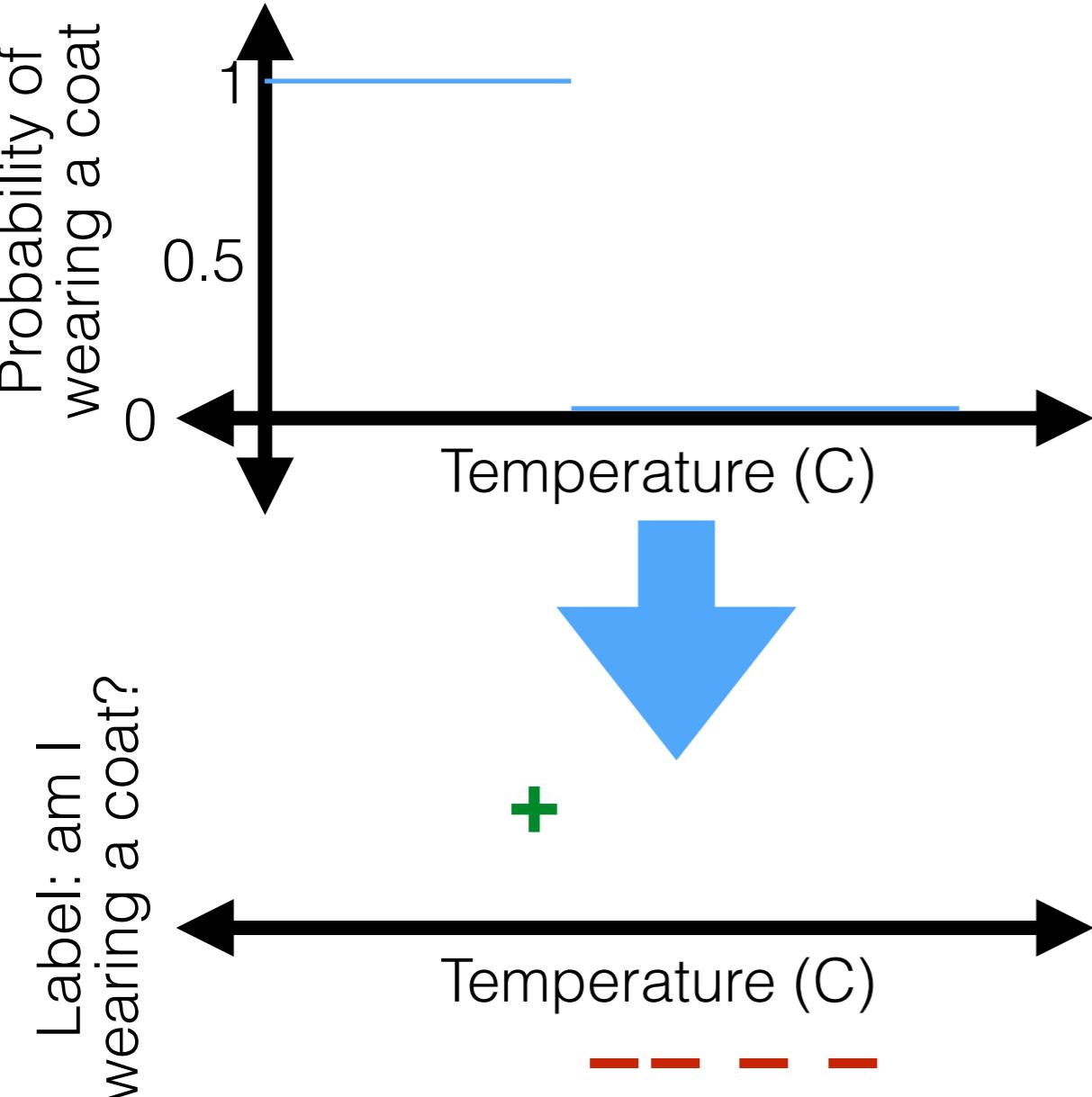
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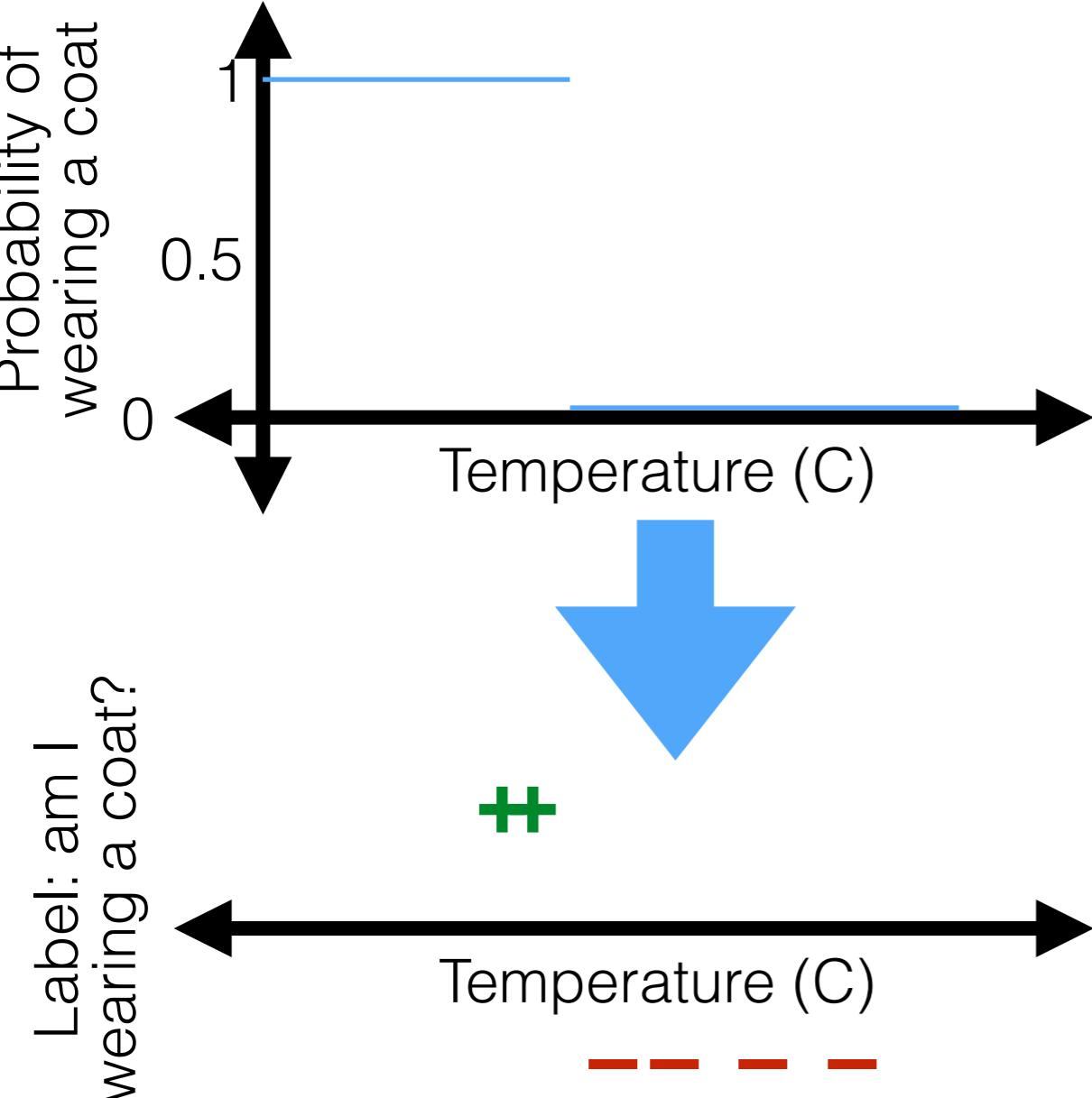
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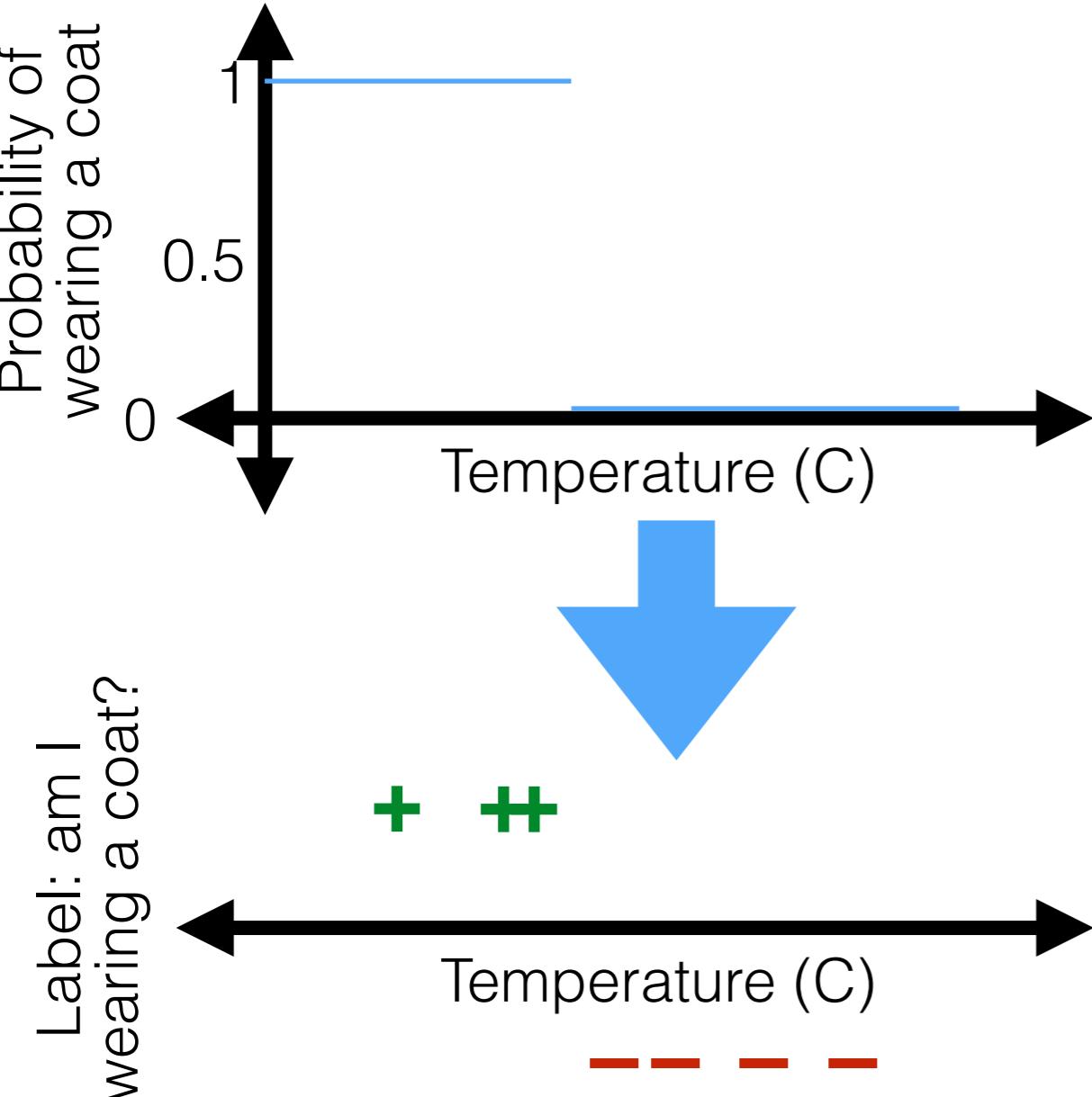
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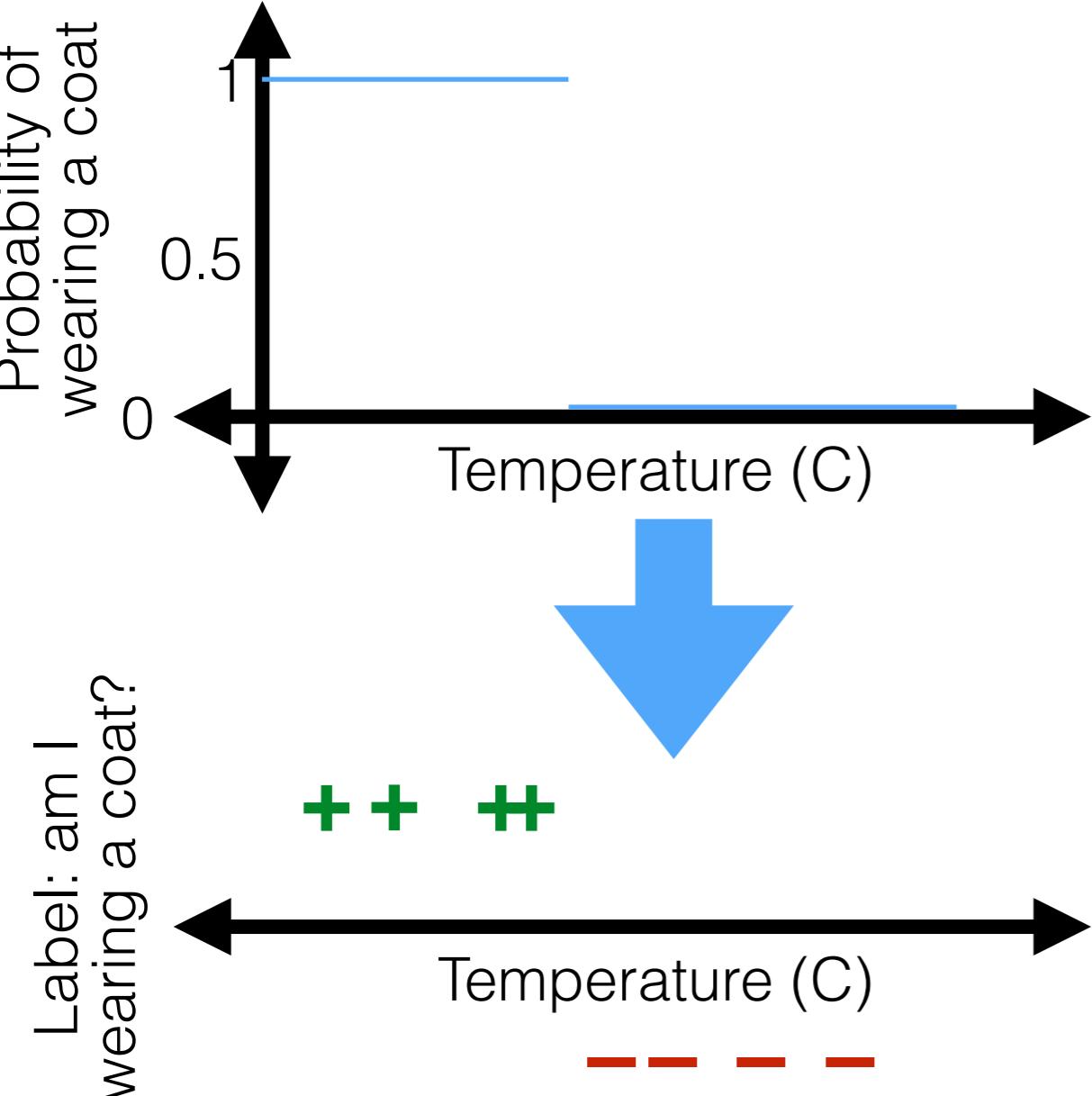
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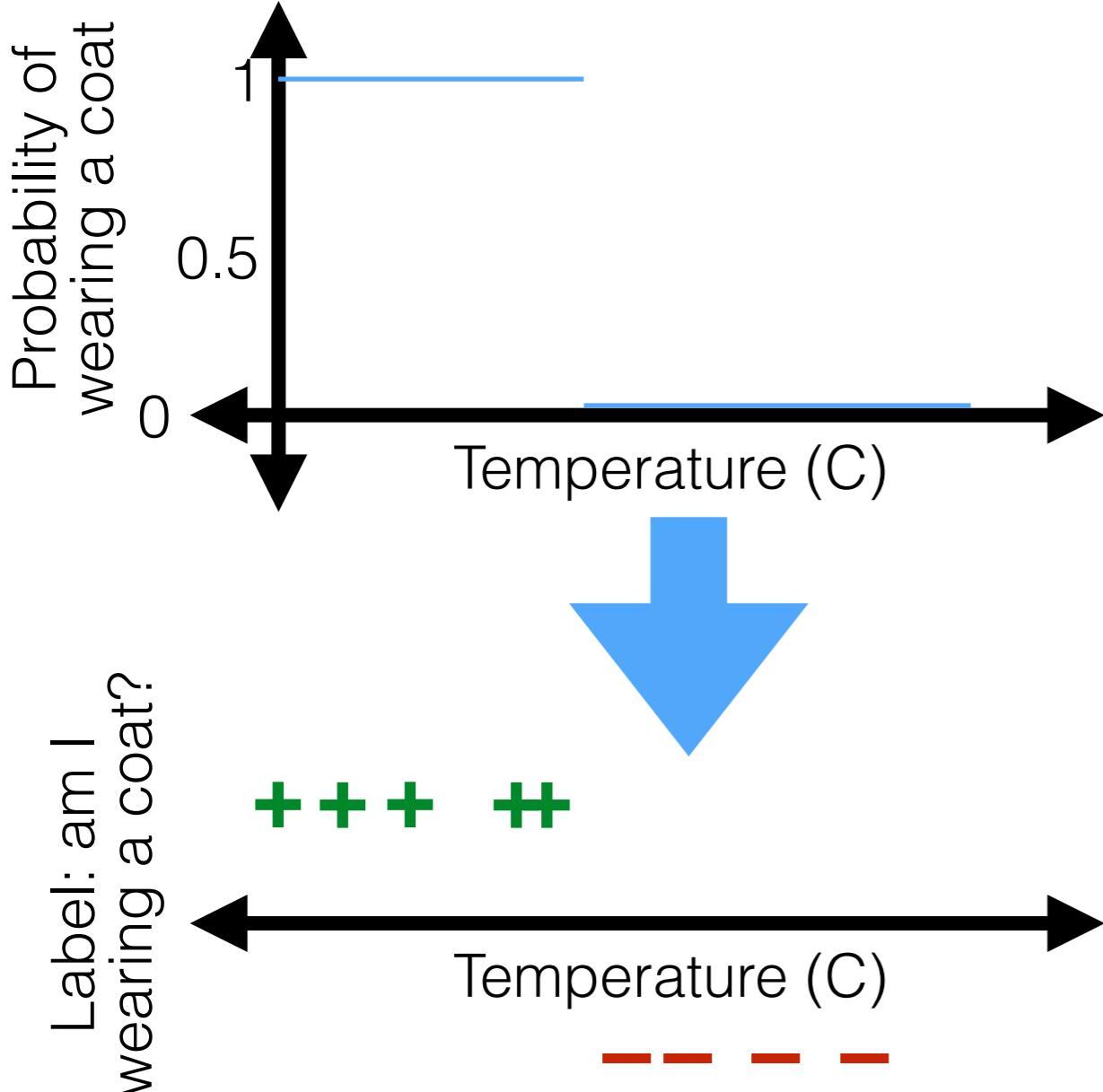
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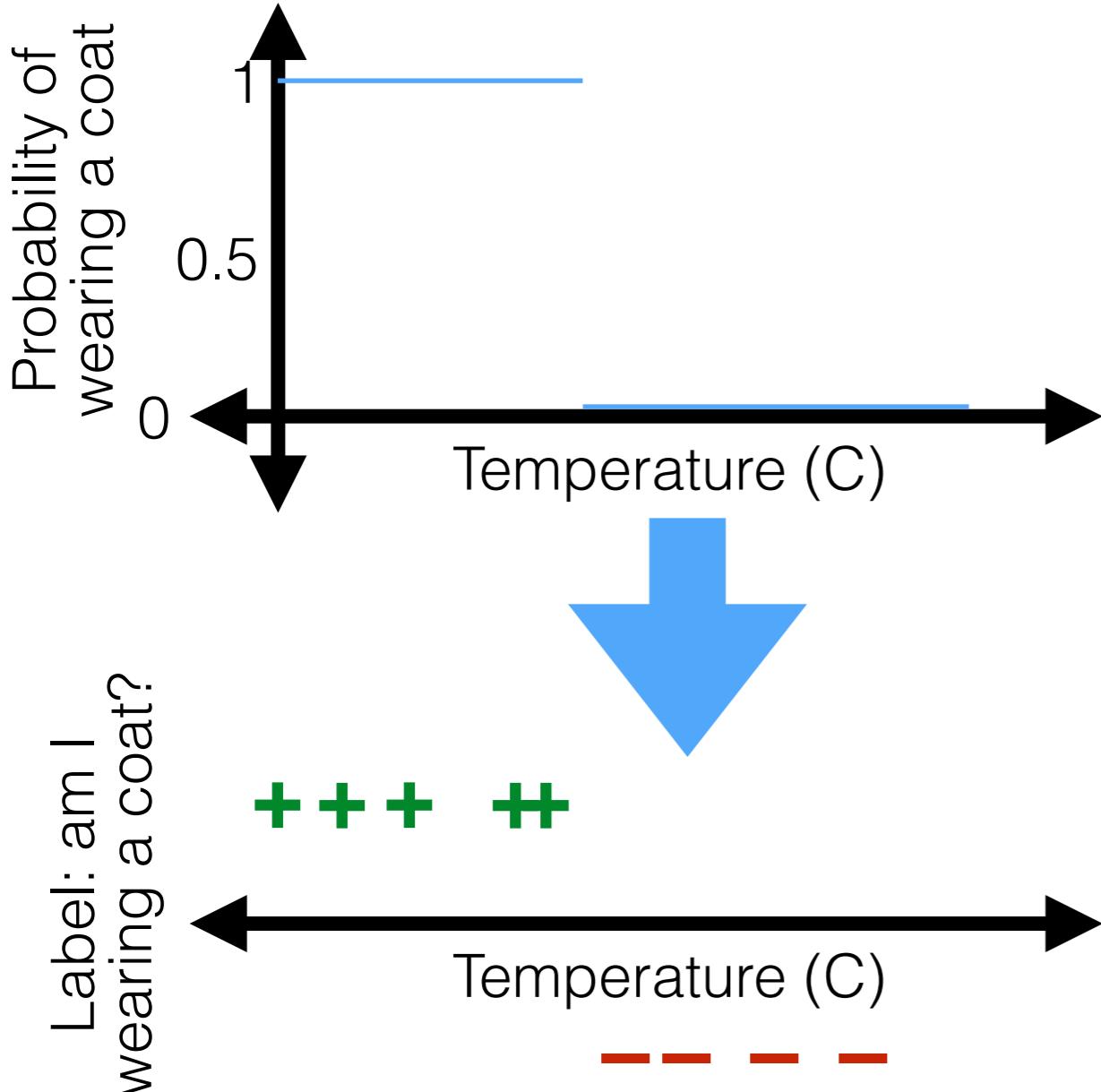
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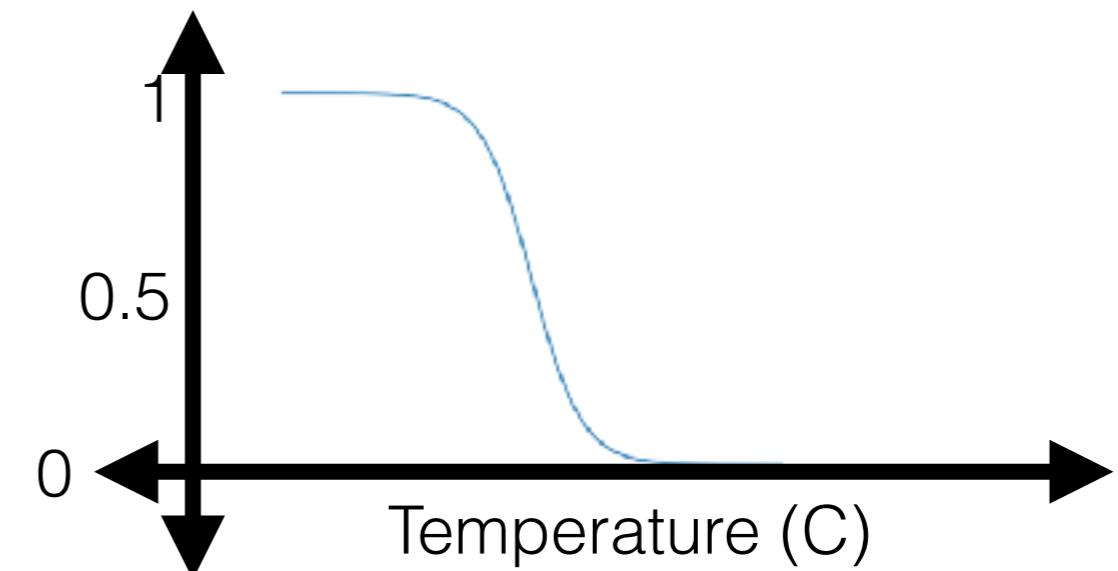
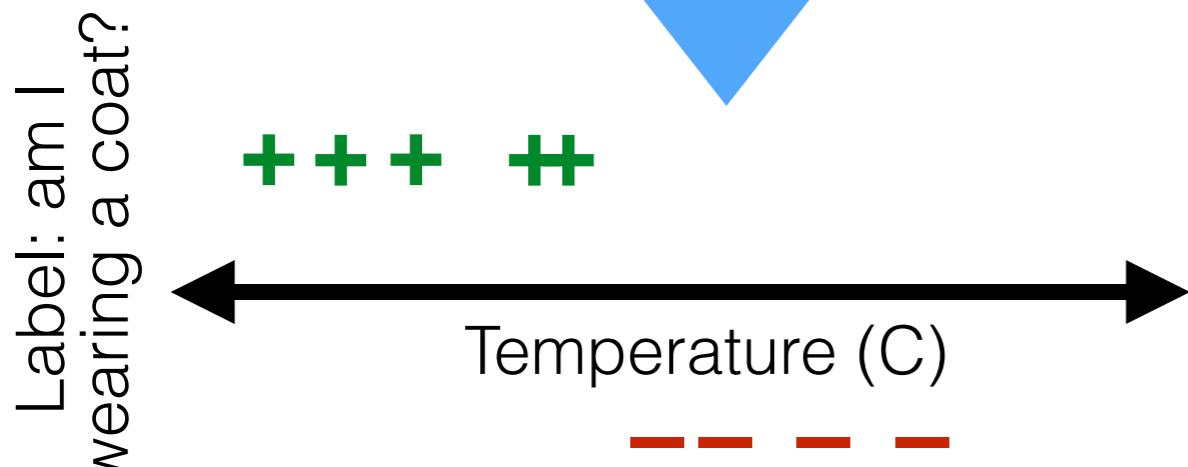
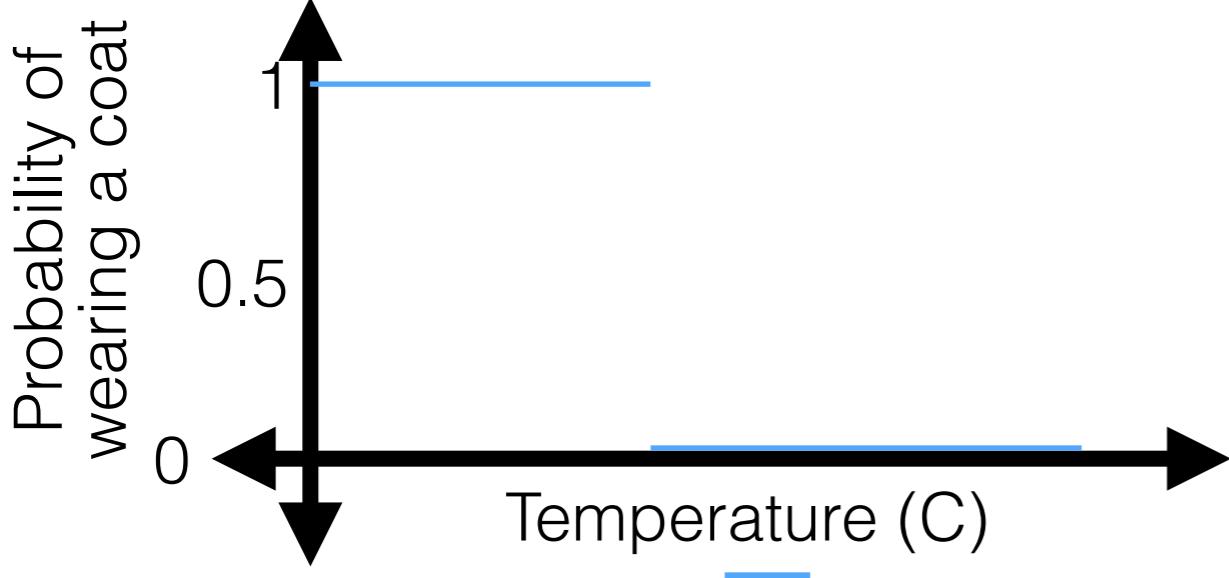
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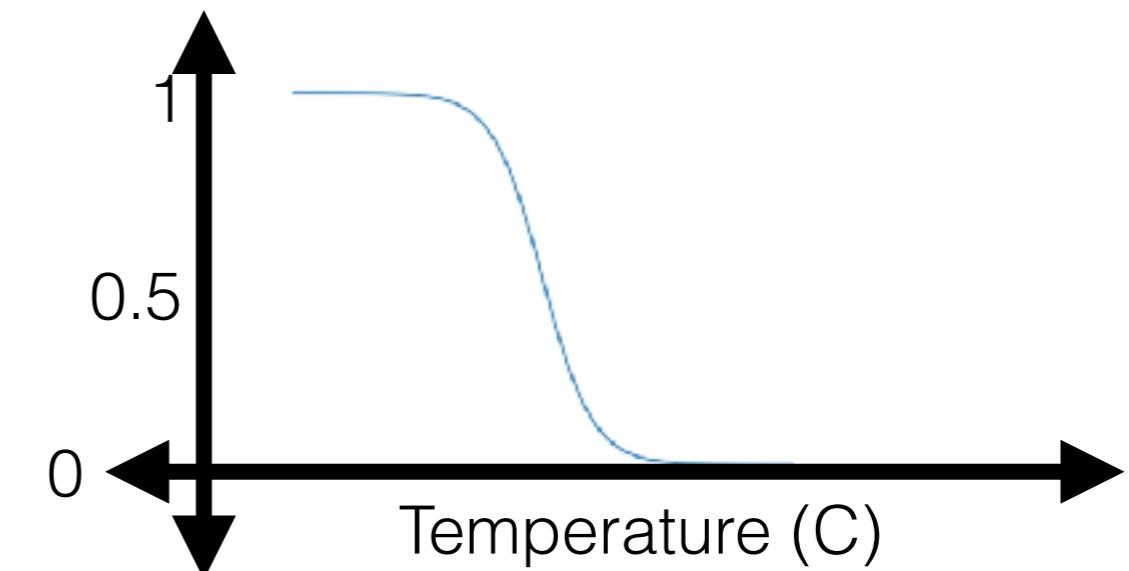
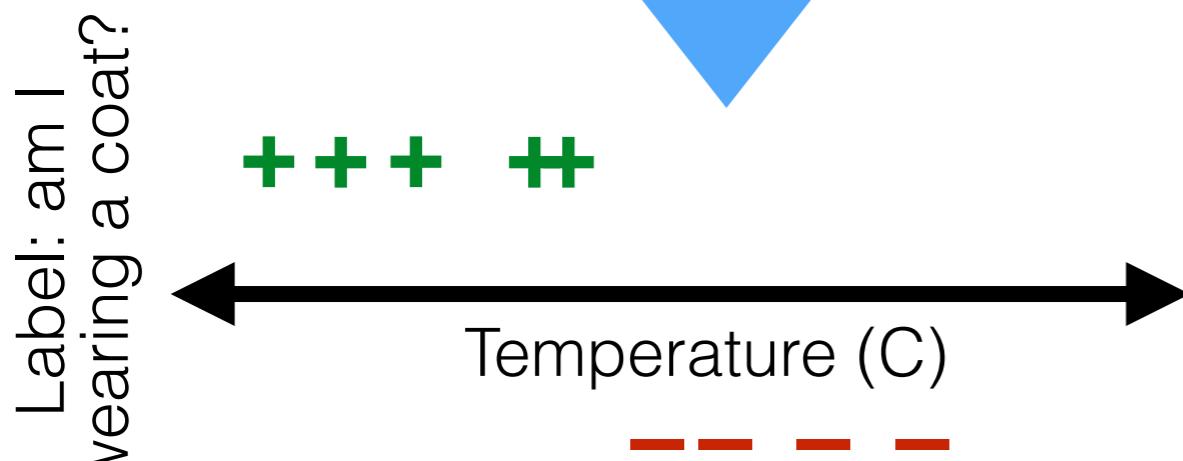
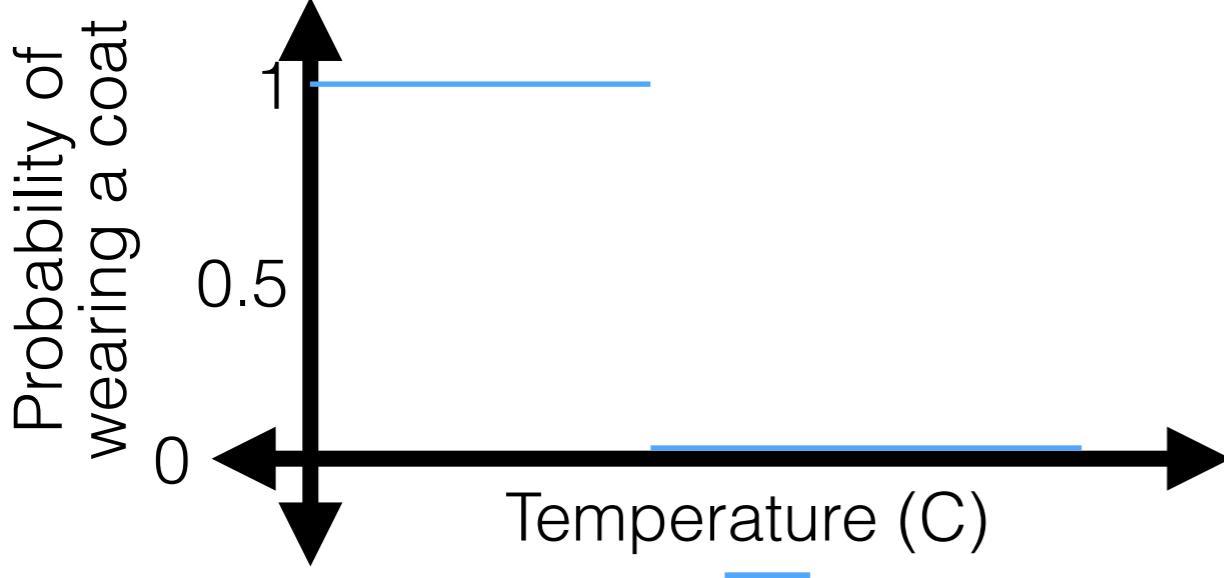
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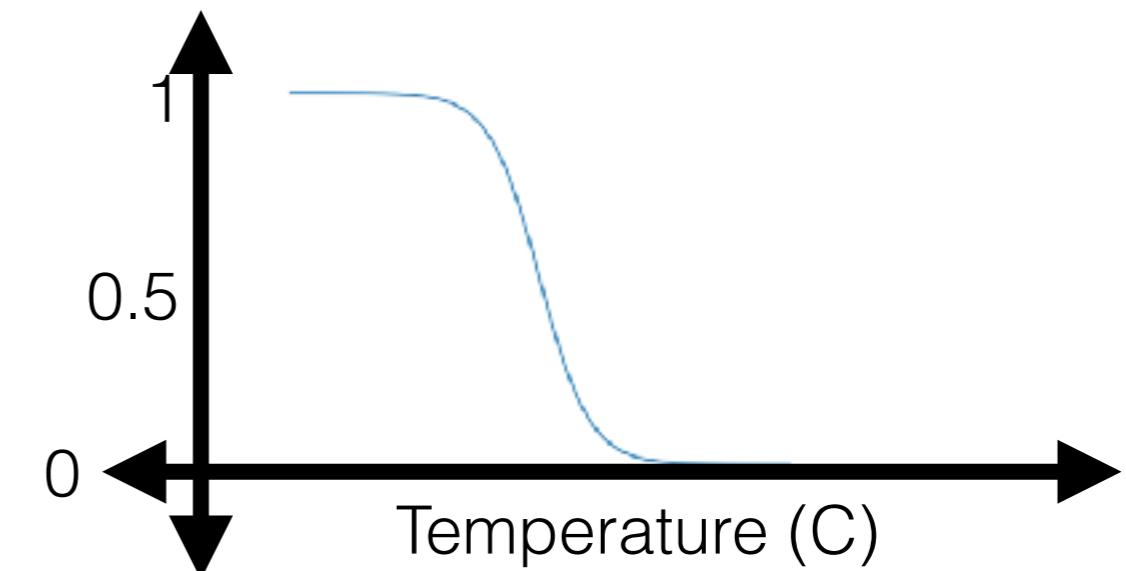
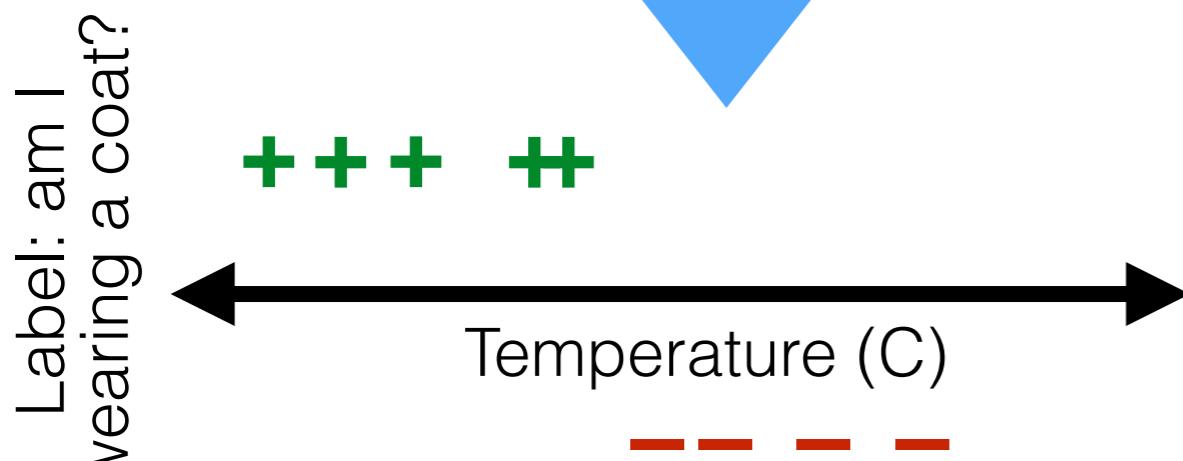
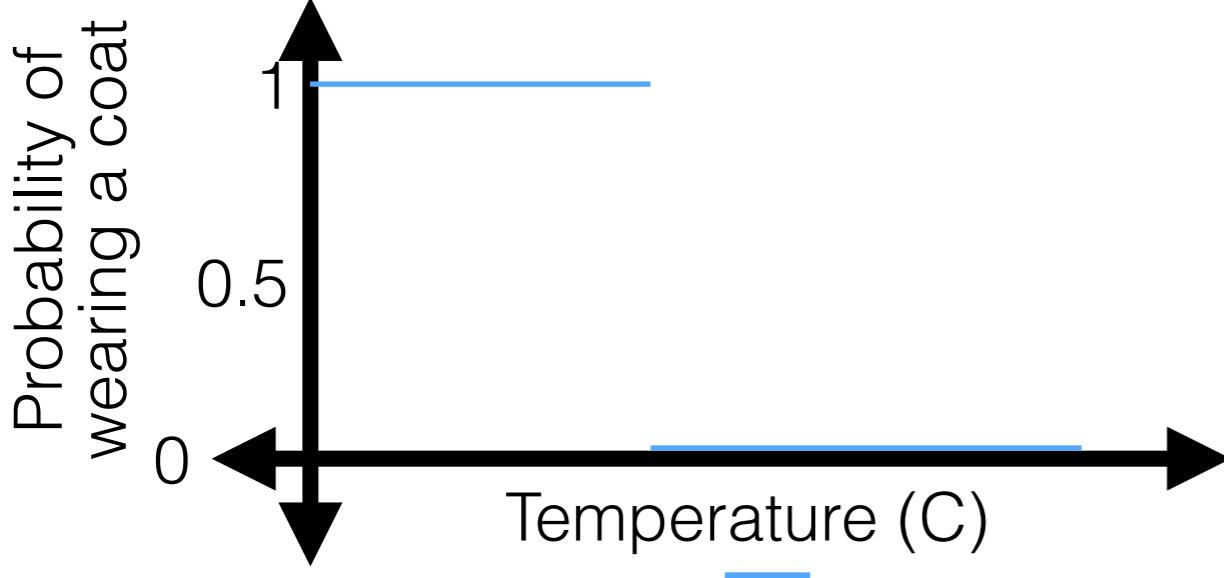
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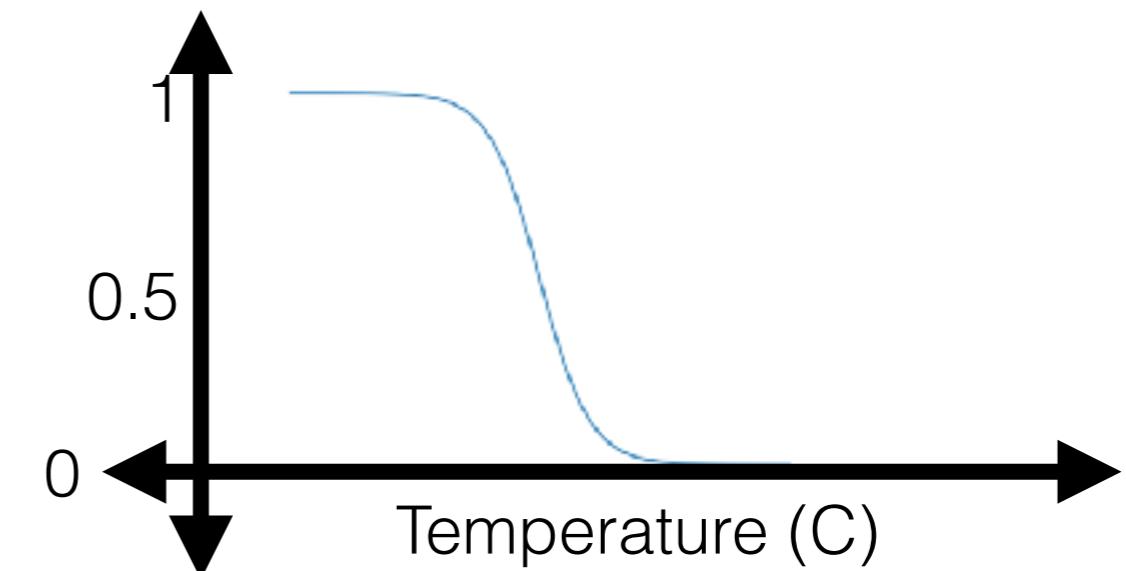
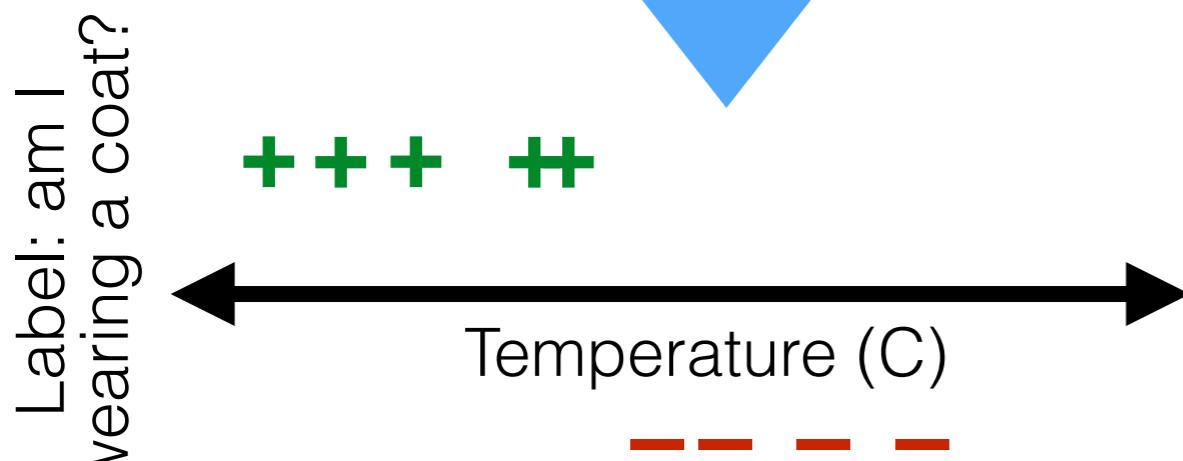
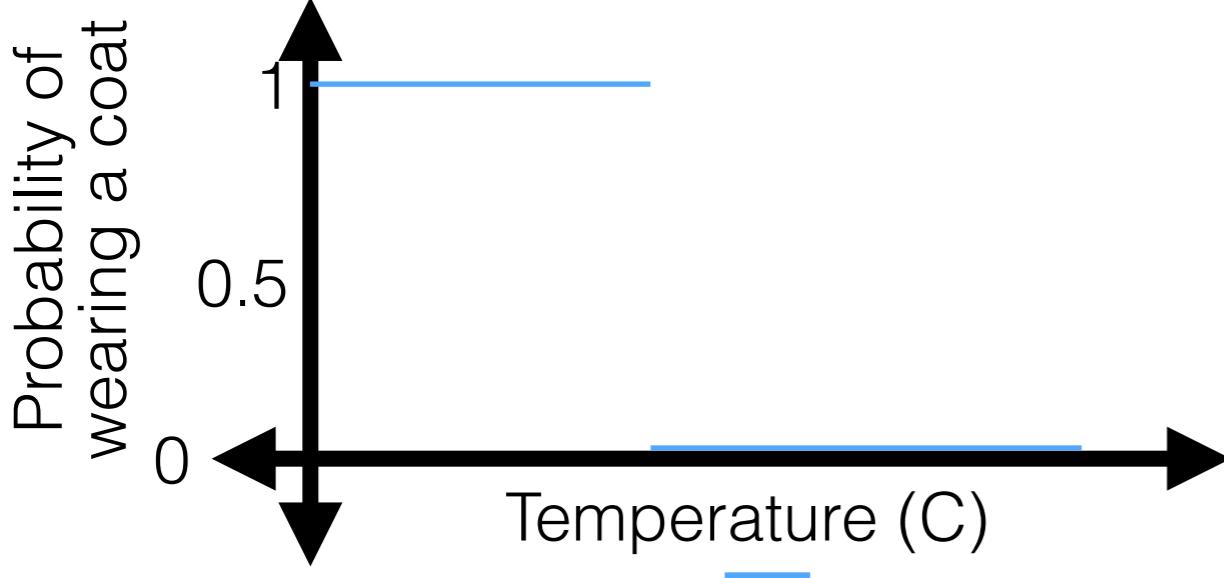
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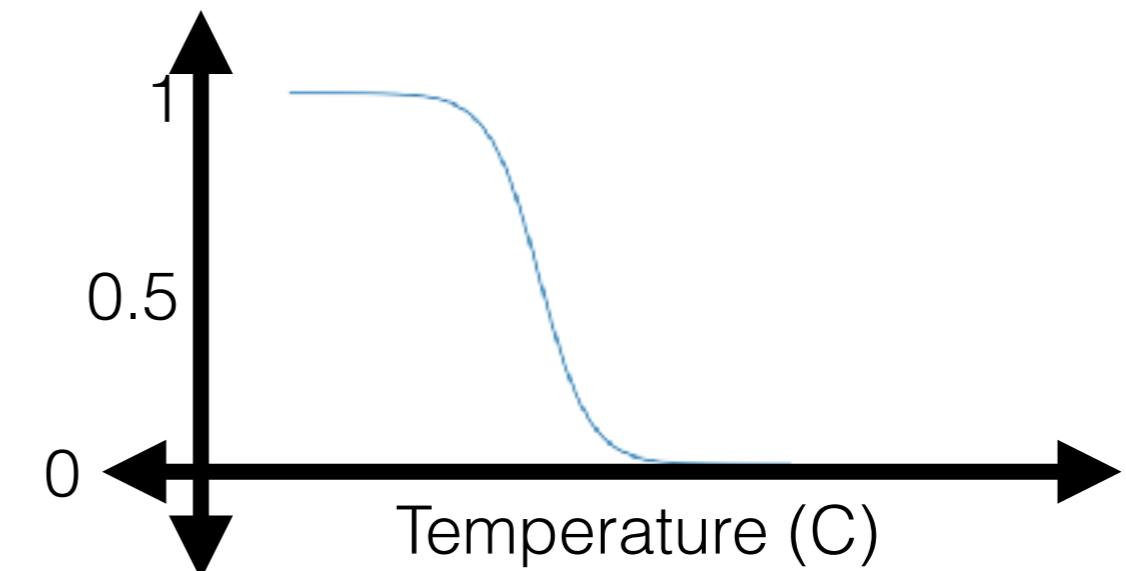
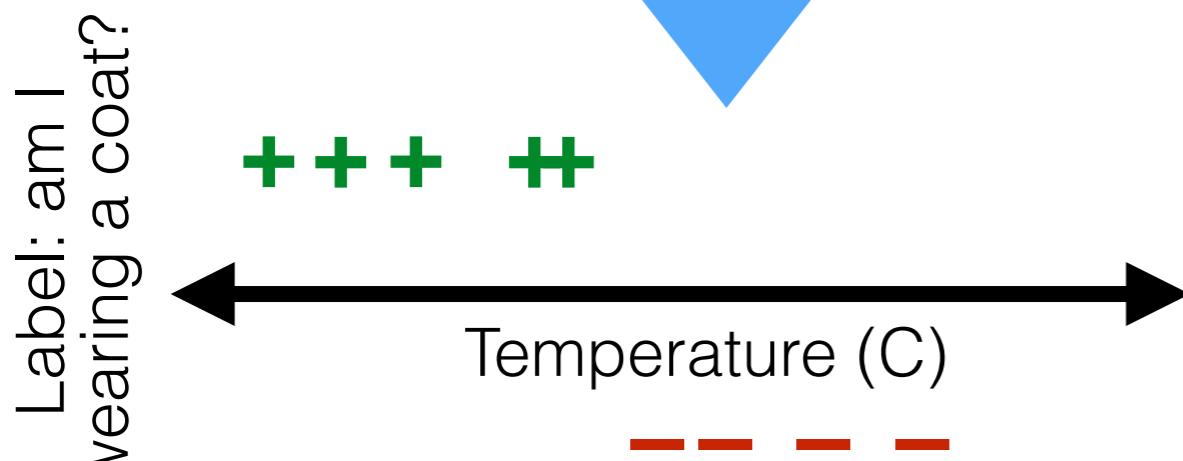
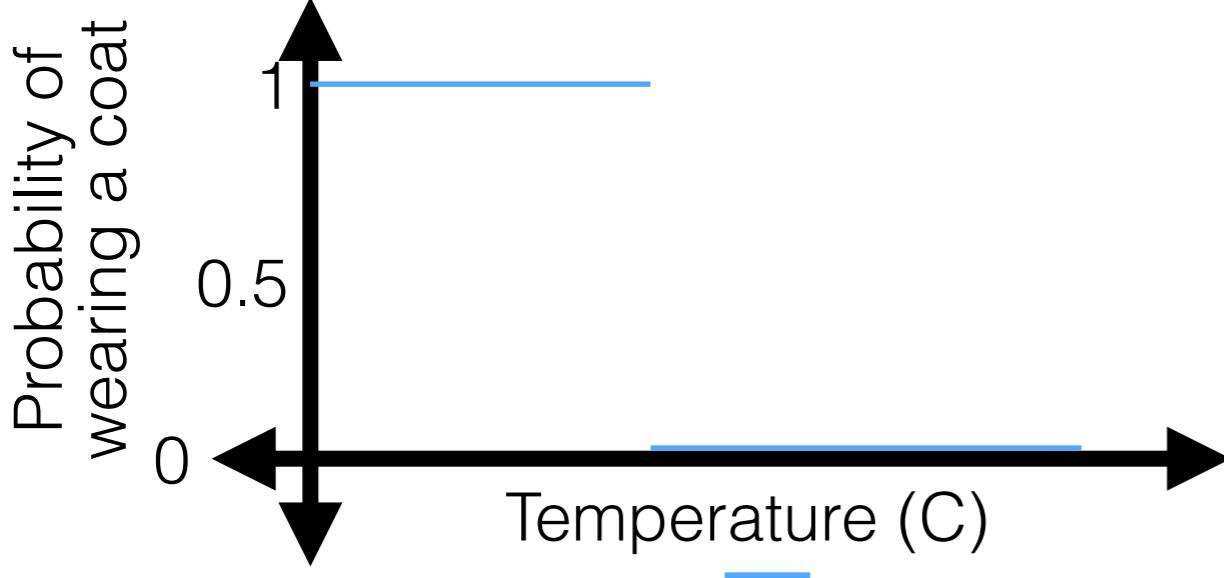
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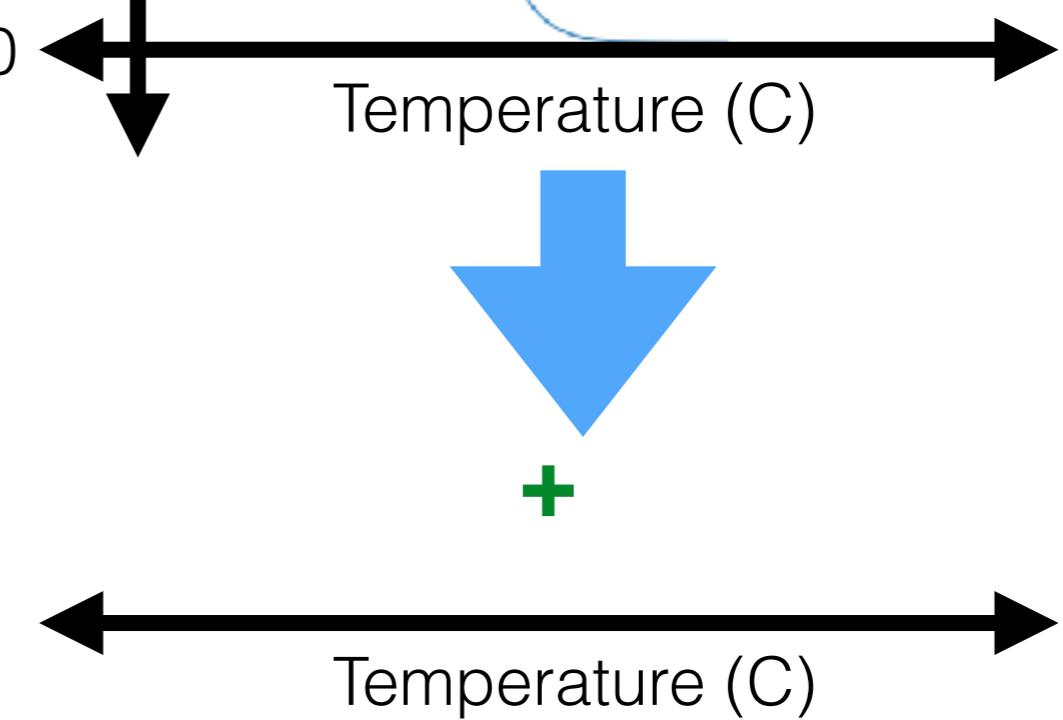
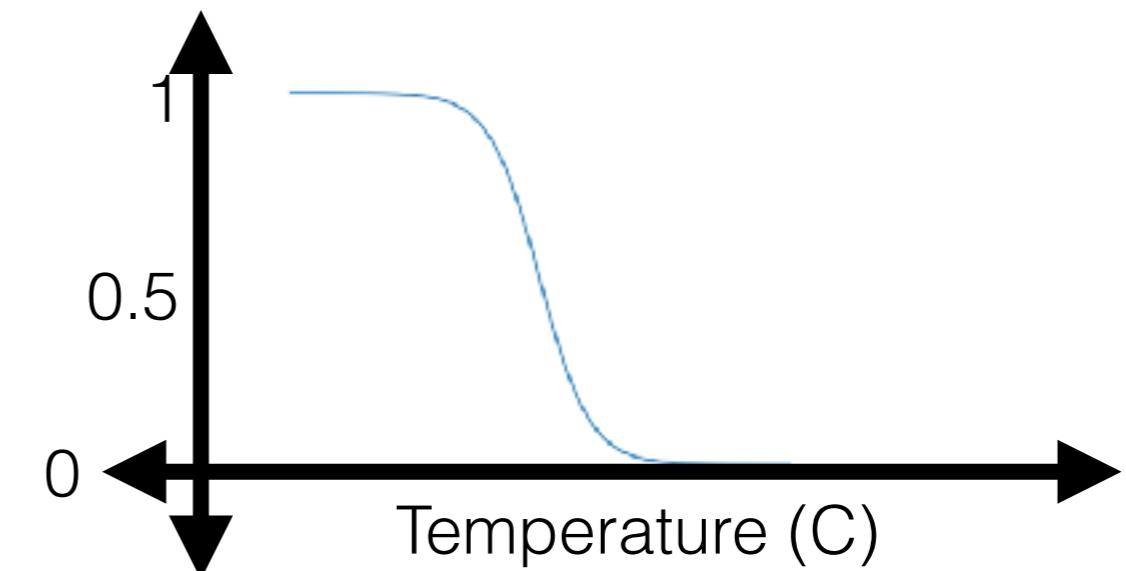
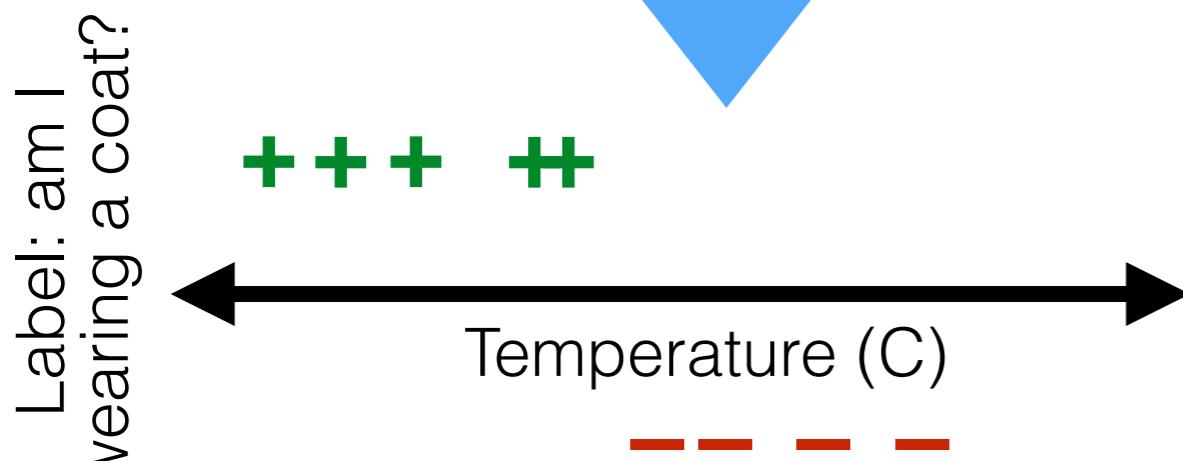
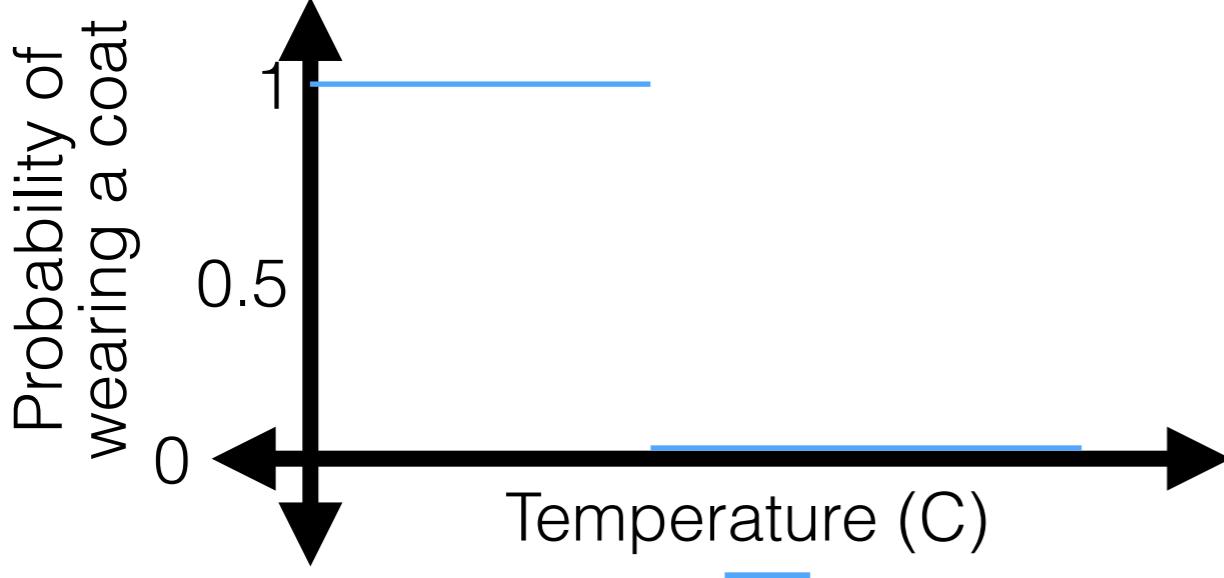
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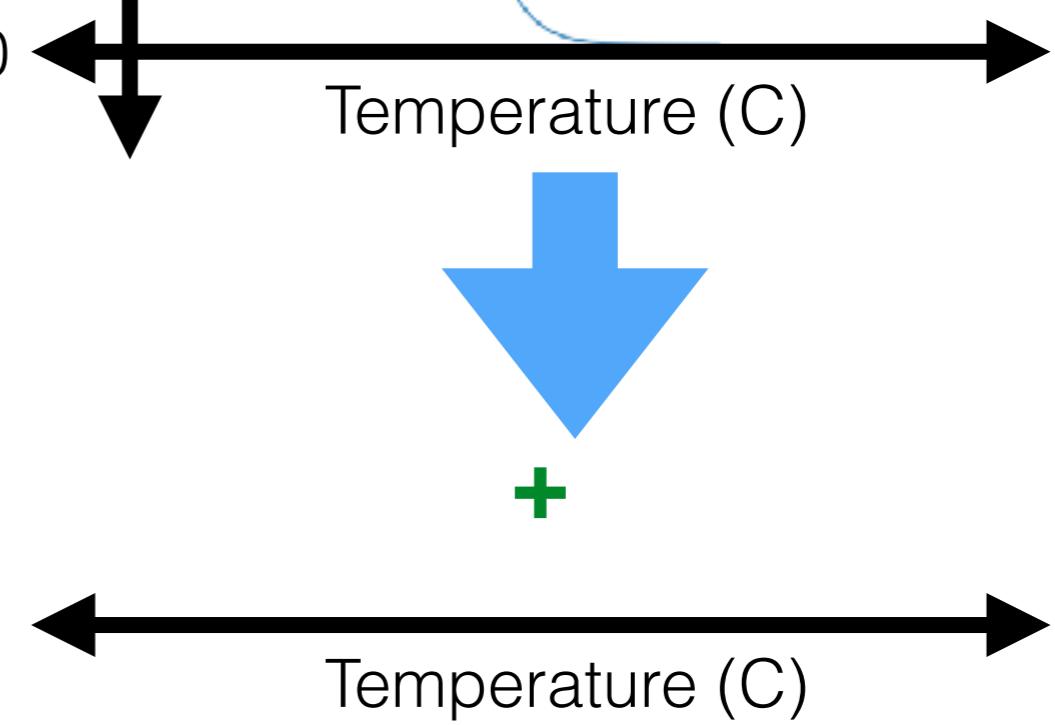
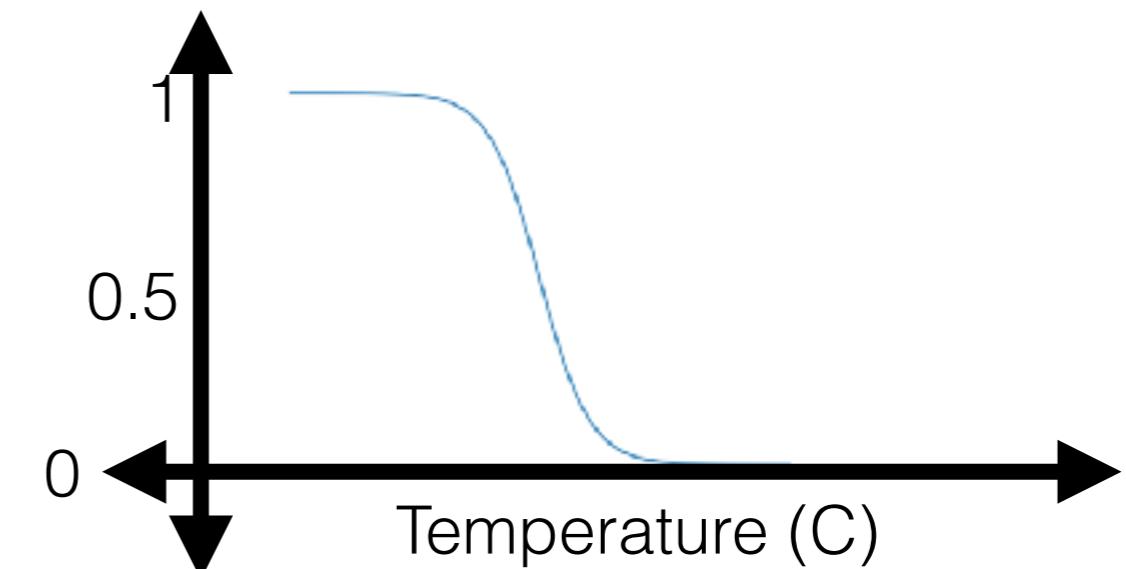
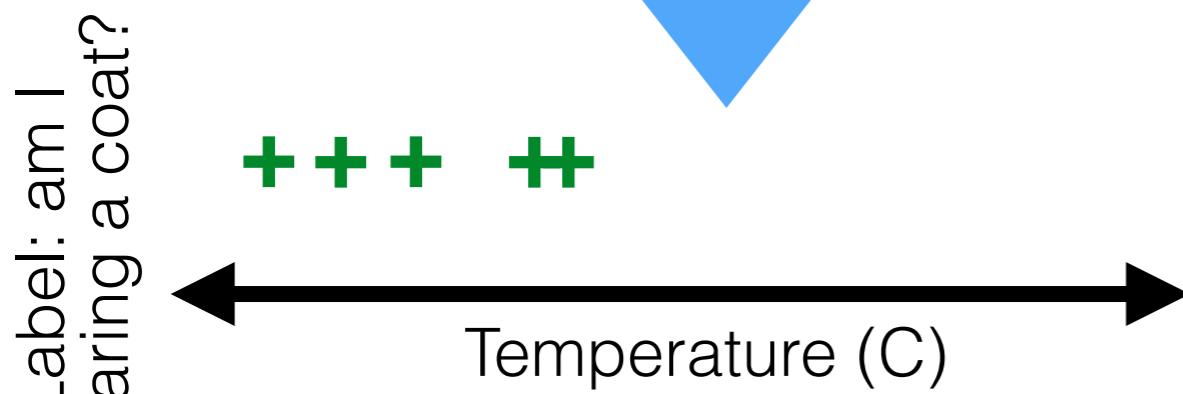
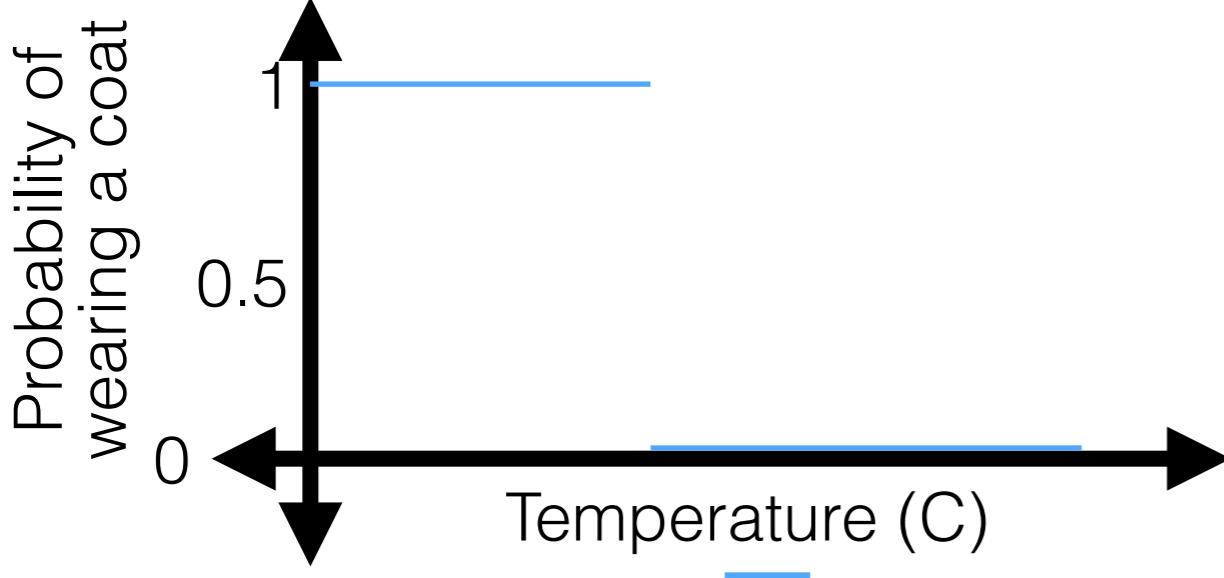
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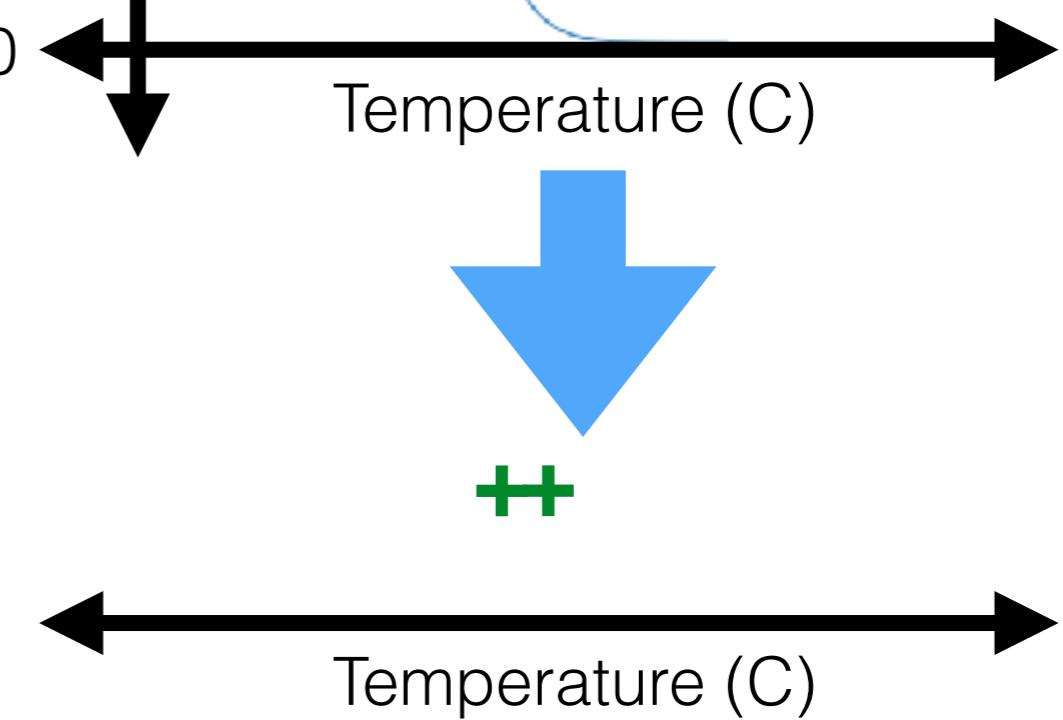
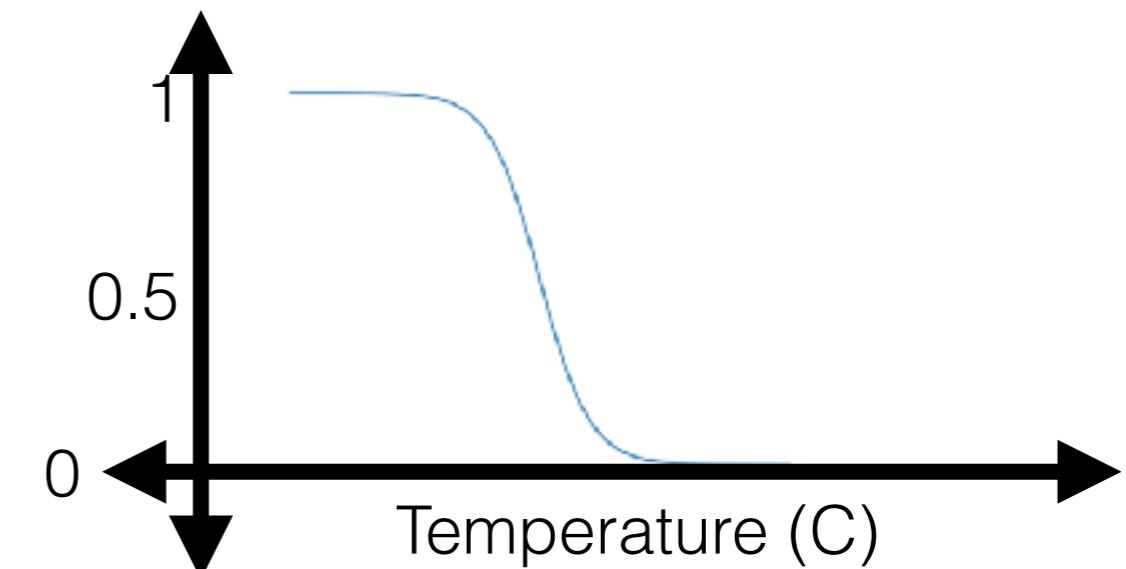
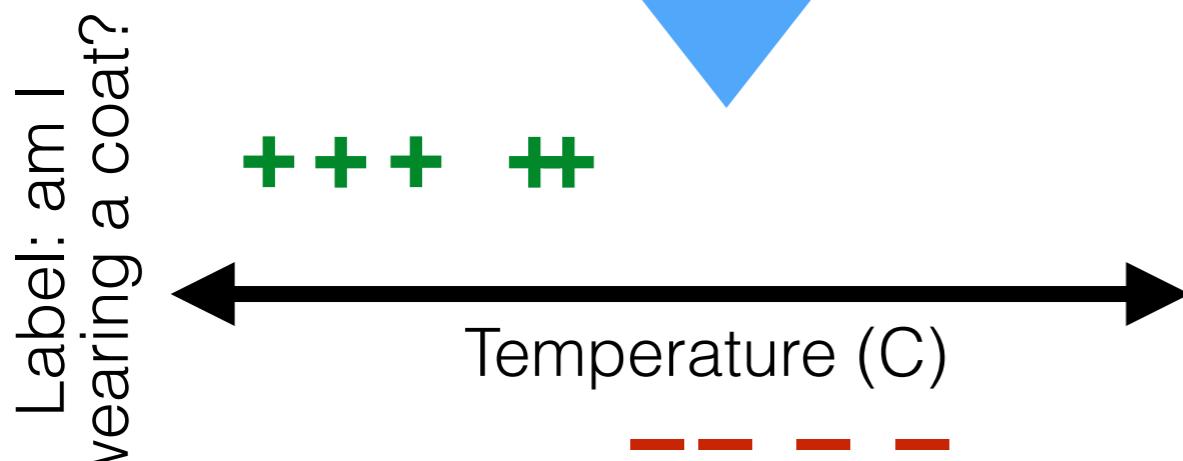
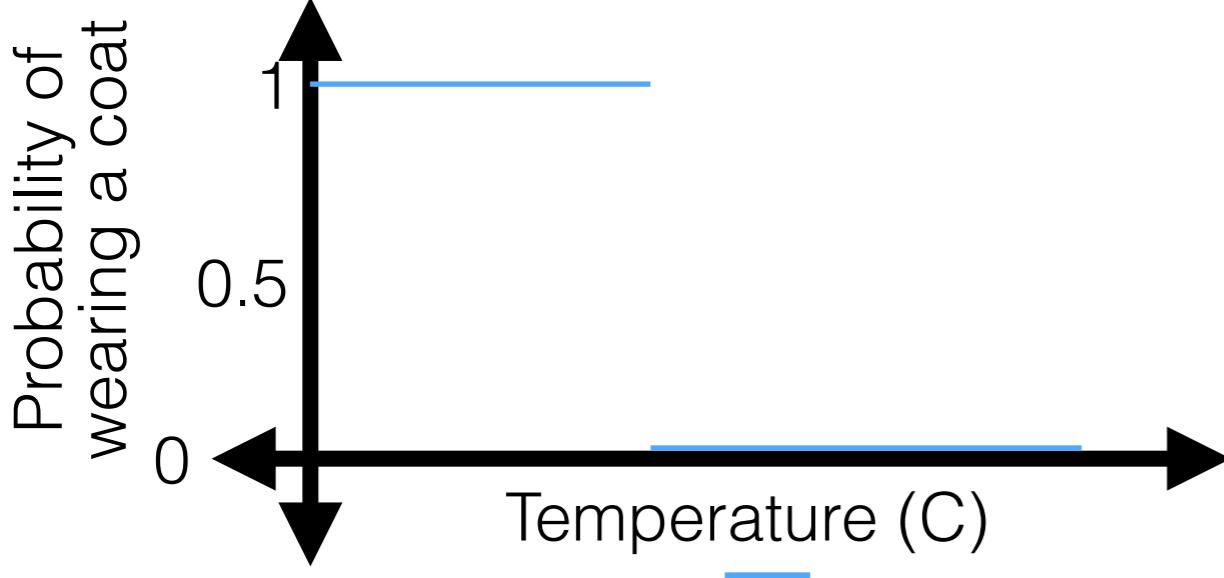
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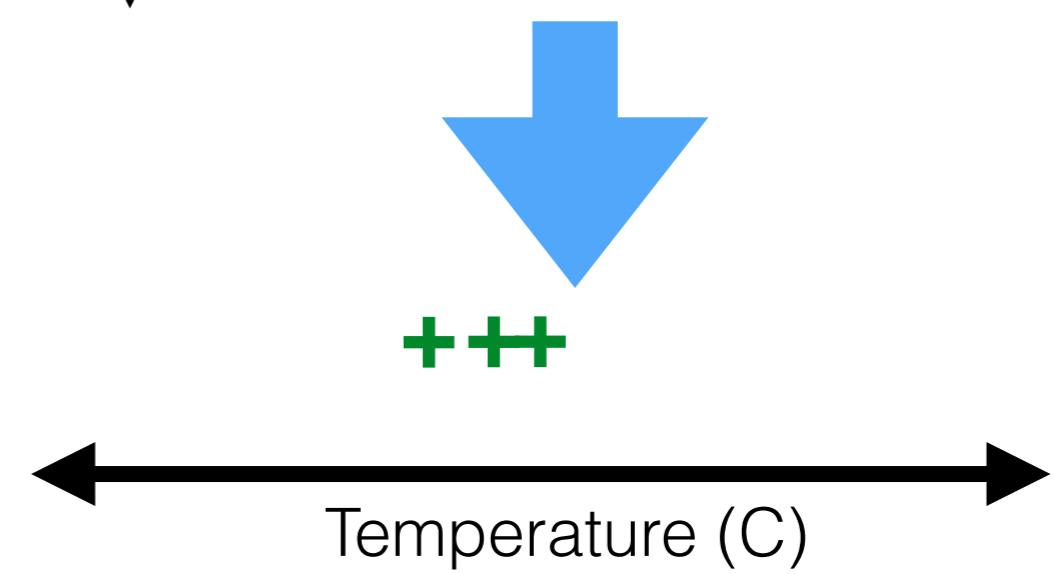
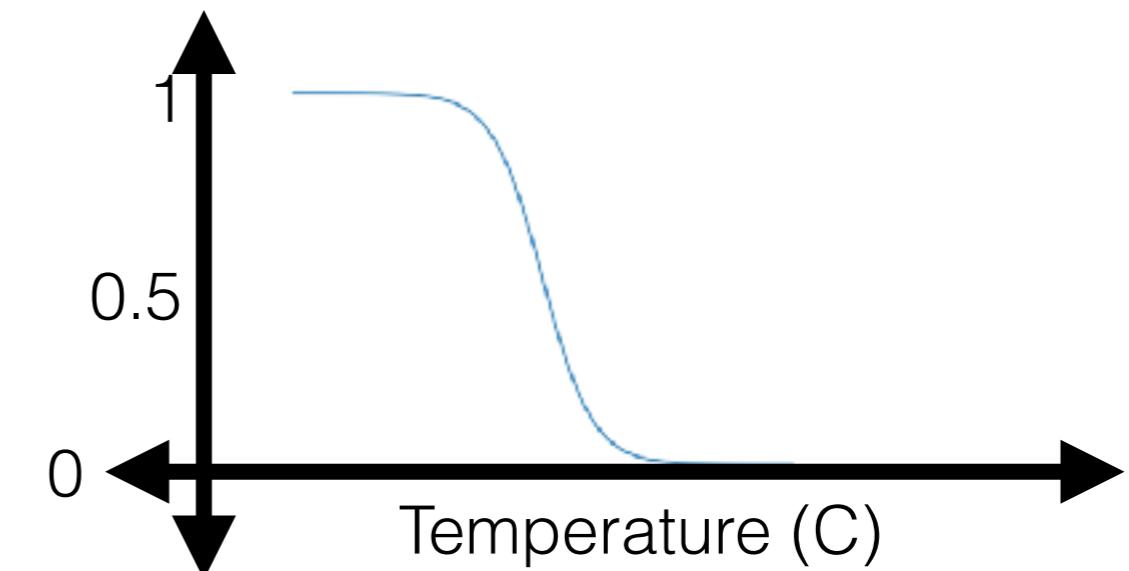
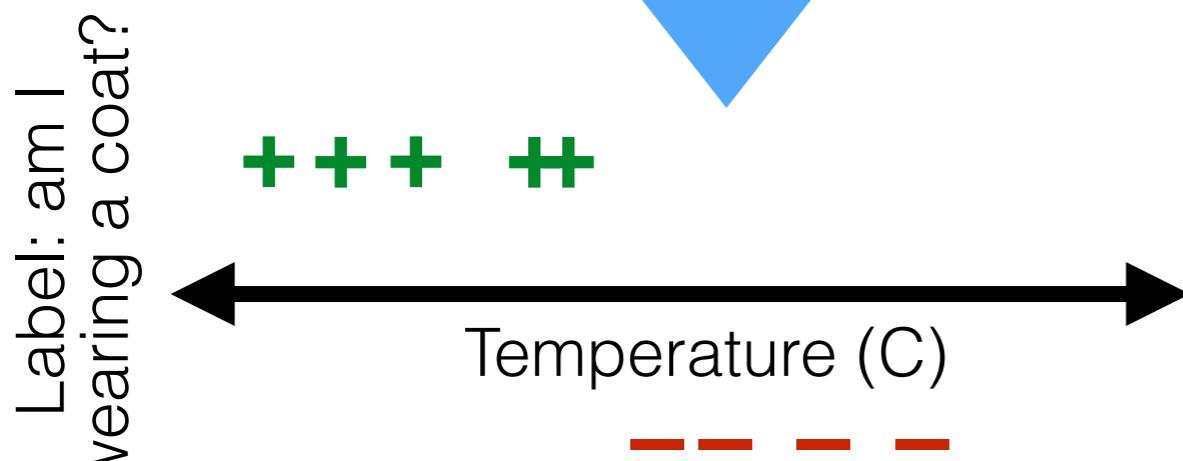
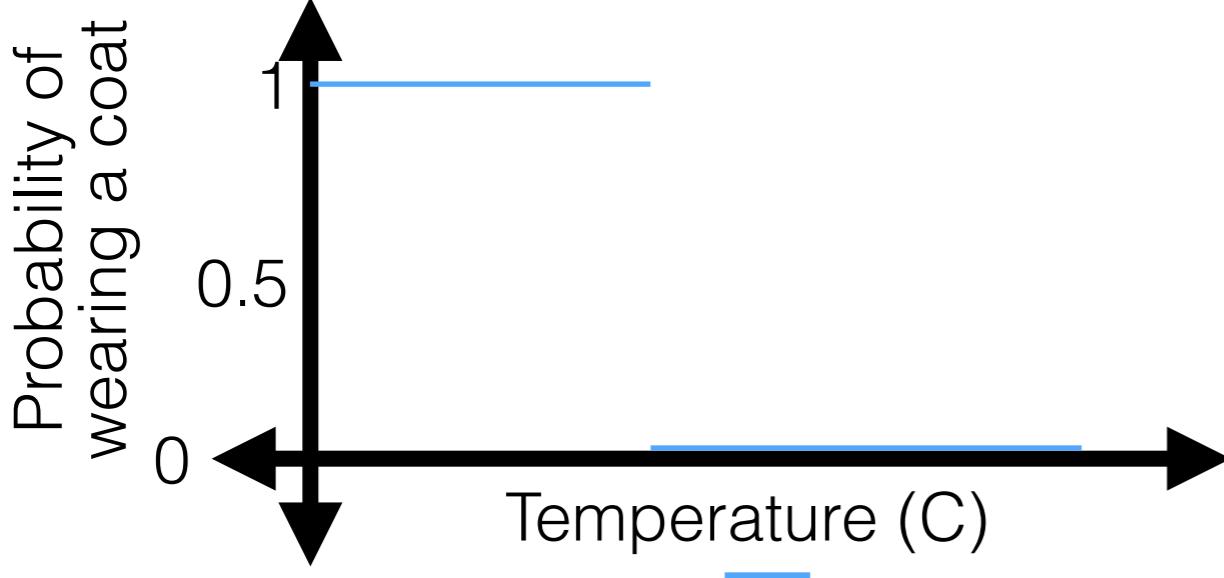
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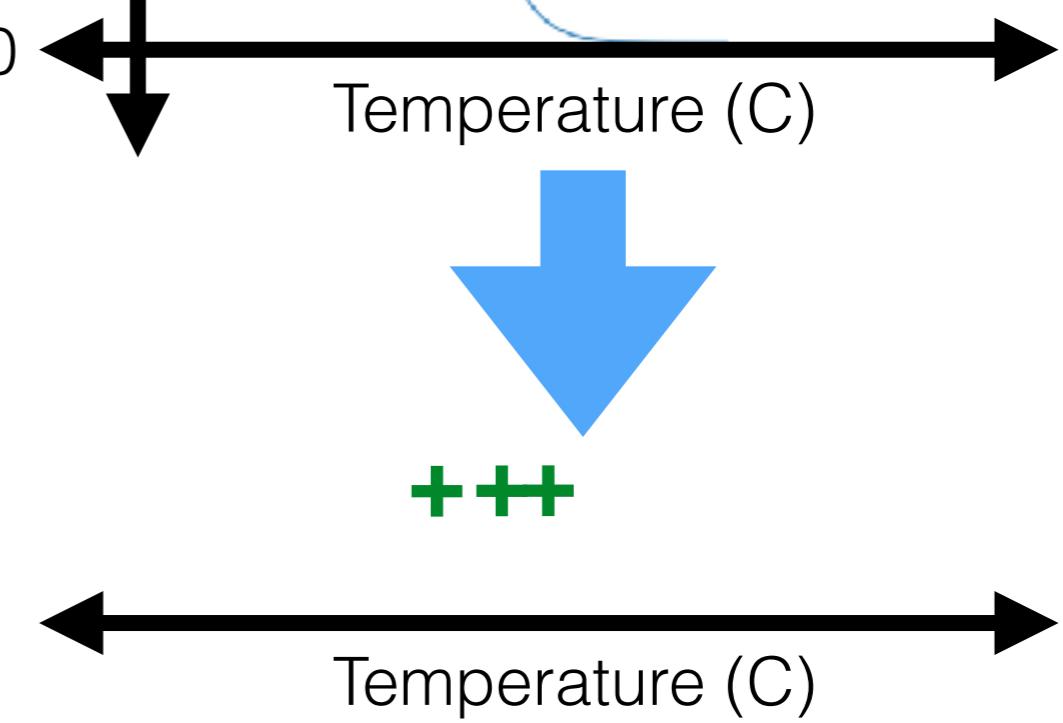
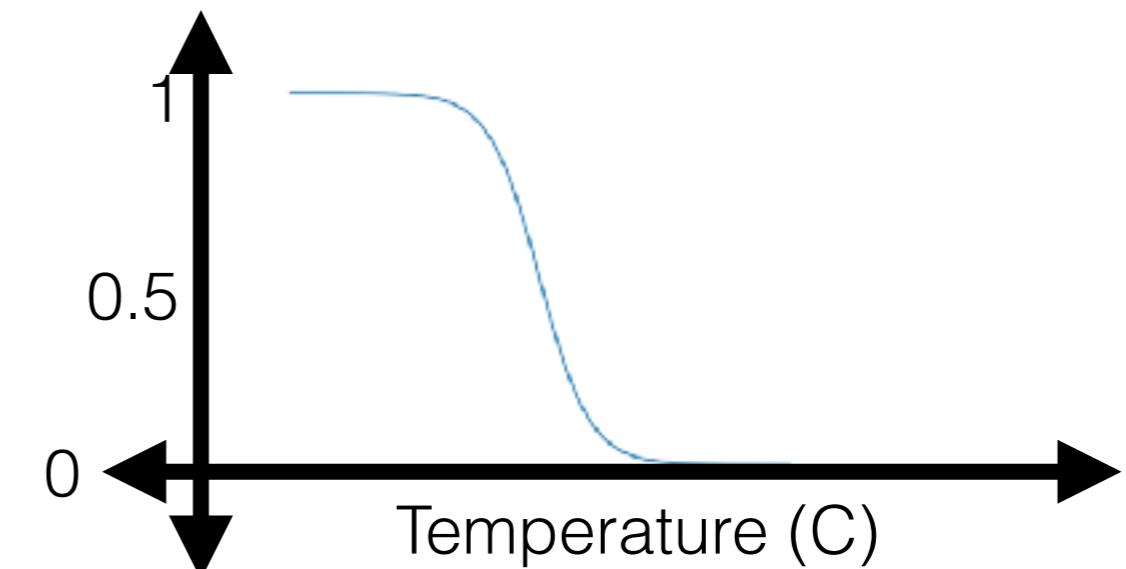
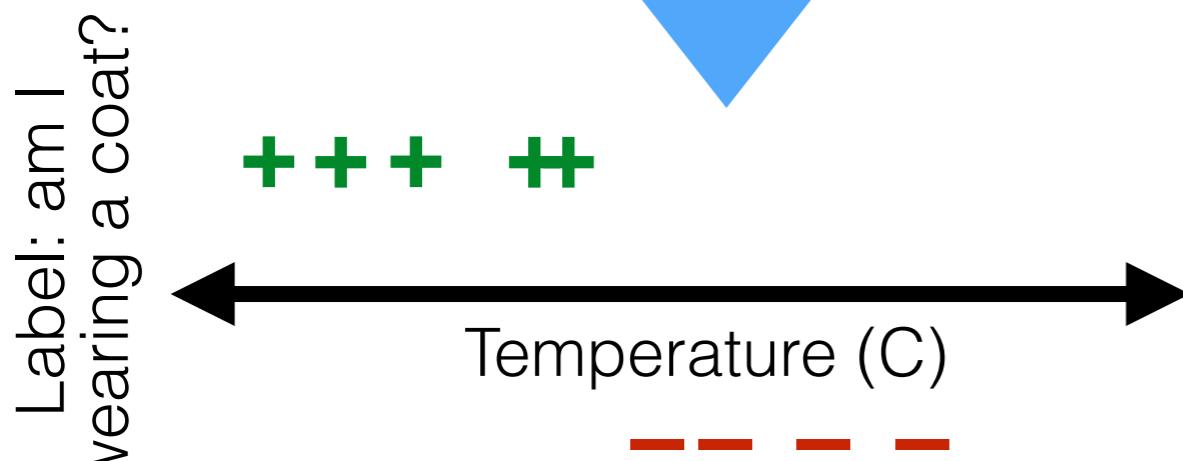
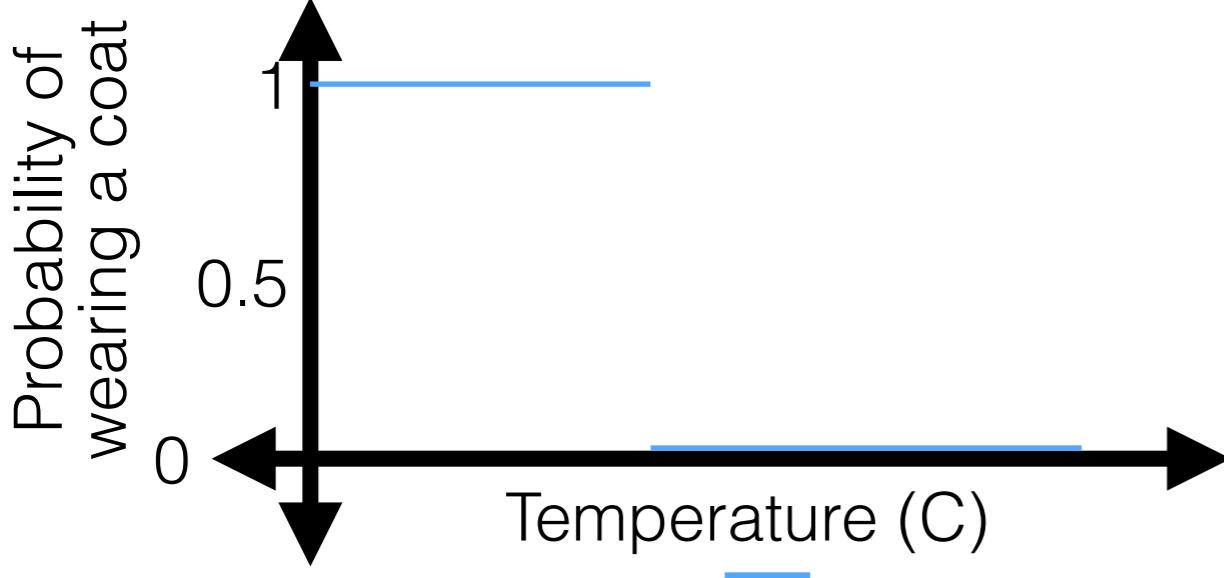
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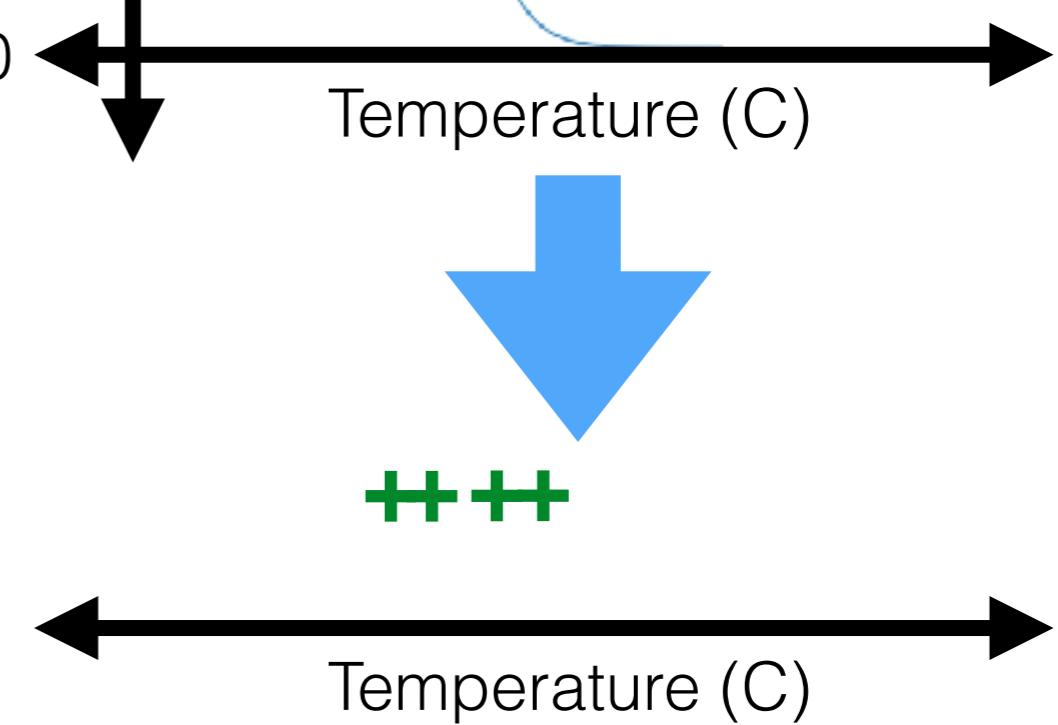
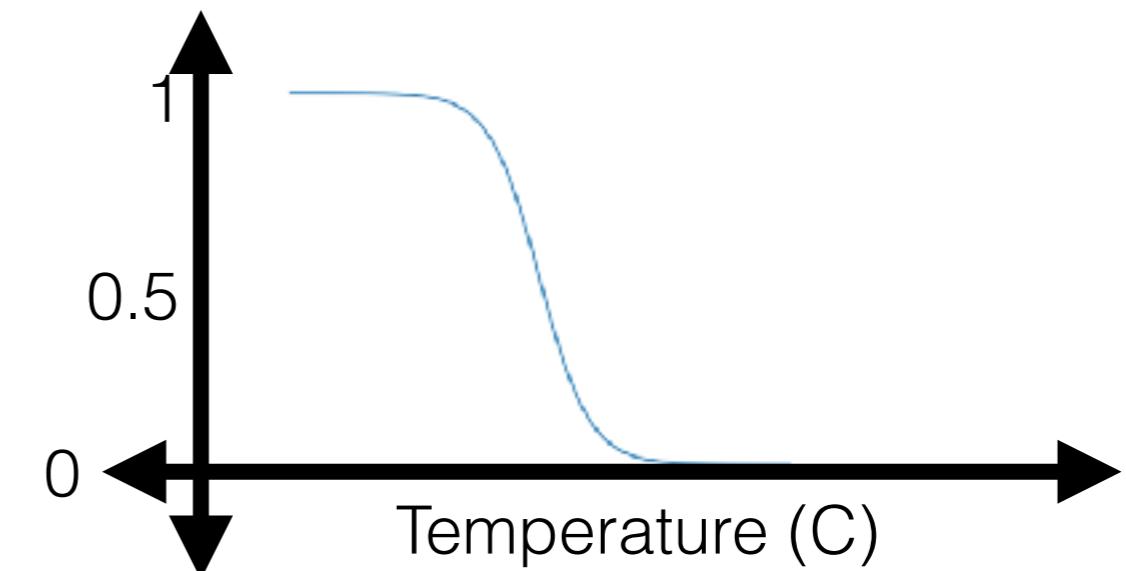
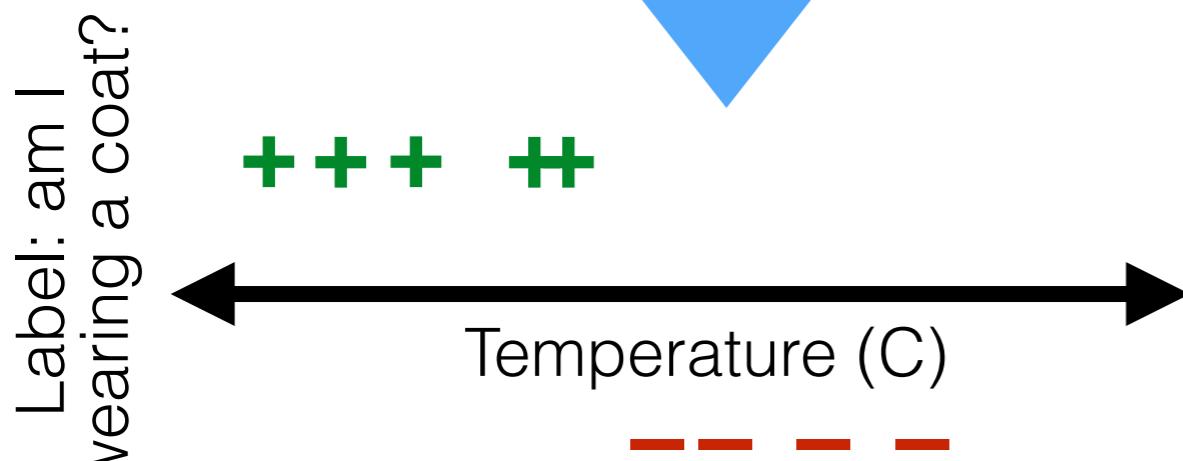
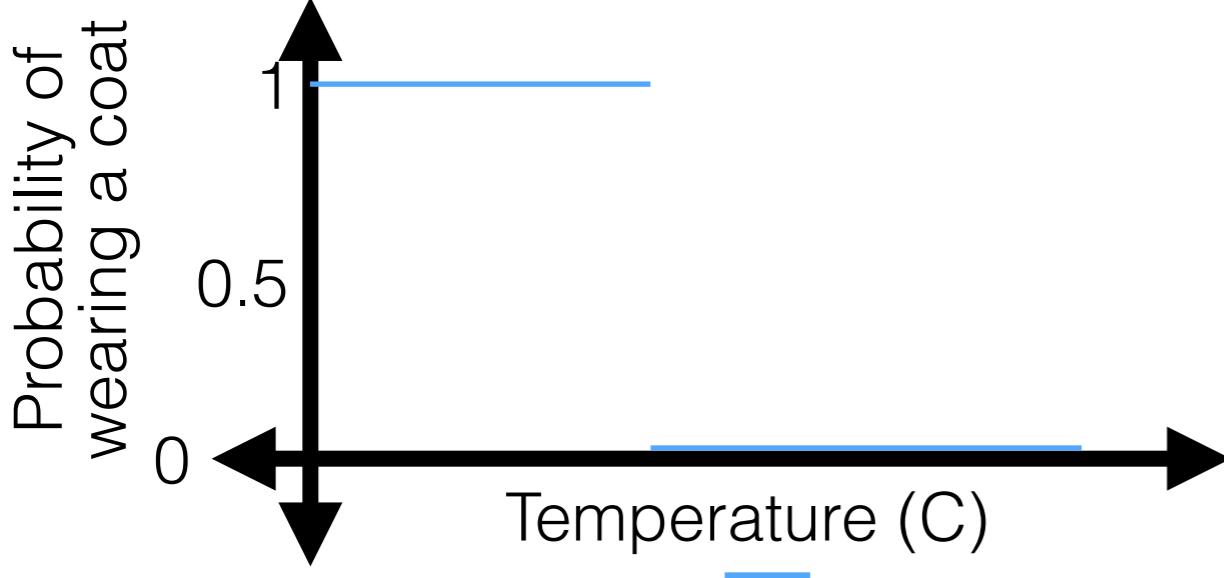
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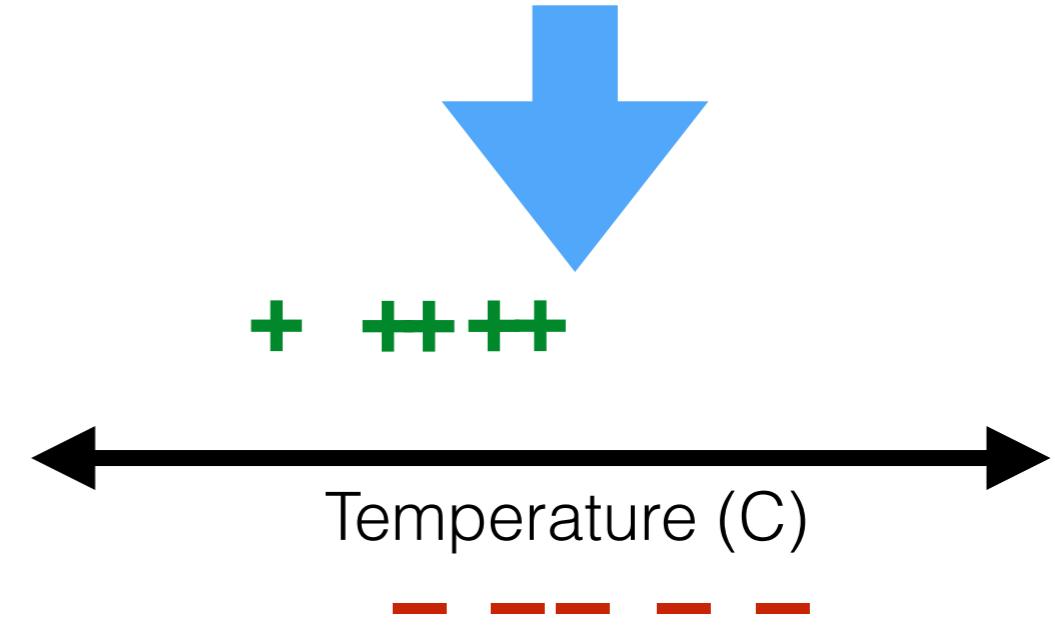
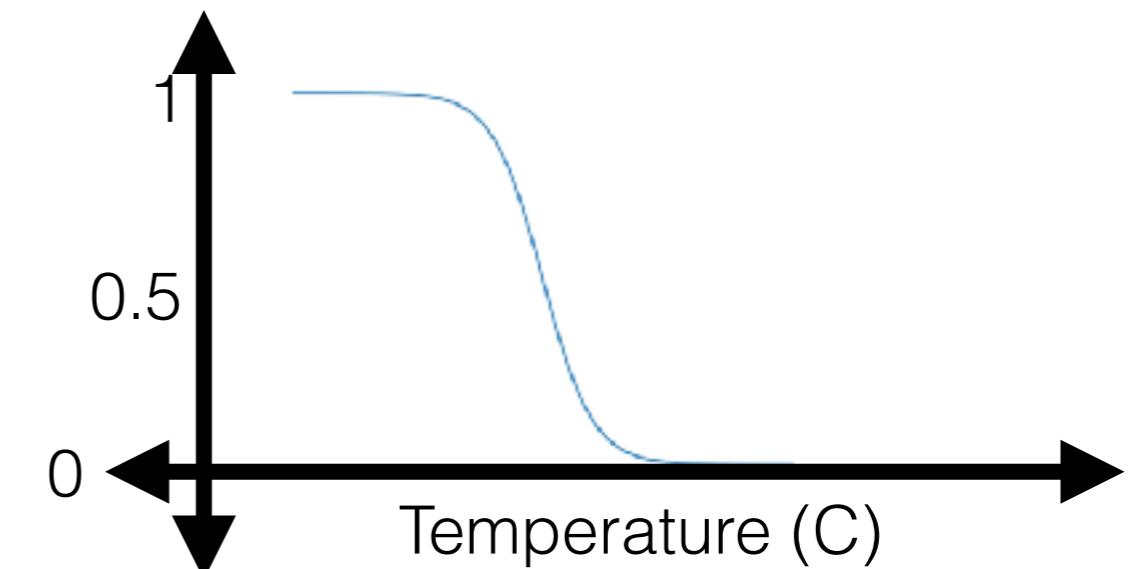
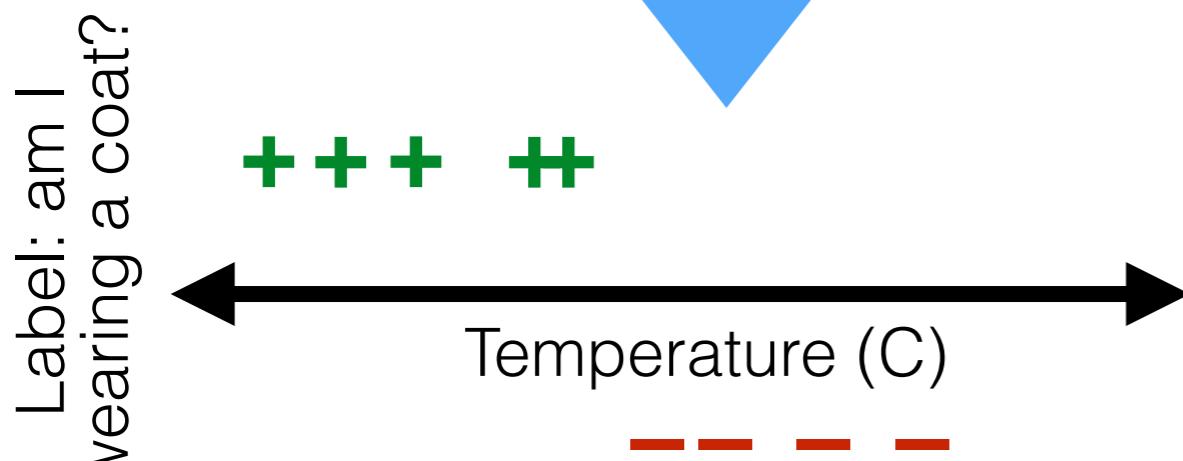
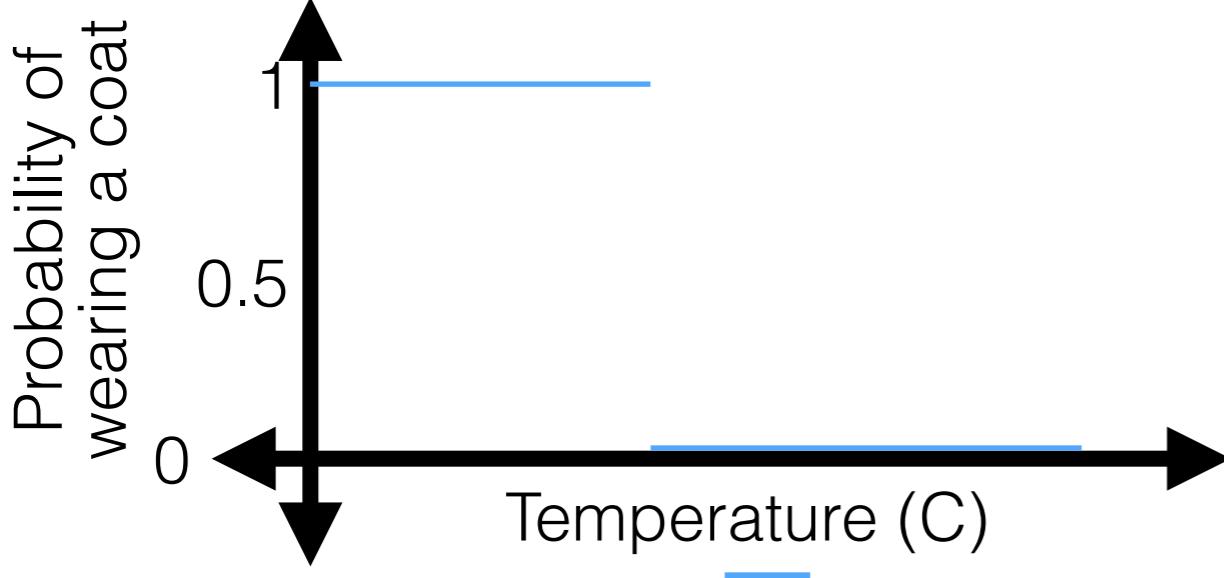
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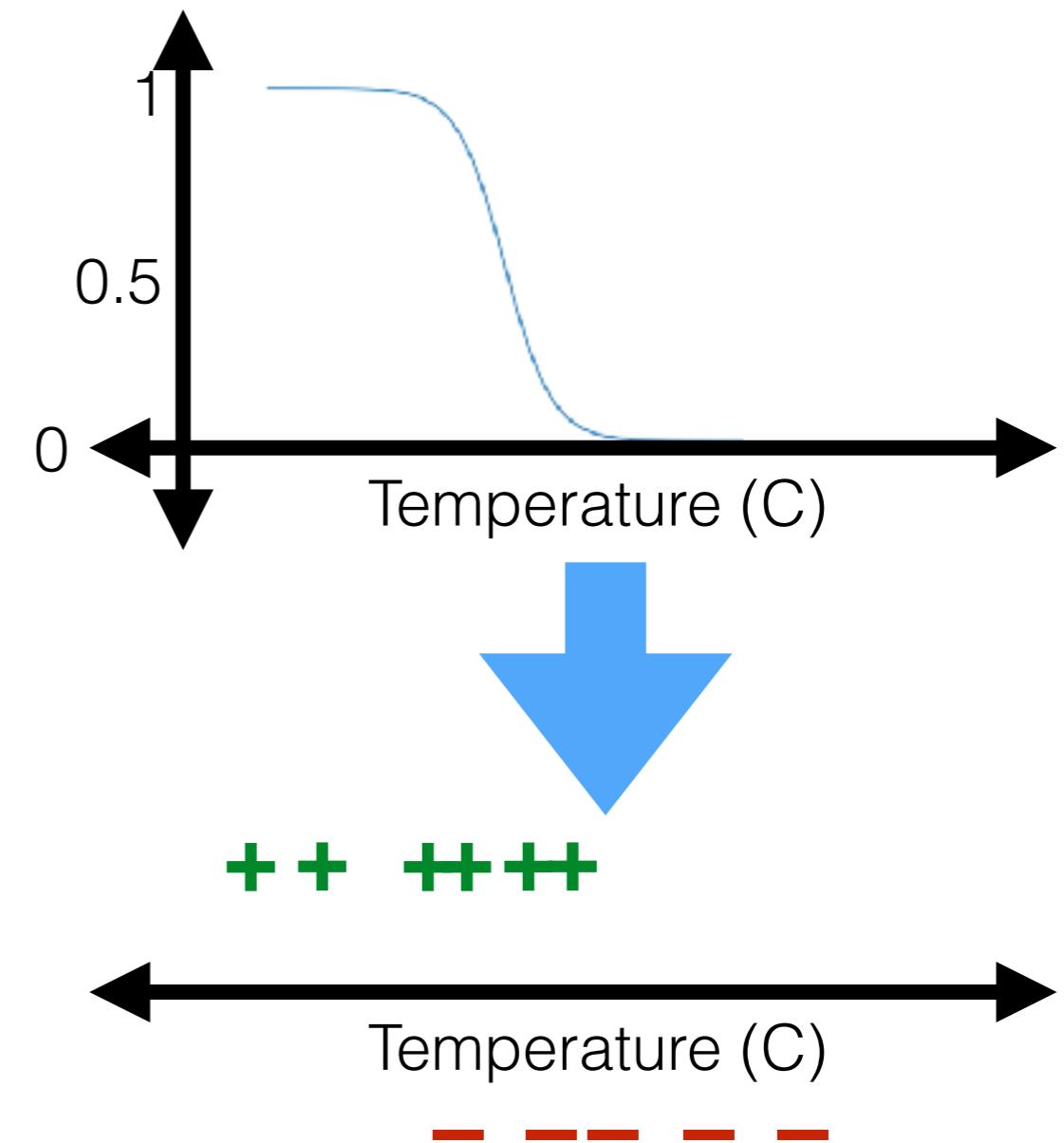
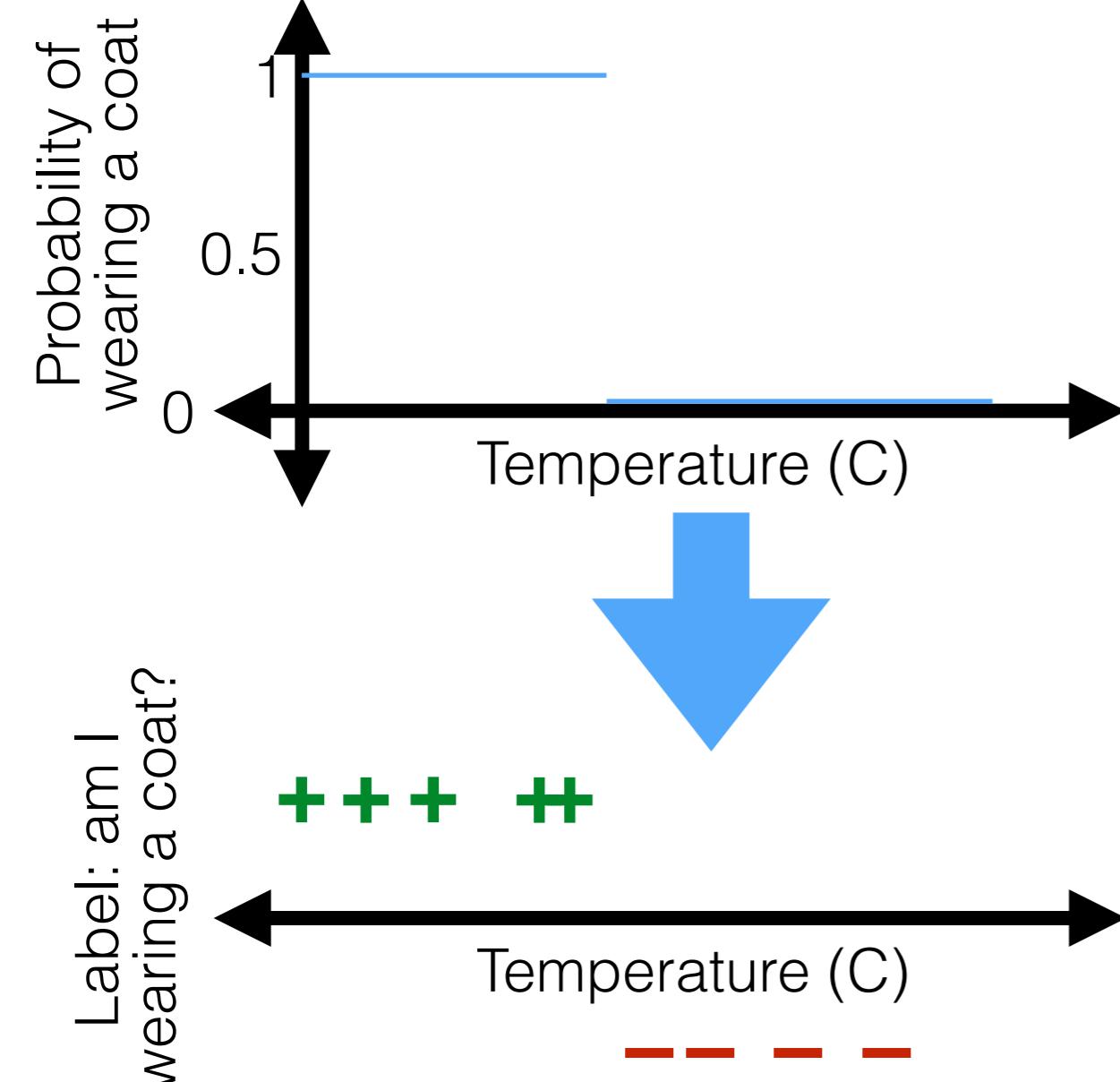
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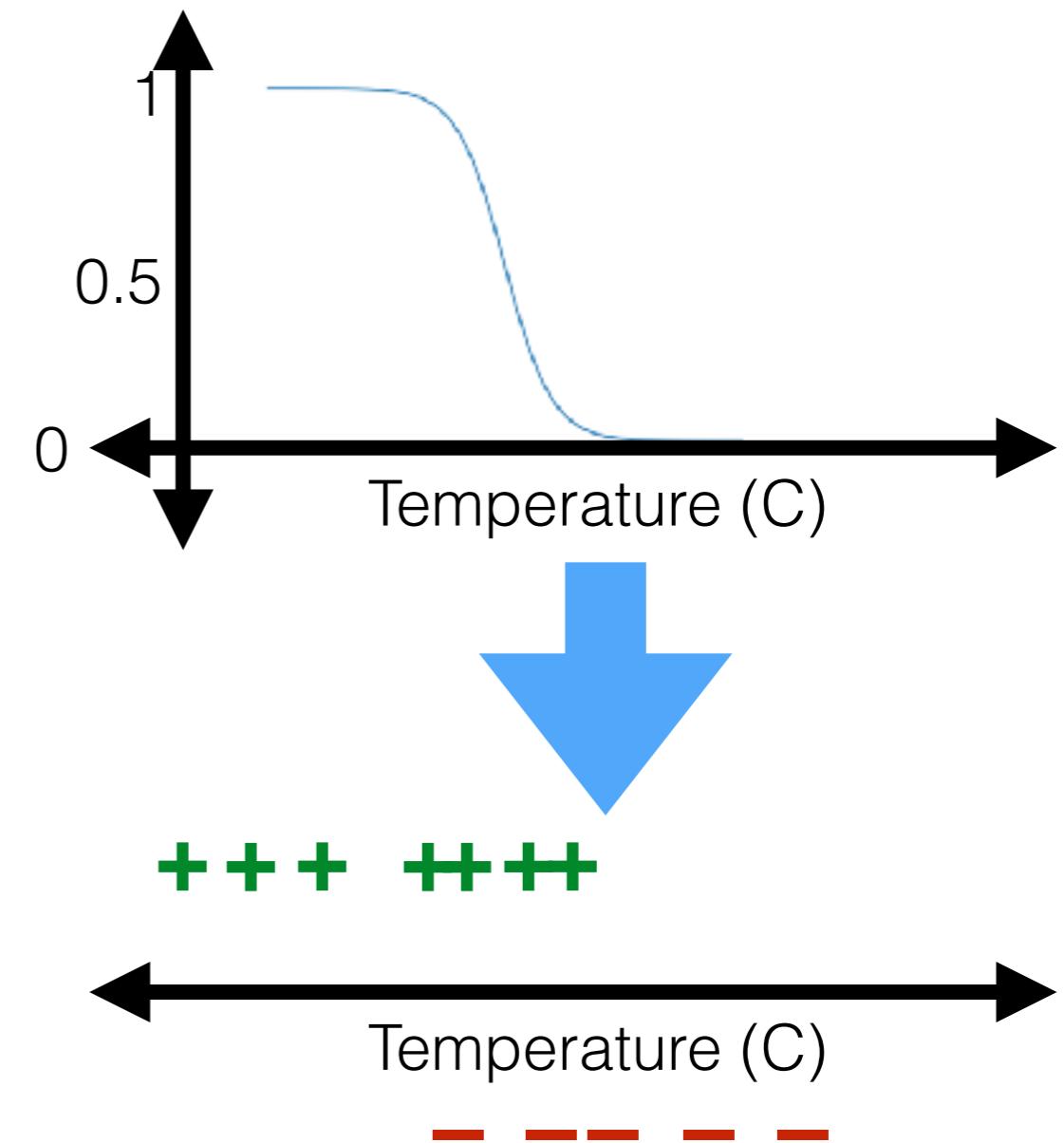
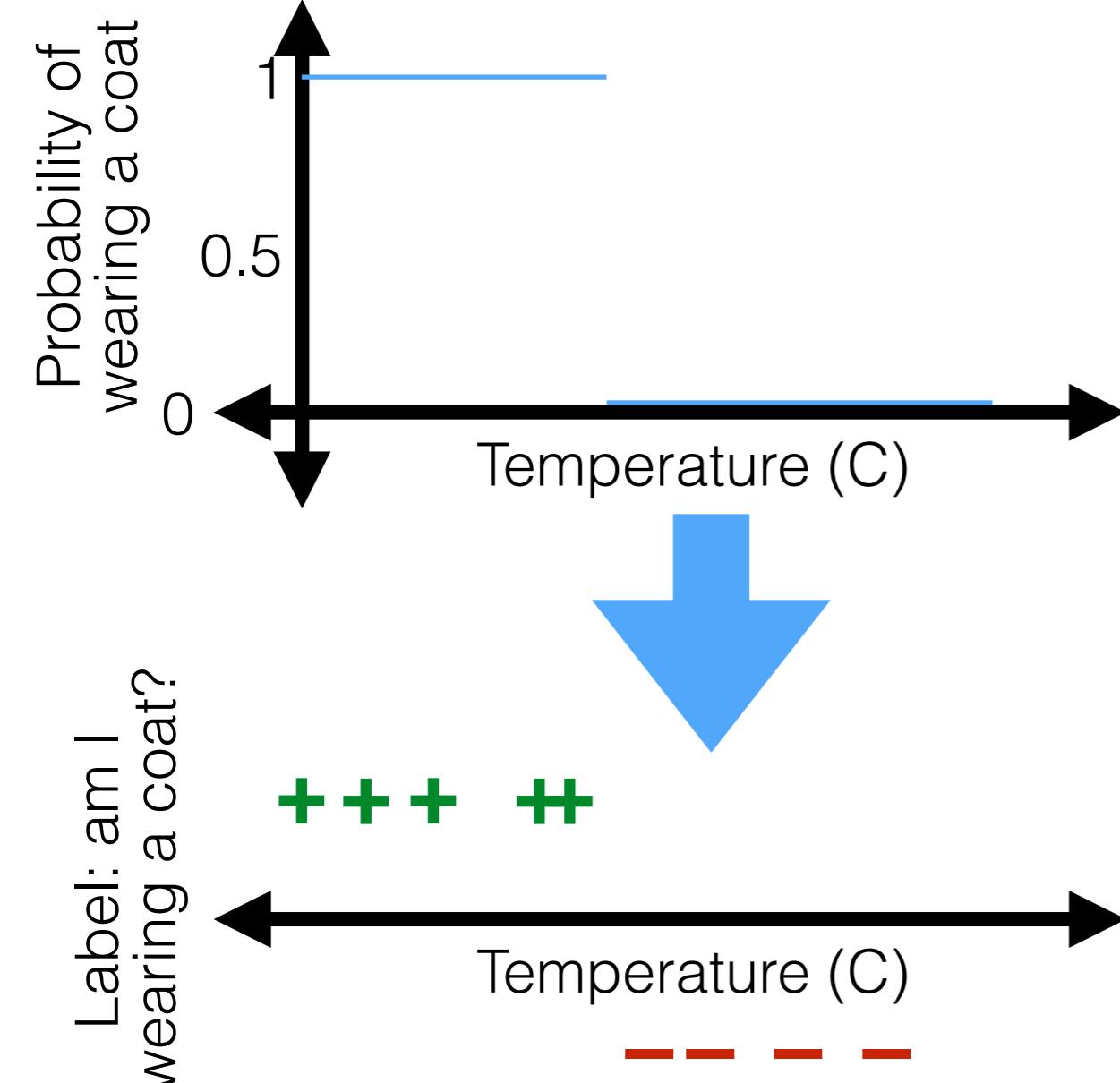
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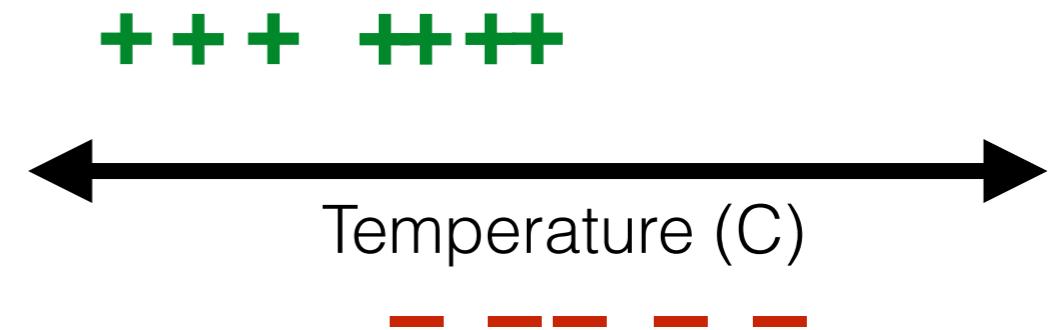
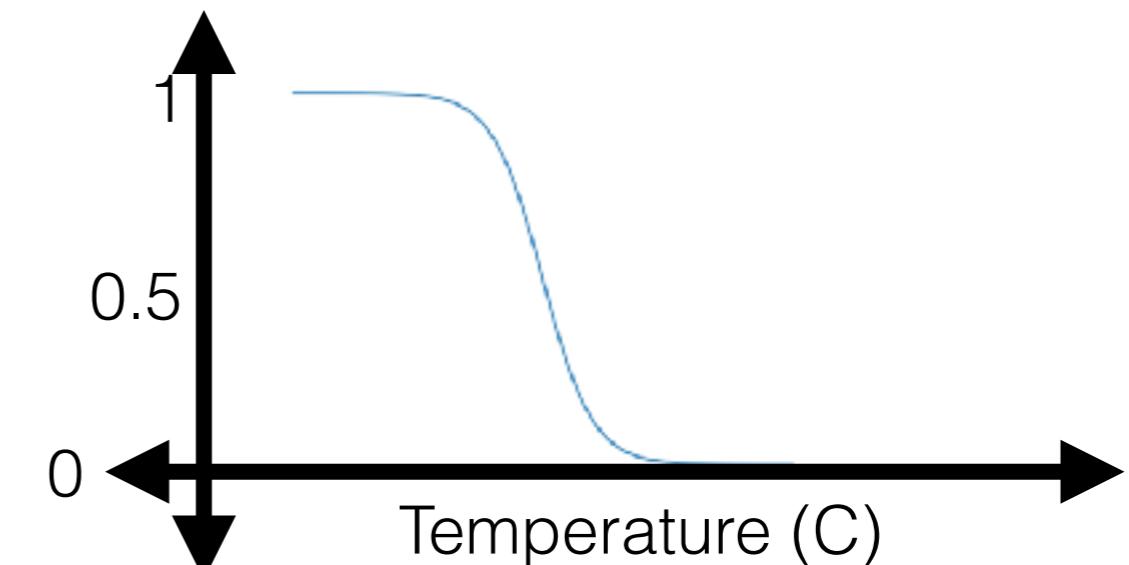
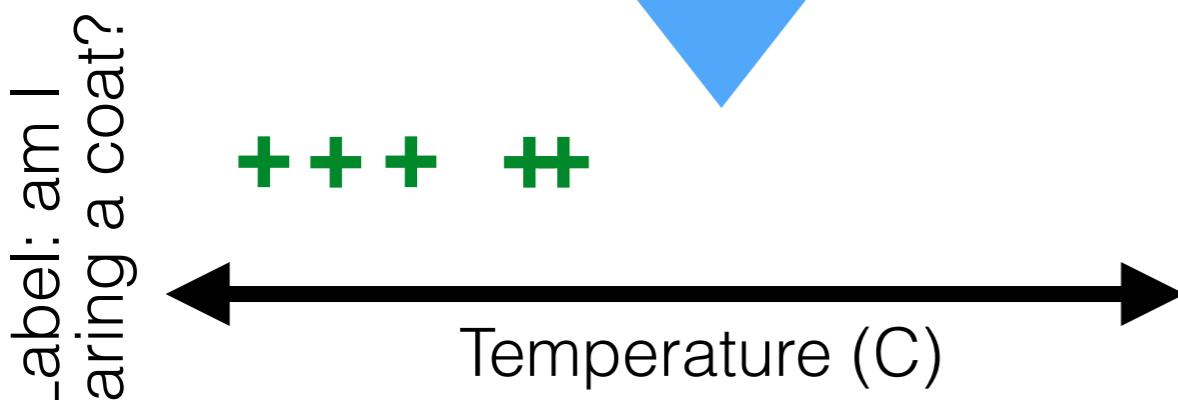
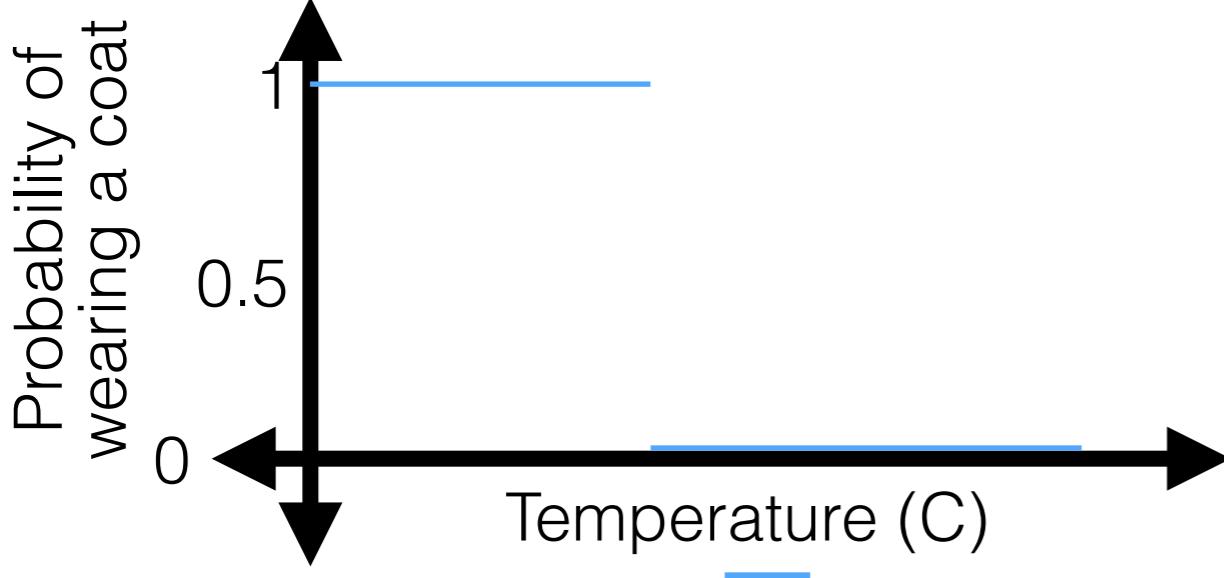
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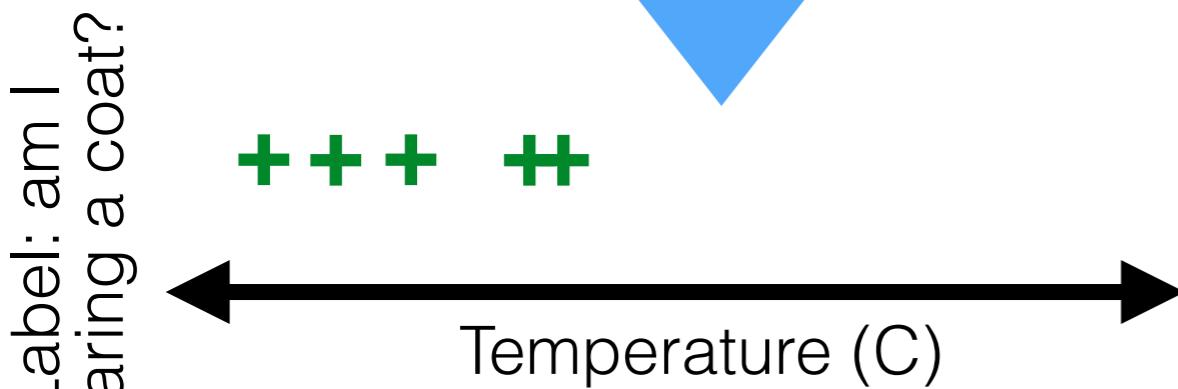
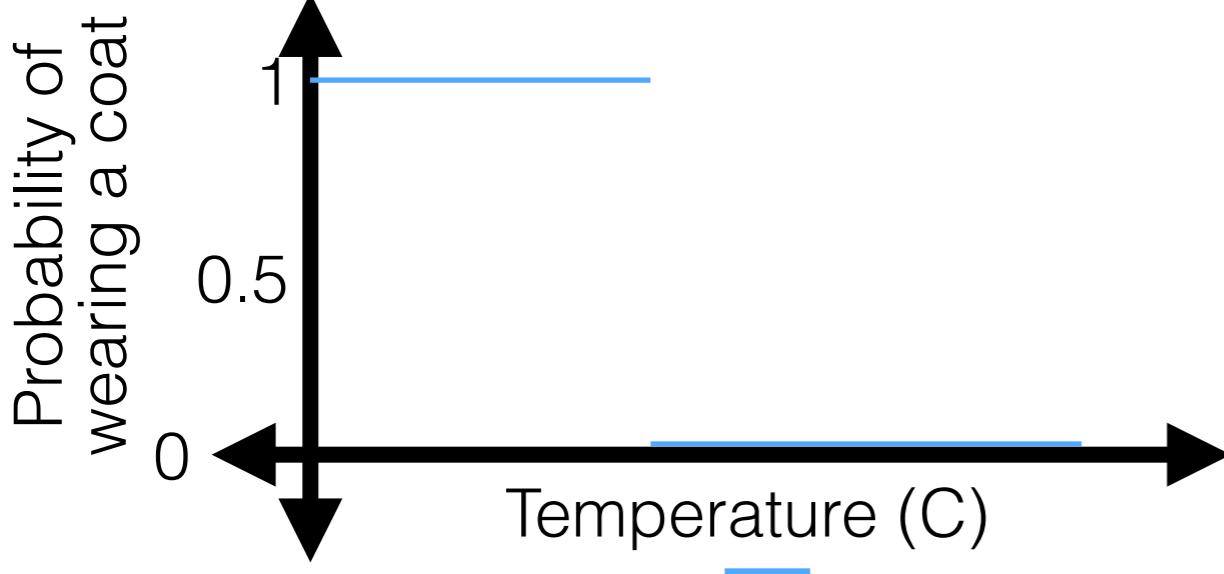


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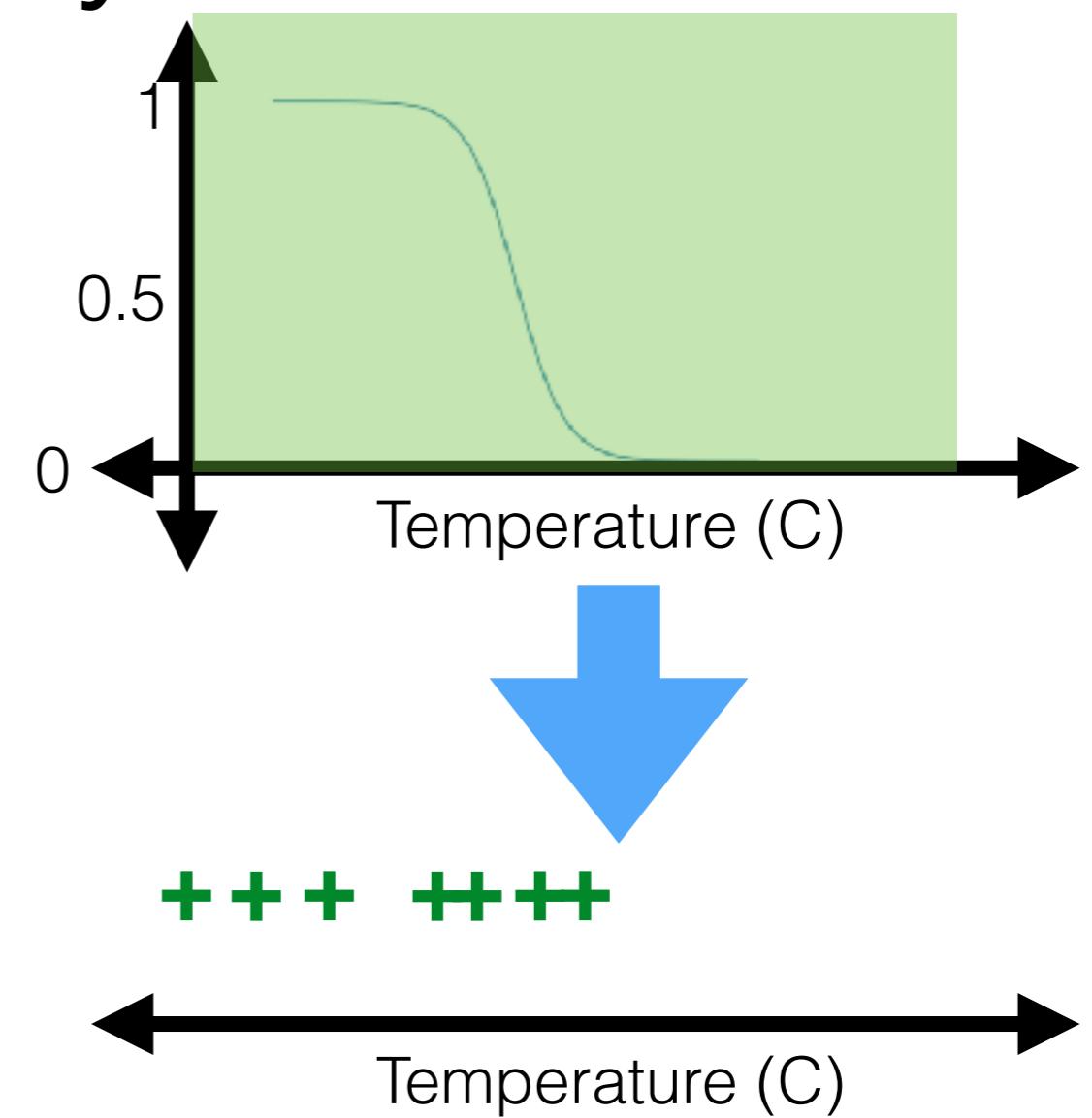


- How to make this shape?

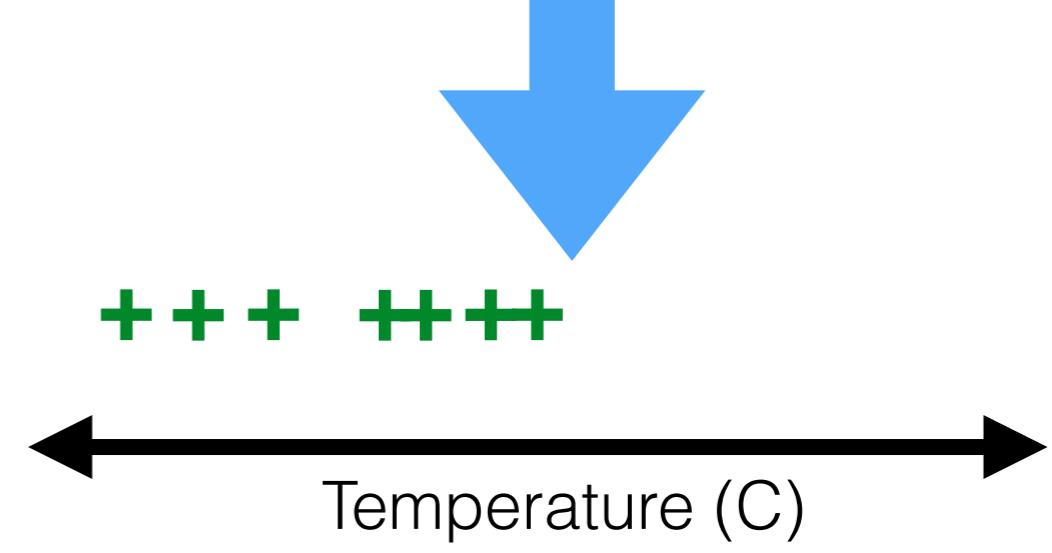
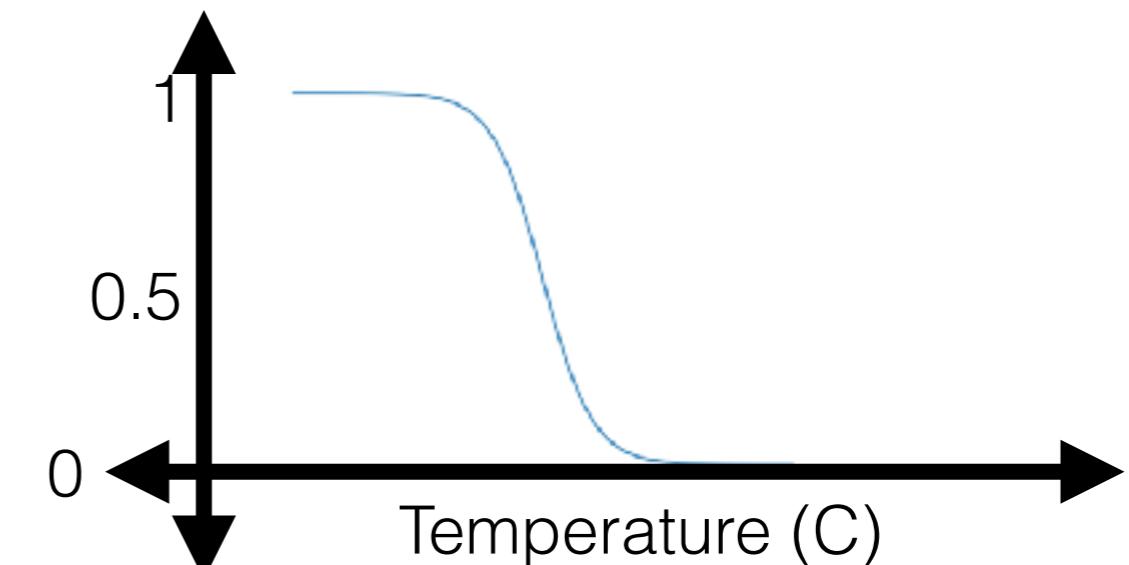
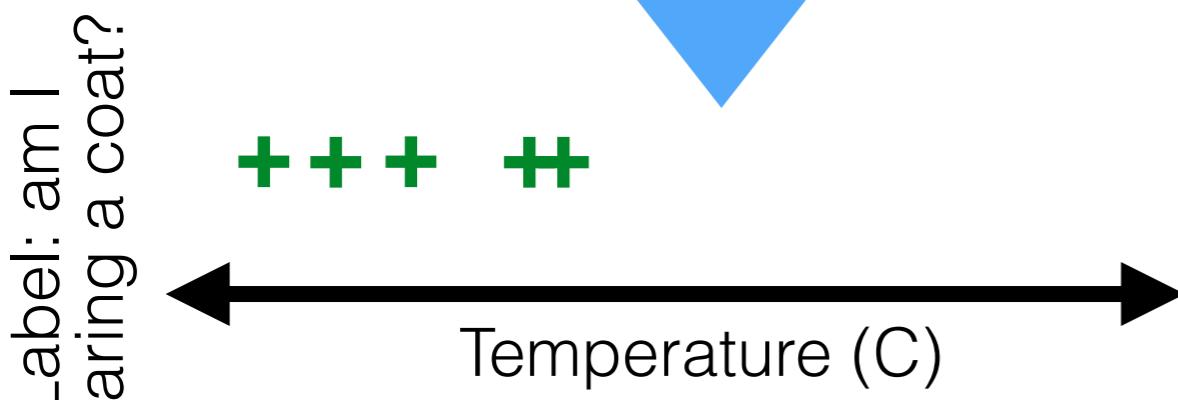
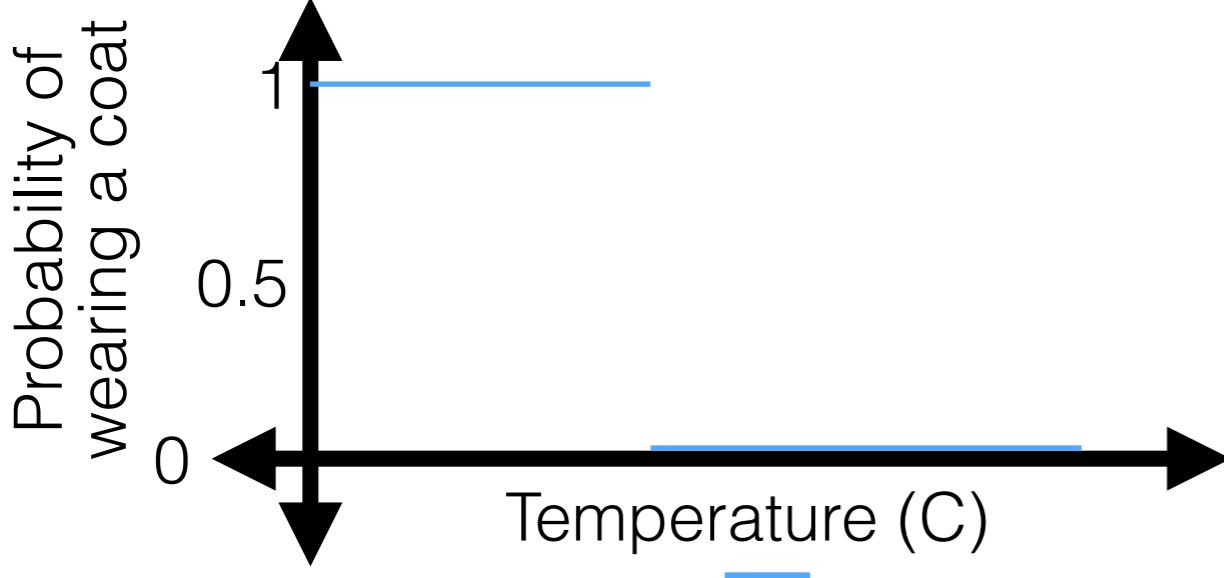
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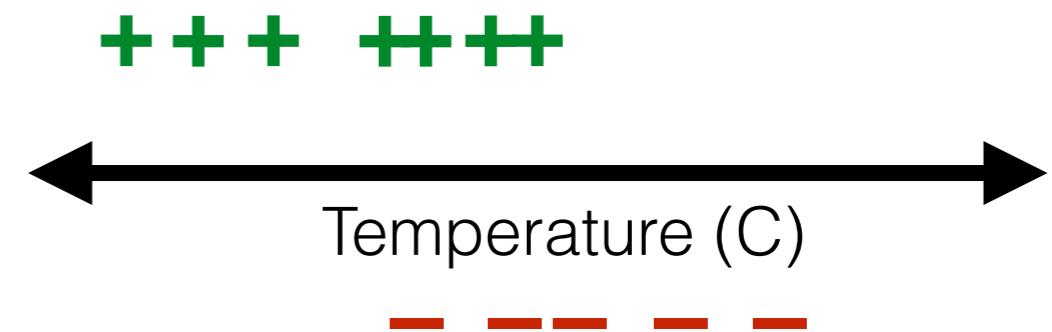
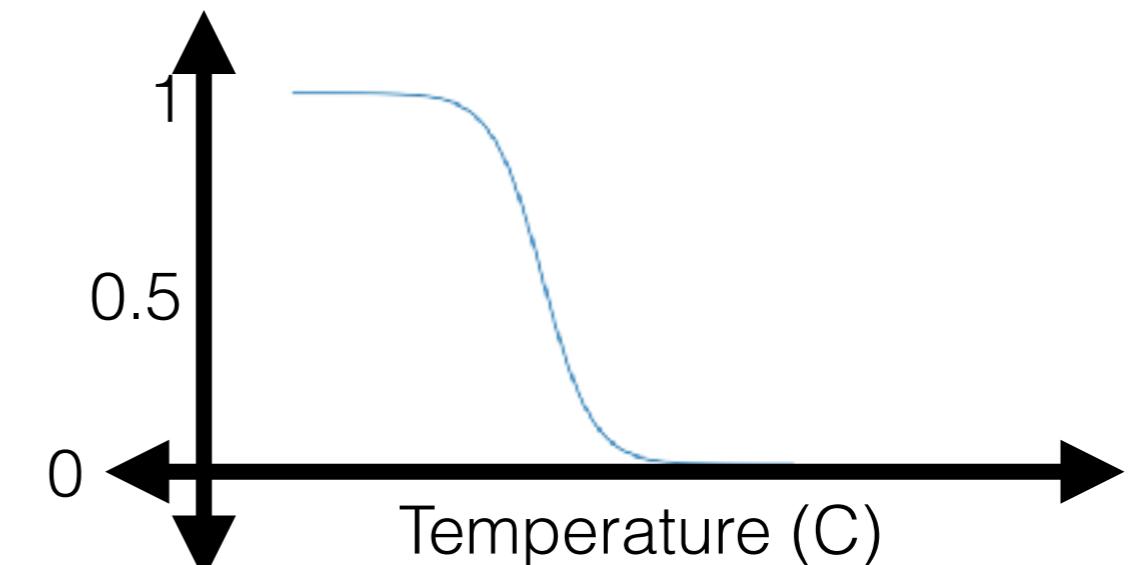
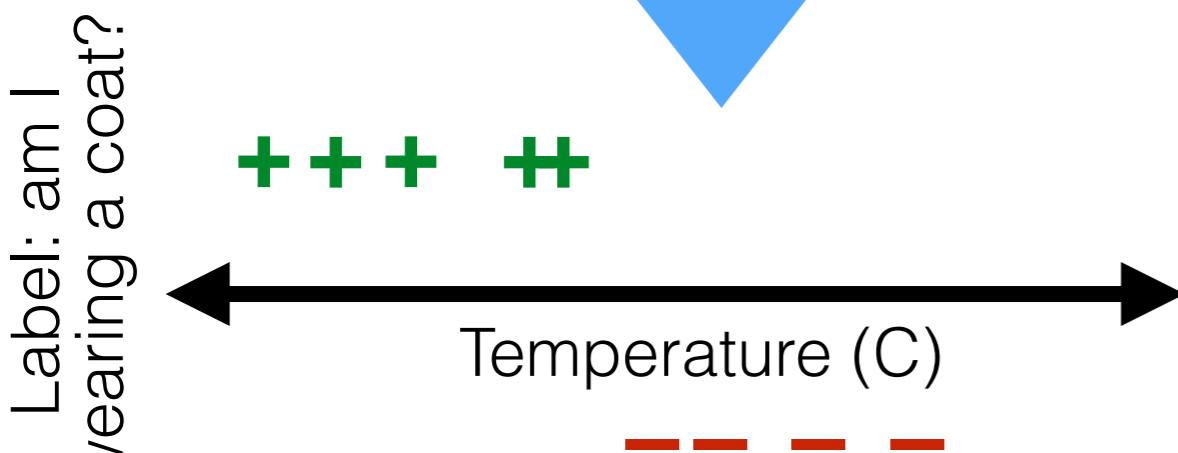
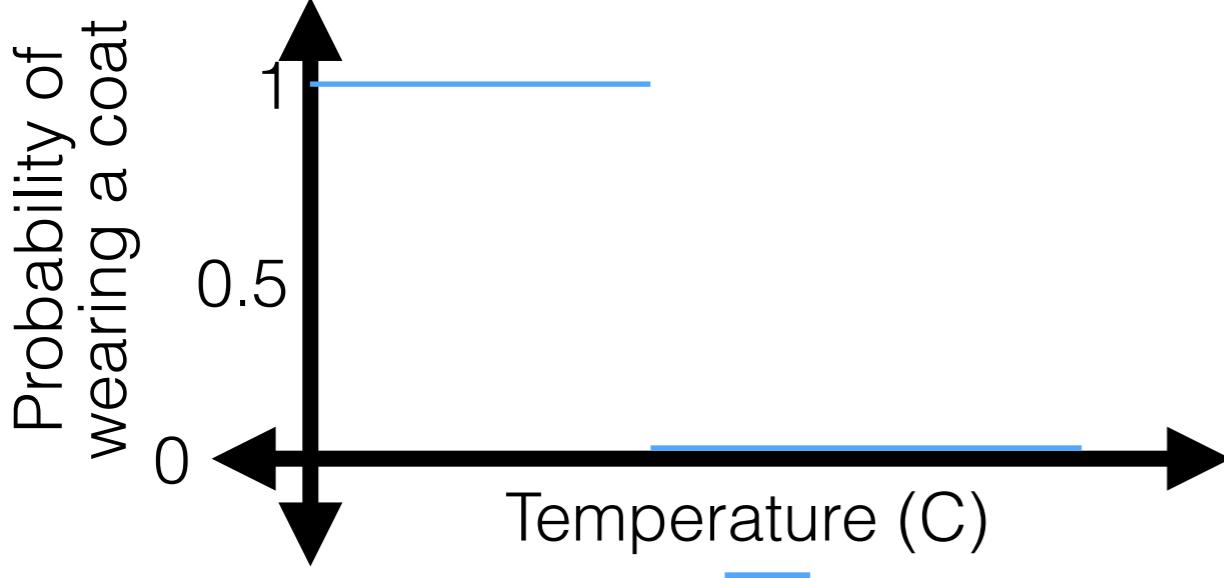


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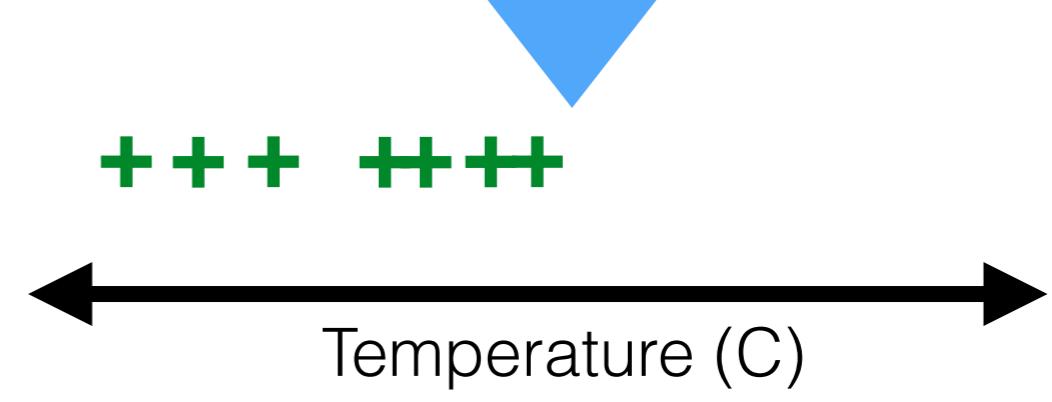
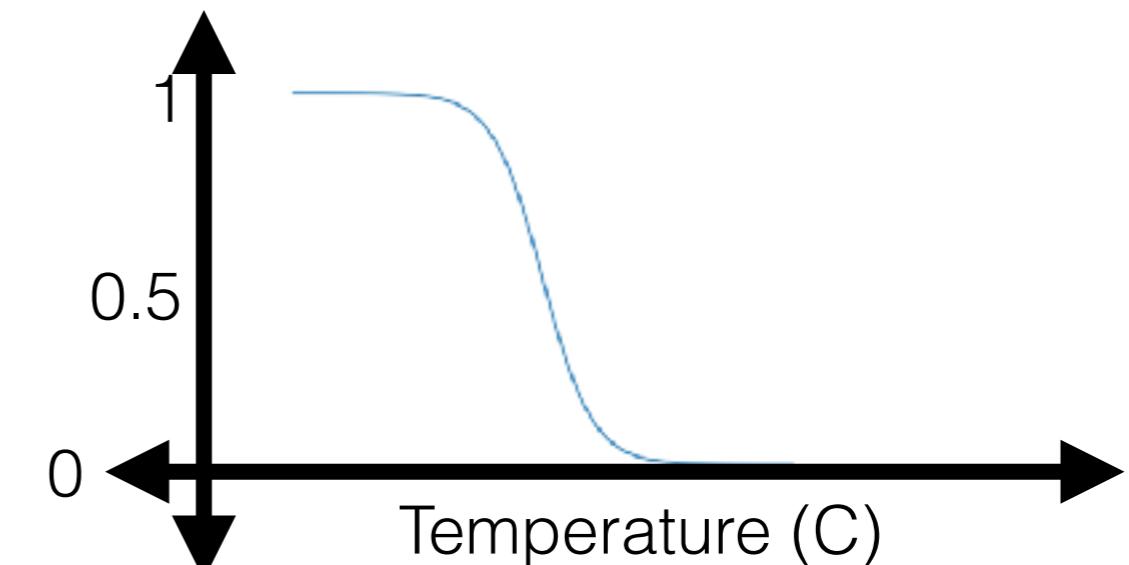
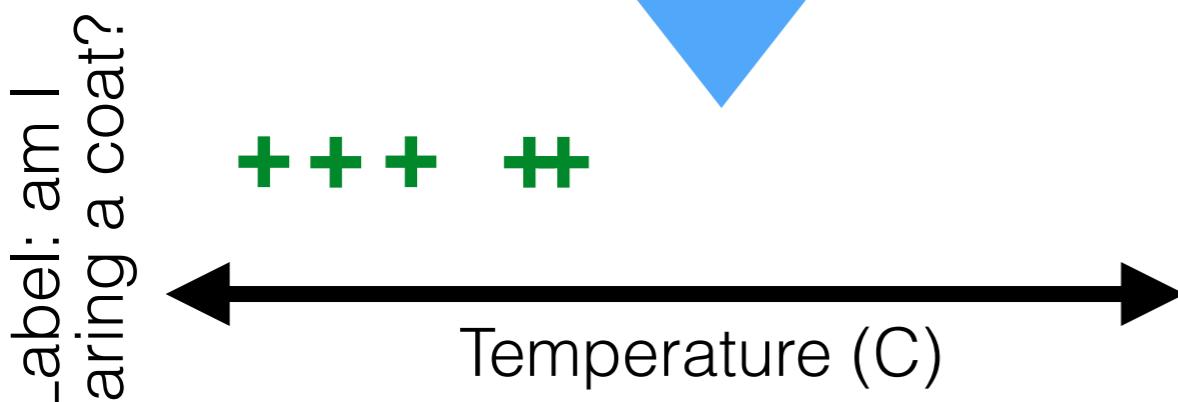
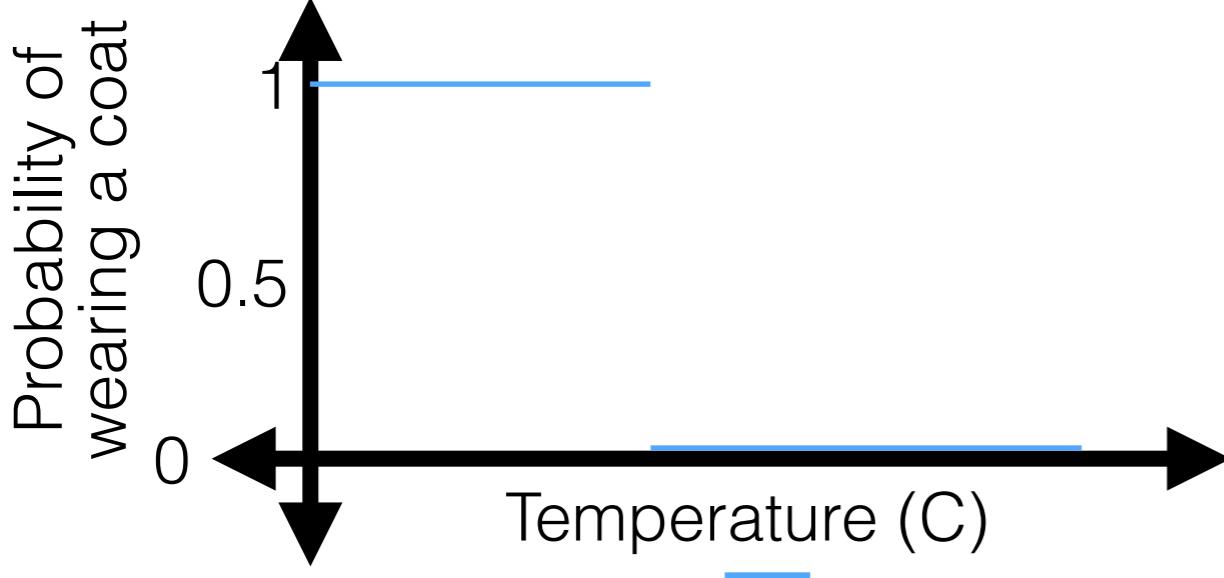
- How to make this shape?

# Capturing uncertainty



- How to make this shape?
  - Sigmoid/logistic function

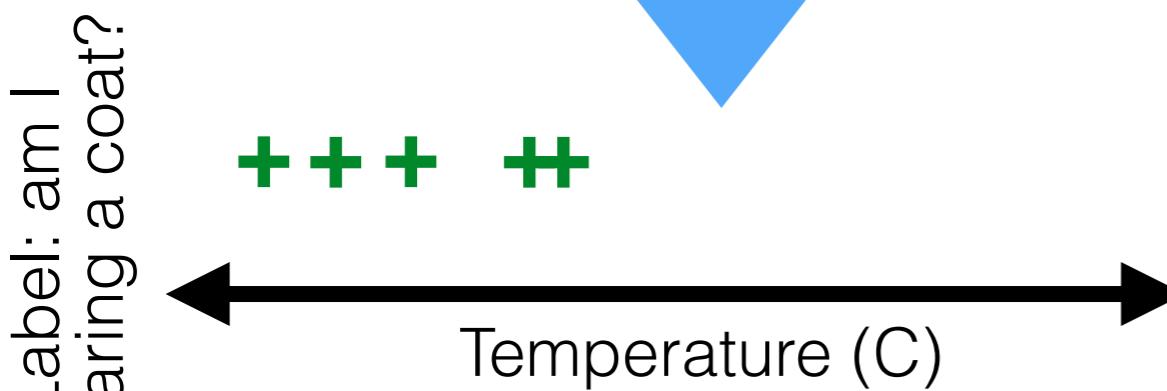
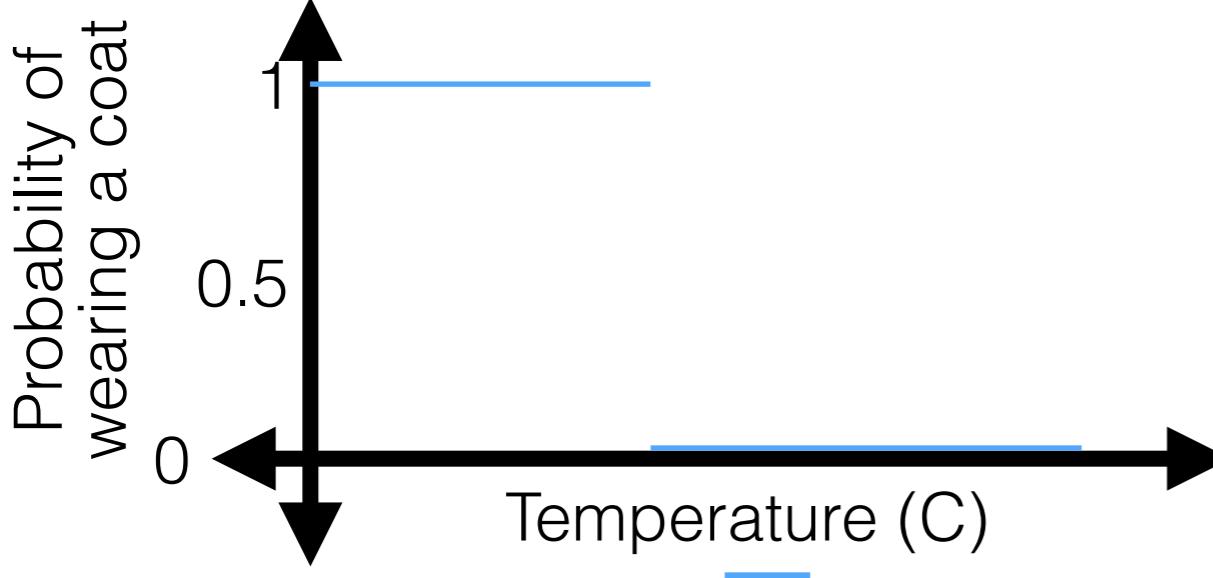
# Capturing uncertainty



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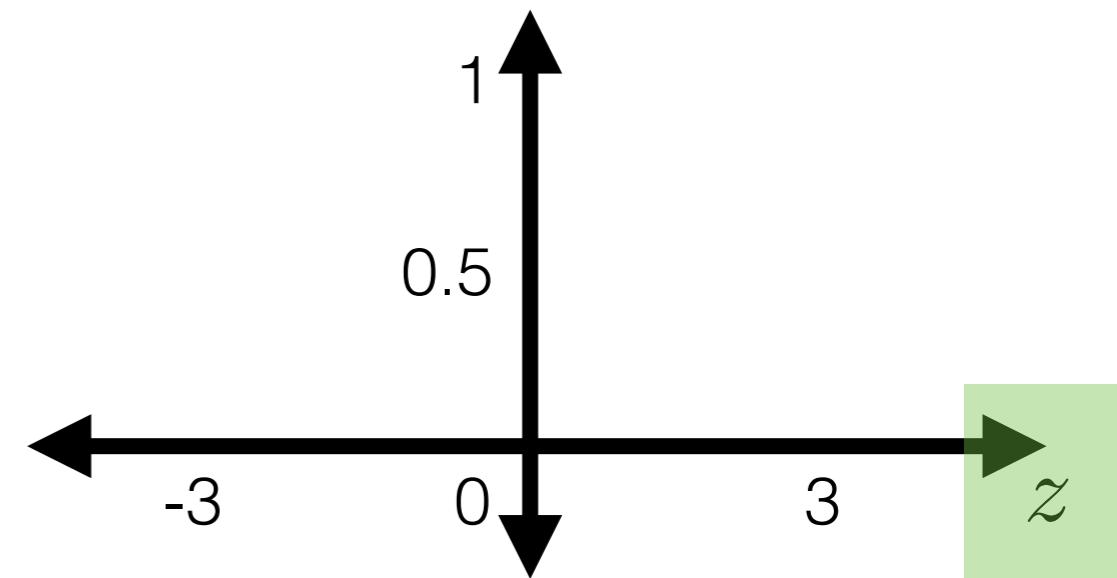
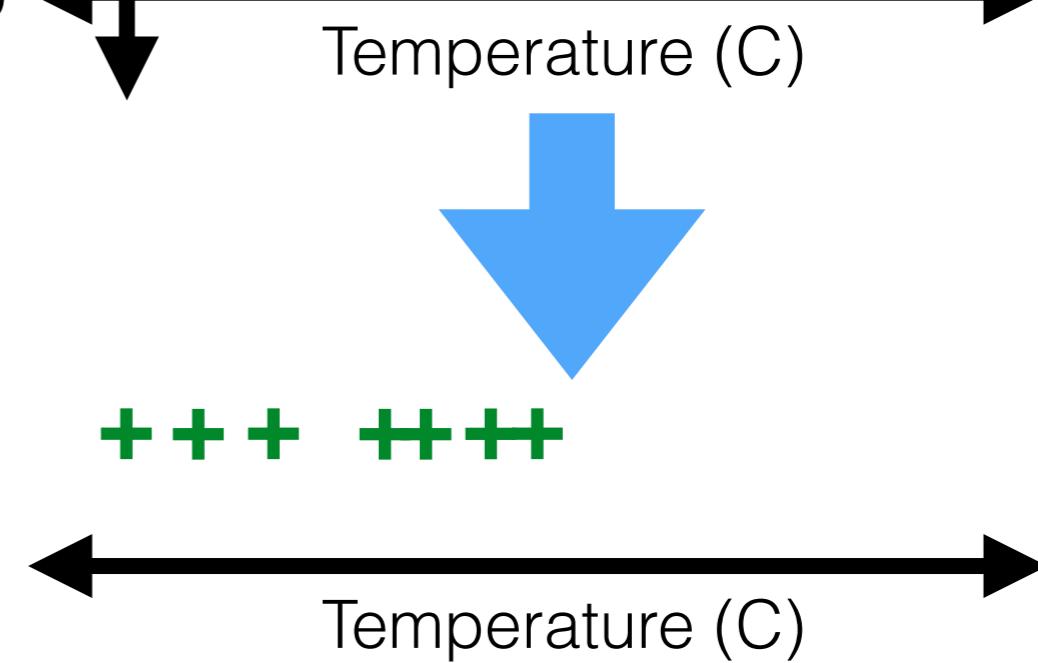
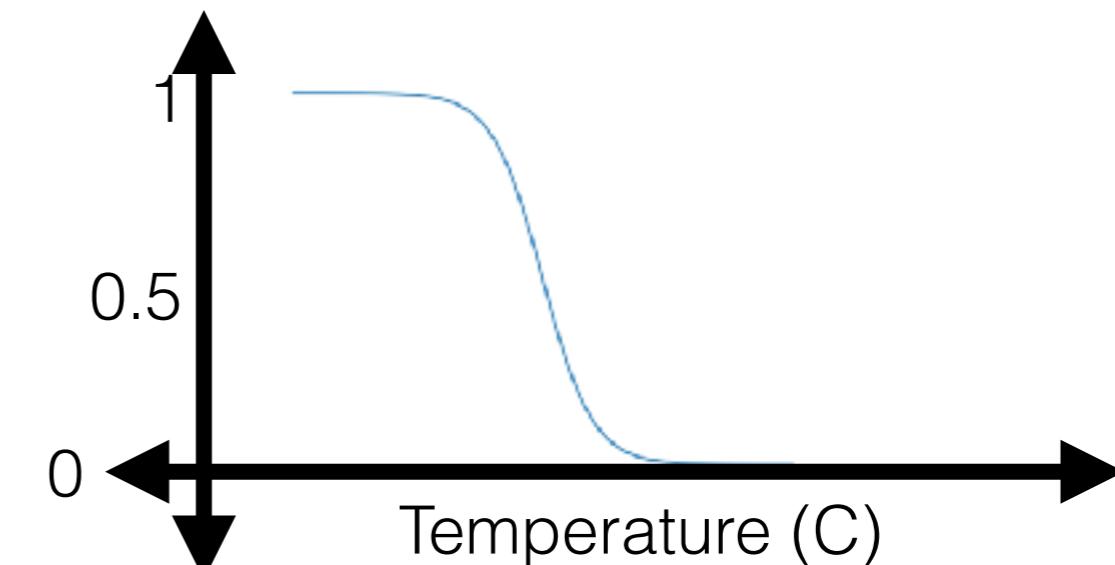
$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$

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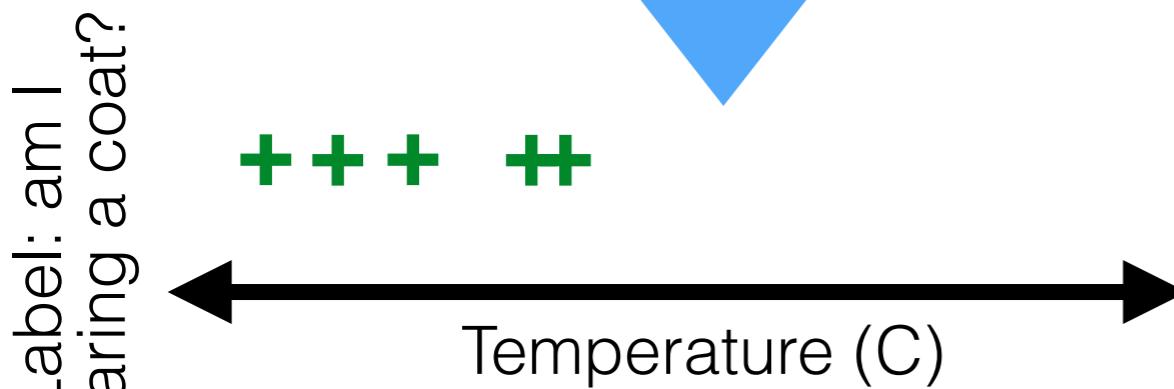
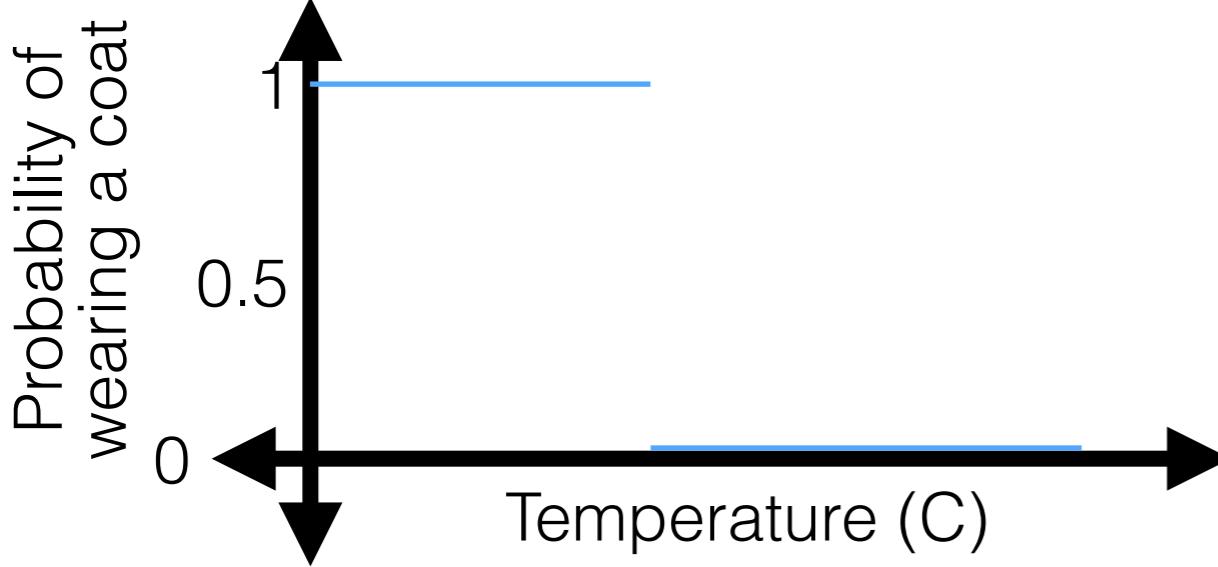


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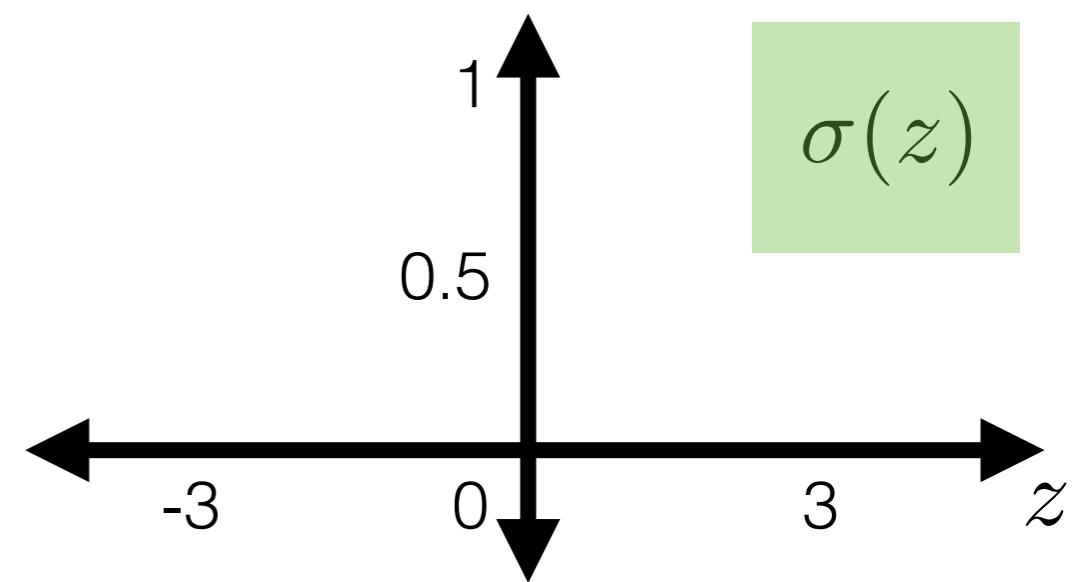
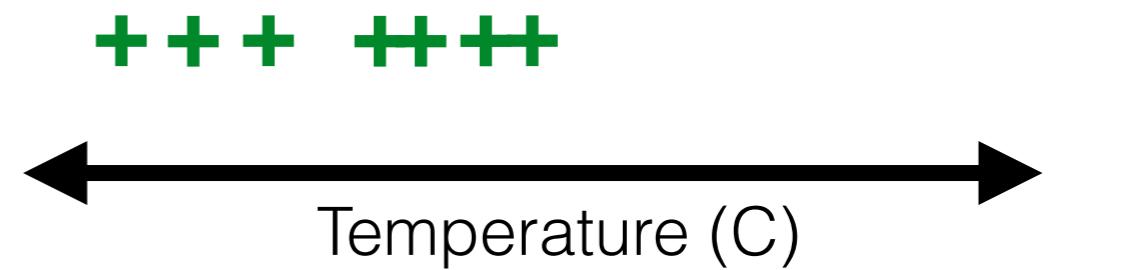
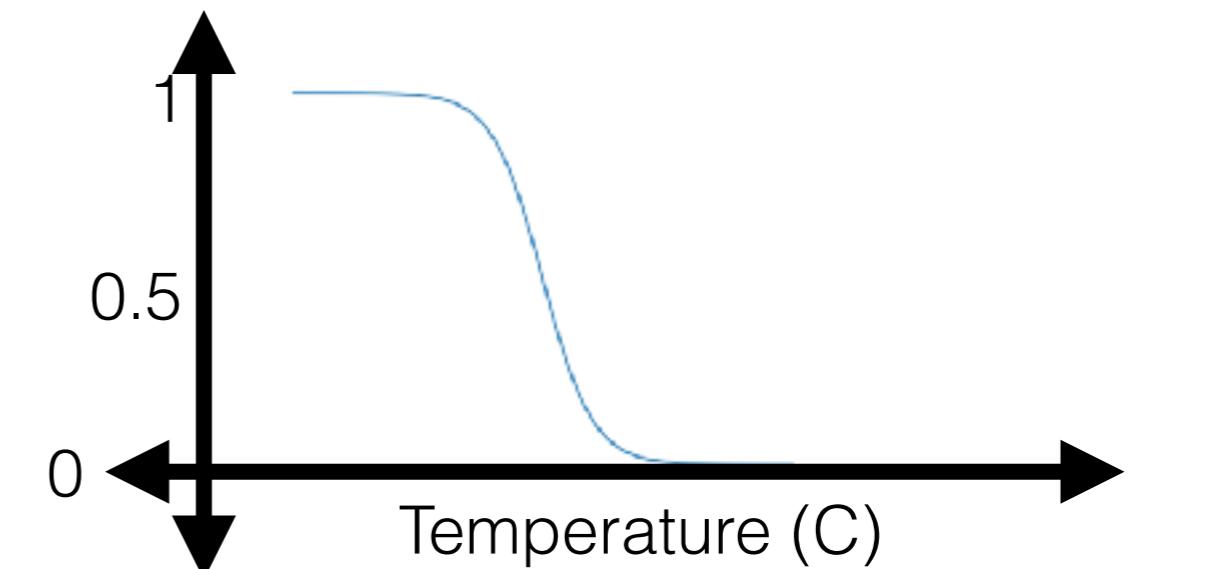


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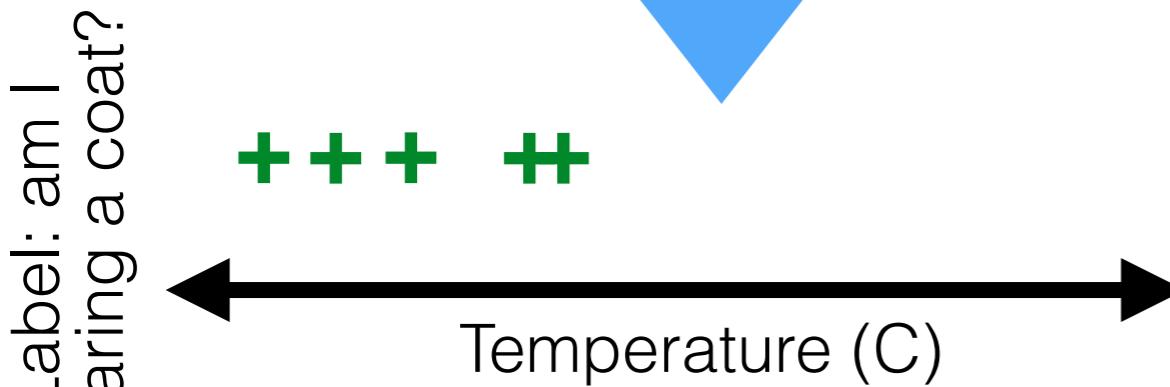
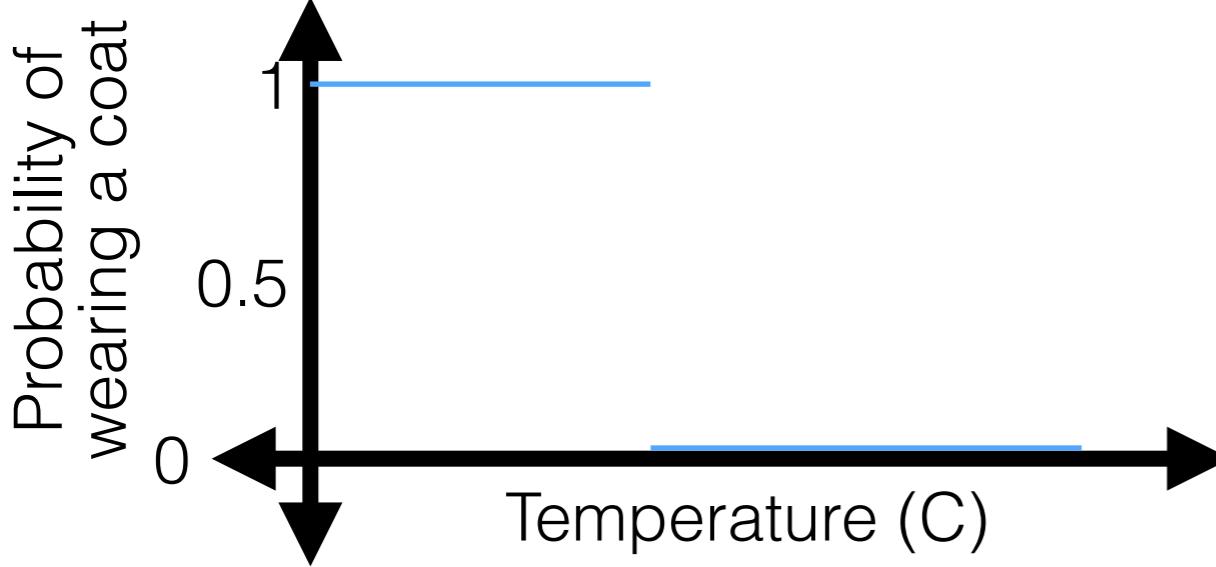


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  - Sigmoid/logistic function

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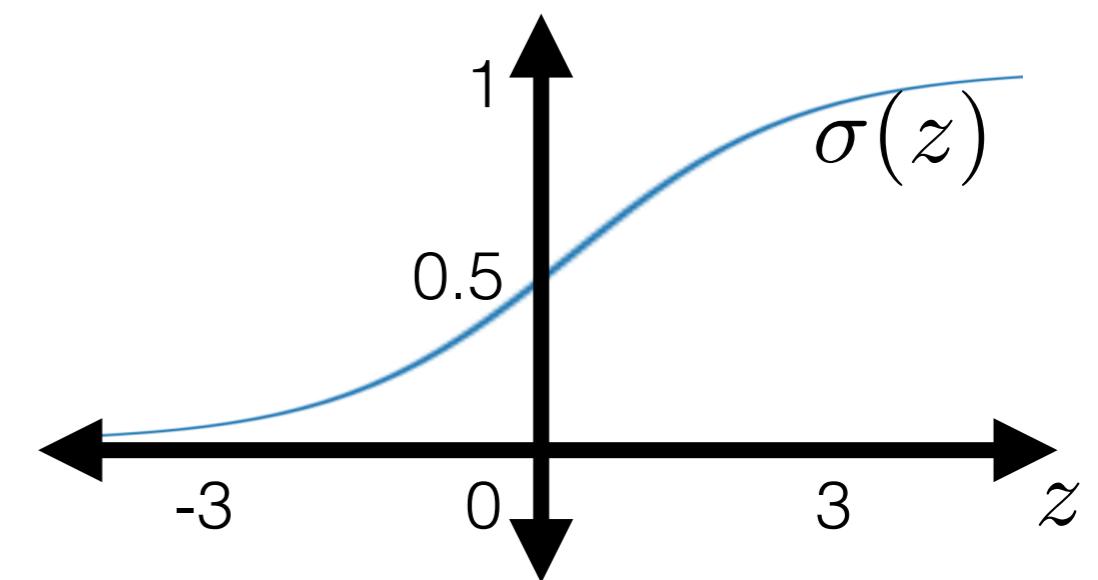
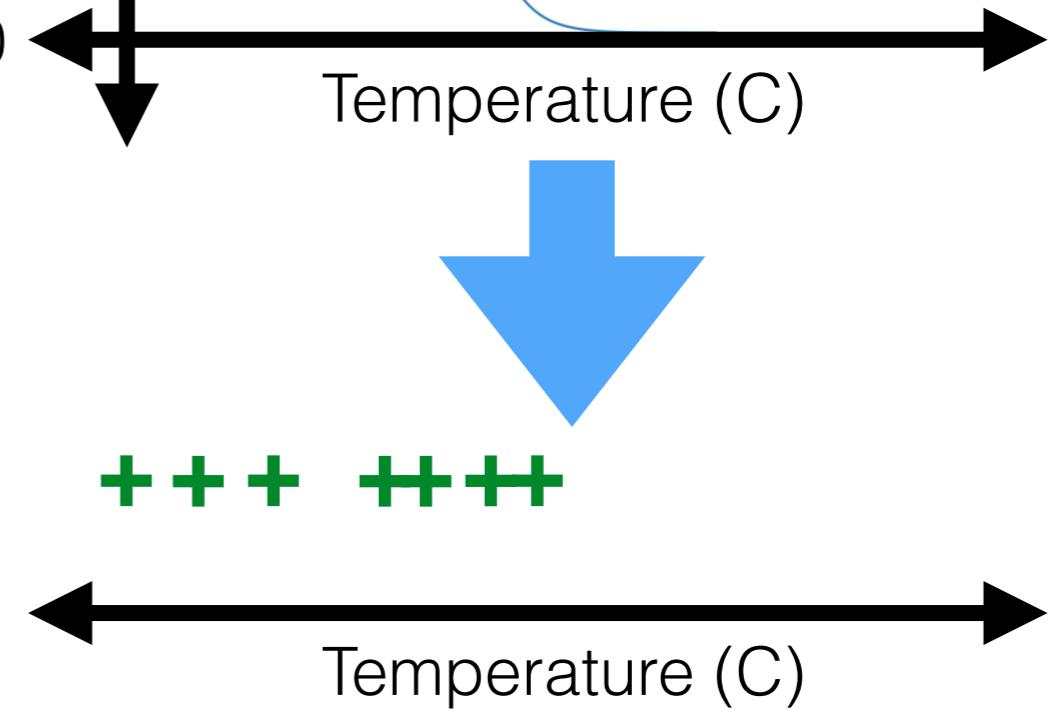
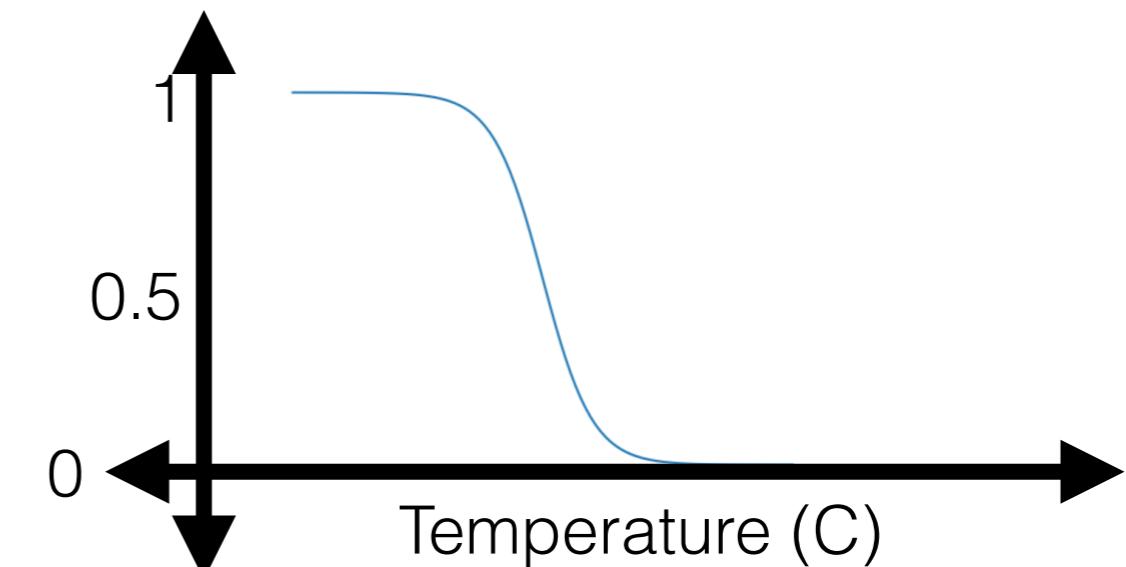


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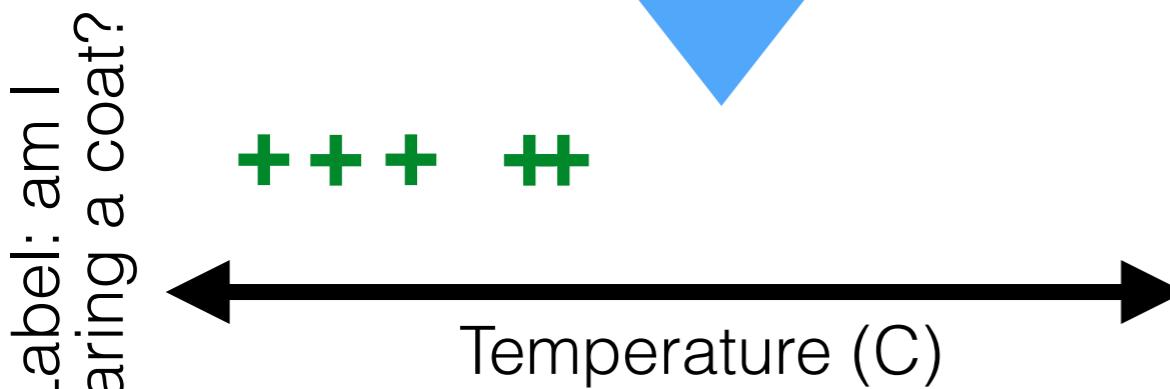
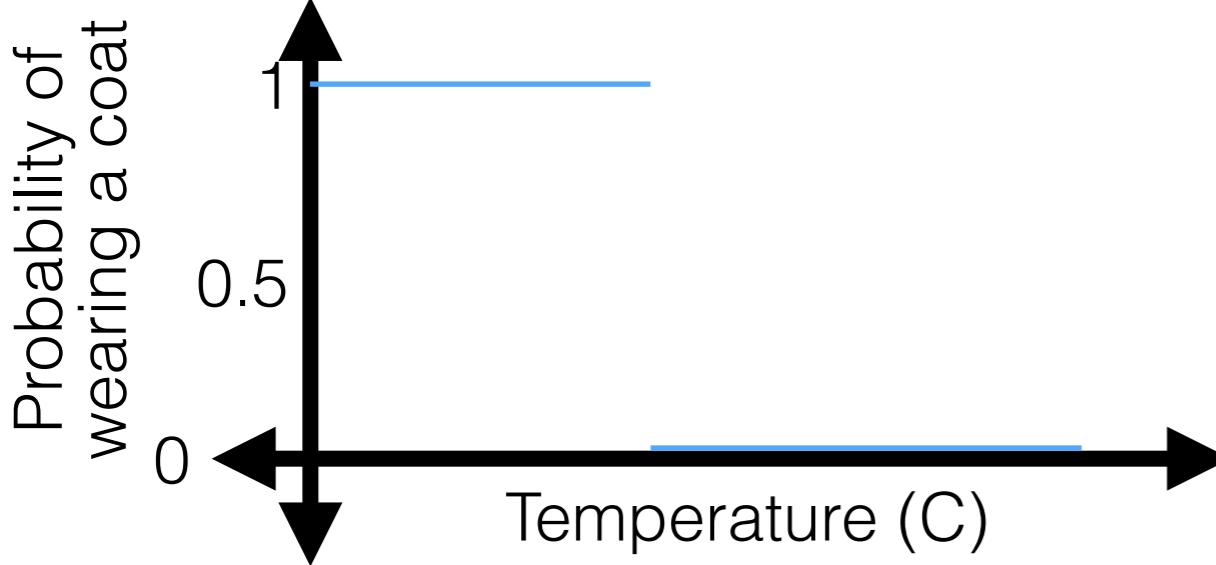


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  - Sigmoid/logistic function

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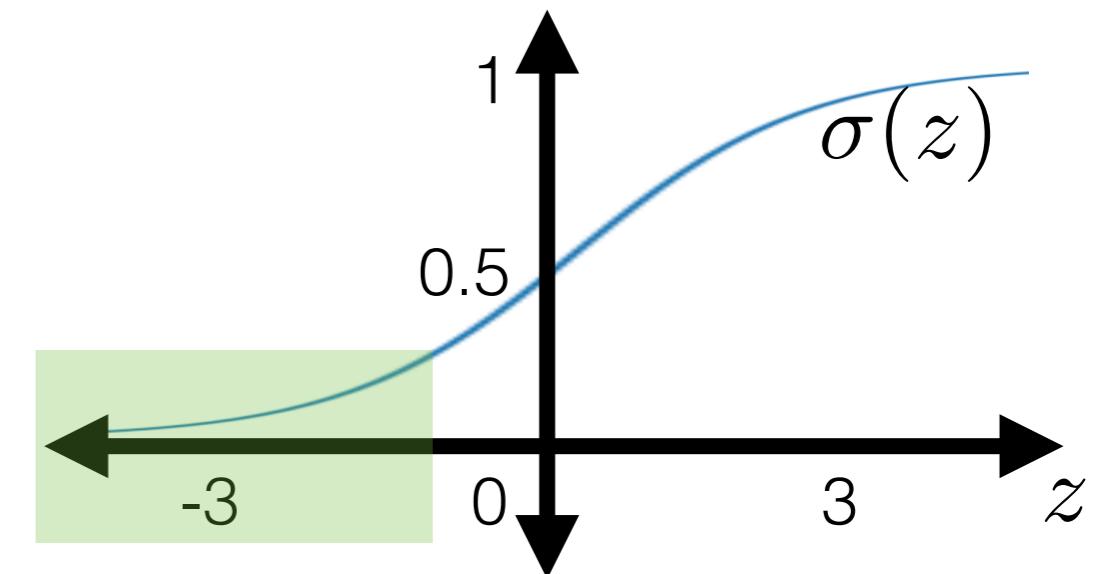
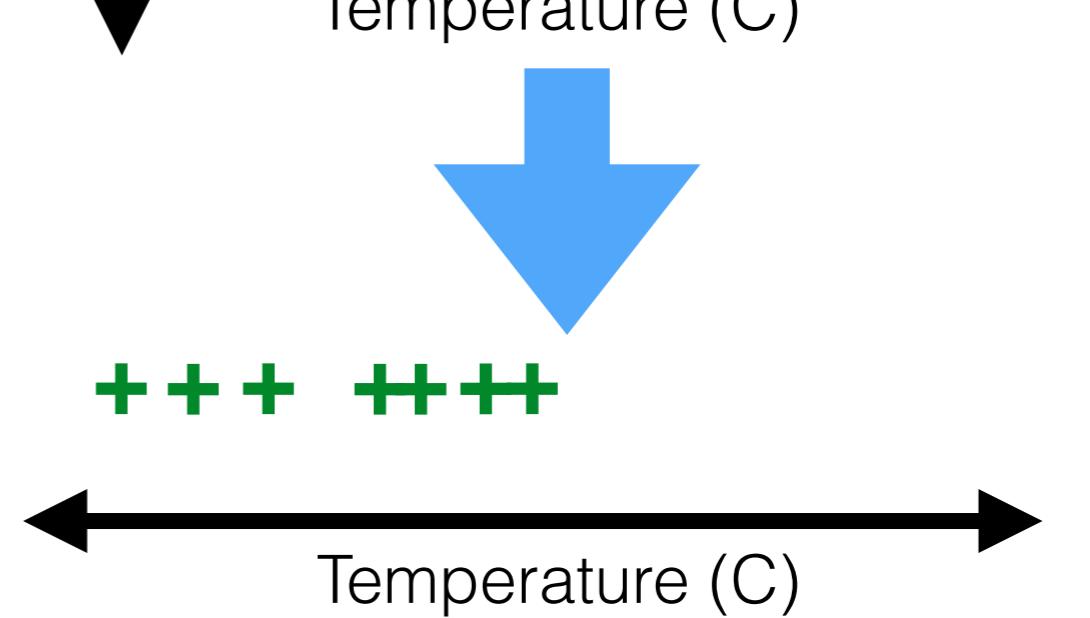
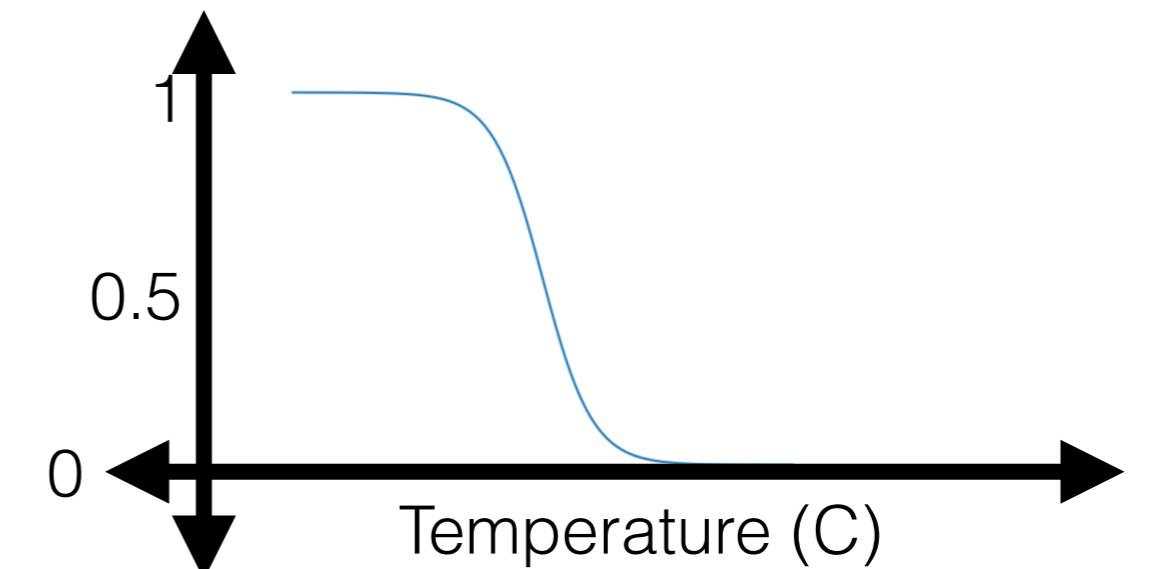


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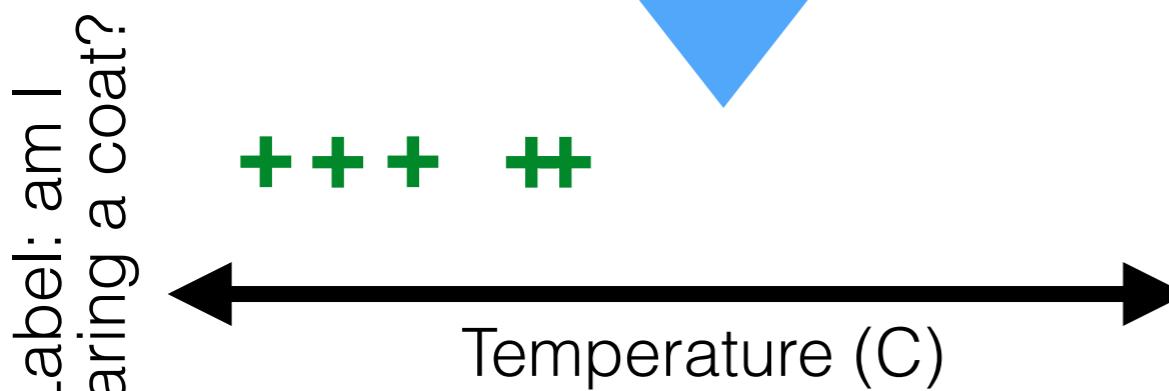
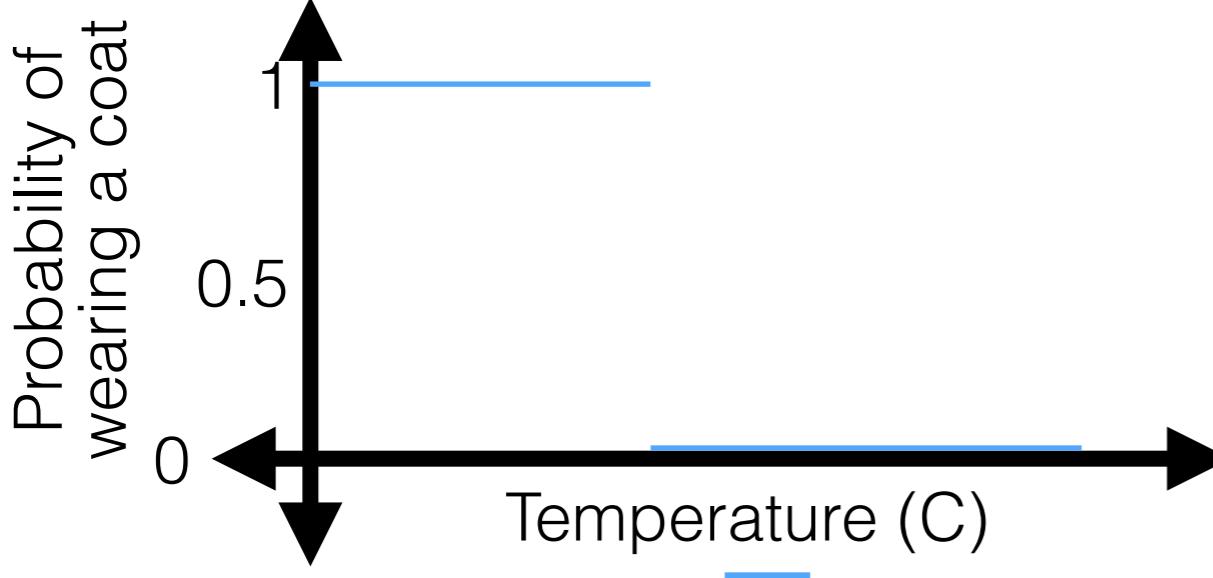


- How to make this shape?
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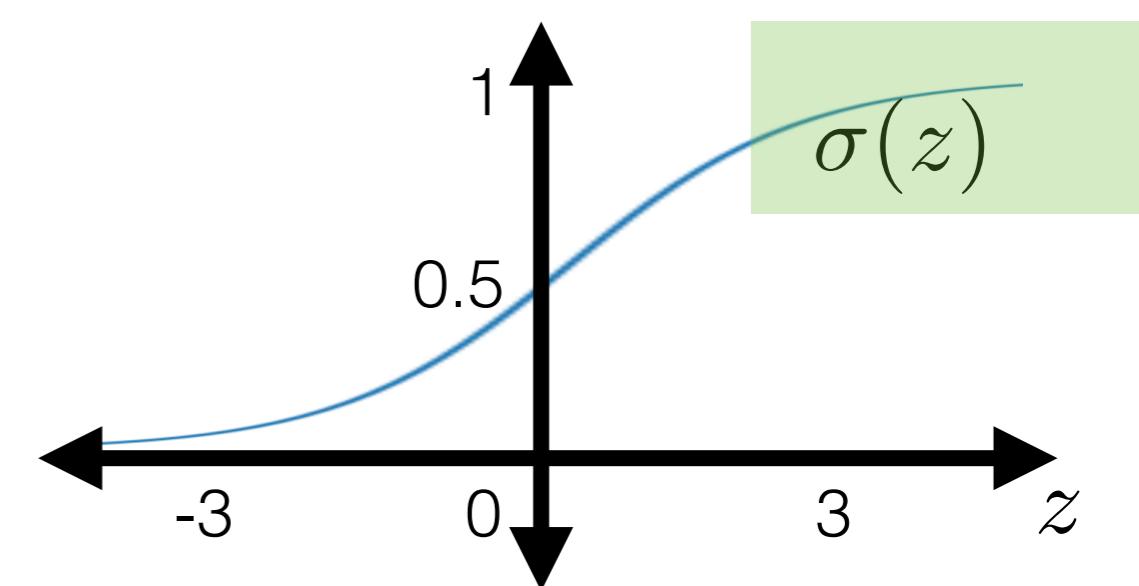
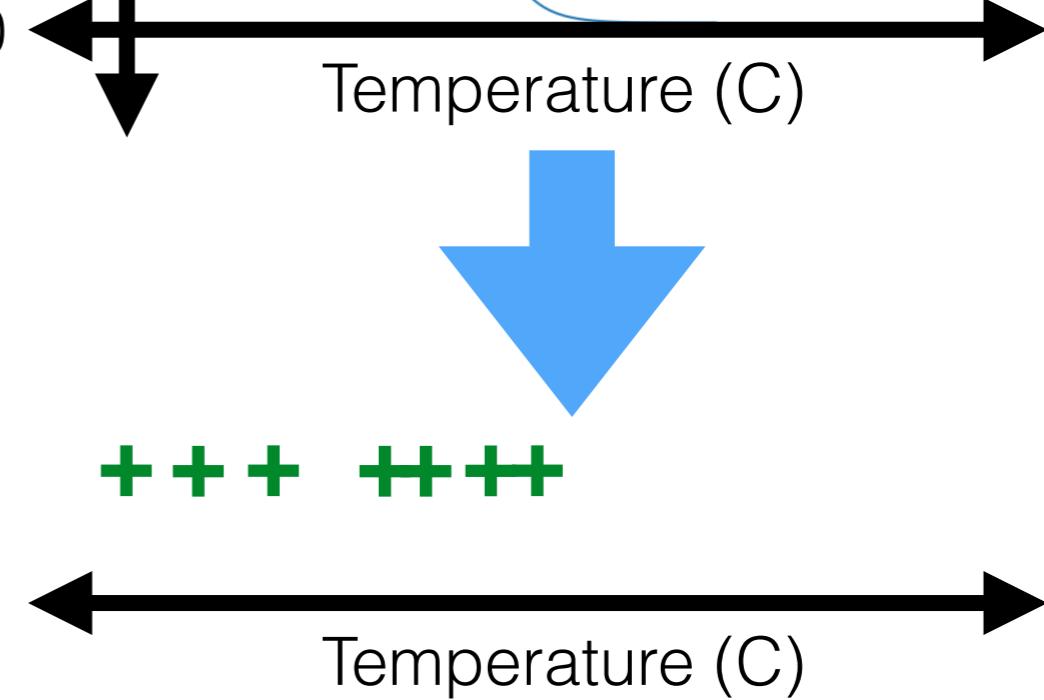
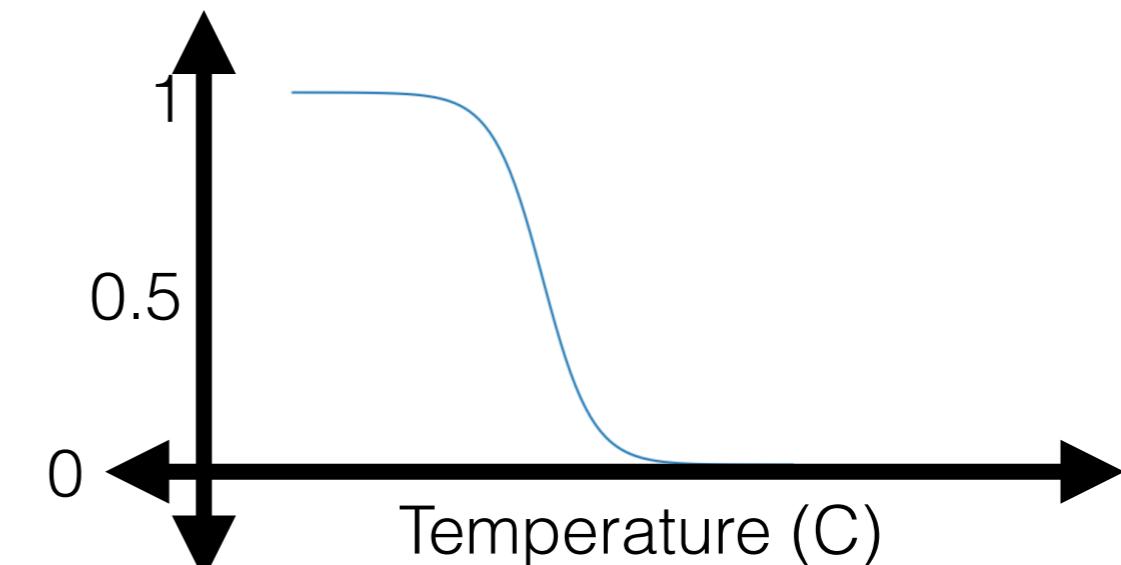


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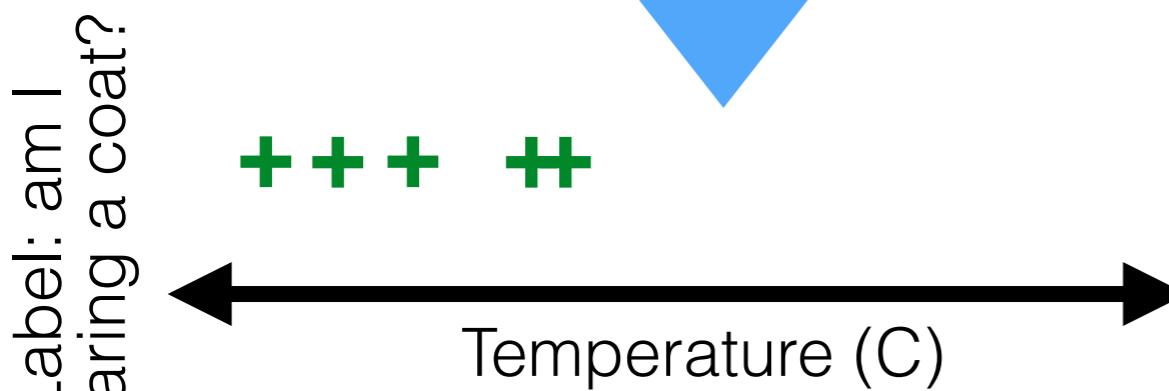
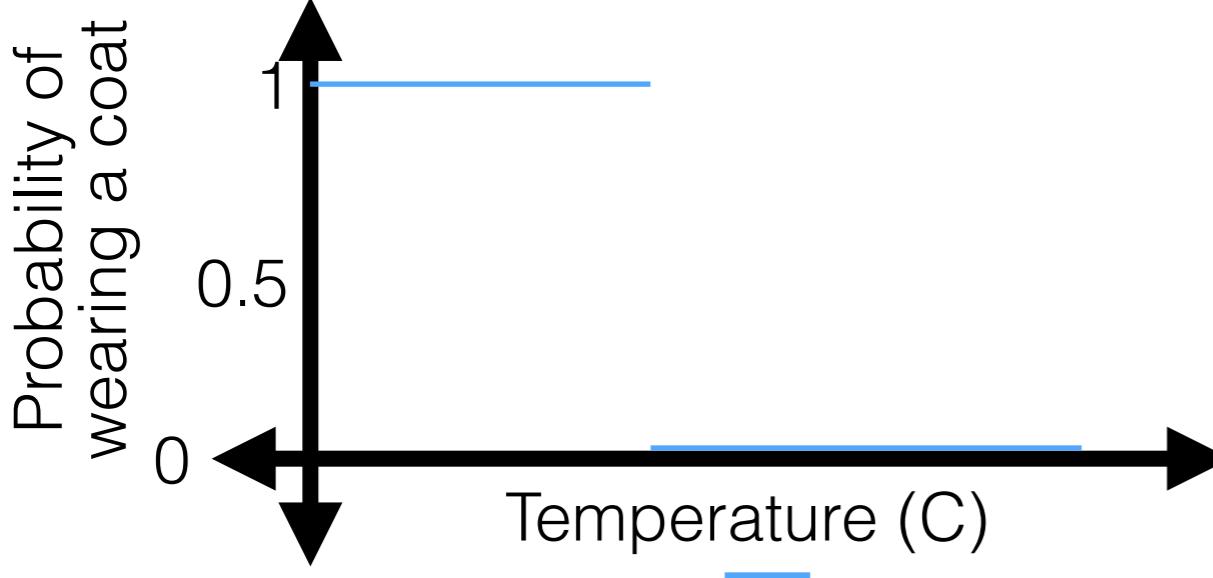


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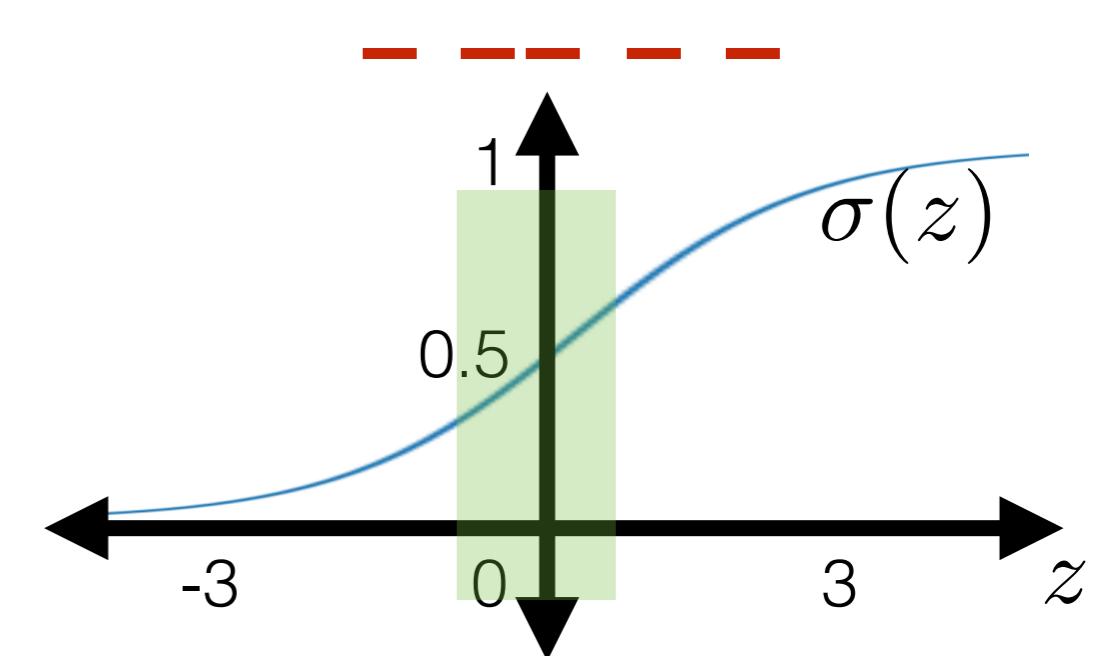
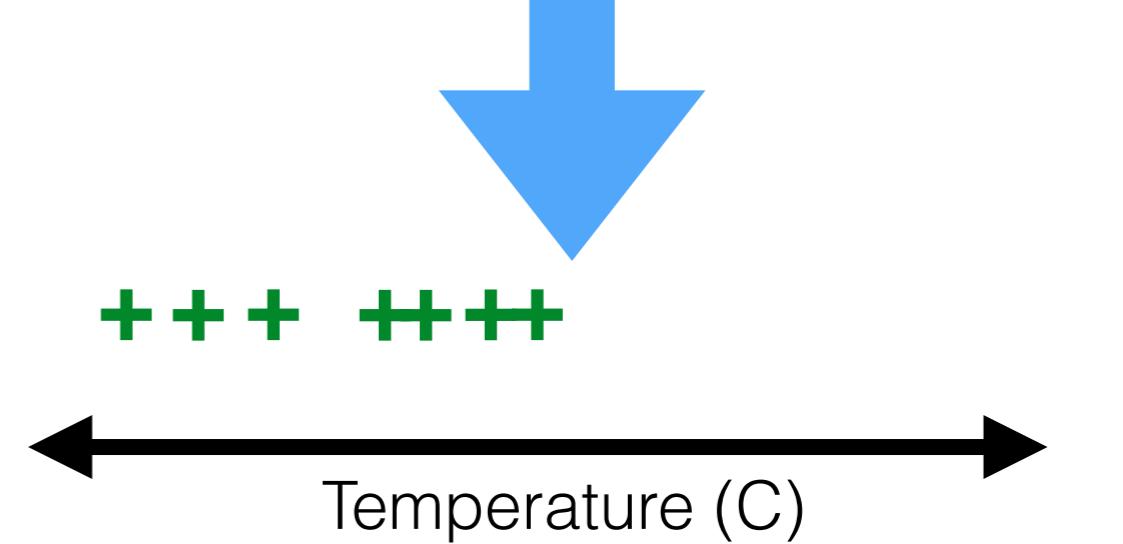
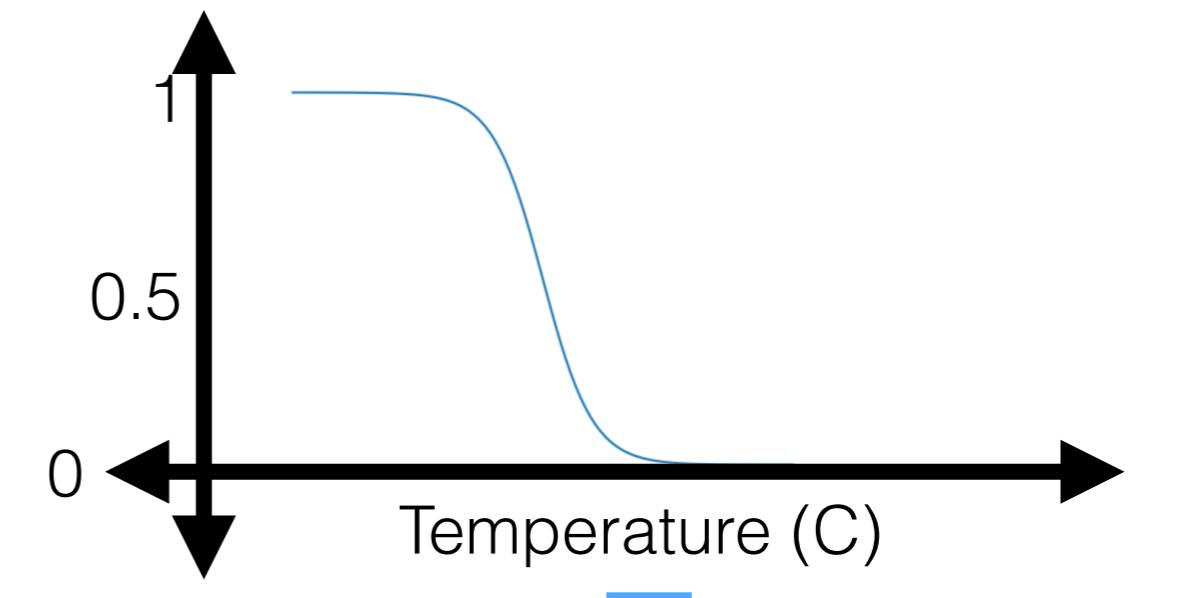


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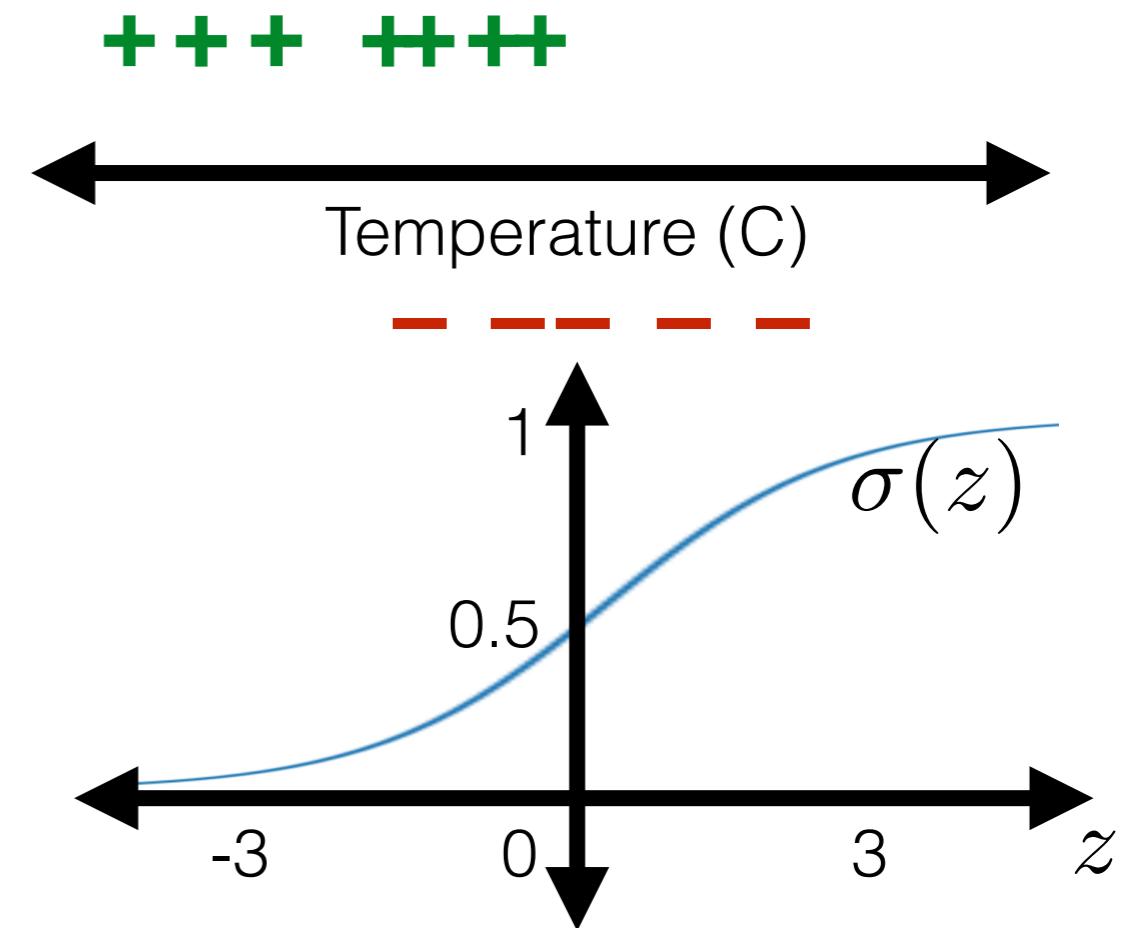
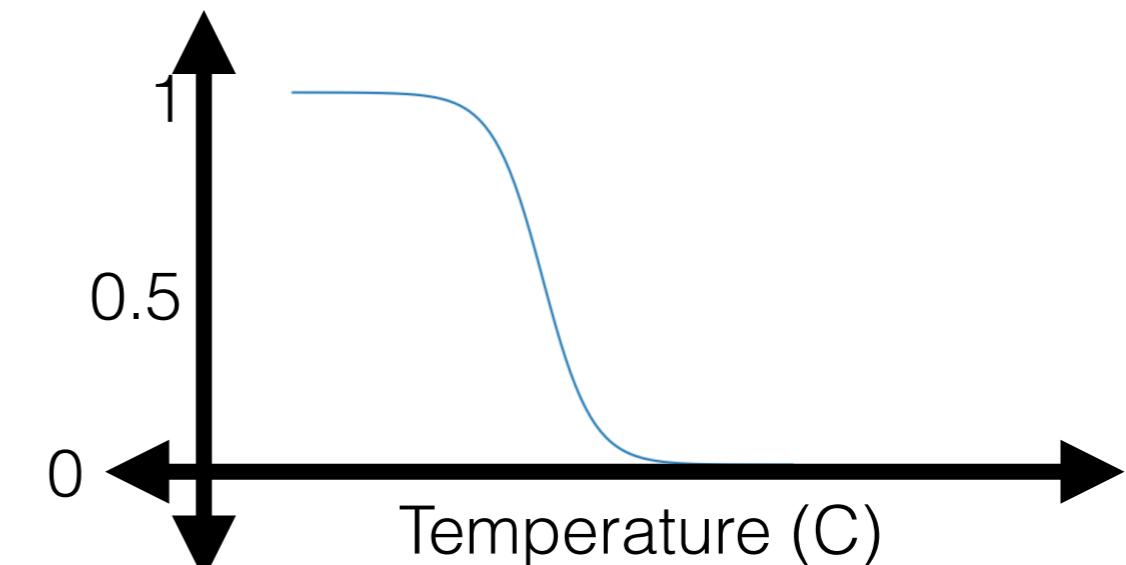
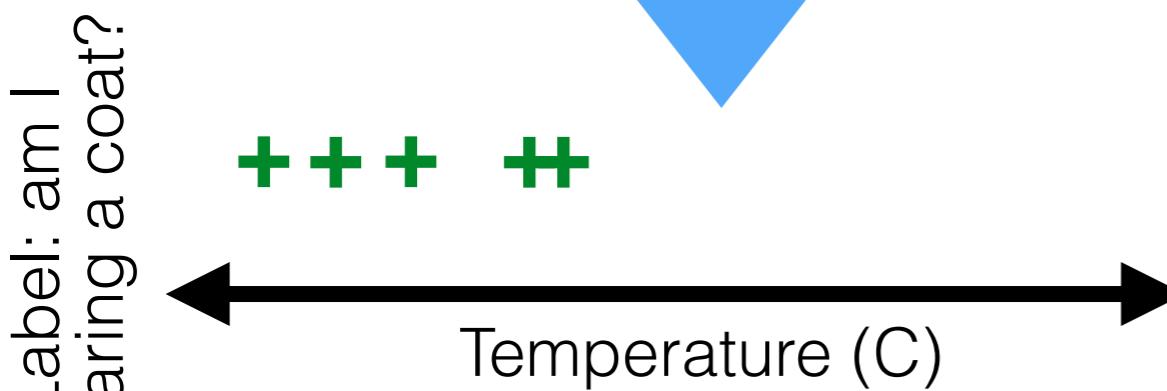
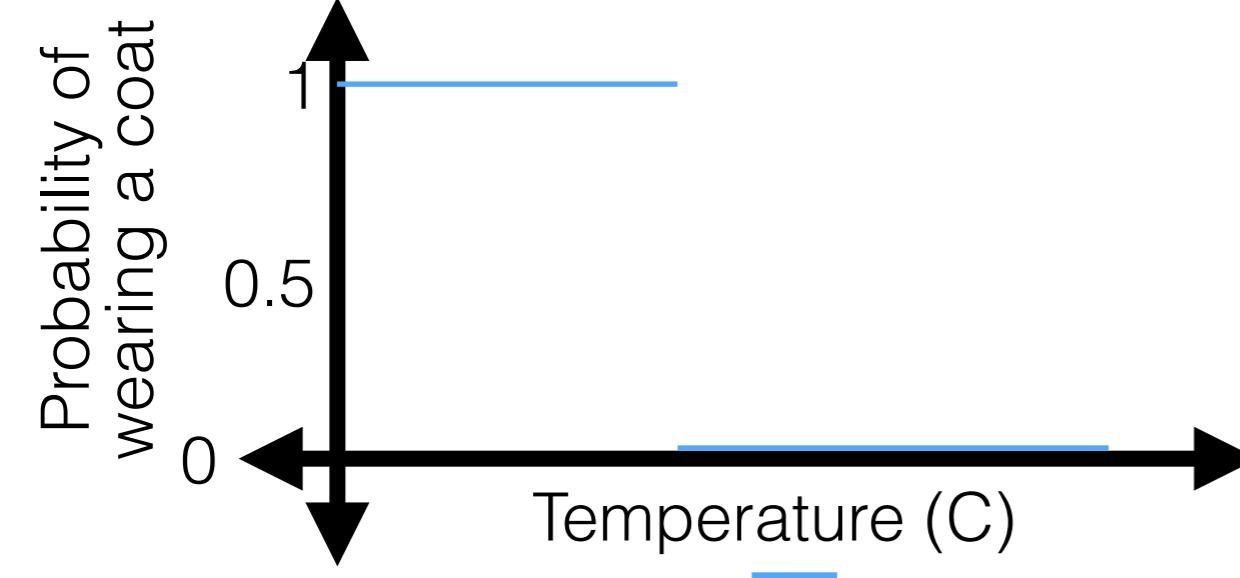


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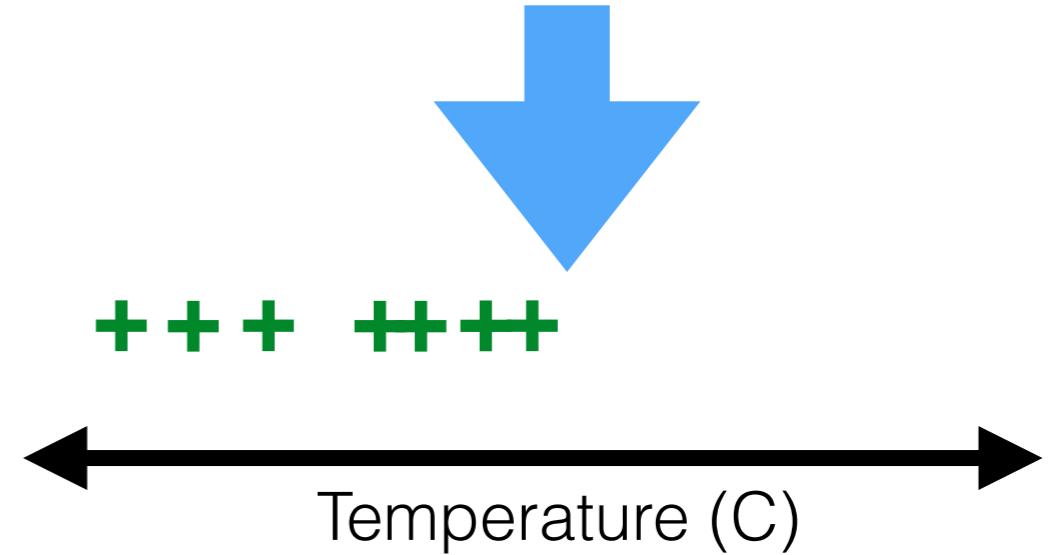
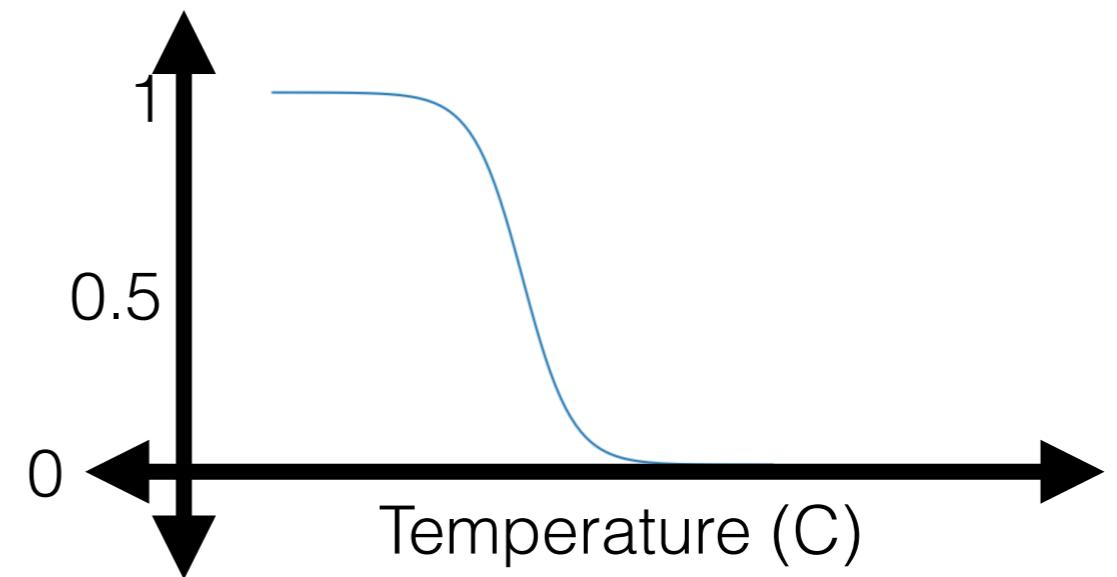
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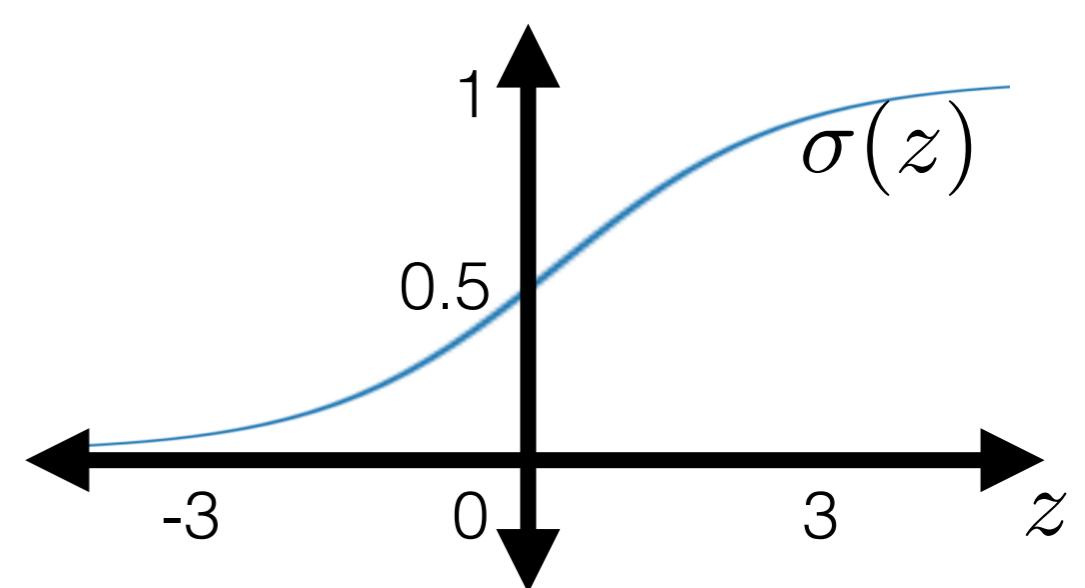
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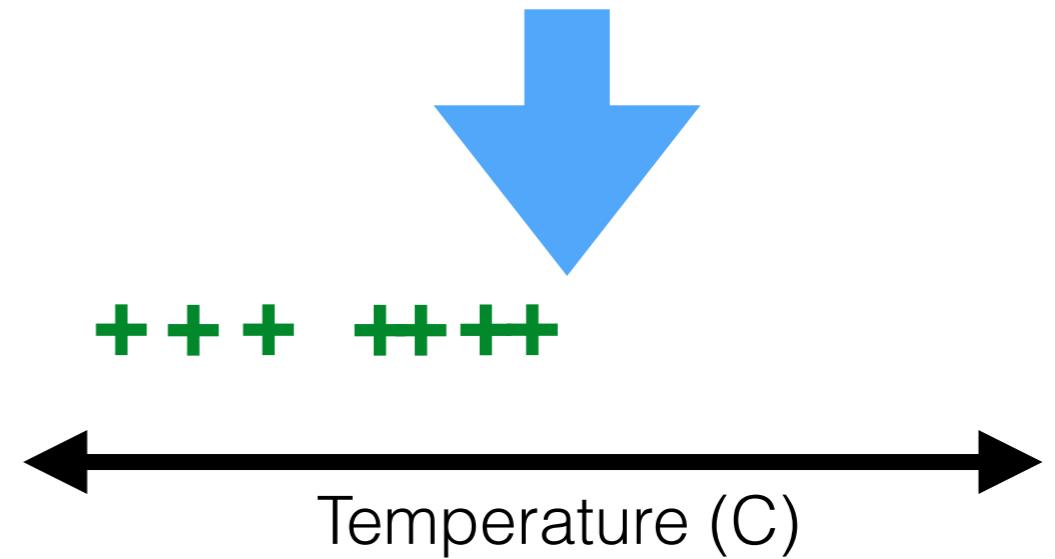
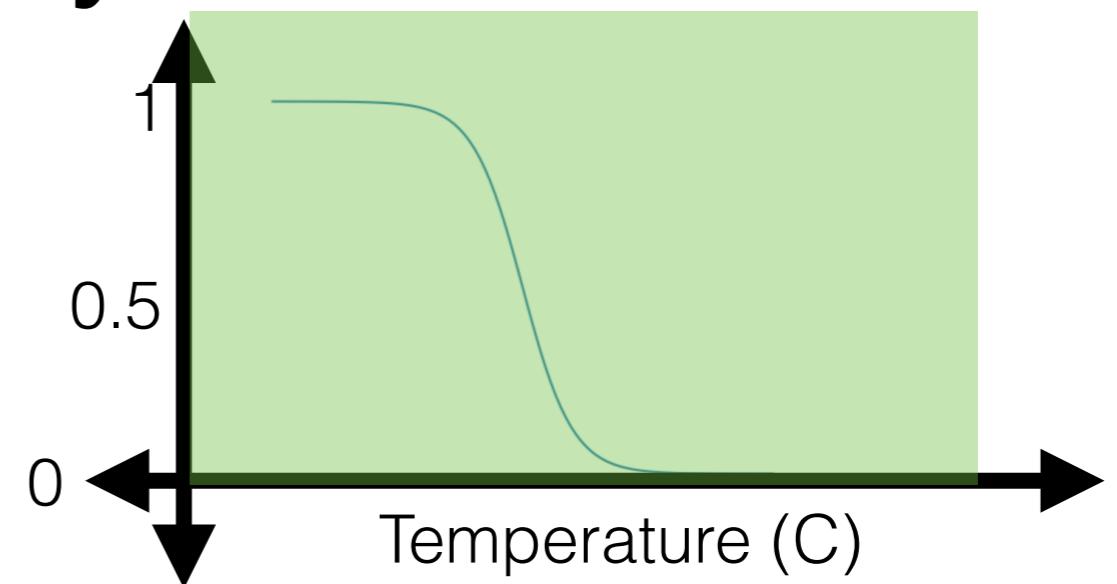


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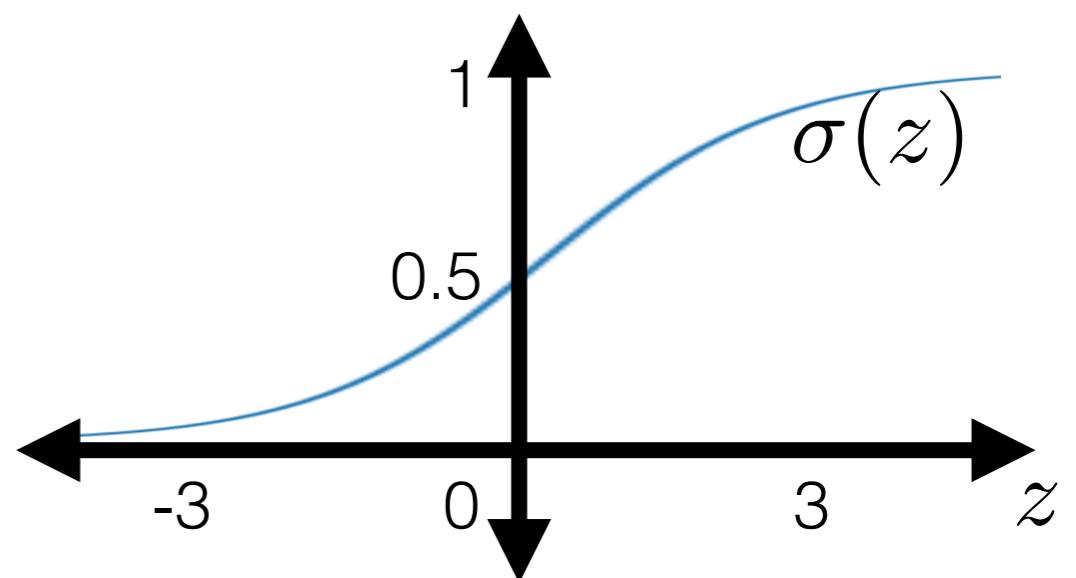


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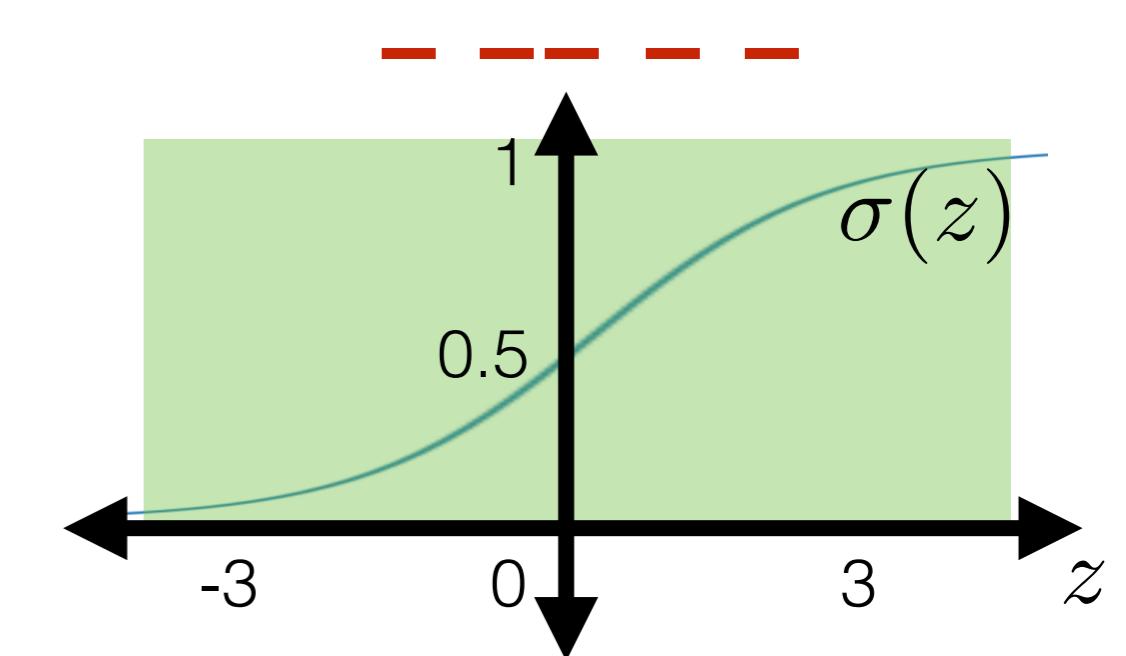
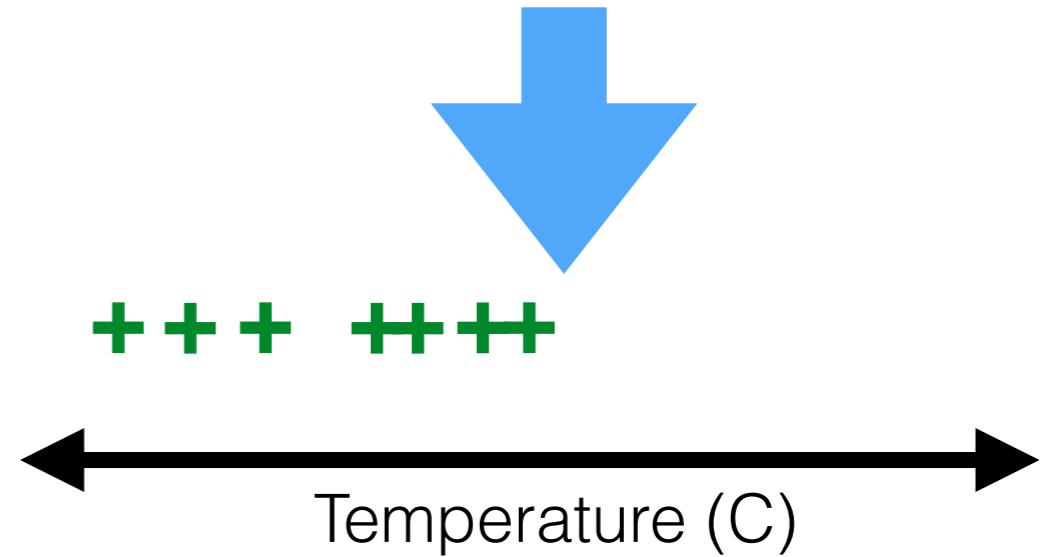
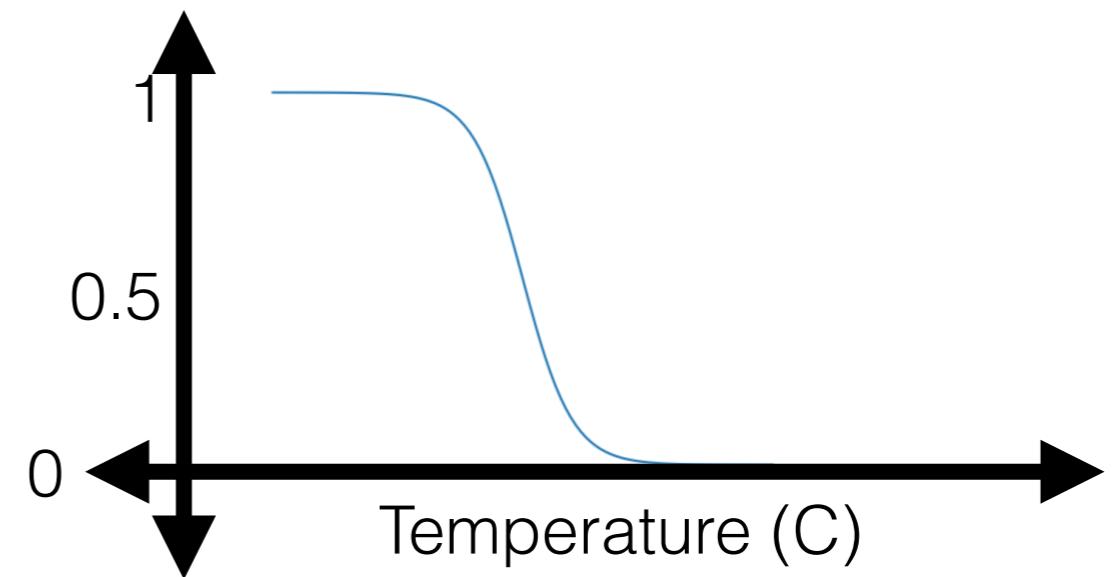


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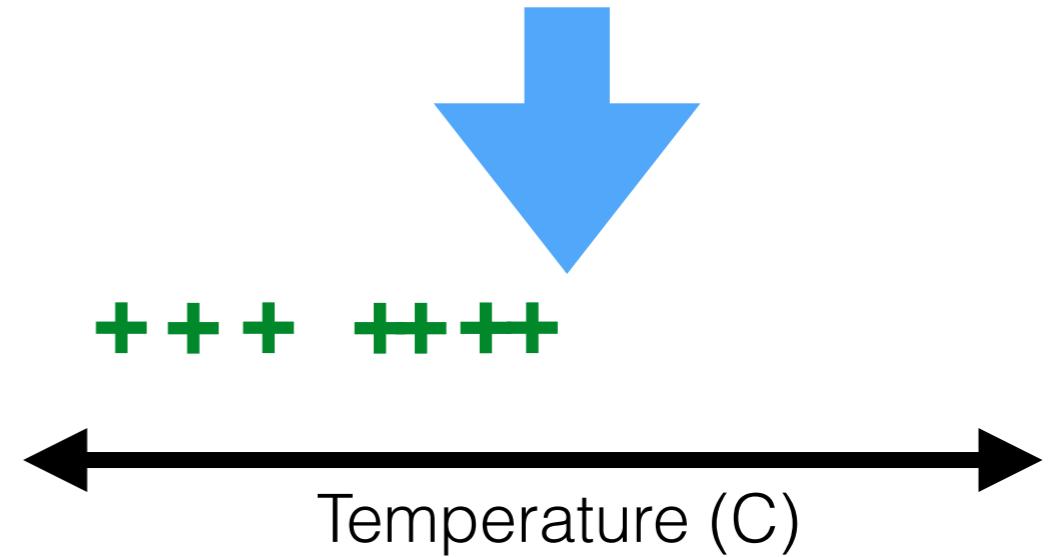
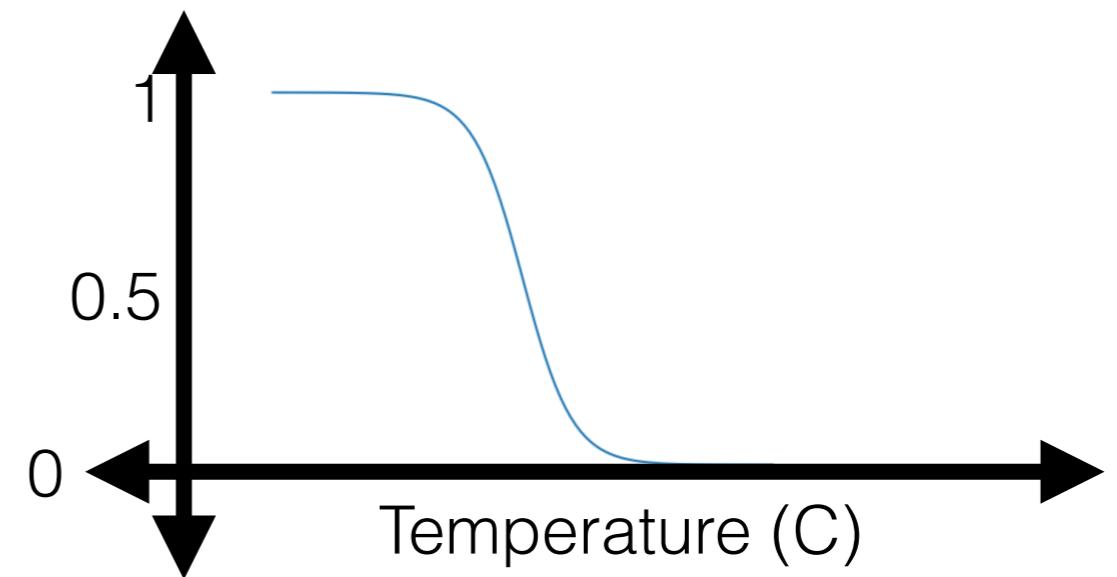
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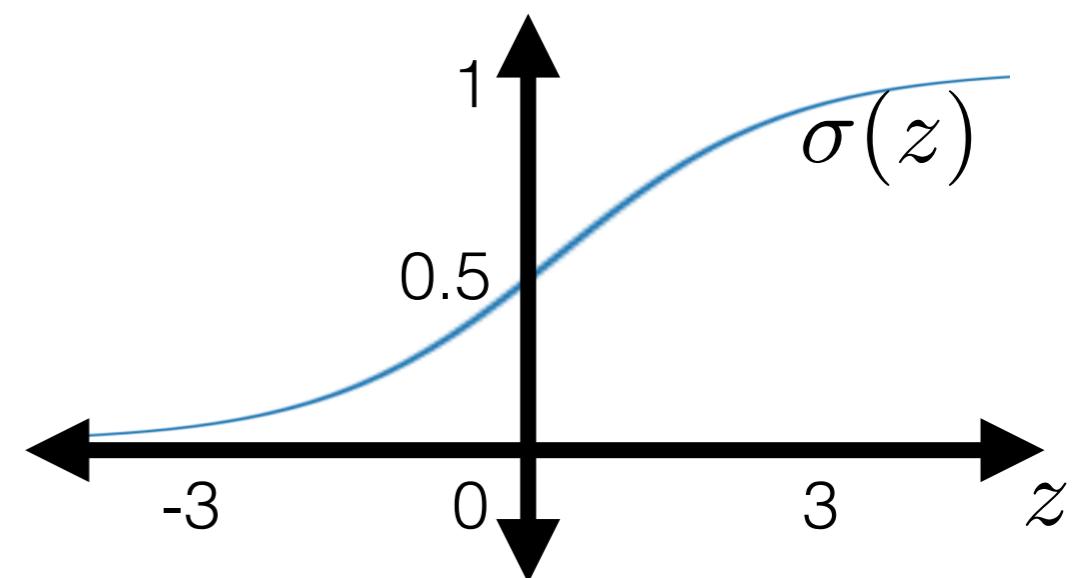
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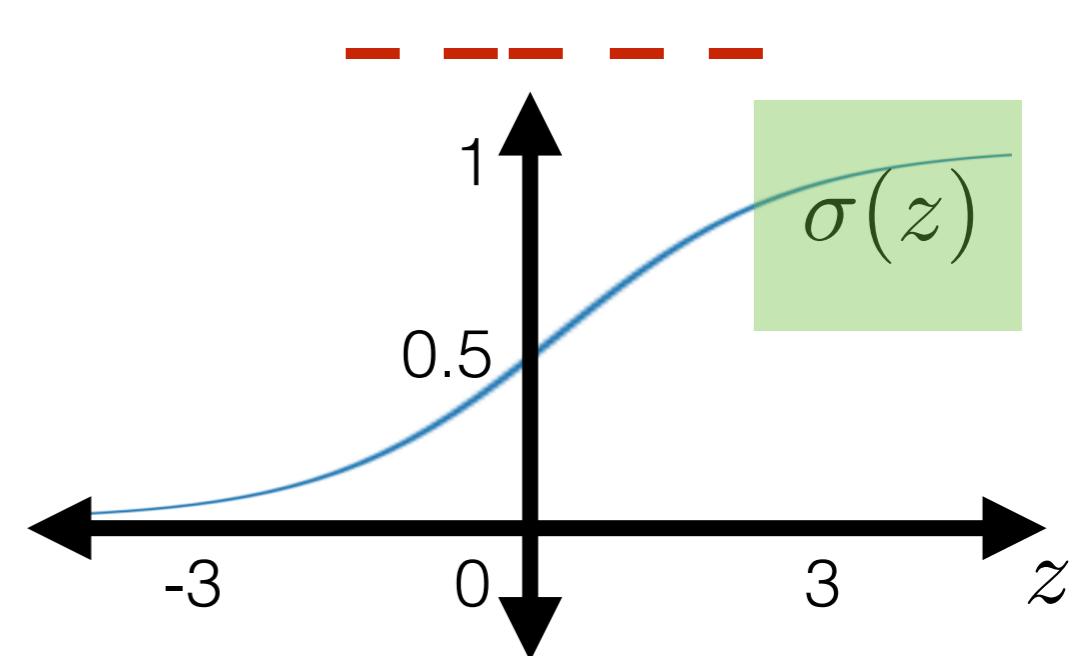
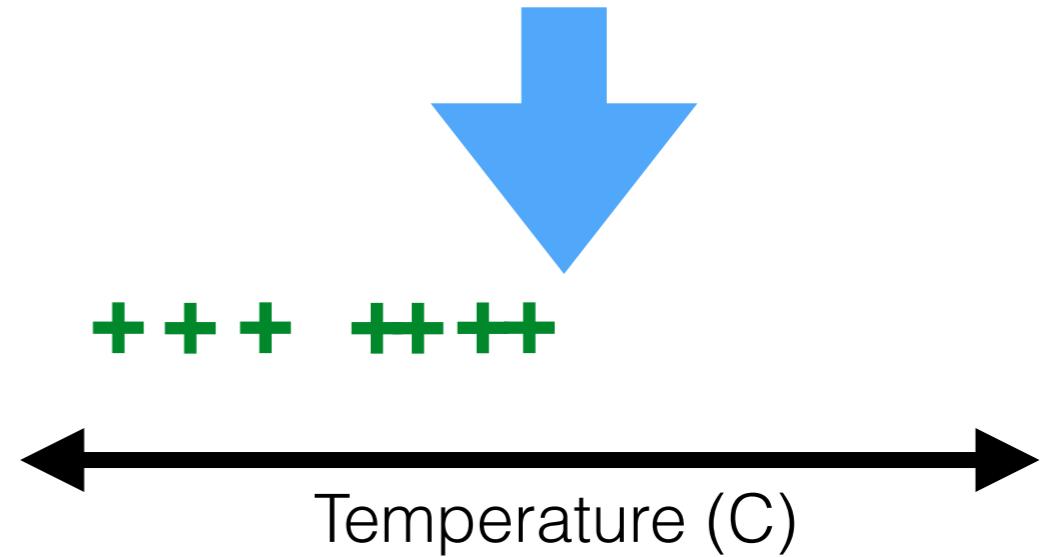
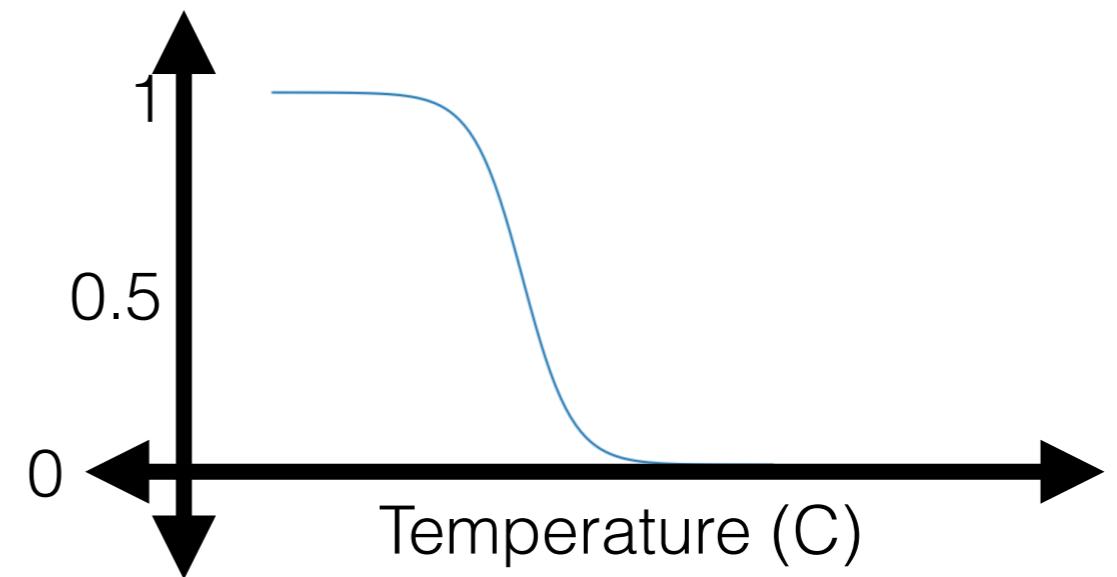


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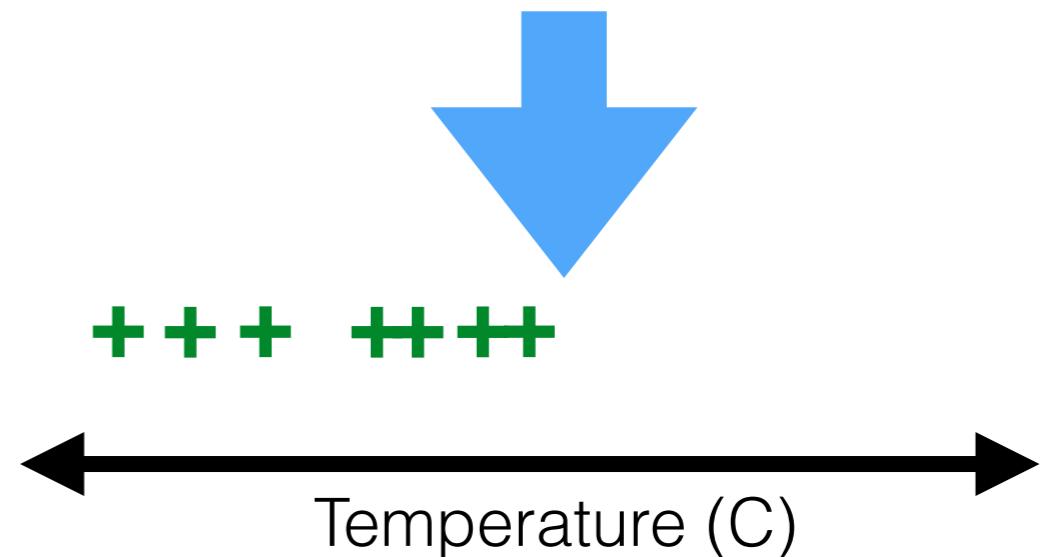
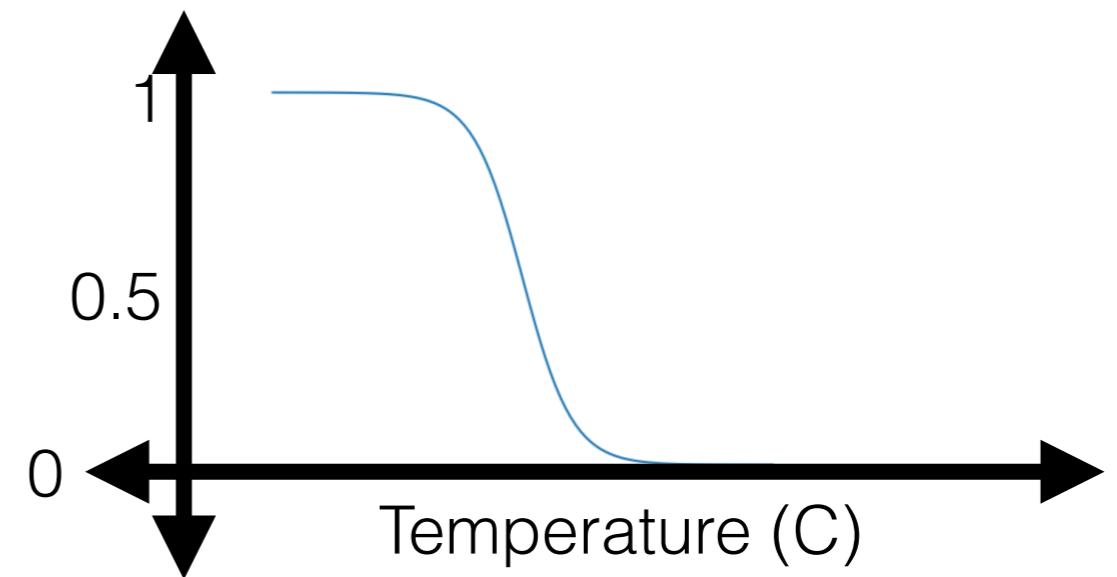
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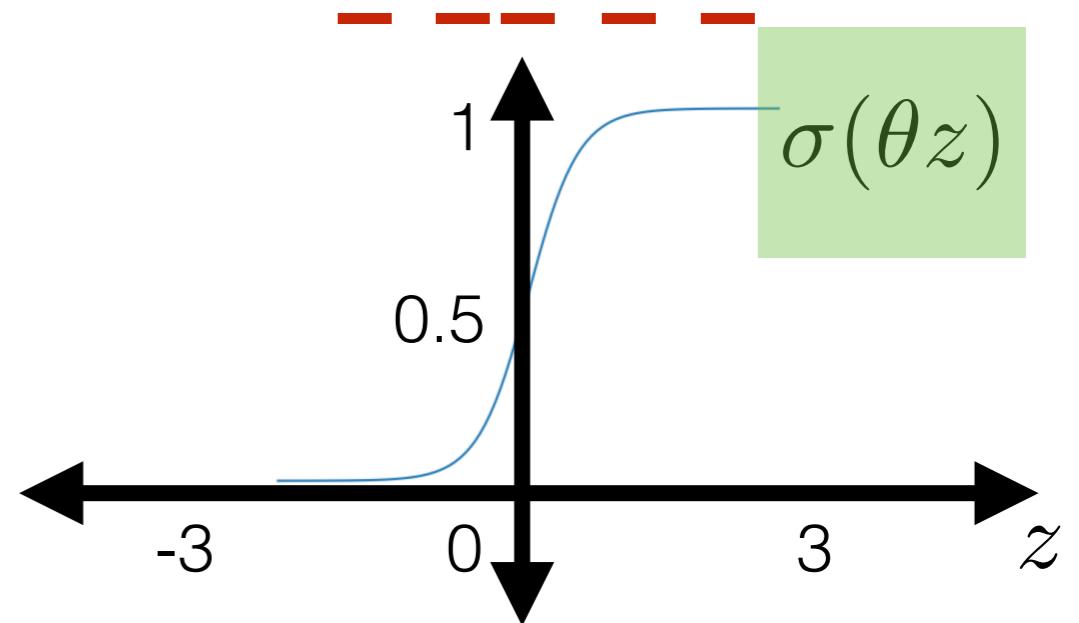
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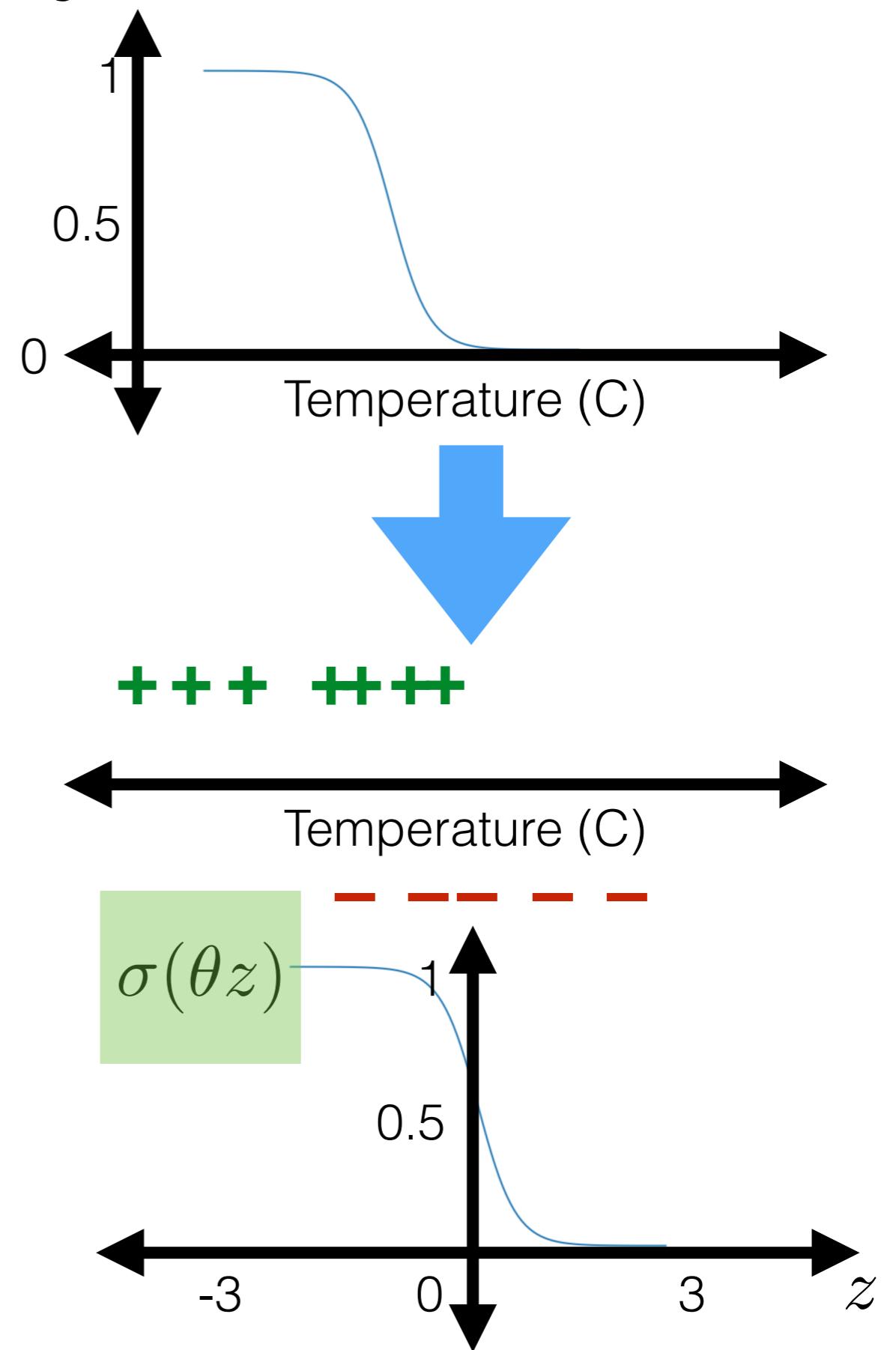
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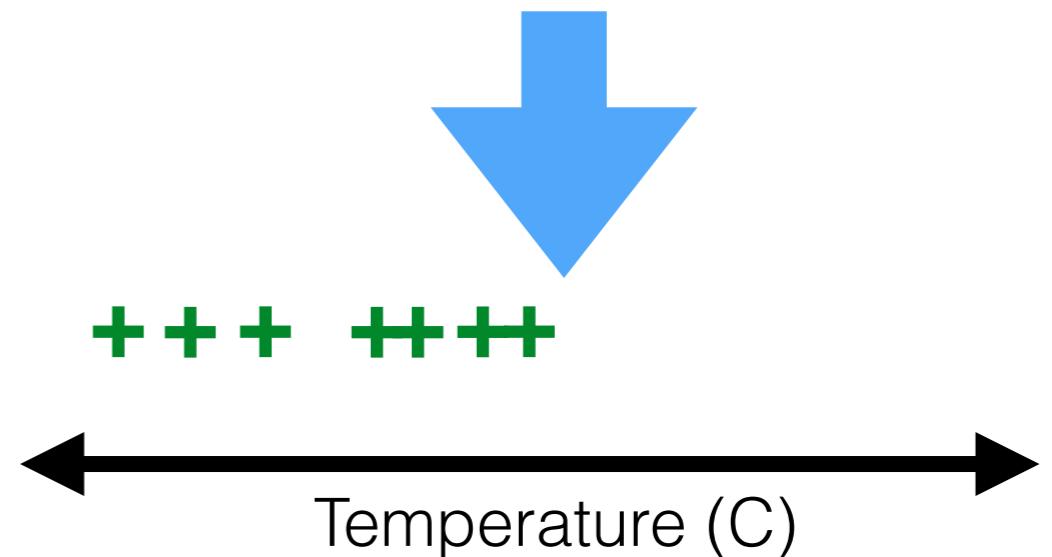
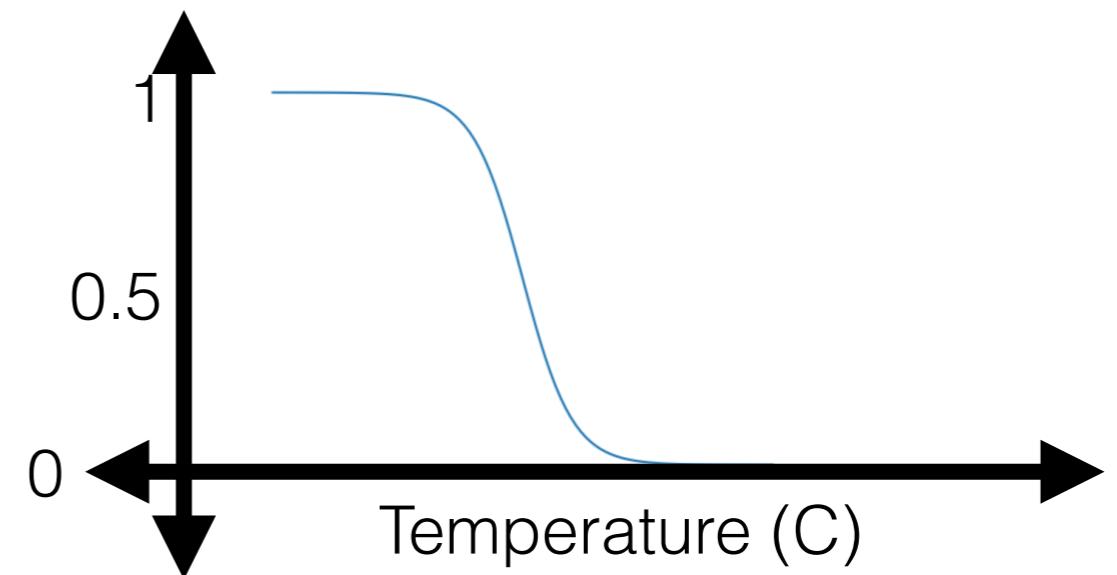
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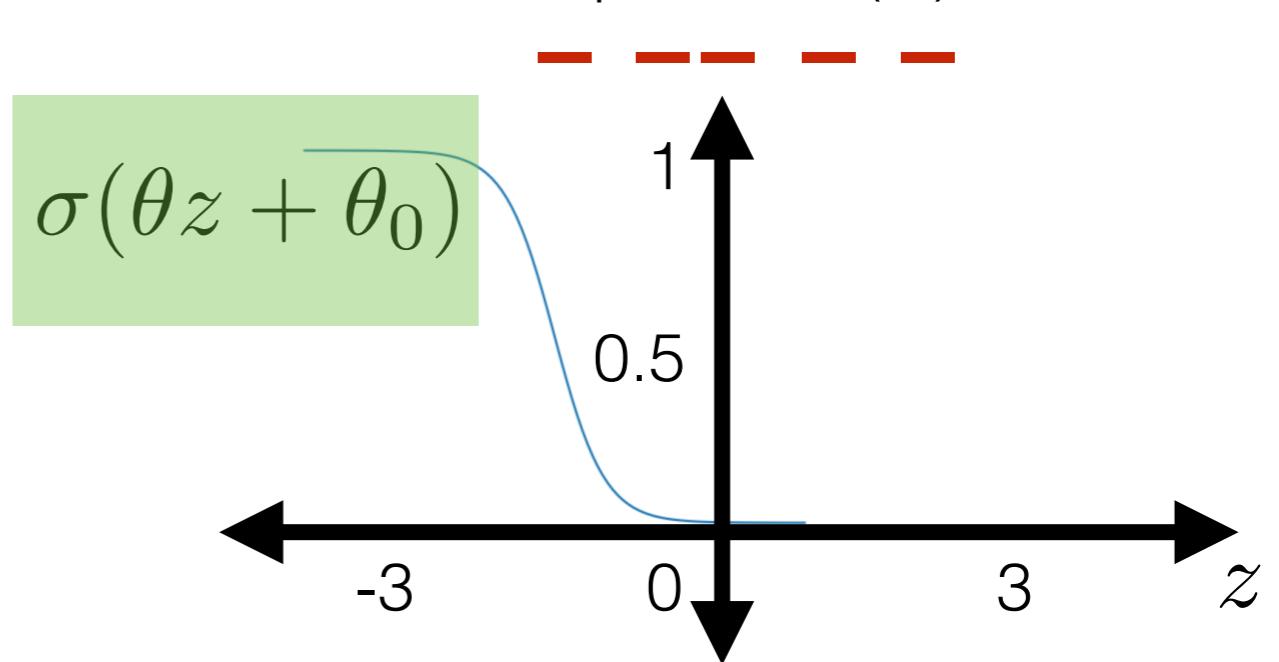


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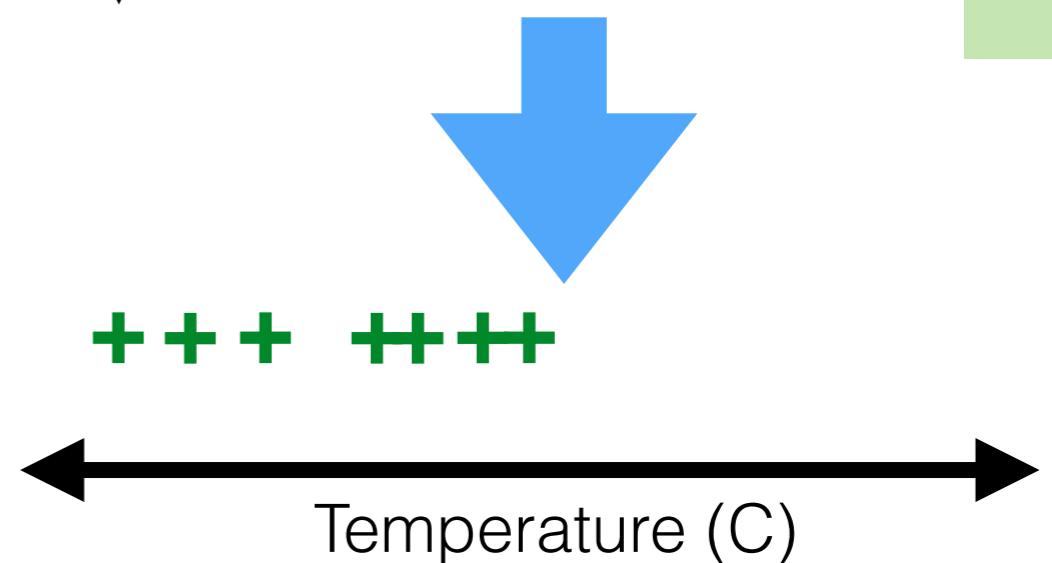
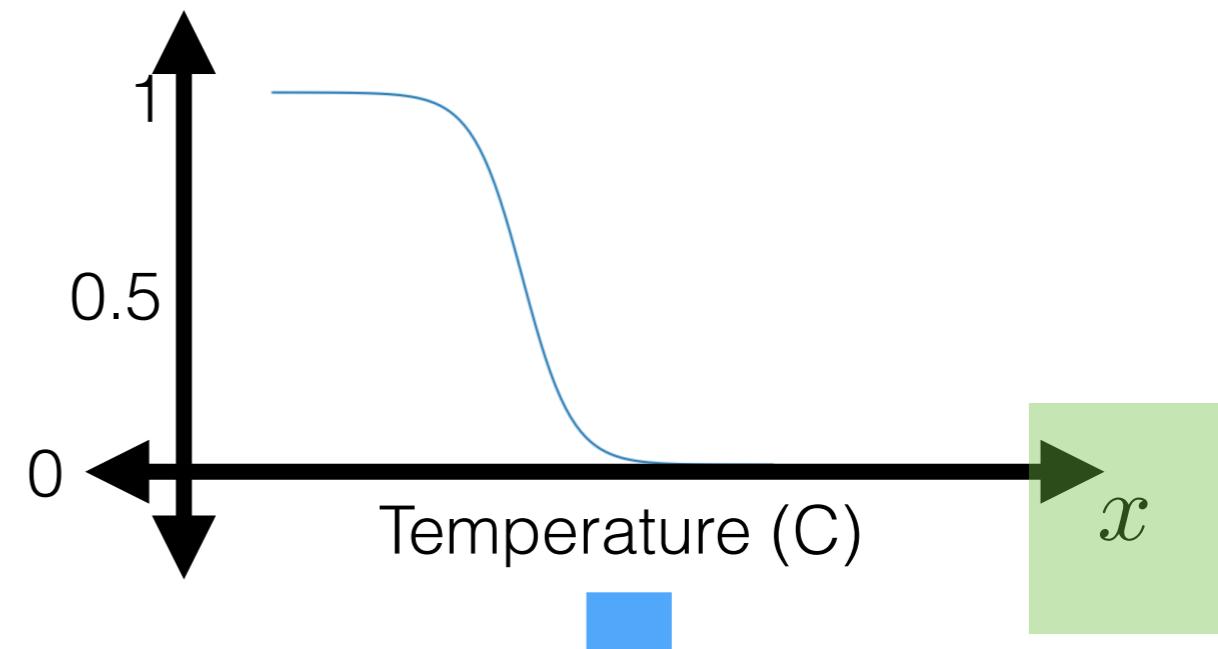


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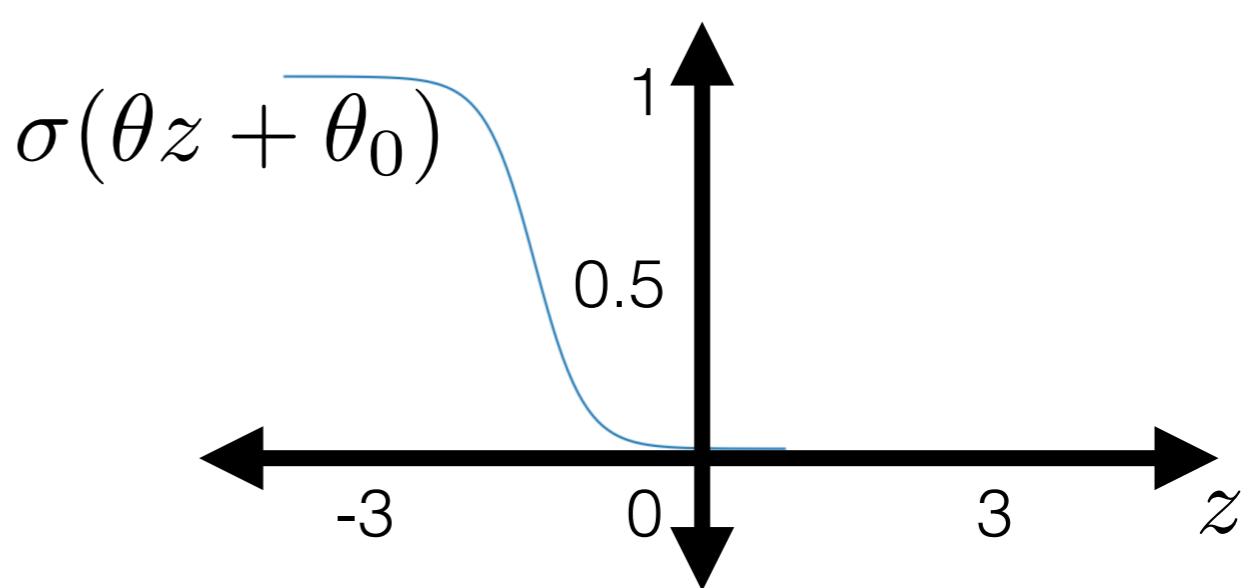


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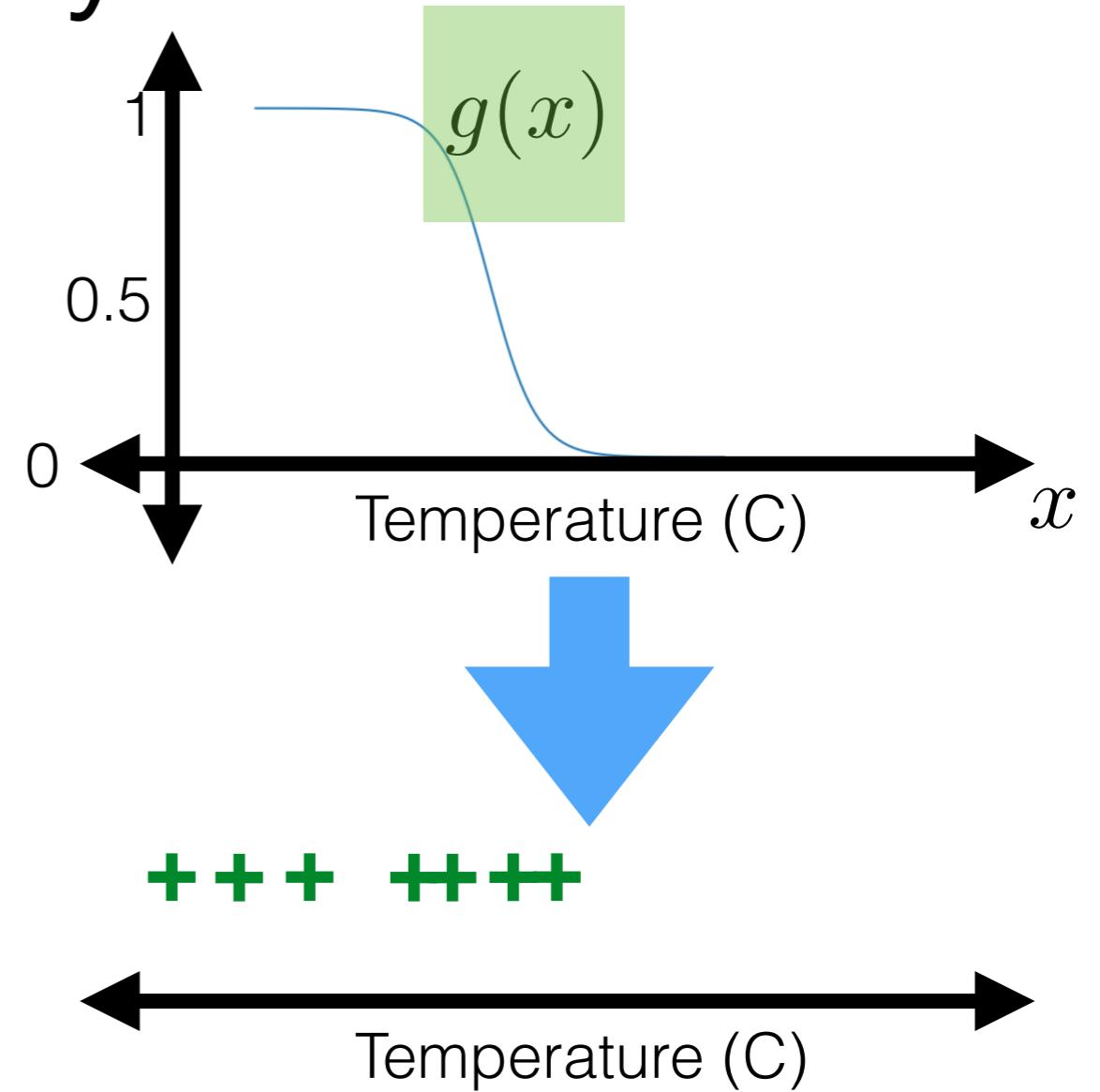


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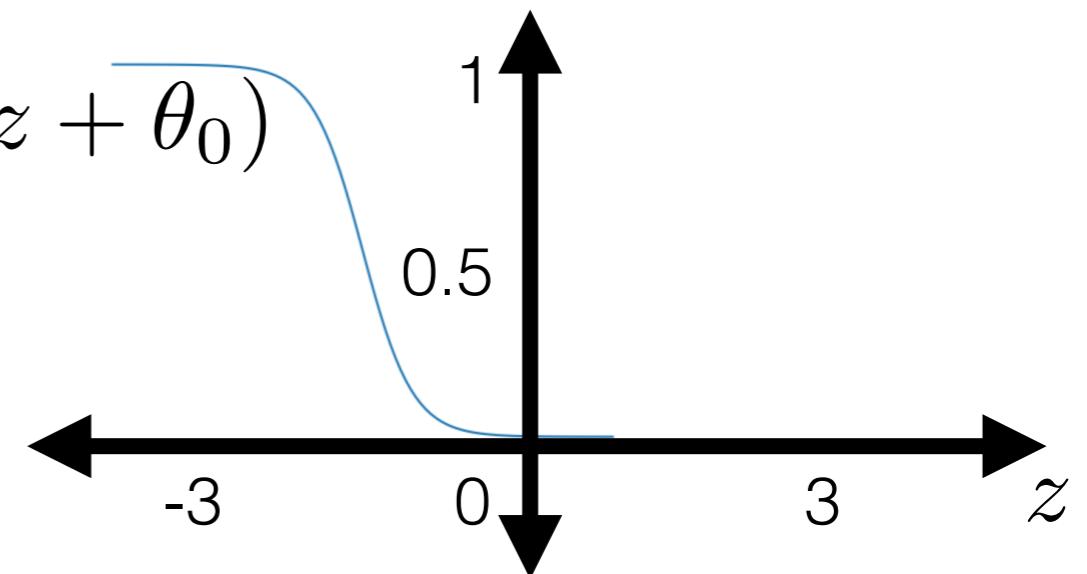


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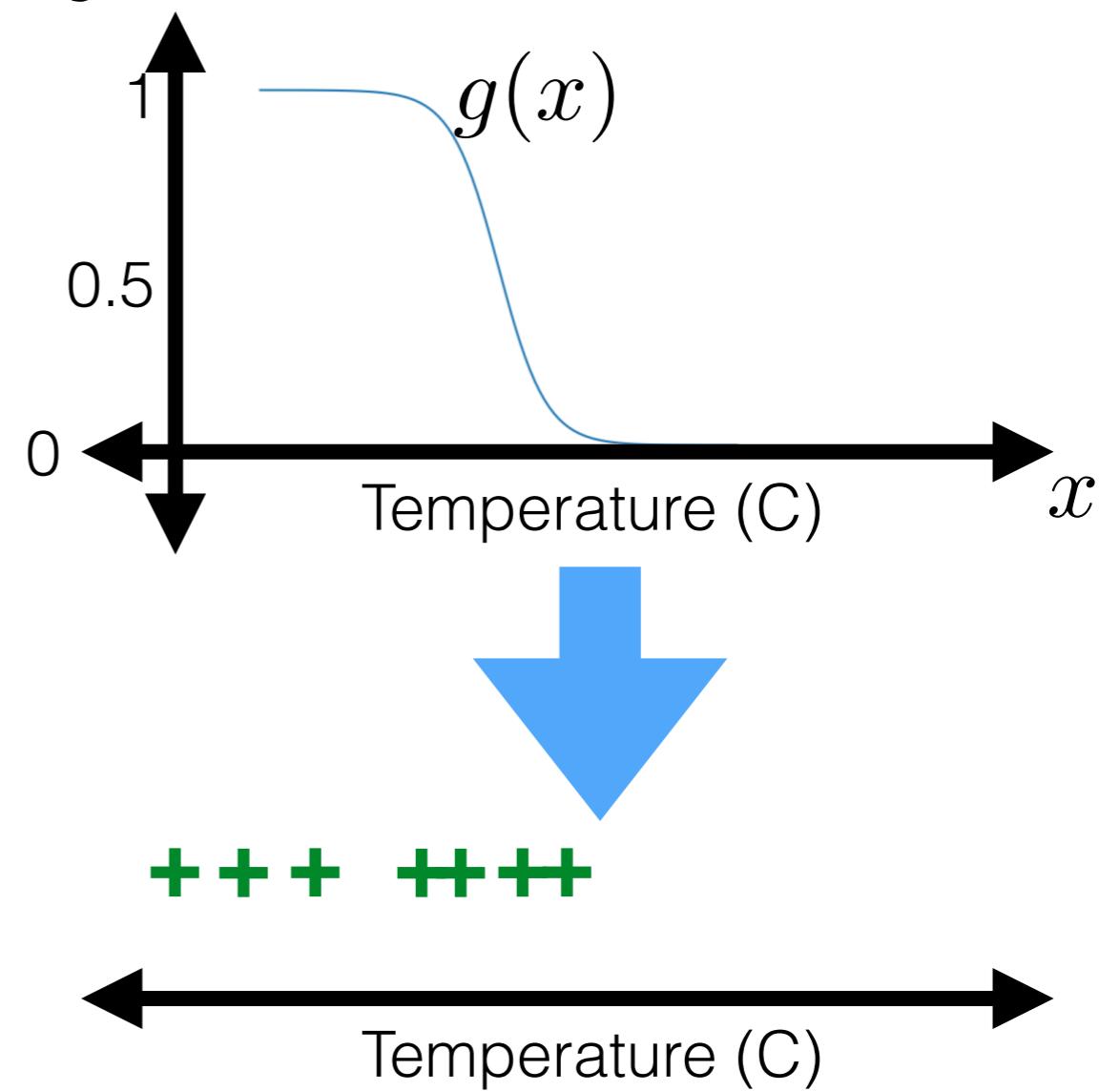
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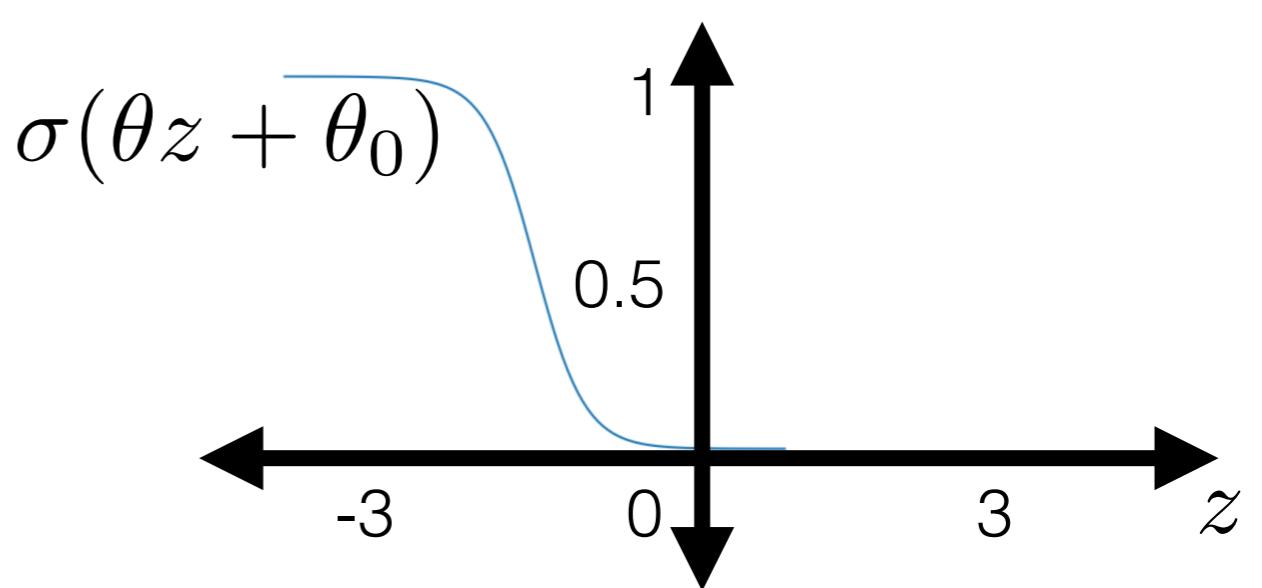
# Capturing uncertainty

$$g(x) = \sigma(\theta x + \theta_0)$$



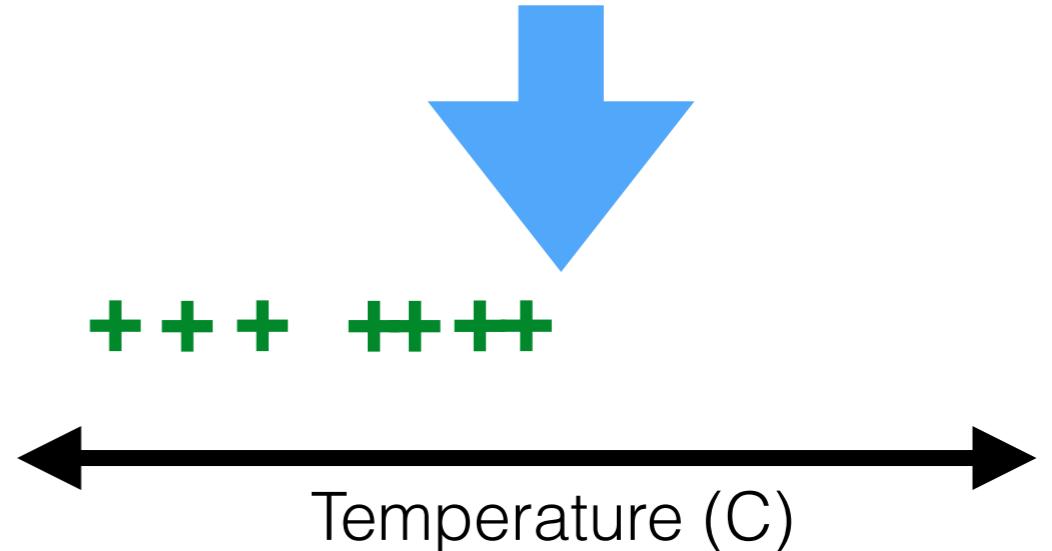
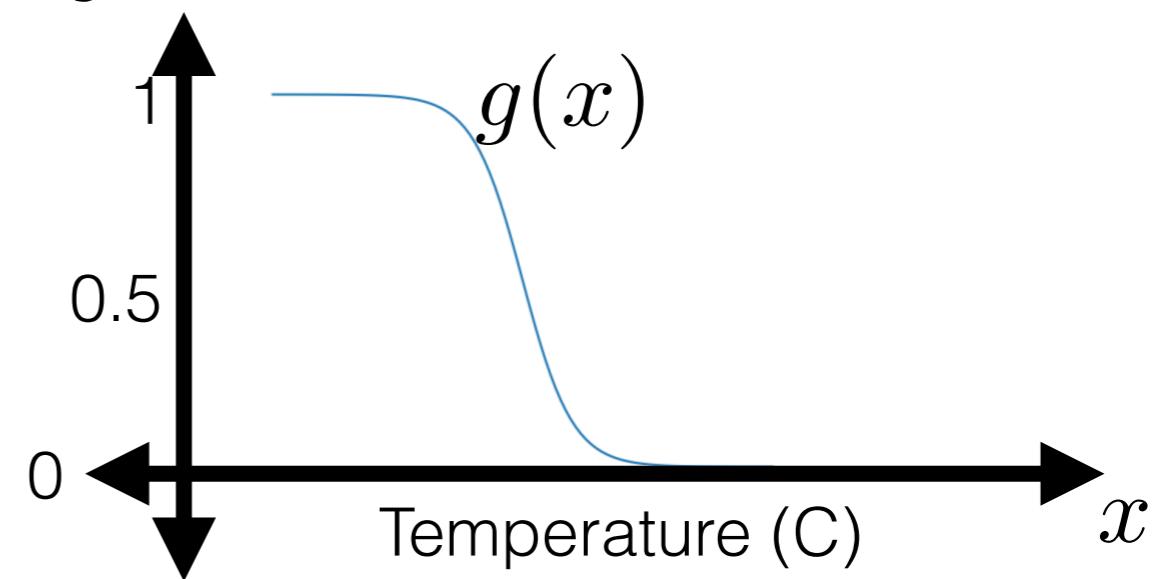
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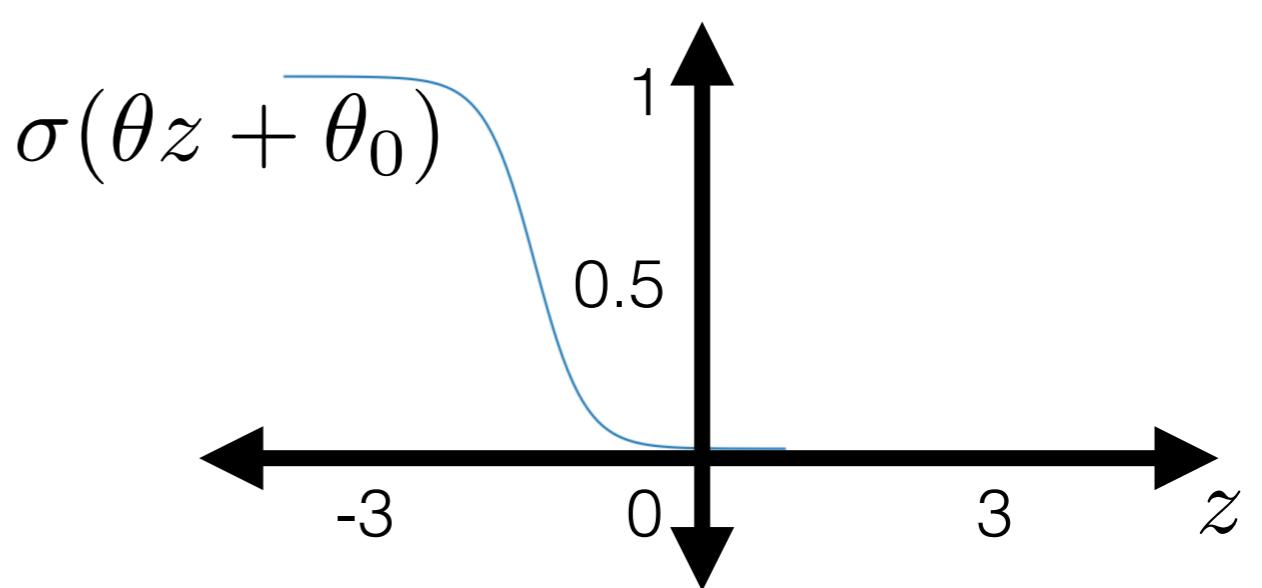
# Capturing uncertainty

$$g(x) = \sigma(\theta x + \theta_0)$$
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- How to make this shape?
  - Sigmoid/logistic function

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# Capturing uncertainty

# Capturing uncertainty

1 feature:

# Capturing uncertainty

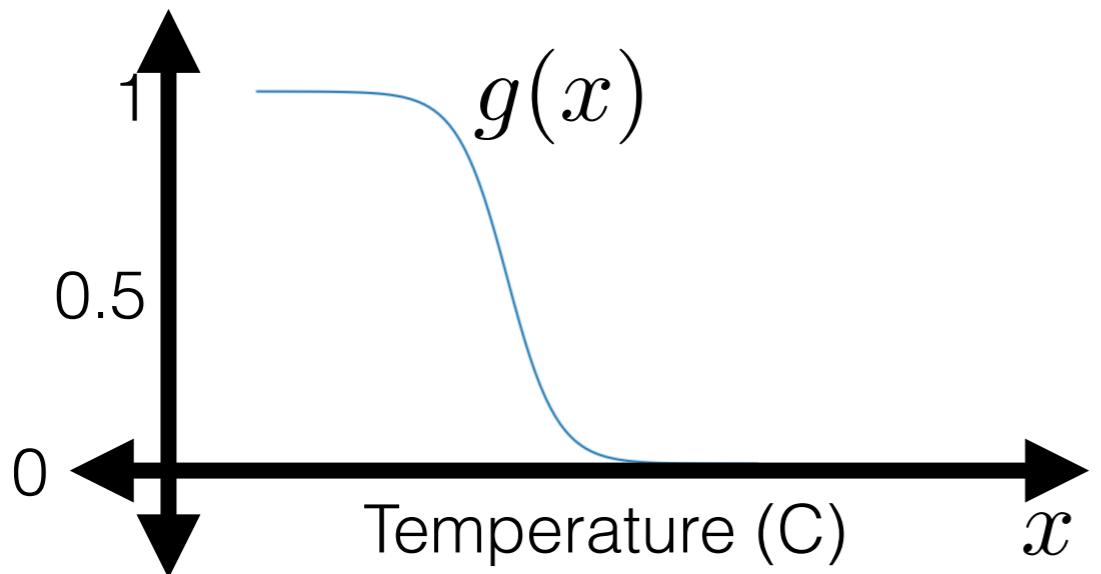
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$$= \frac{1}{1 + \exp \{-(\theta x + \theta_0)\}}$$

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1 feature:

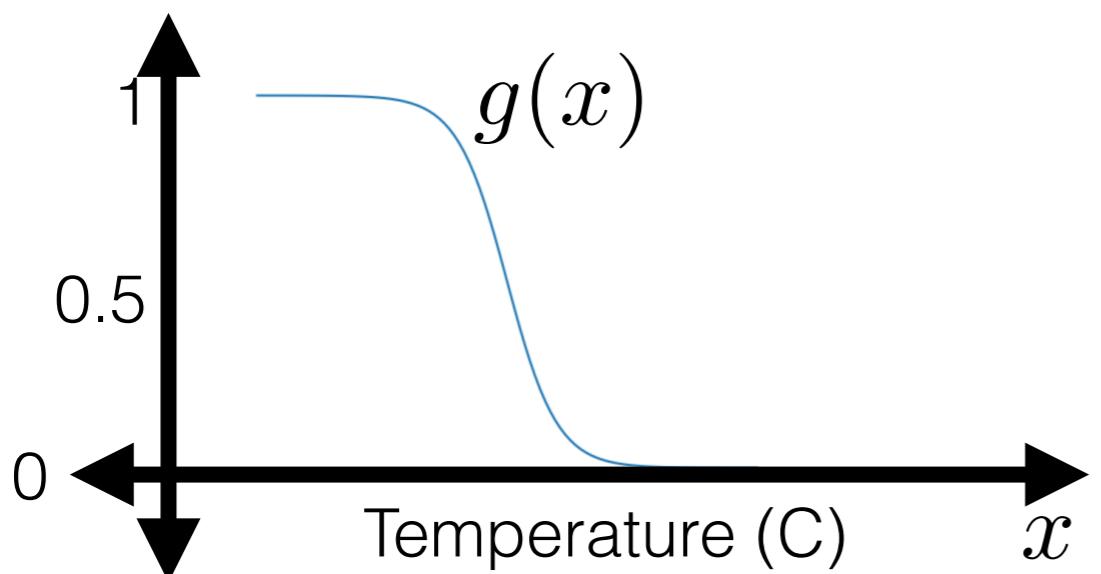
$$g(x) = \sigma(\theta x + \theta_0)$$
$$= \frac{1}{1 + \exp \{-(\theta x + \theta_0)\}}$$



# Capturing uncertainty

1 feature:

$$g(x) = \sigma(\theta x + \theta_0)$$
$$= \frac{1}{1 + \exp \{-(\theta x + \theta_0)\}}$$



+++ +++

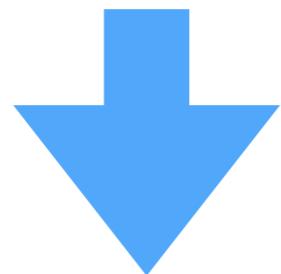
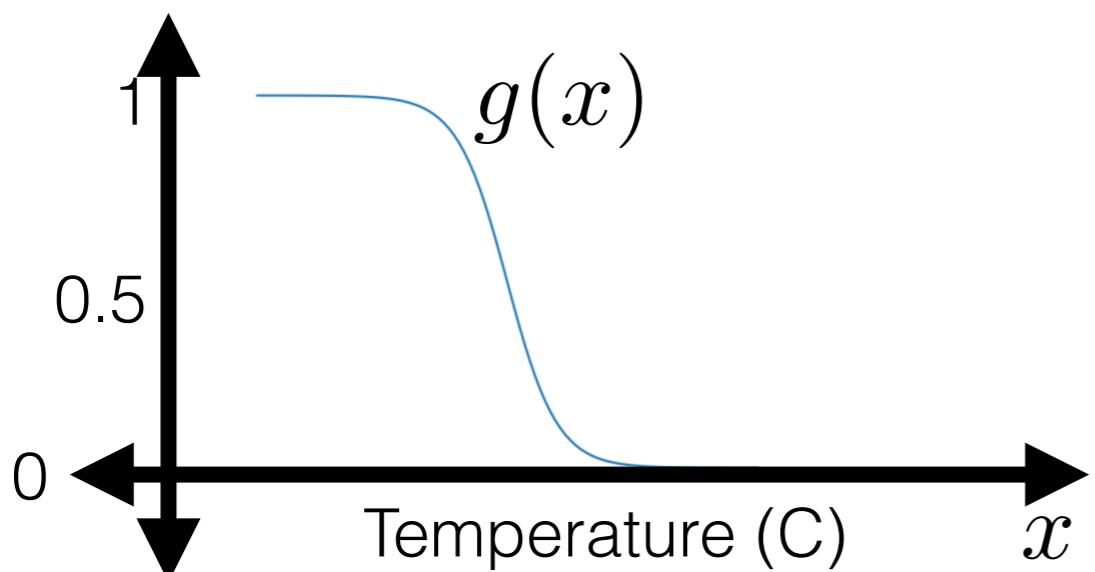


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+++ +++



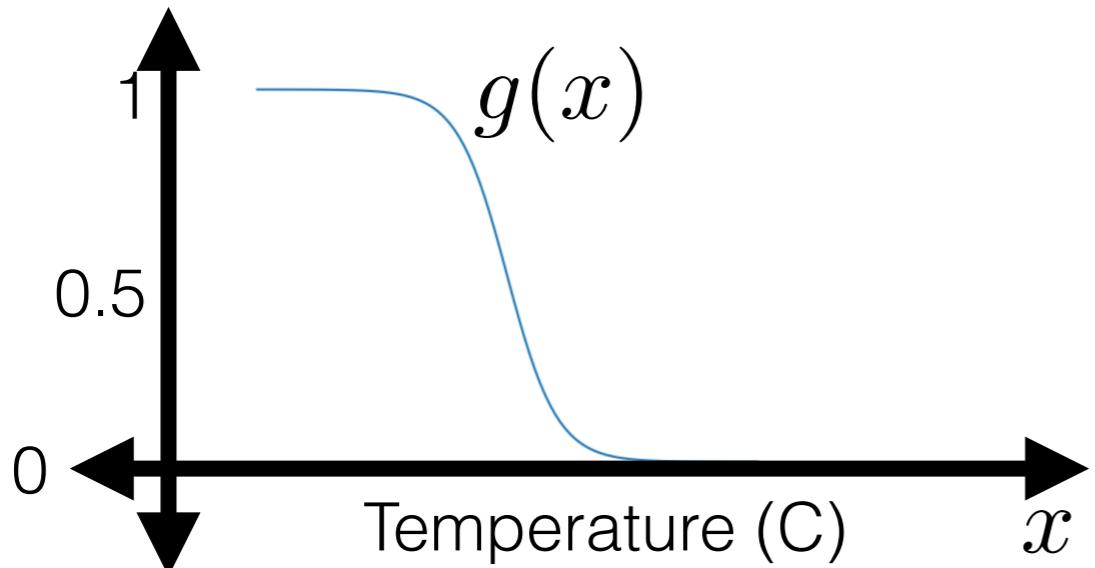
— — — —

# Capturing uncertainty

2 features:

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+++ +++



$$g(x) = \sigma(\theta^\top x + \theta_0)$$
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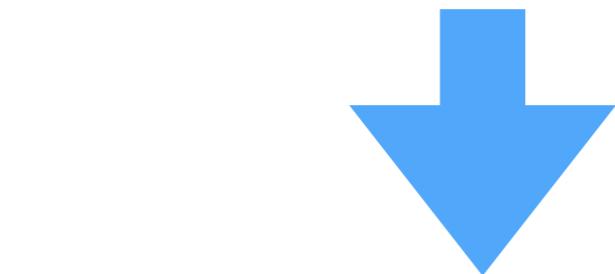
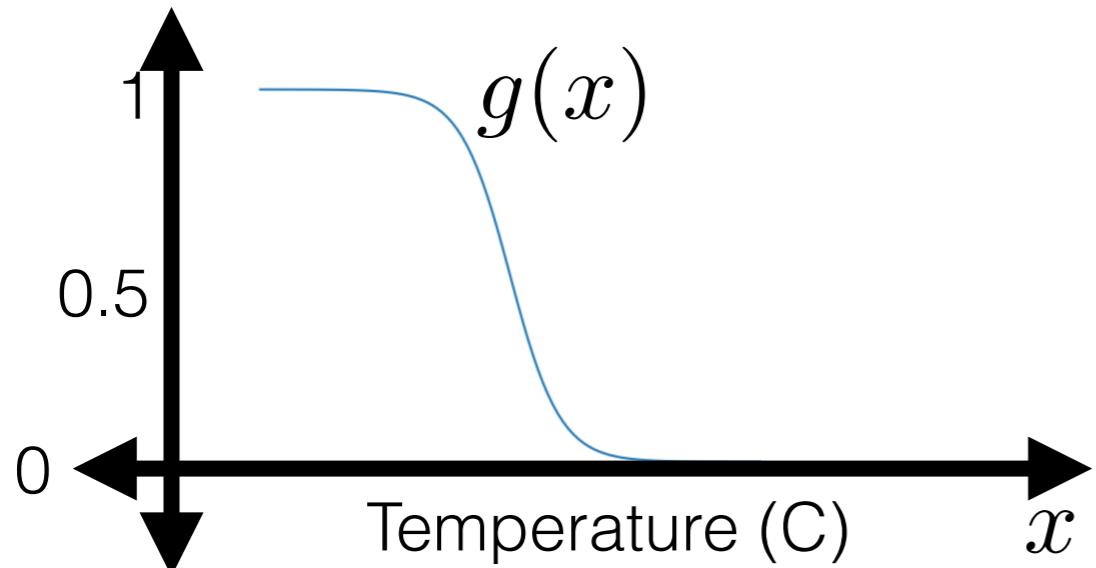
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2 features:

1 feature:

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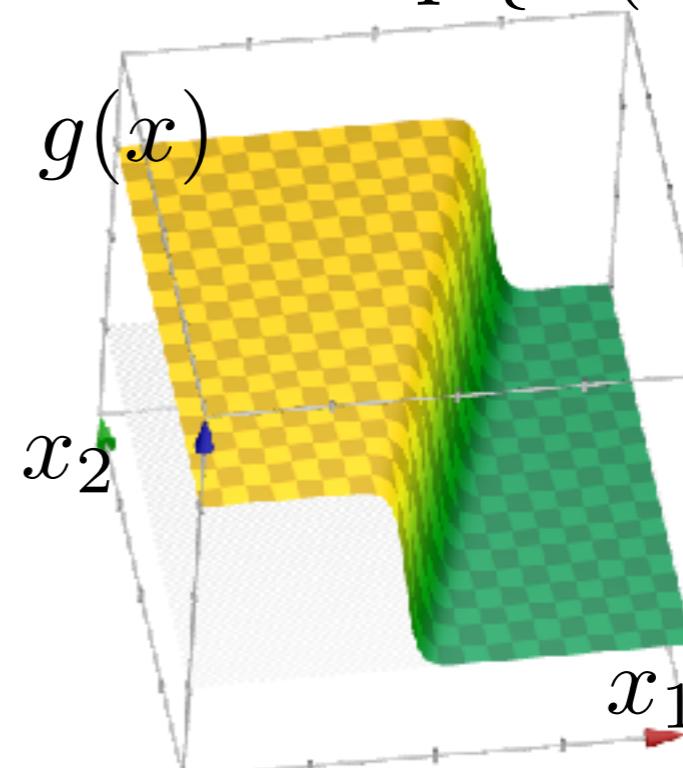
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+++ +++



$$\begin{aligned} g(x) &= \sigma(\theta^\top x + \theta_0) \\ &= \frac{1}{1 + \exp \{-(\theta^\top x + \theta_0)\}} \end{aligned}$$

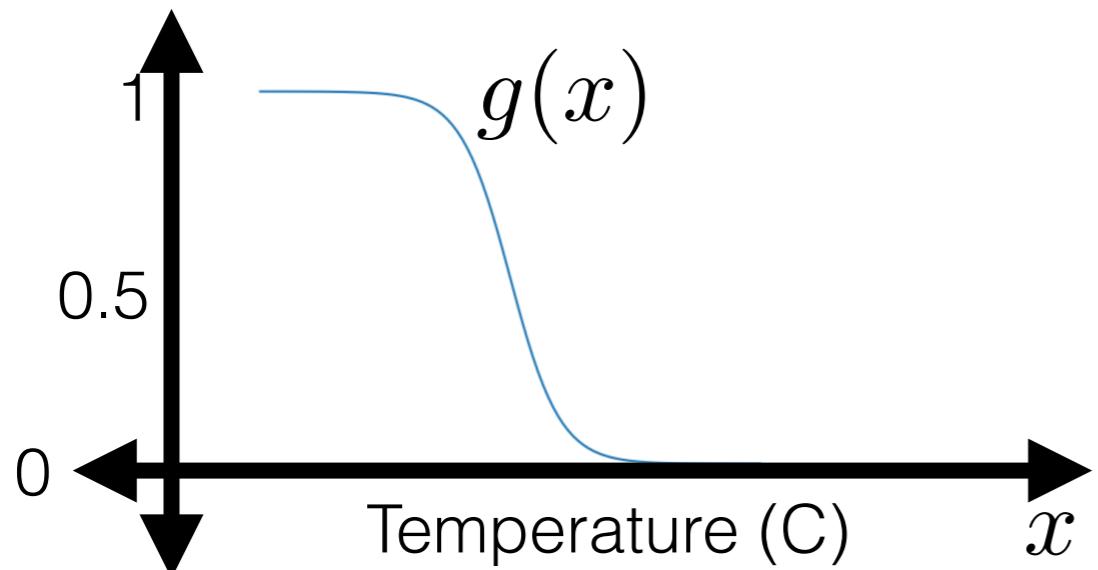


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2 features:

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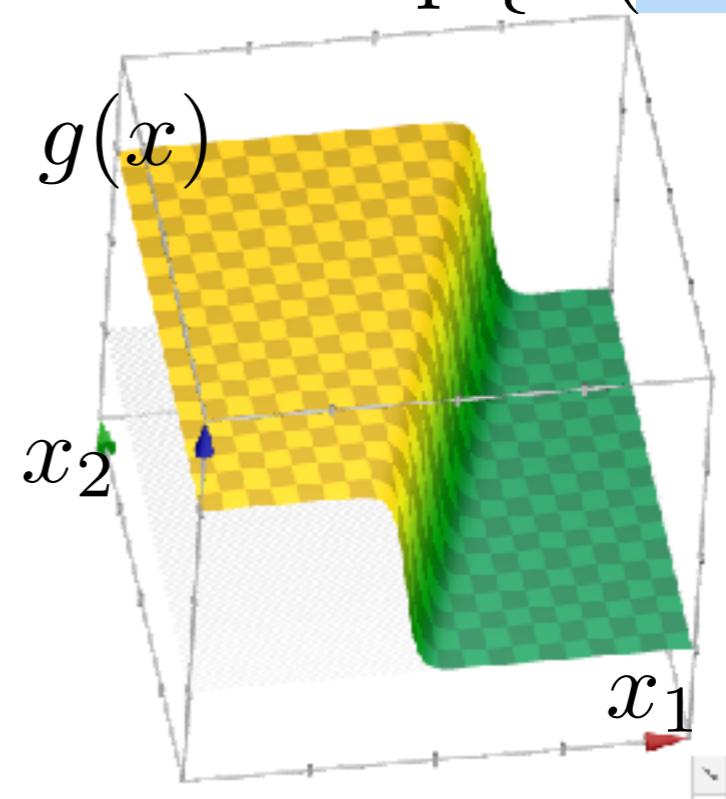
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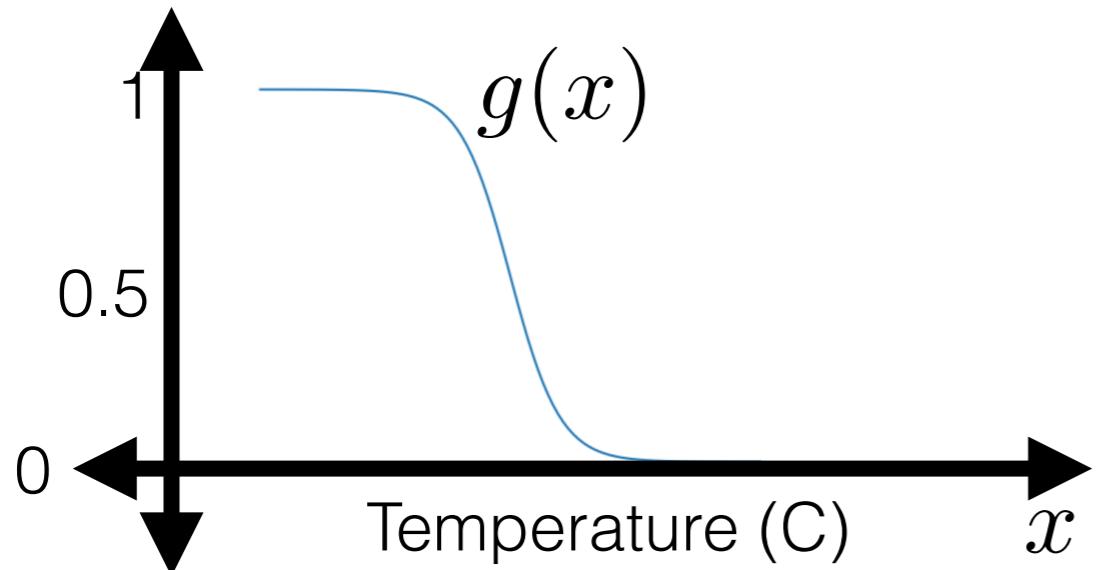


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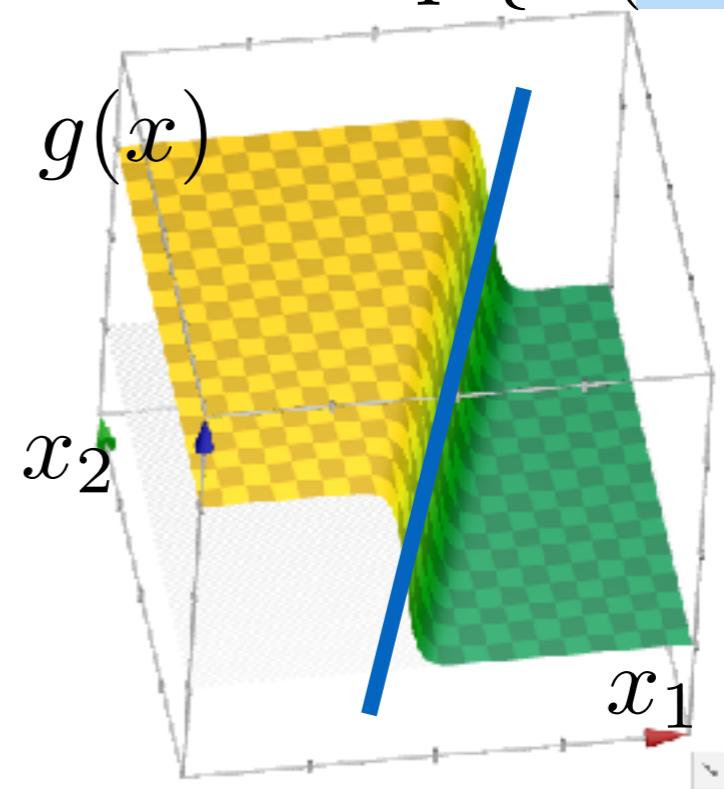
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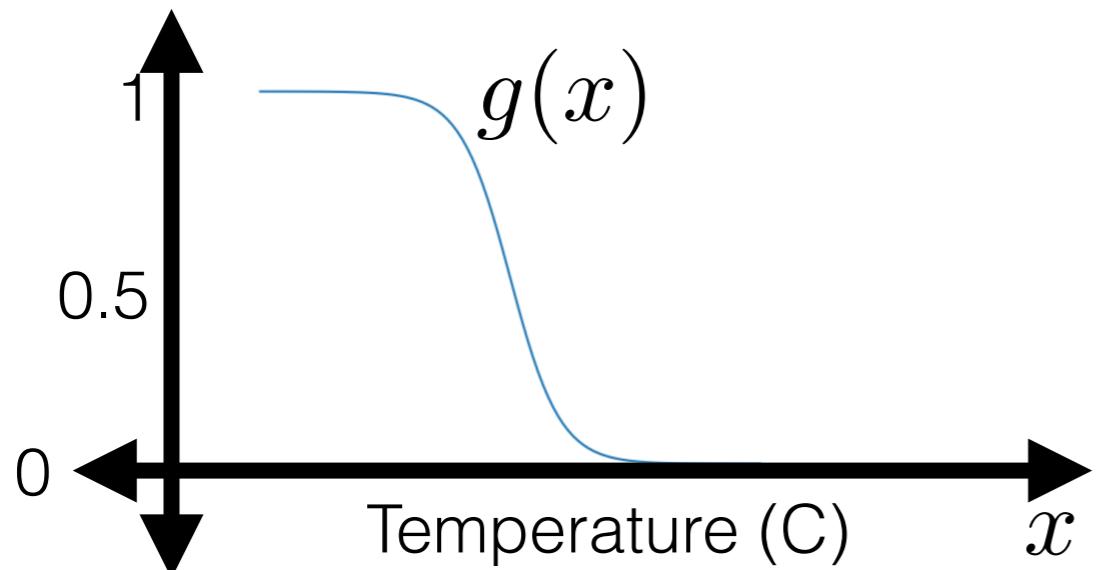
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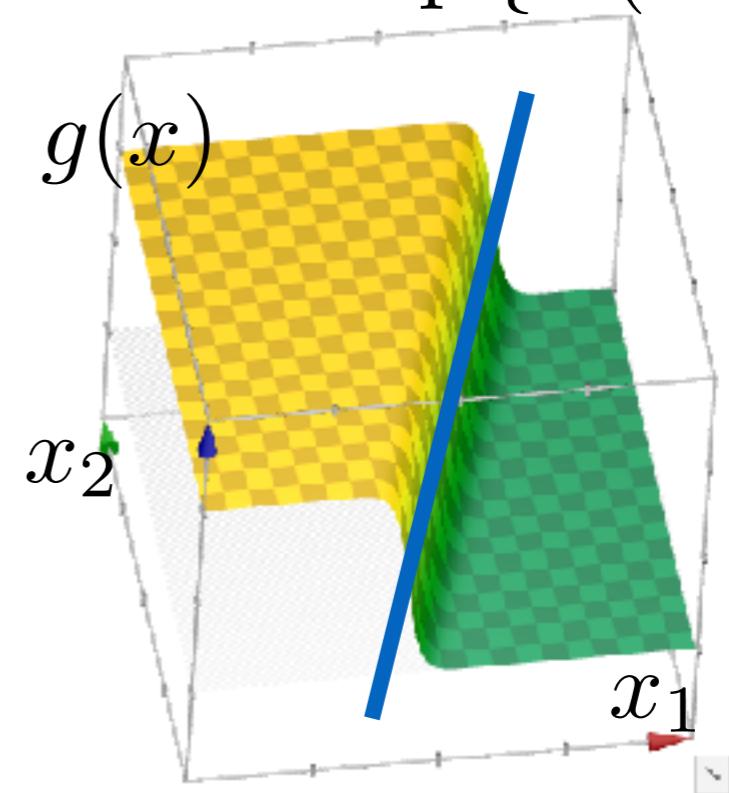
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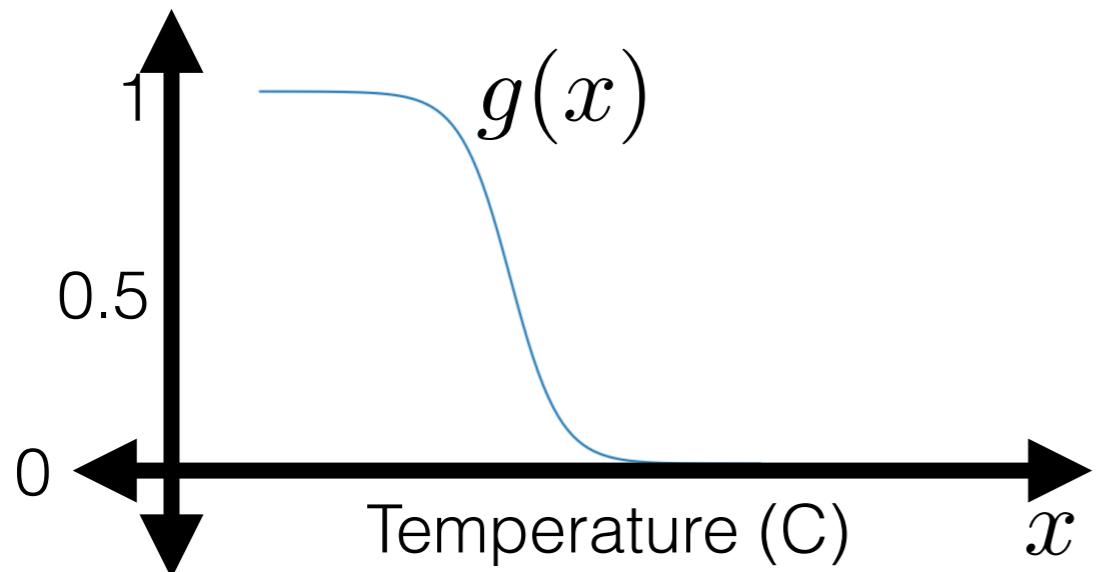


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2 features:

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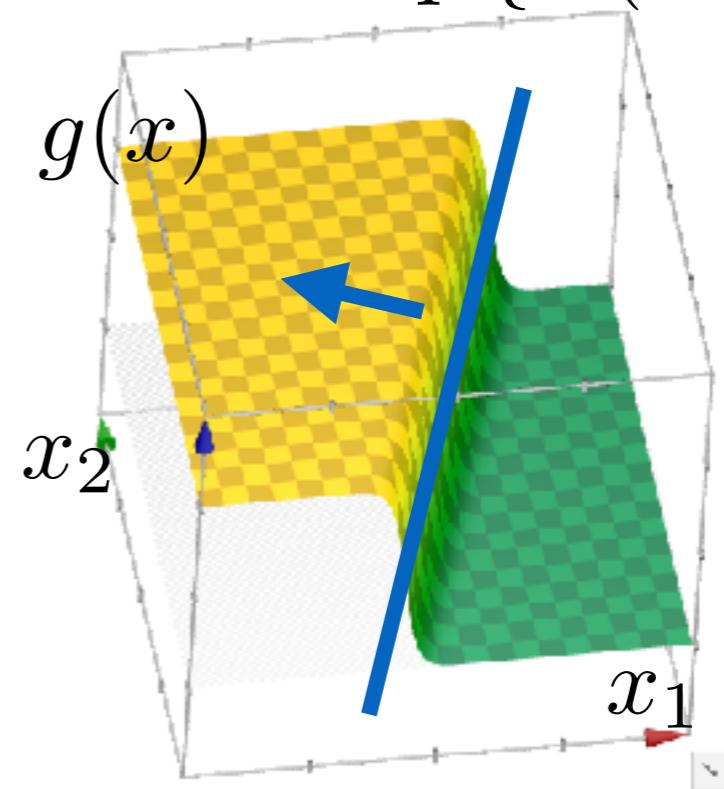
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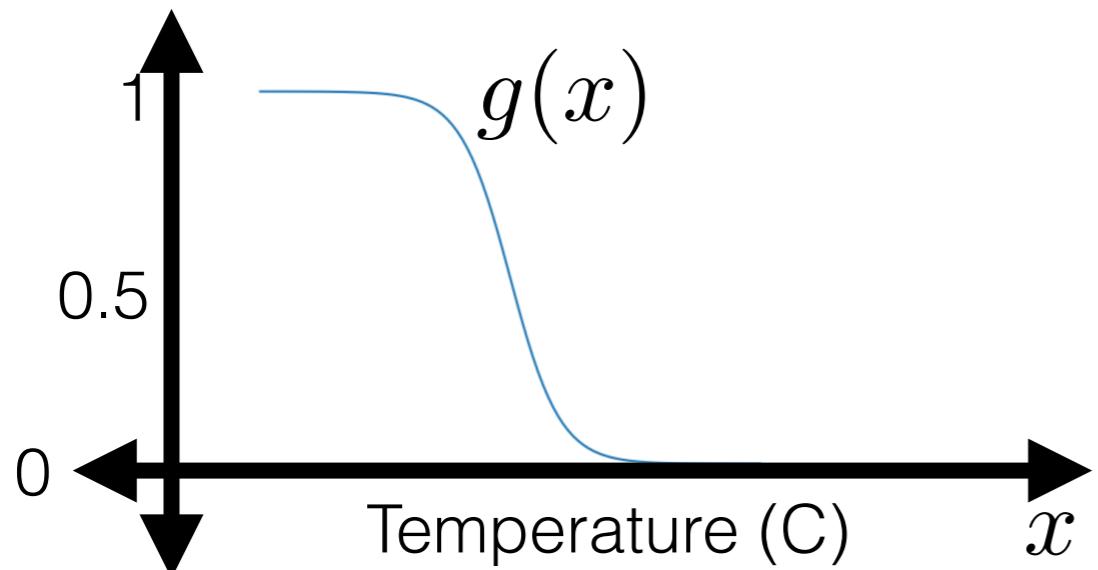


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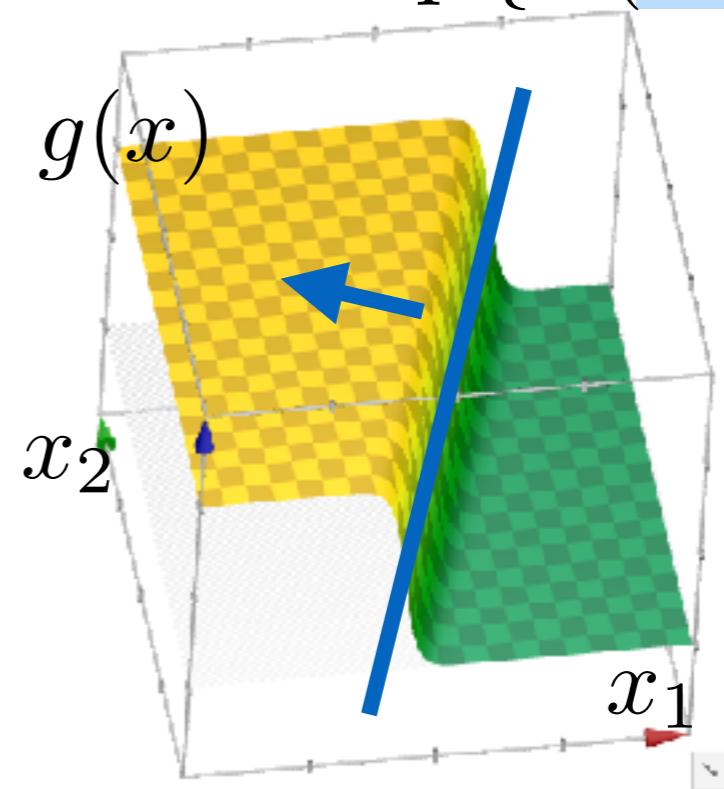
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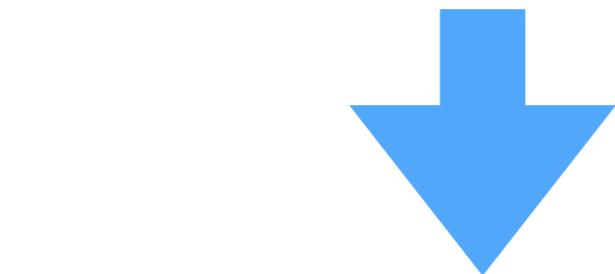
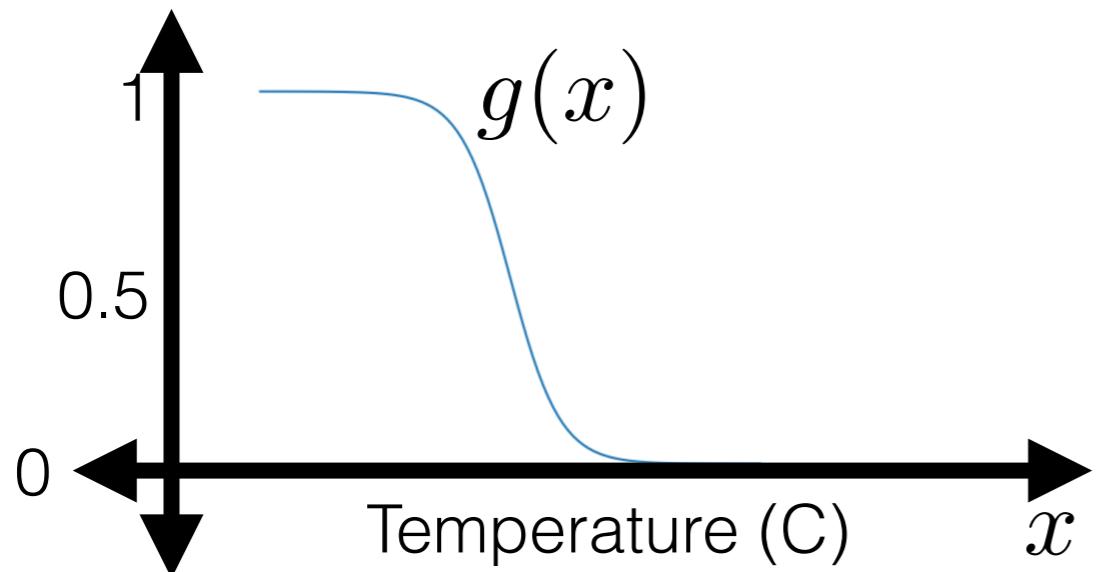


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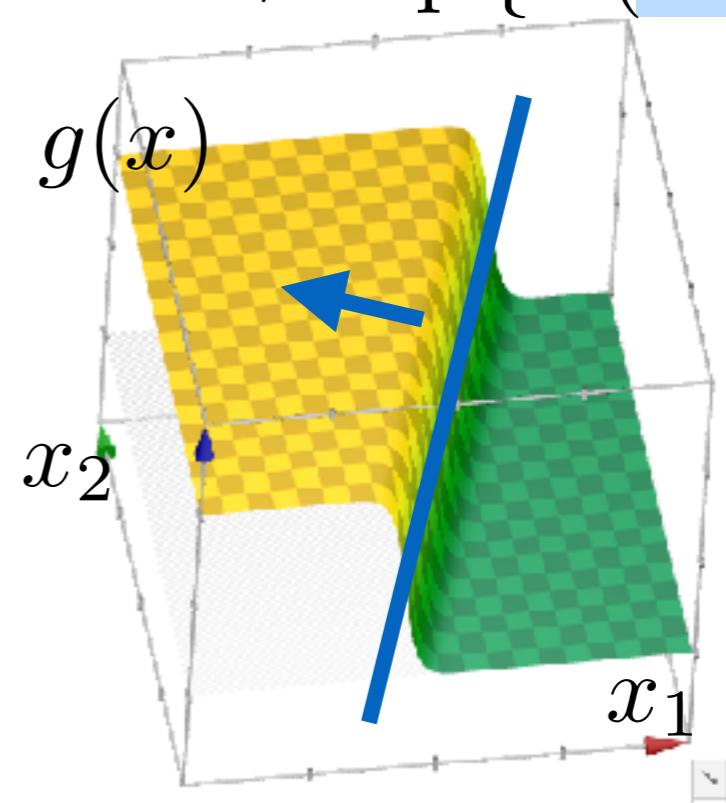
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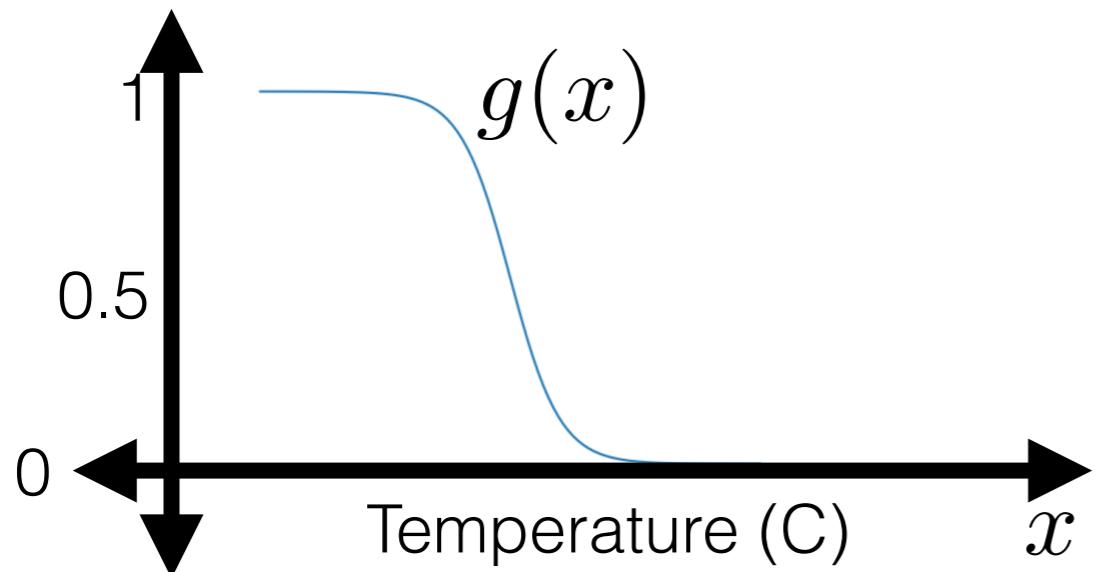


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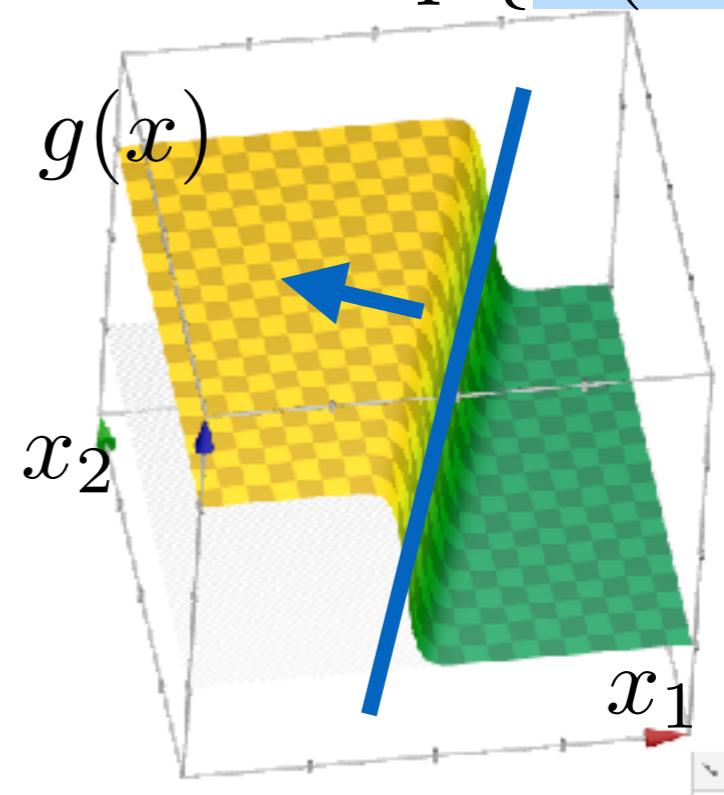
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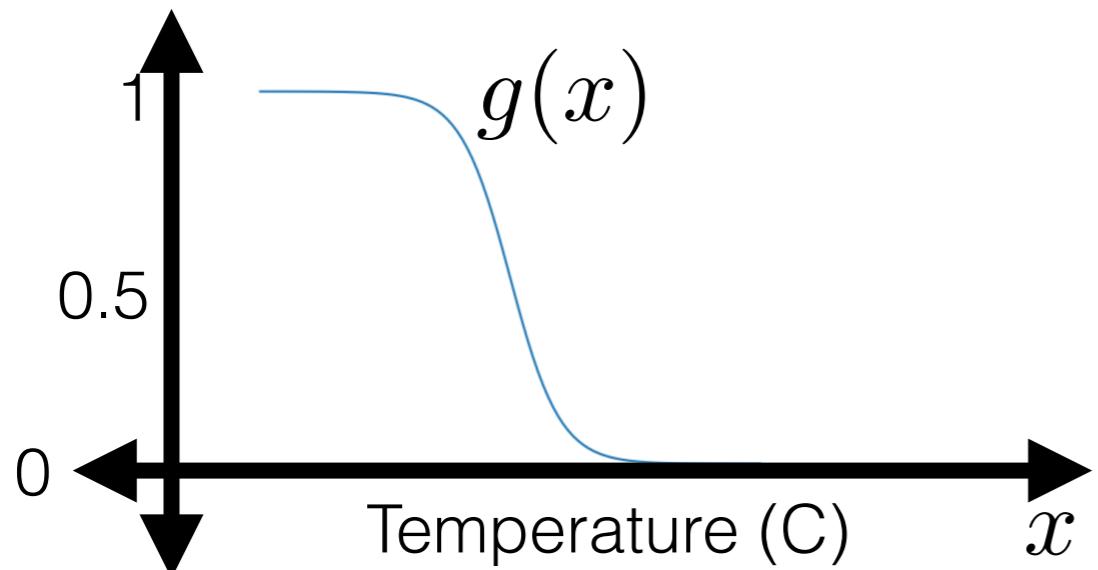


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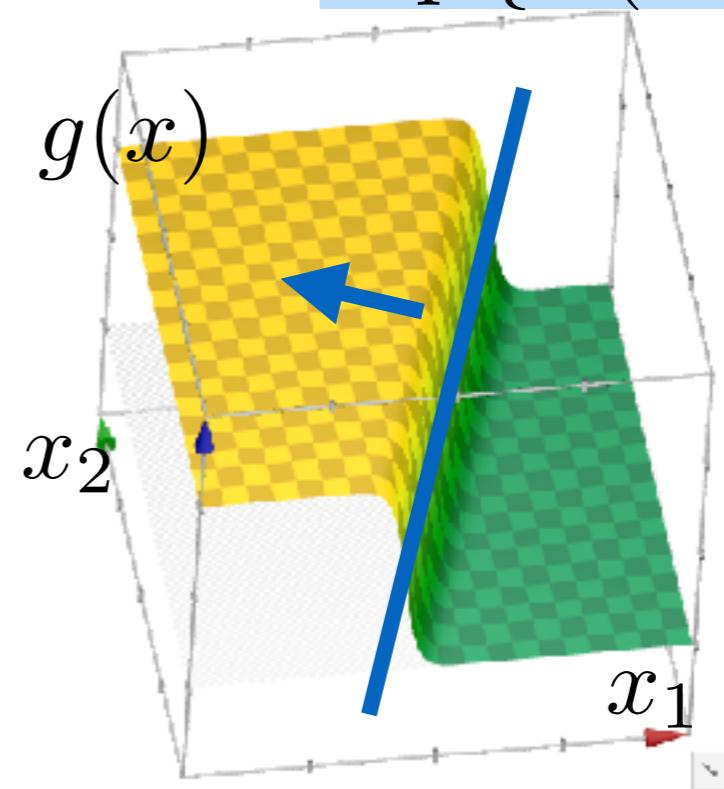
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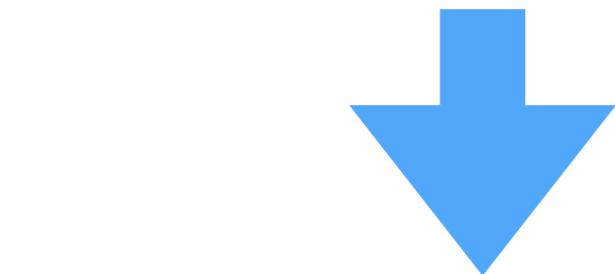
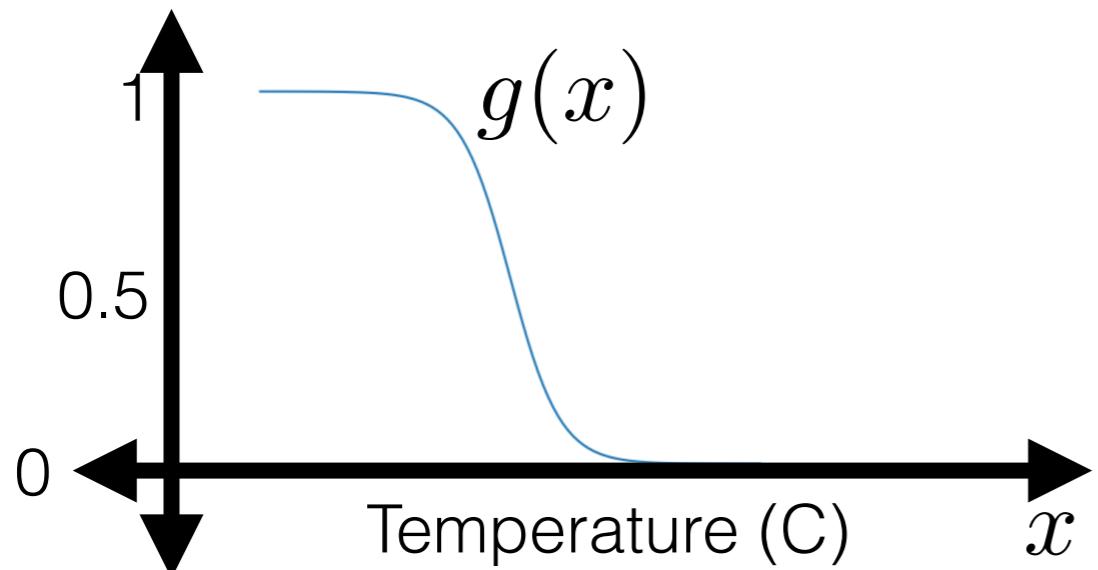
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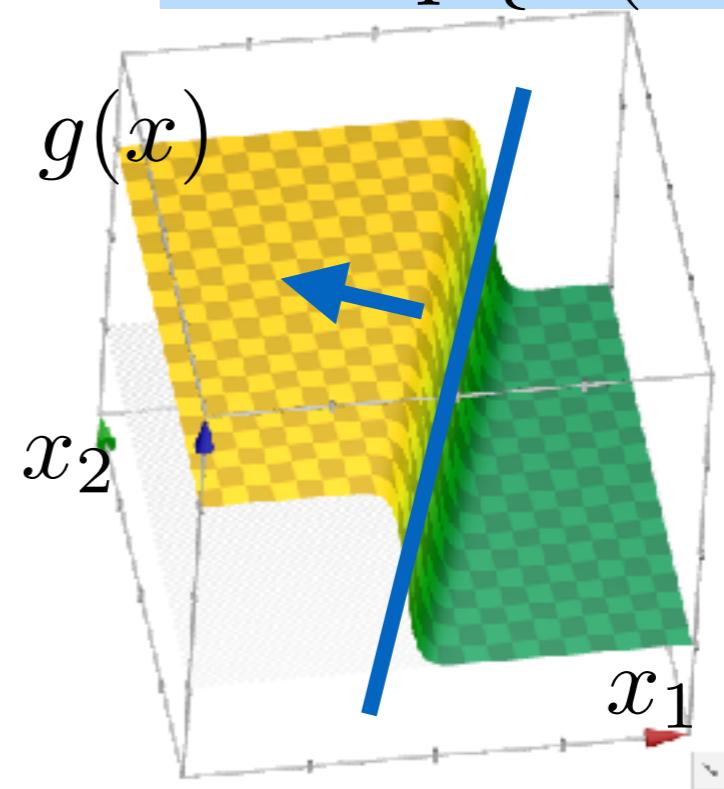
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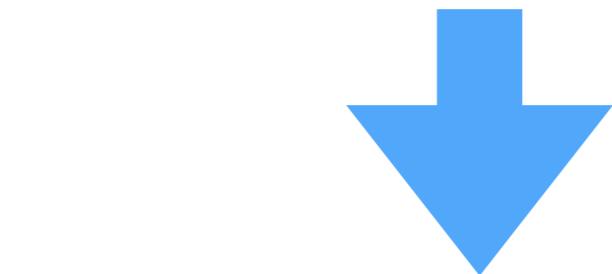
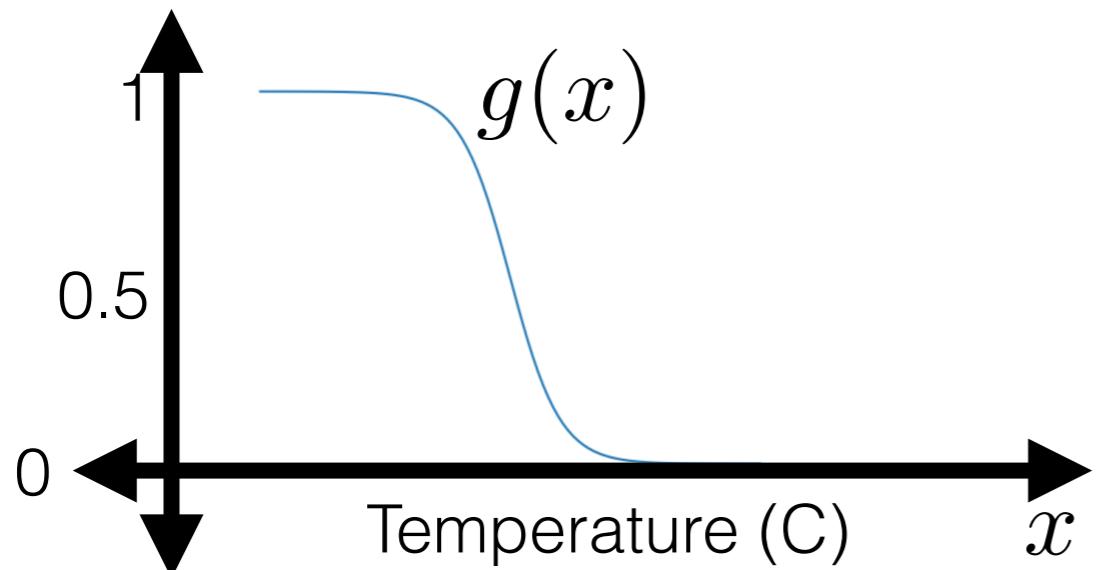
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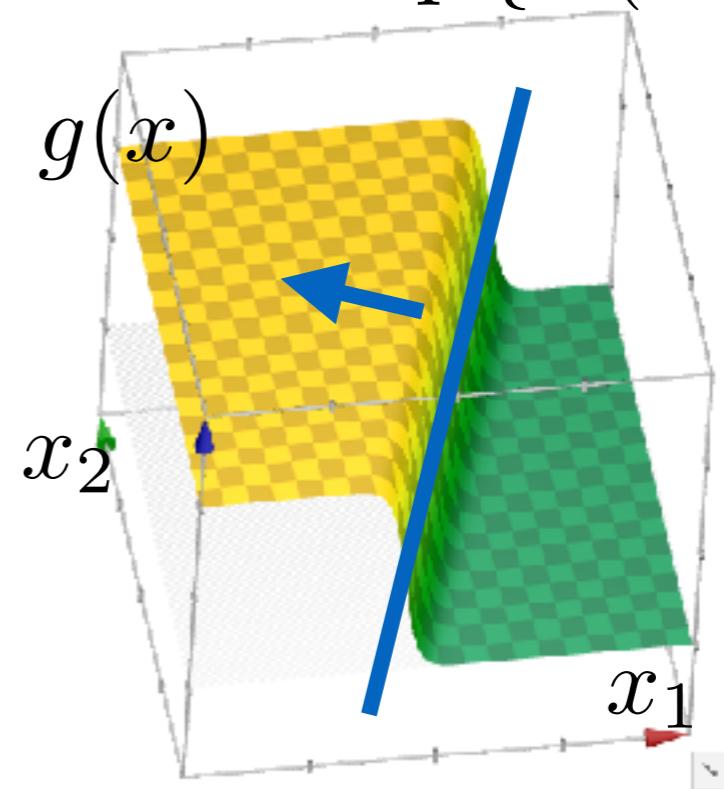
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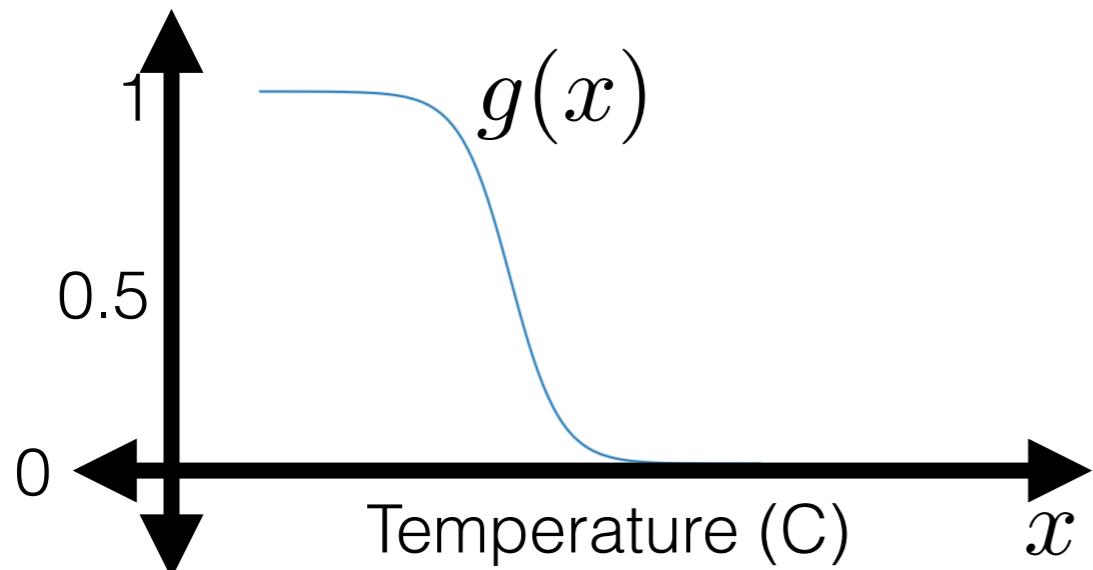
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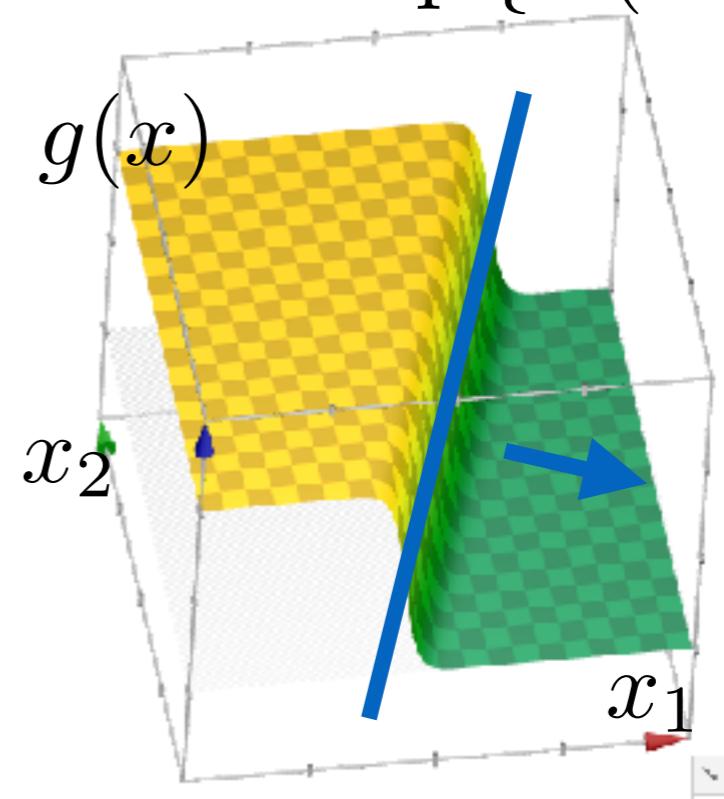
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+++ +++



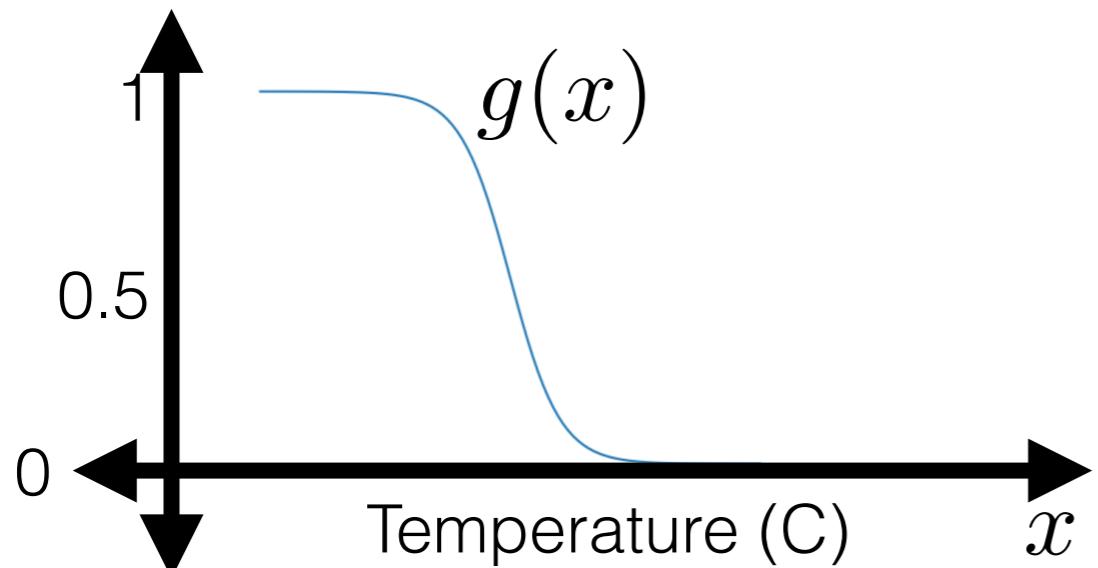
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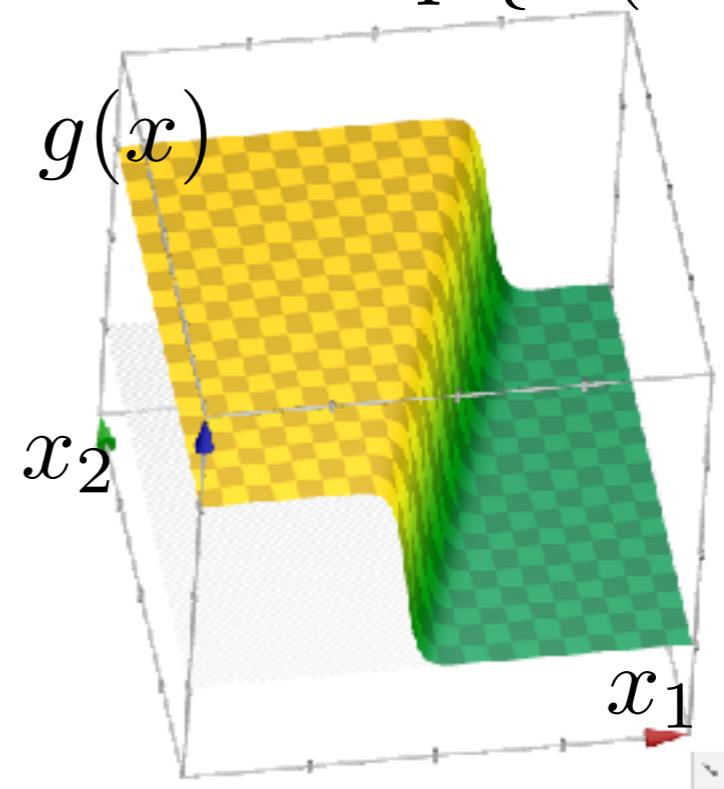
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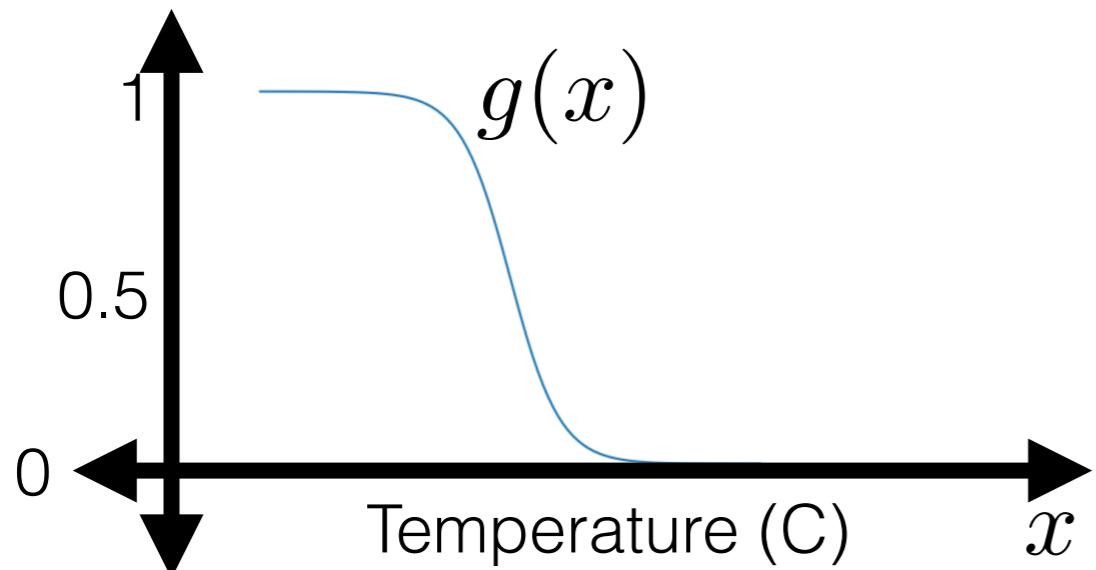
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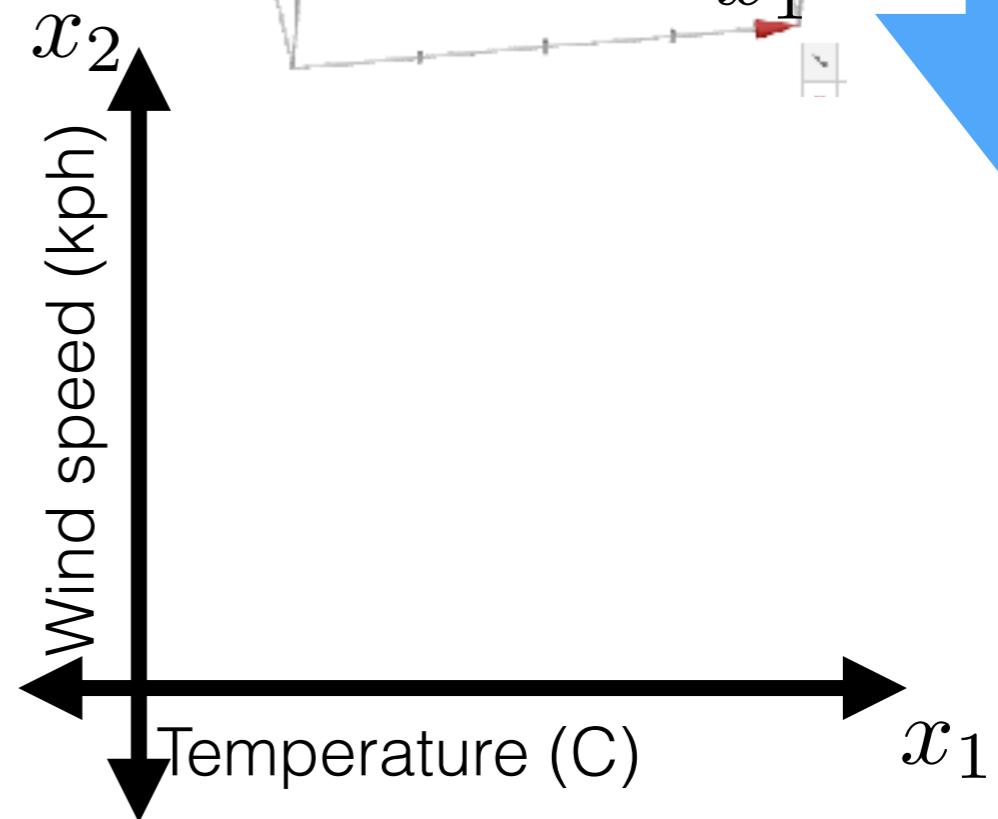
$$= \frac{1}{1 + \exp \{-(\theta^T x + \theta_0)\}}$$

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+++ +++



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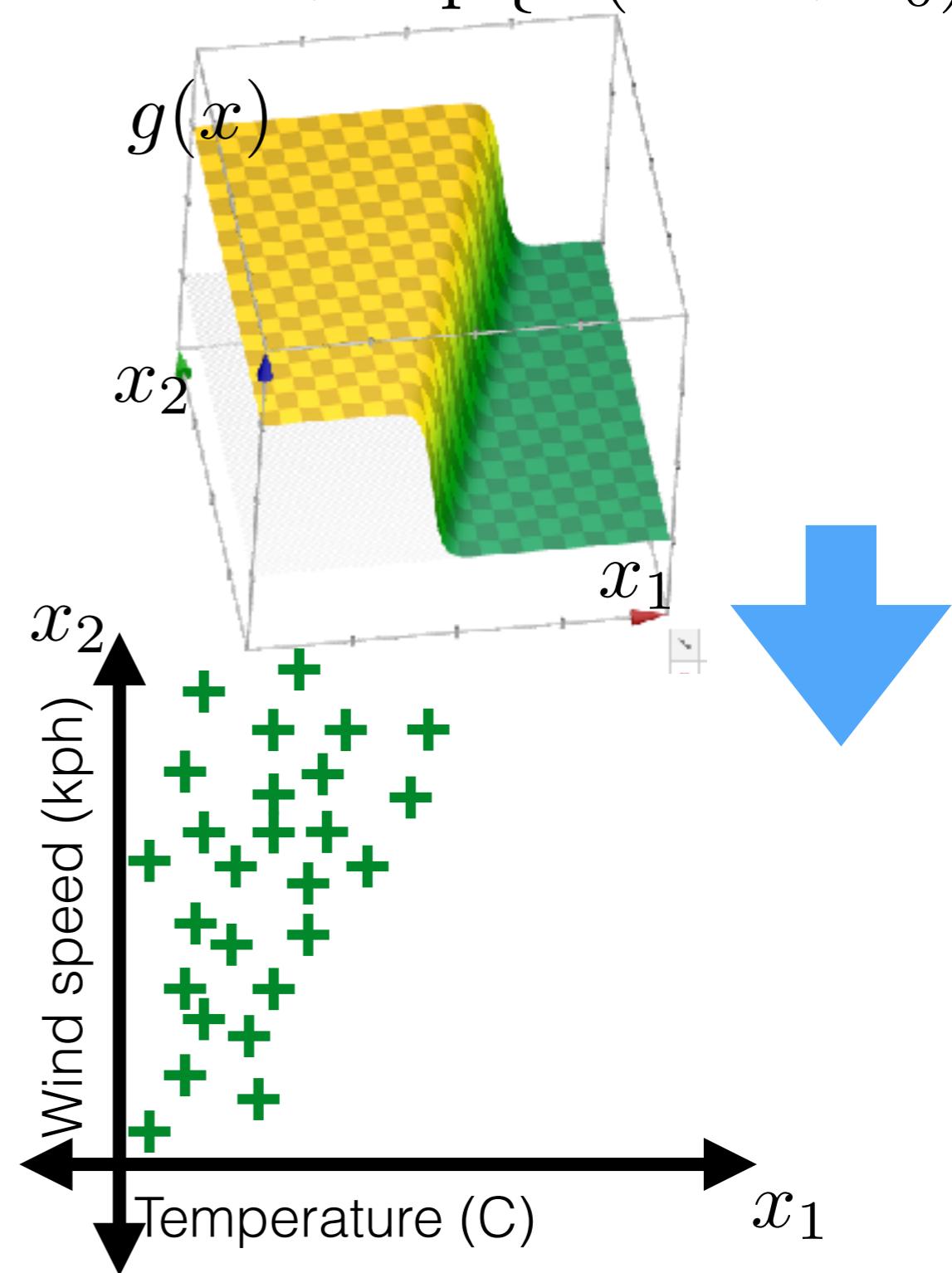
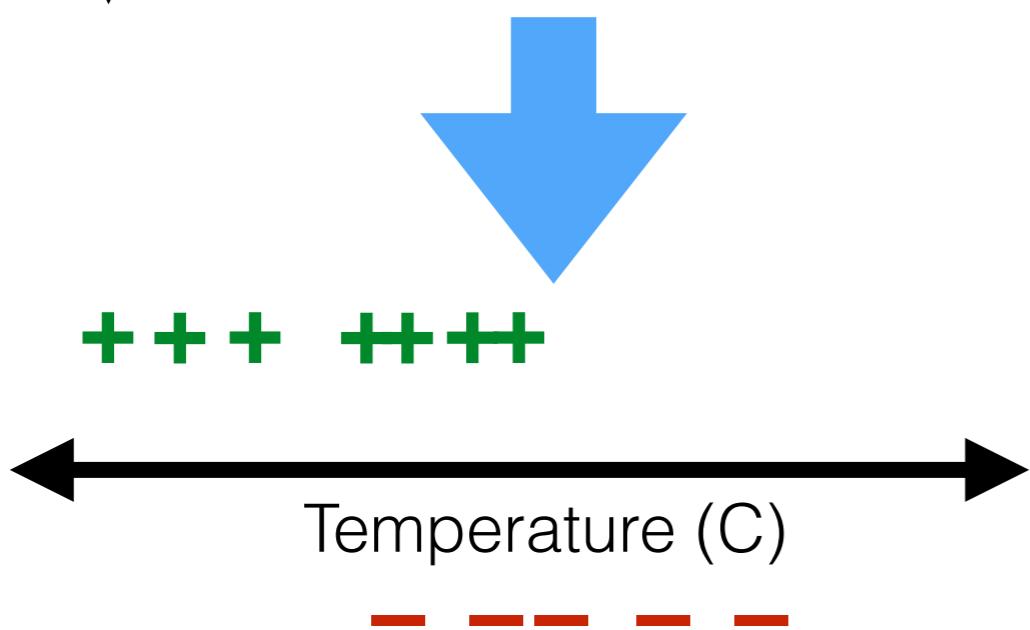
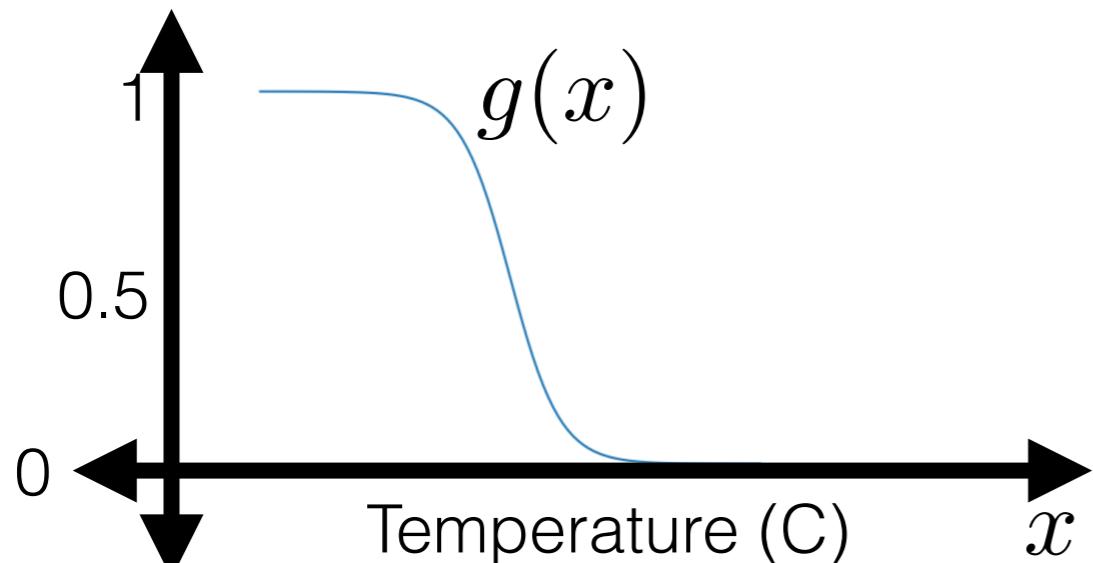
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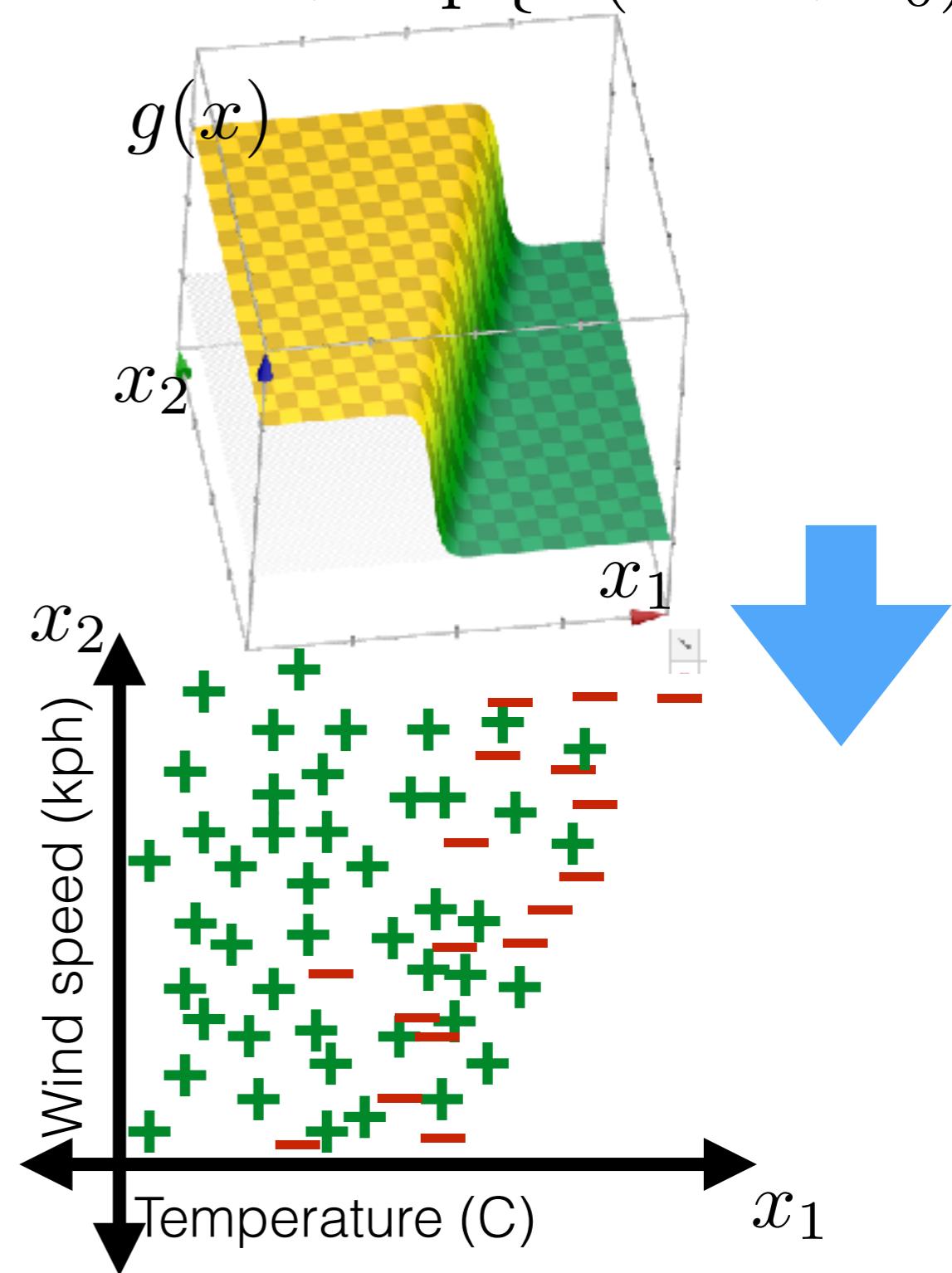
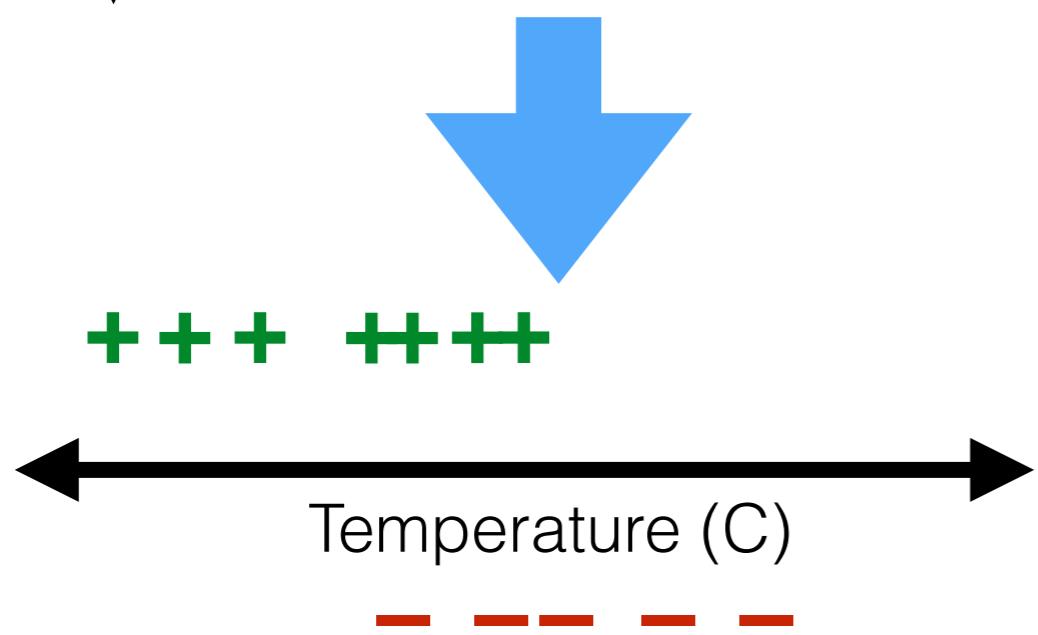
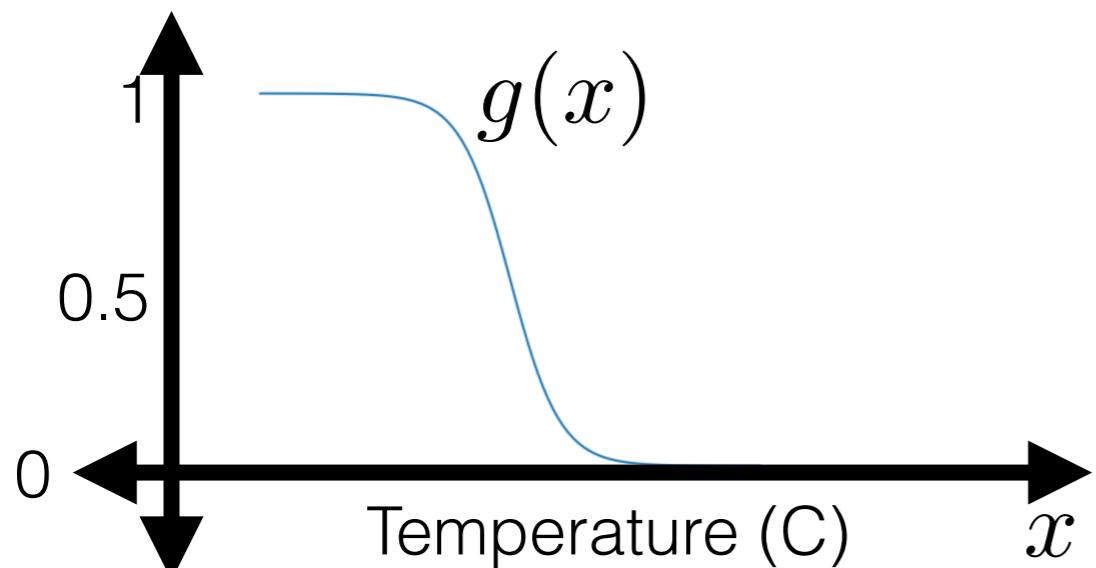
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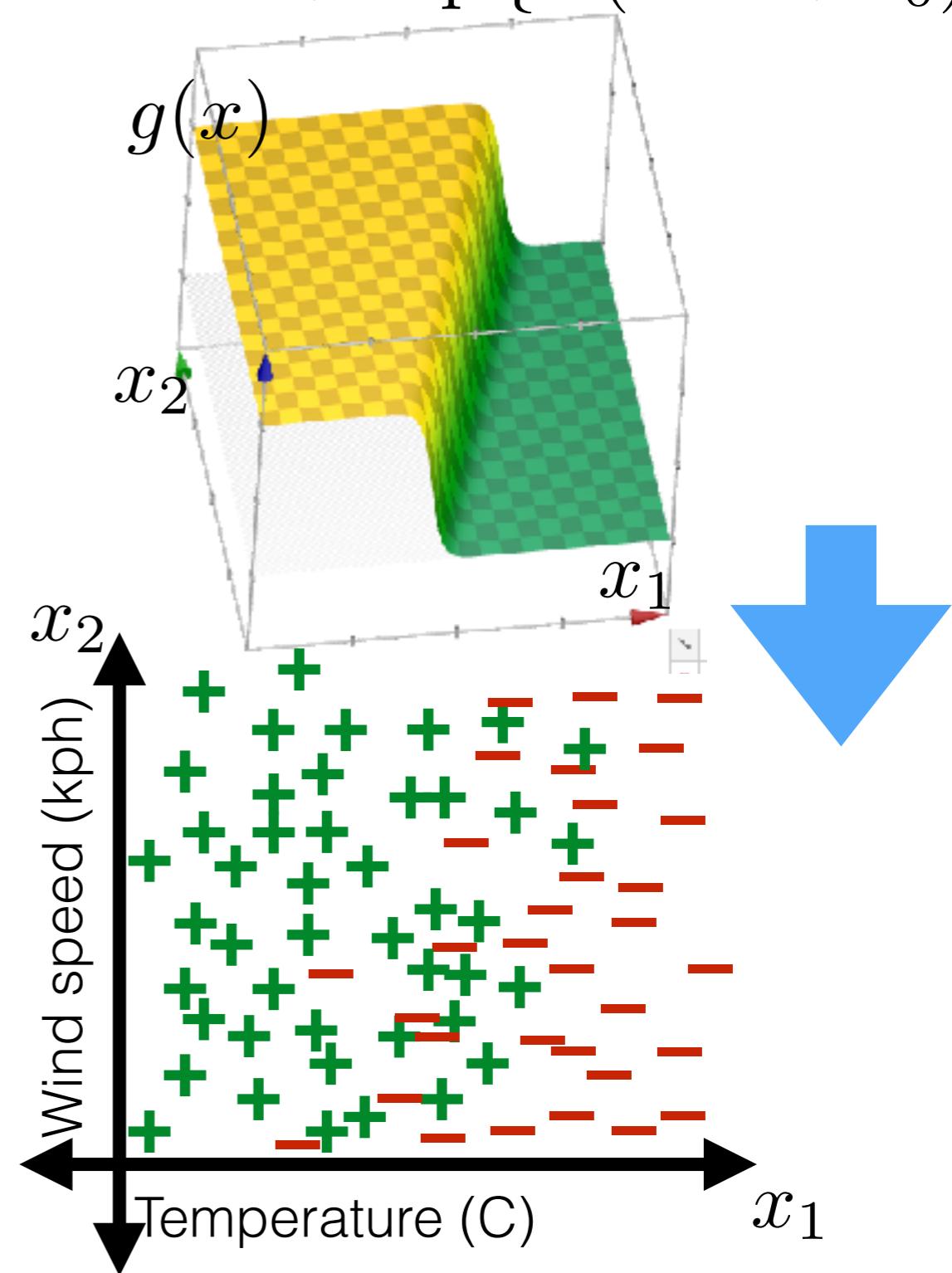
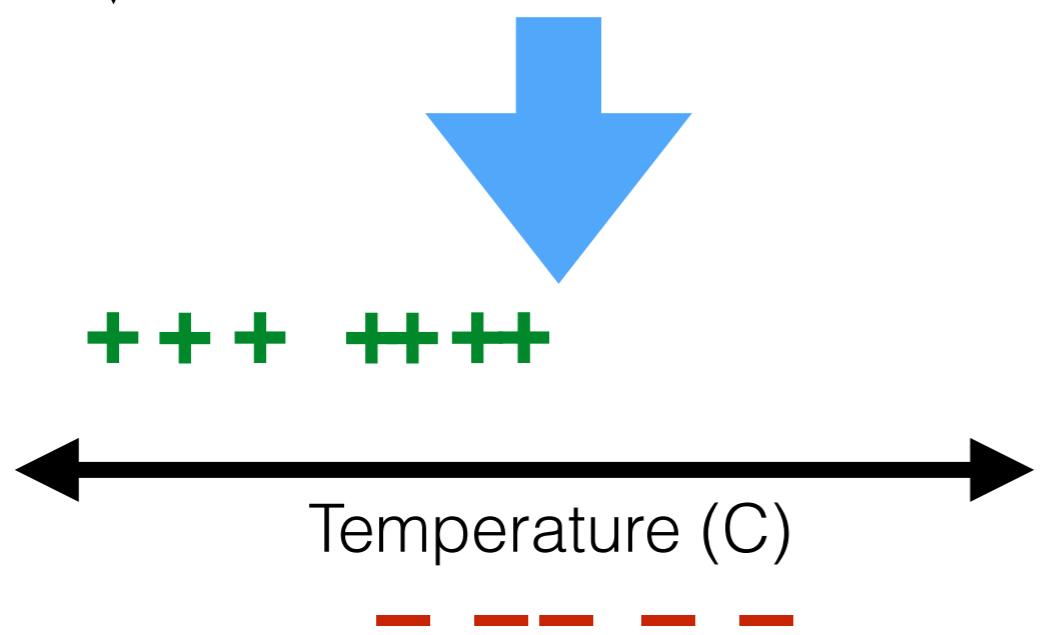
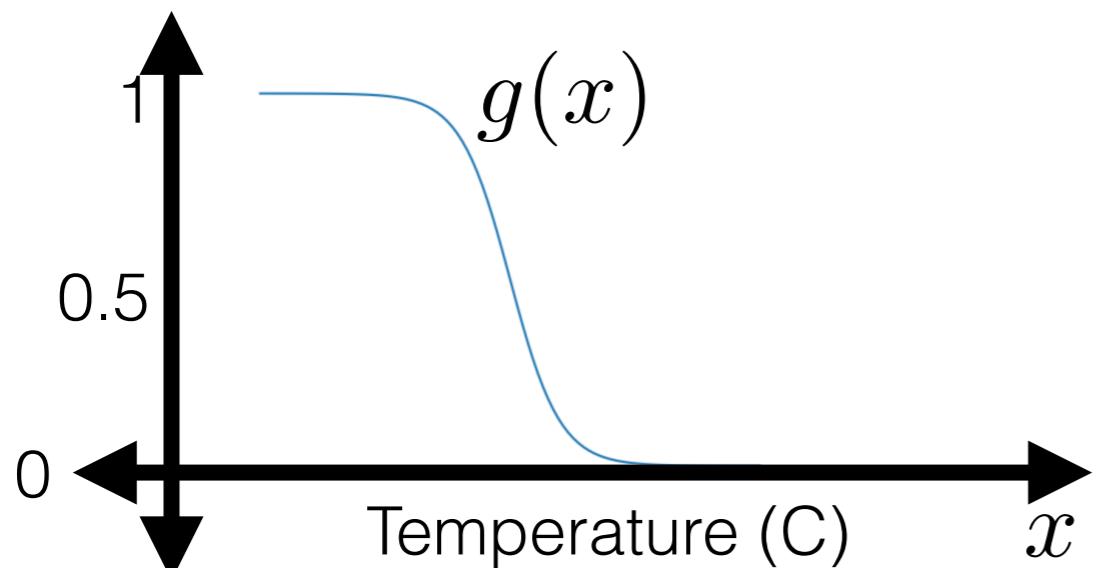
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# Linear logistic classification

aka logistic regression

# Linear logistic classification

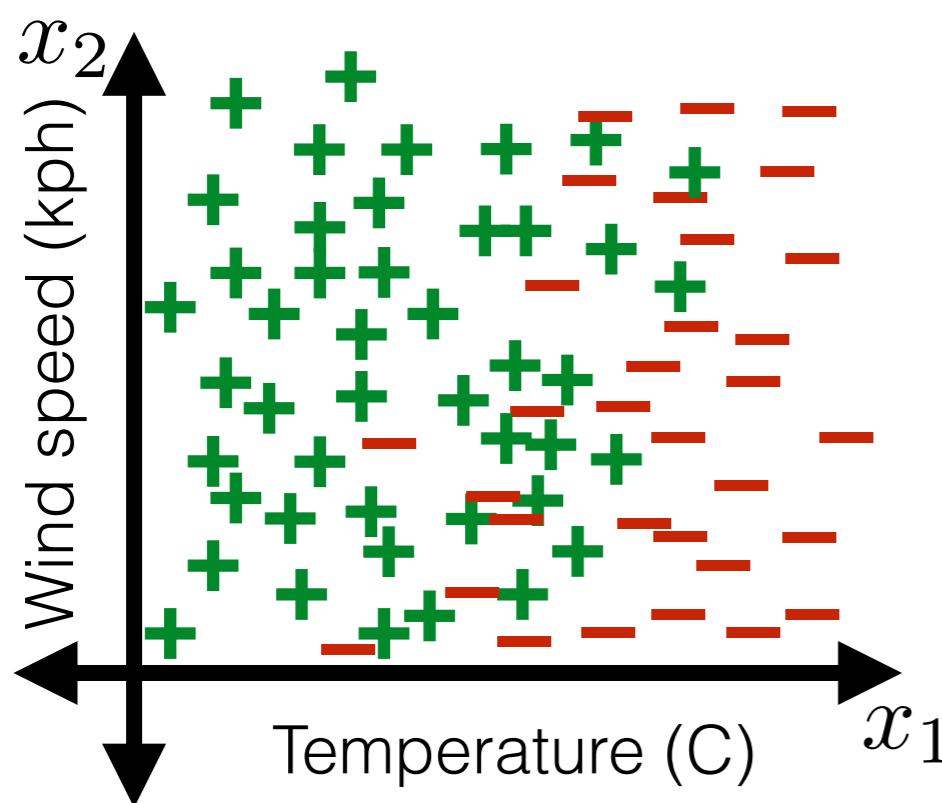
- How do we learn a classifier (i.e. learn  $\theta, \theta_0$ )?

aka logistic regression

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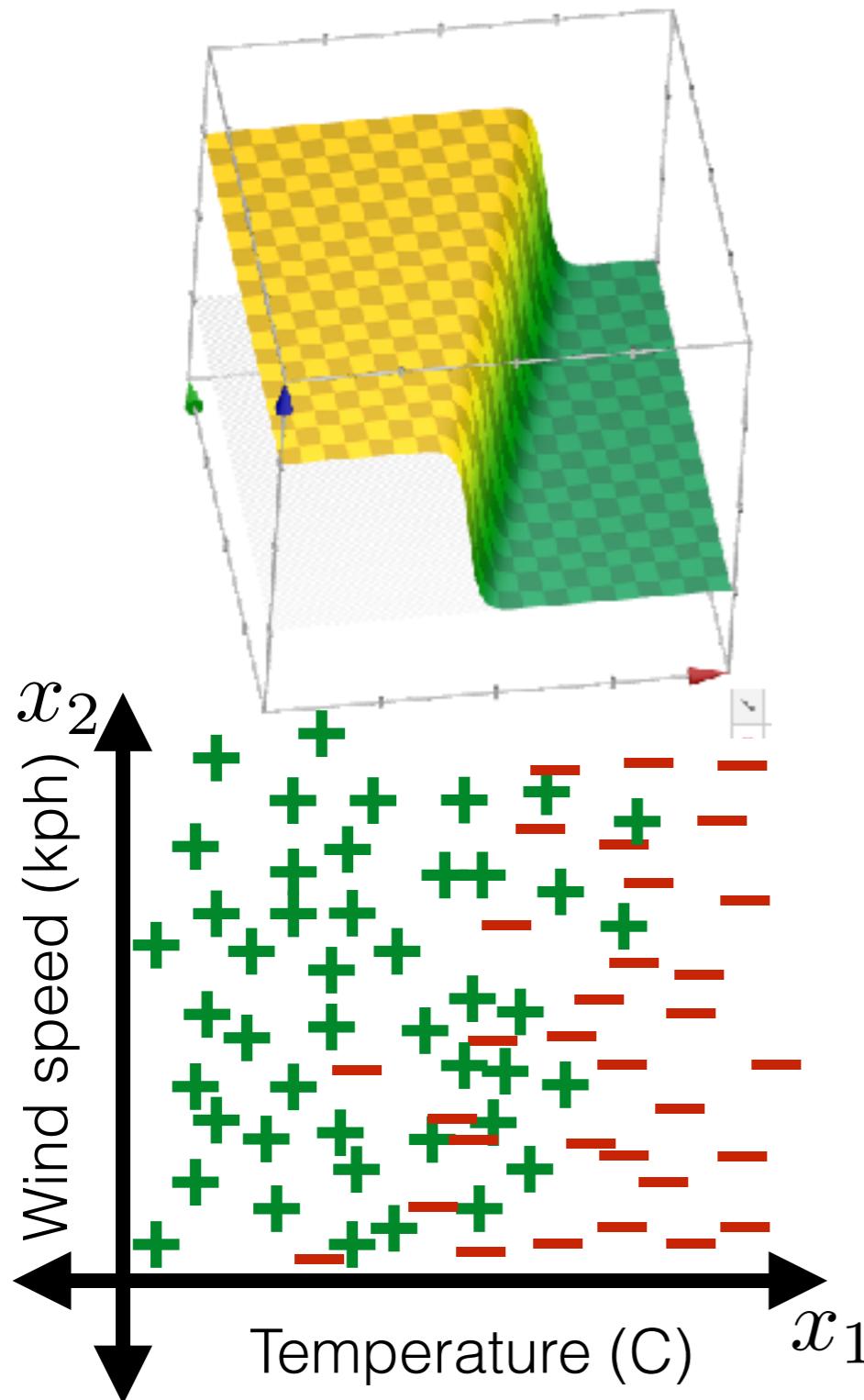
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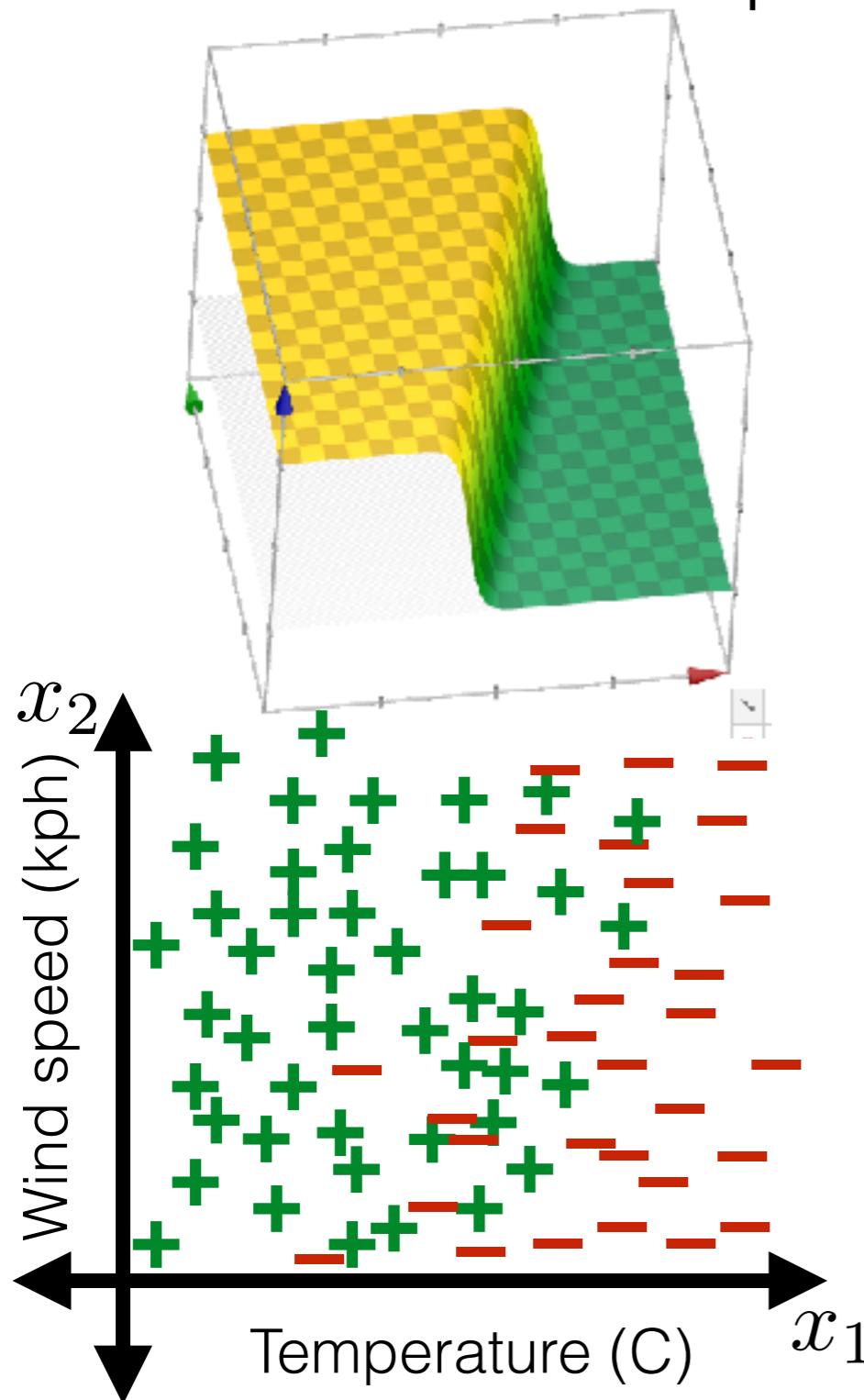
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# Linear logistic classification

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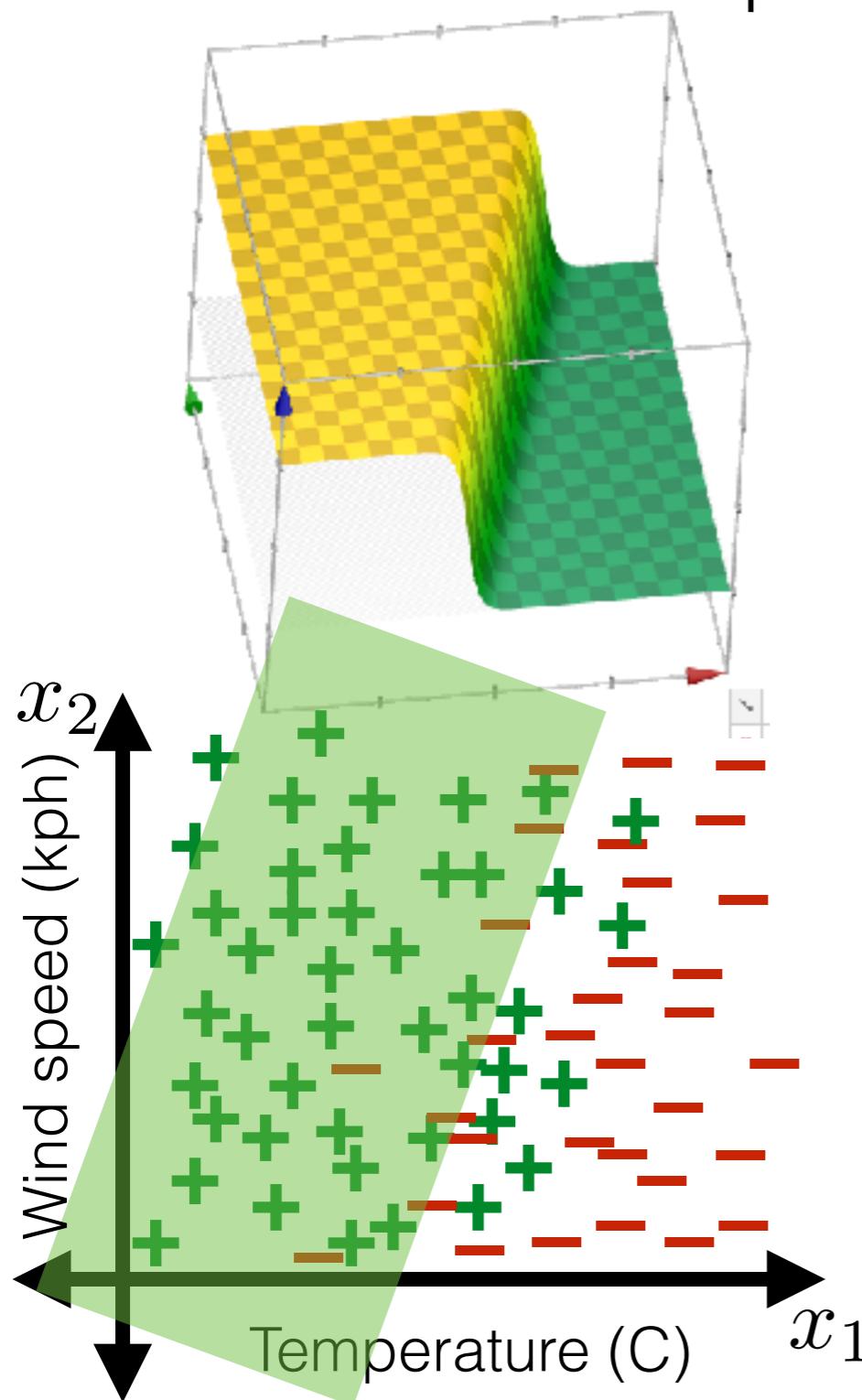
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# Linear logistic classification

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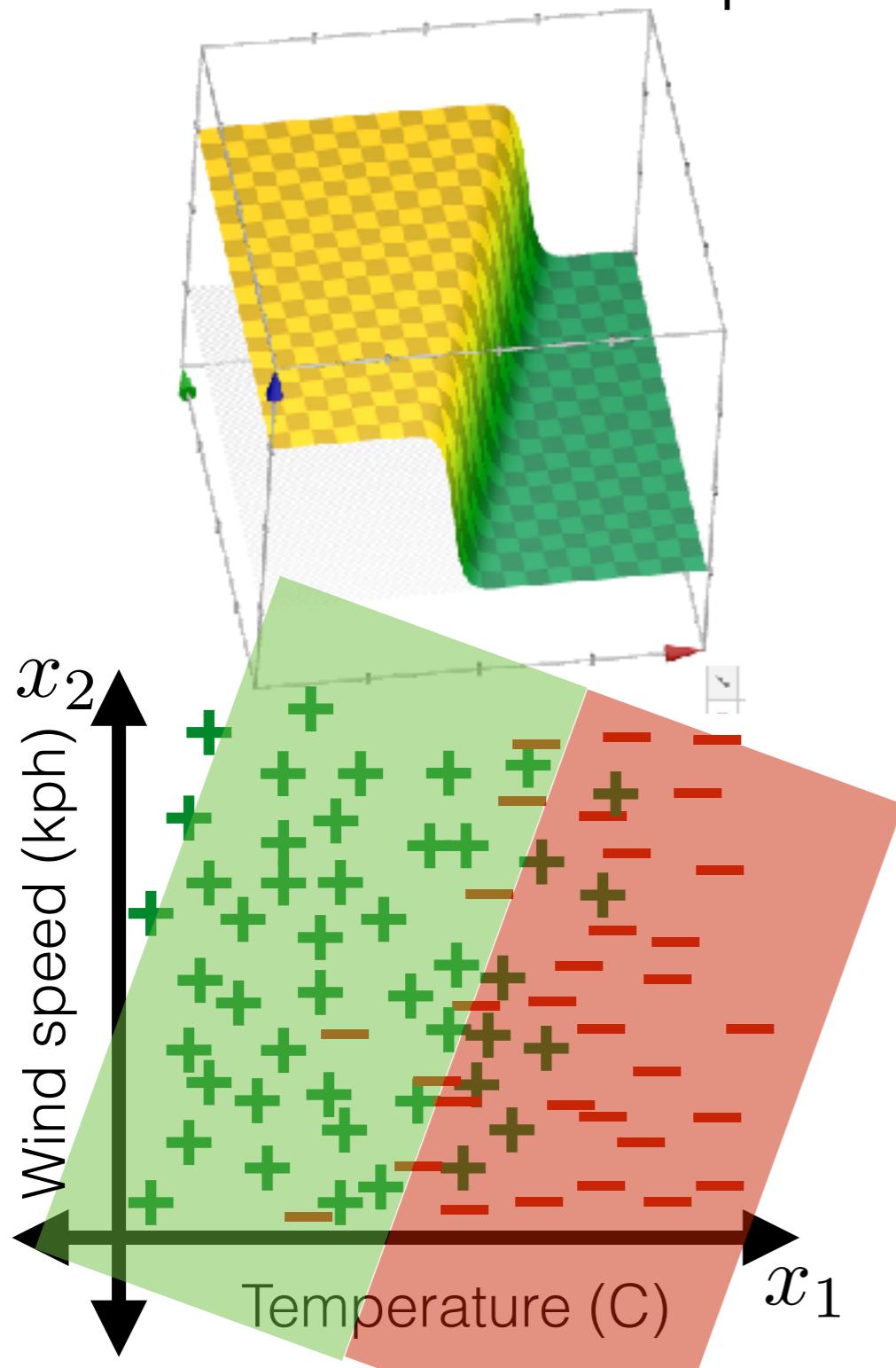
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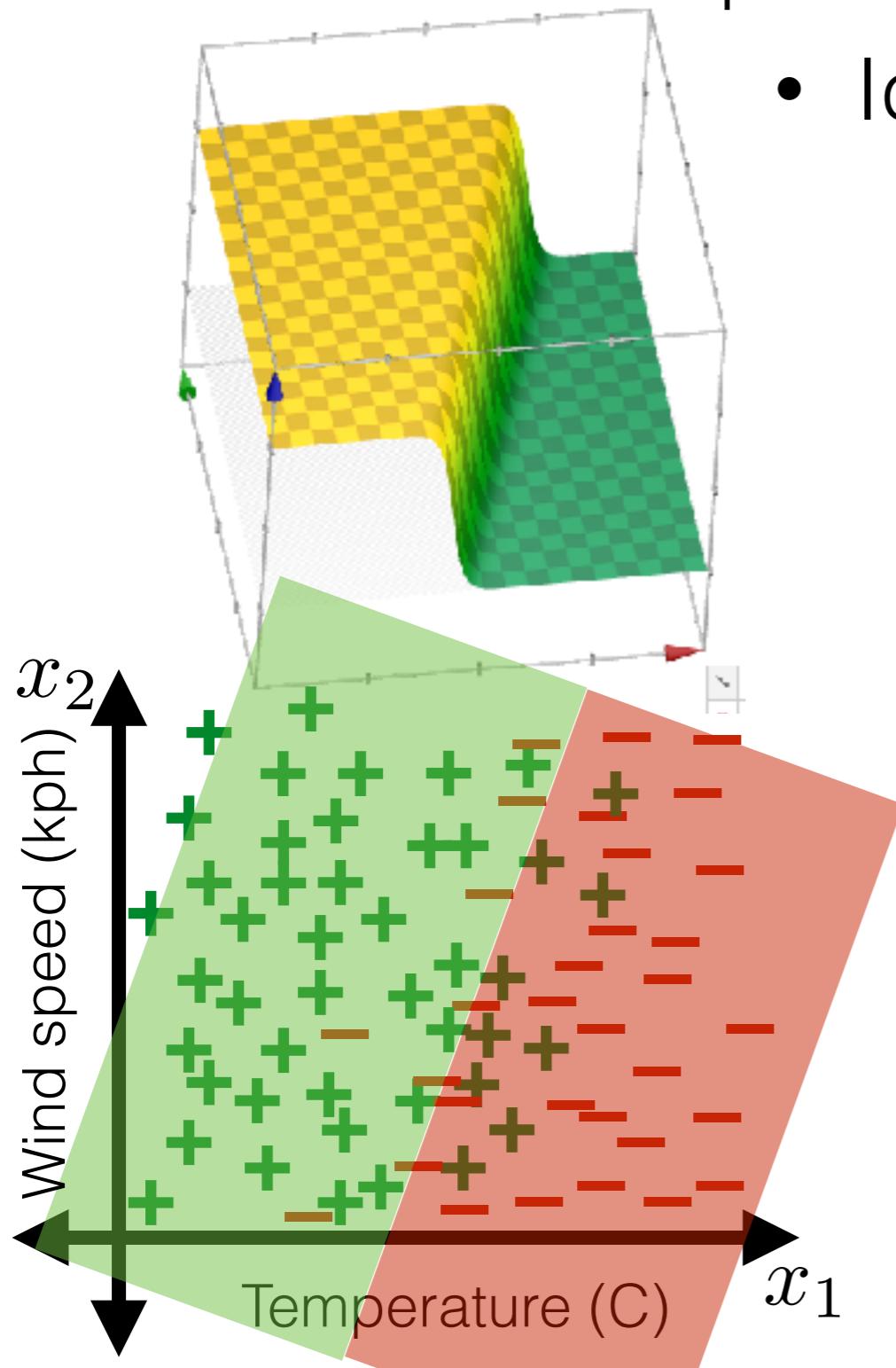


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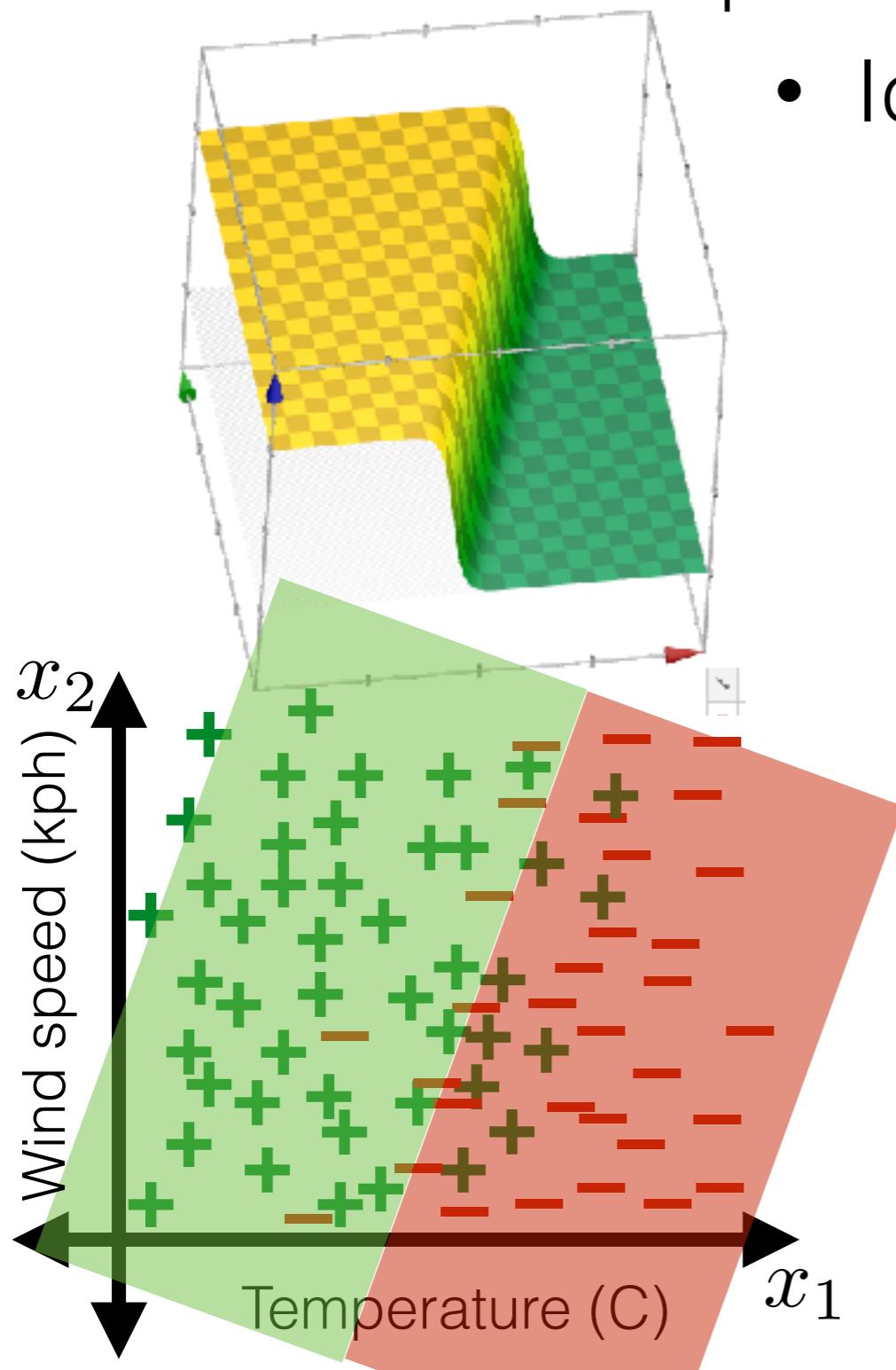
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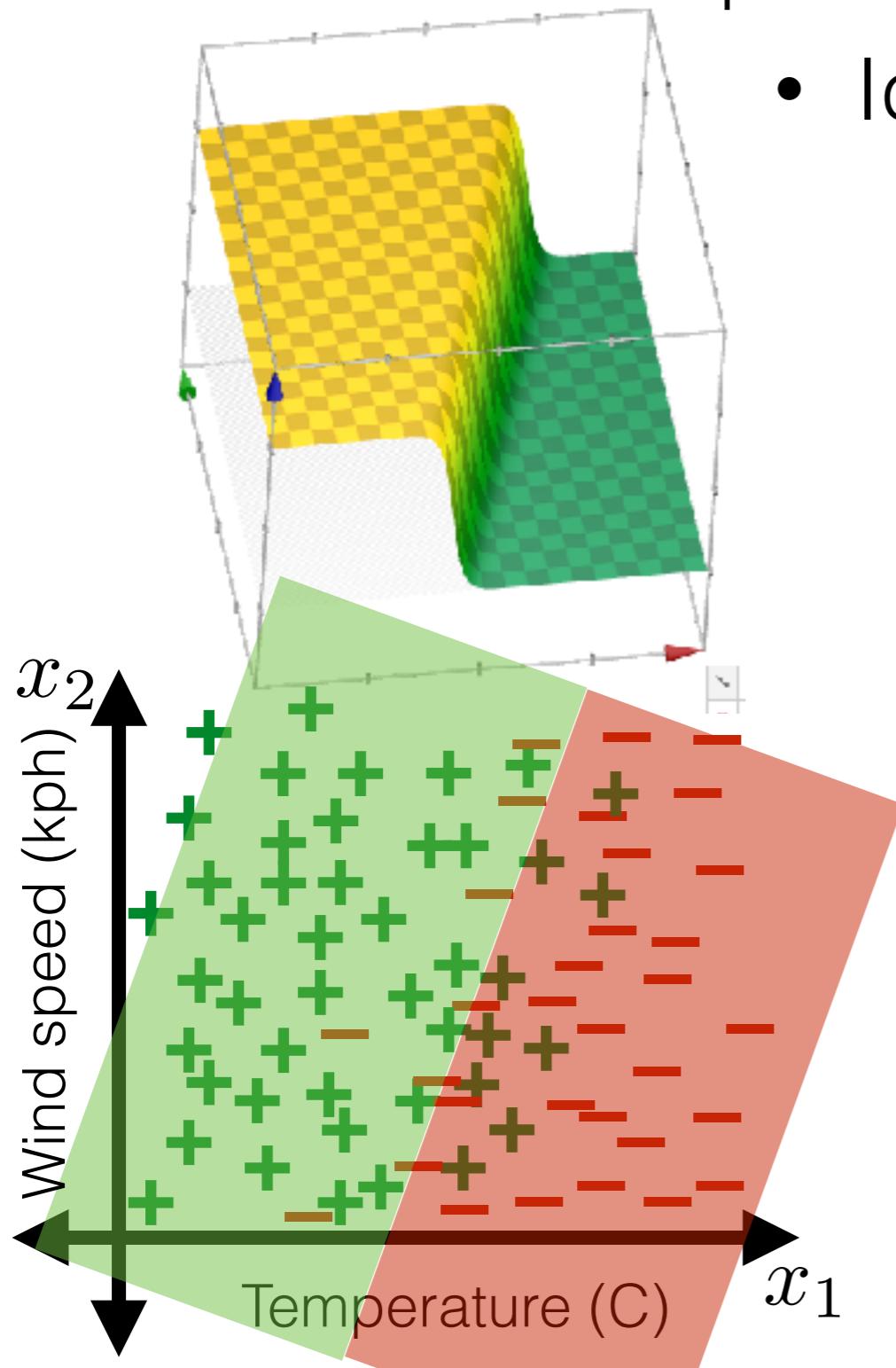


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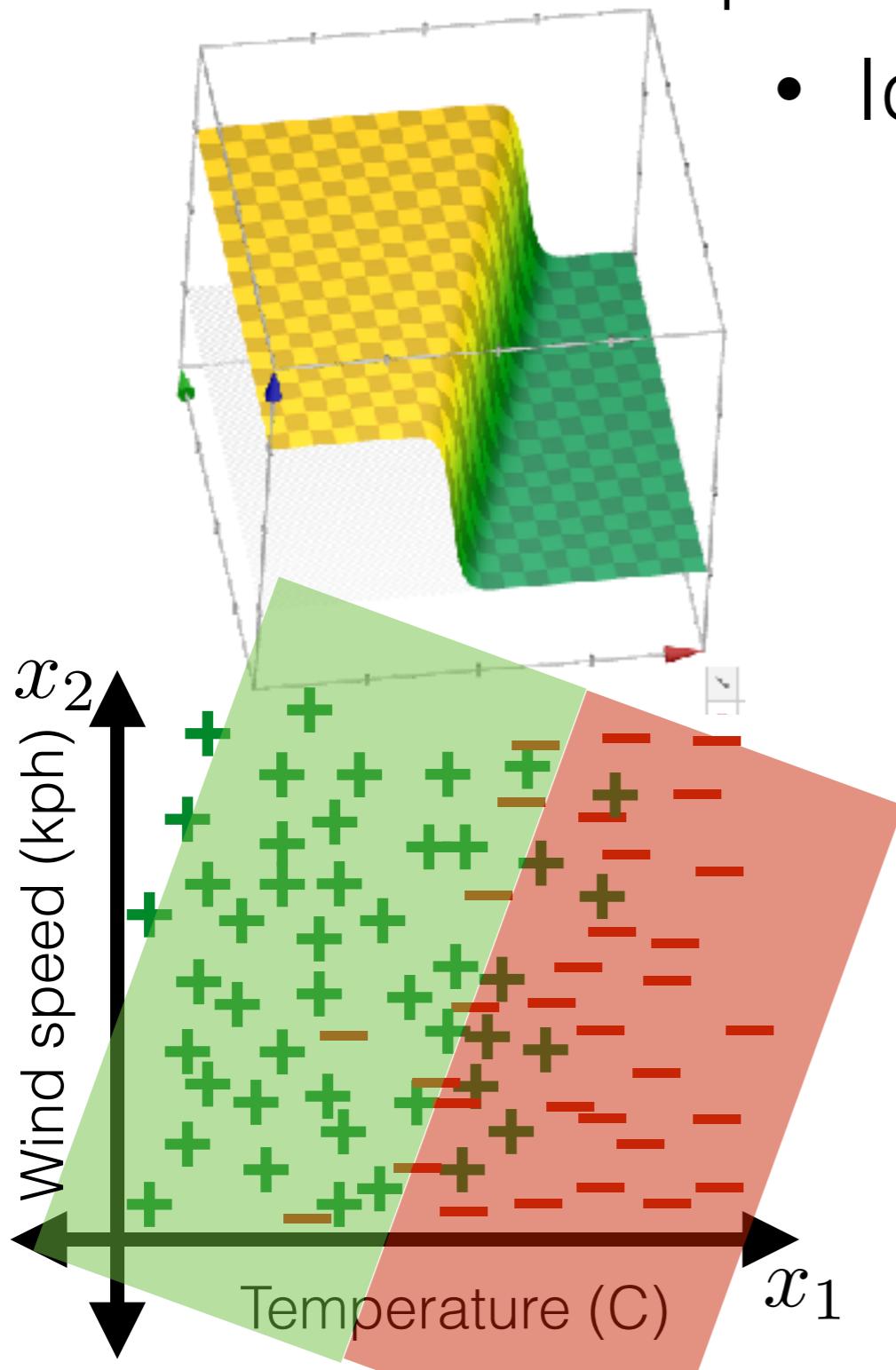
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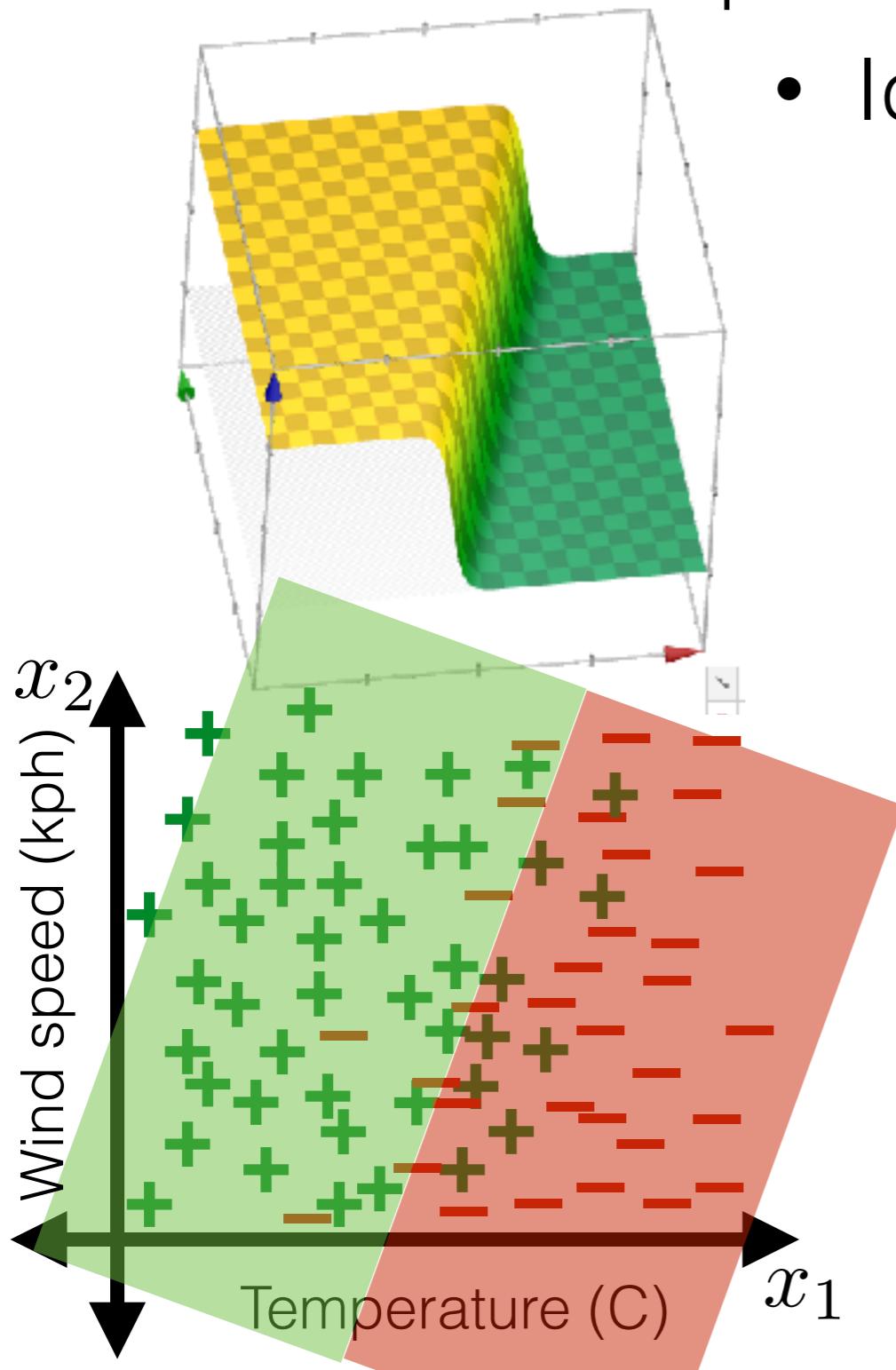


- Idea: predict +1 if: probability  $> 0.5$   
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$$\frac{1}{1 + \exp\{-(\theta^\top x + \theta_0)\}} > 0.5$$

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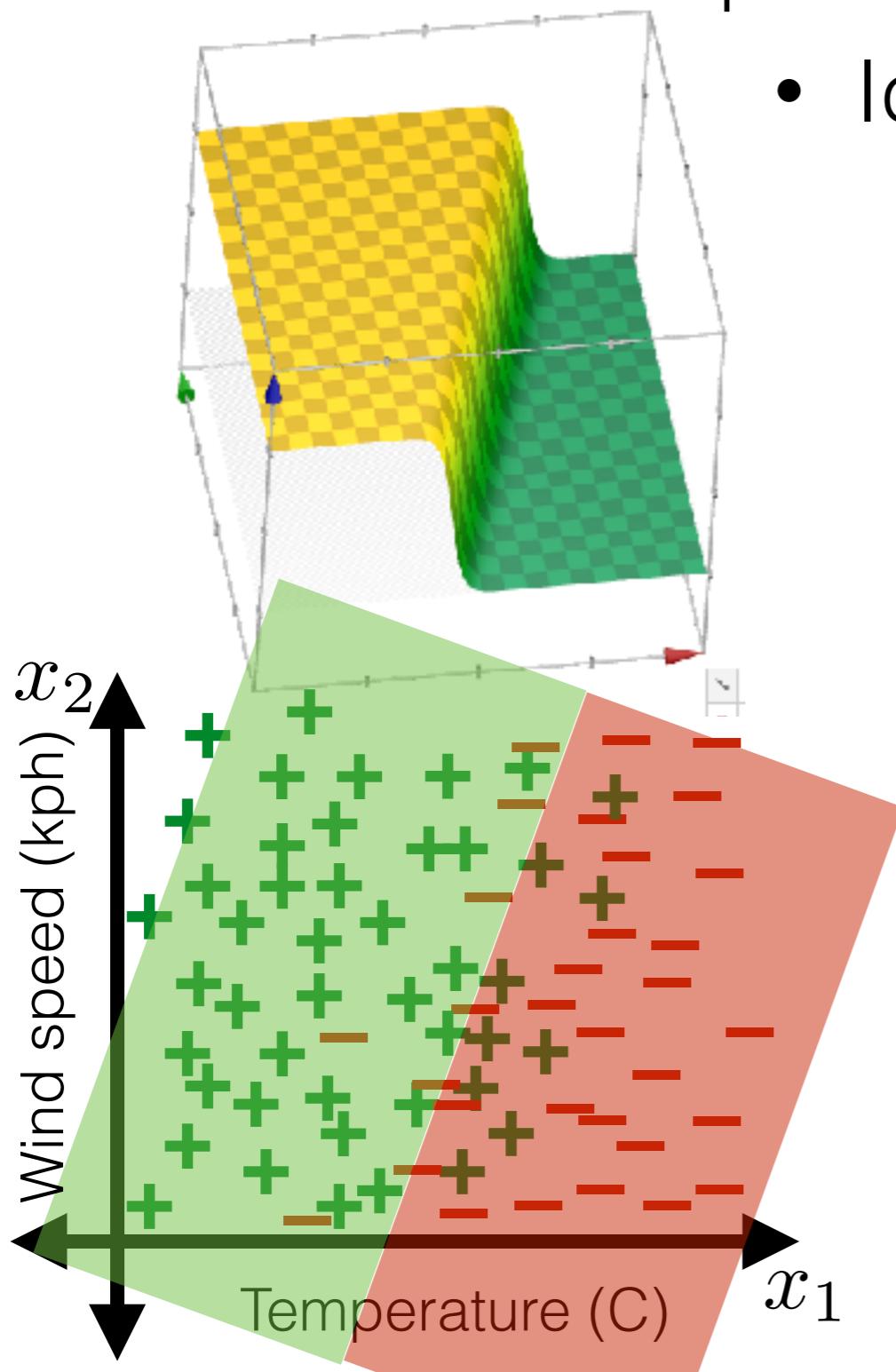


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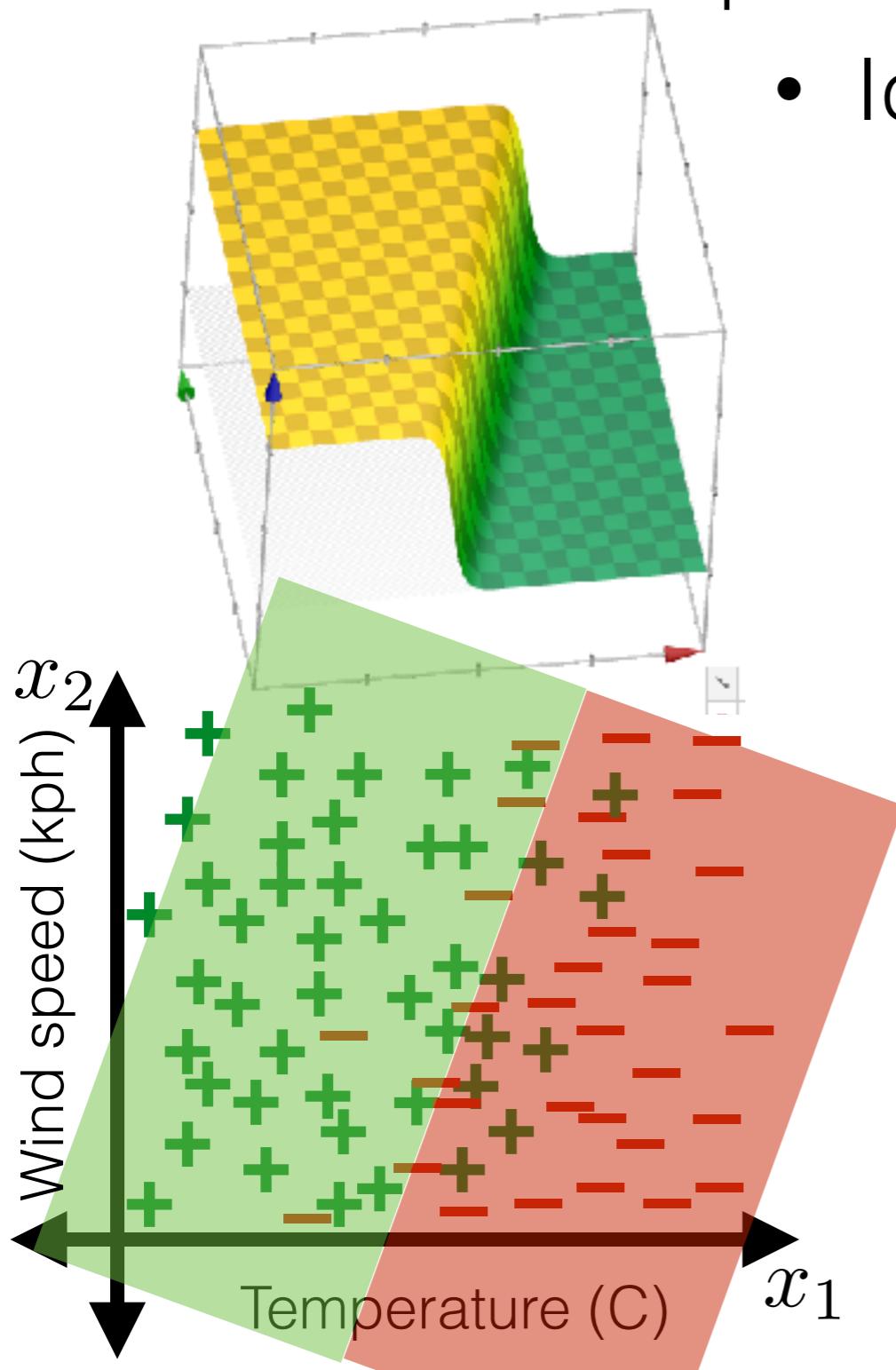


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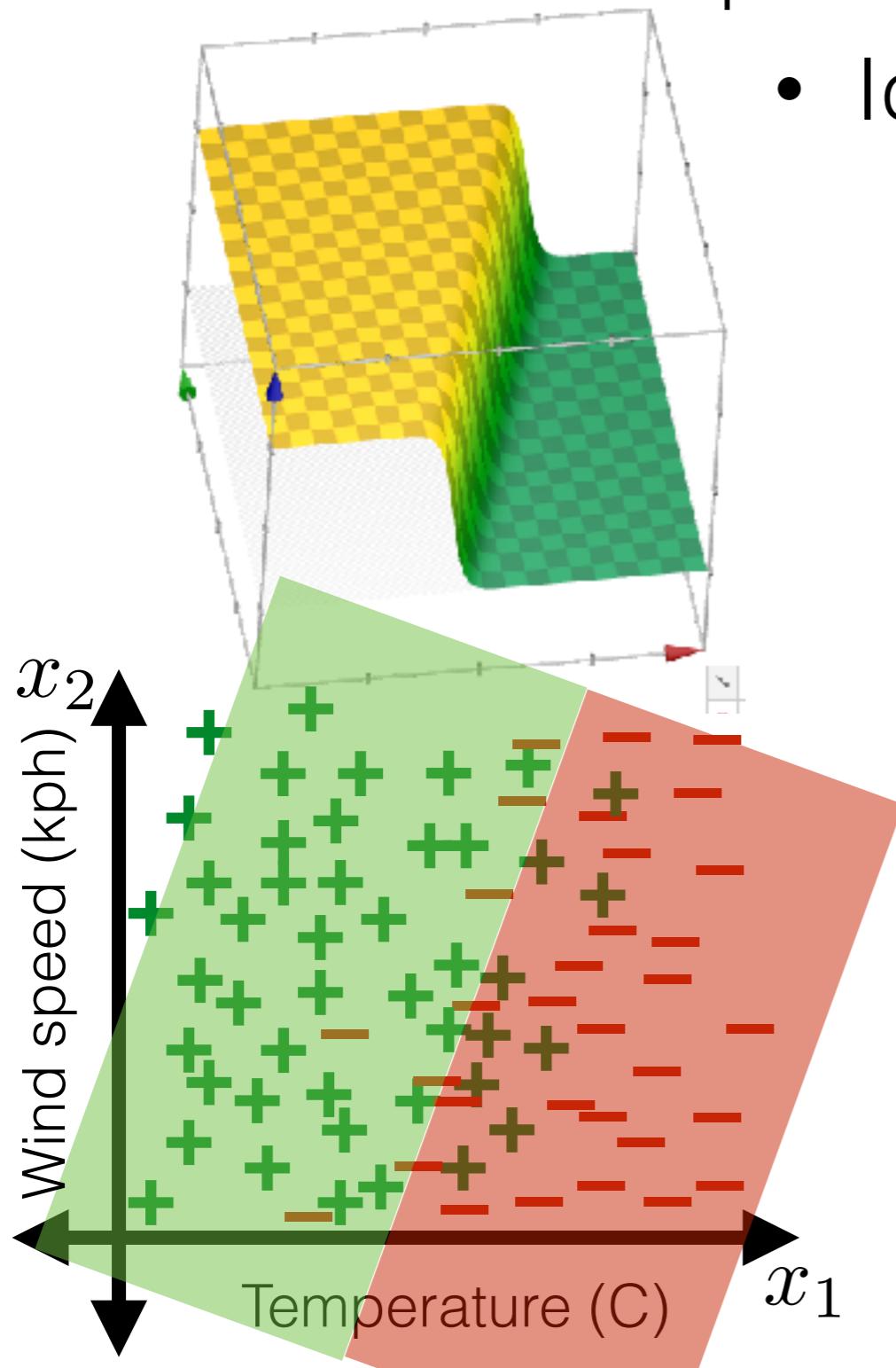


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$$\exp\{-(\theta^\top x + \theta_0)\} < 1$$
  
$$\theta^\top x + \theta_0 > 0$$
- Same hypothesis class as before!

# Linear logistic classification

aka logistic regression

- How do we learn a classifier (i.e. learn  $\theta, \theta_0$ )?
- How do we make predictions?

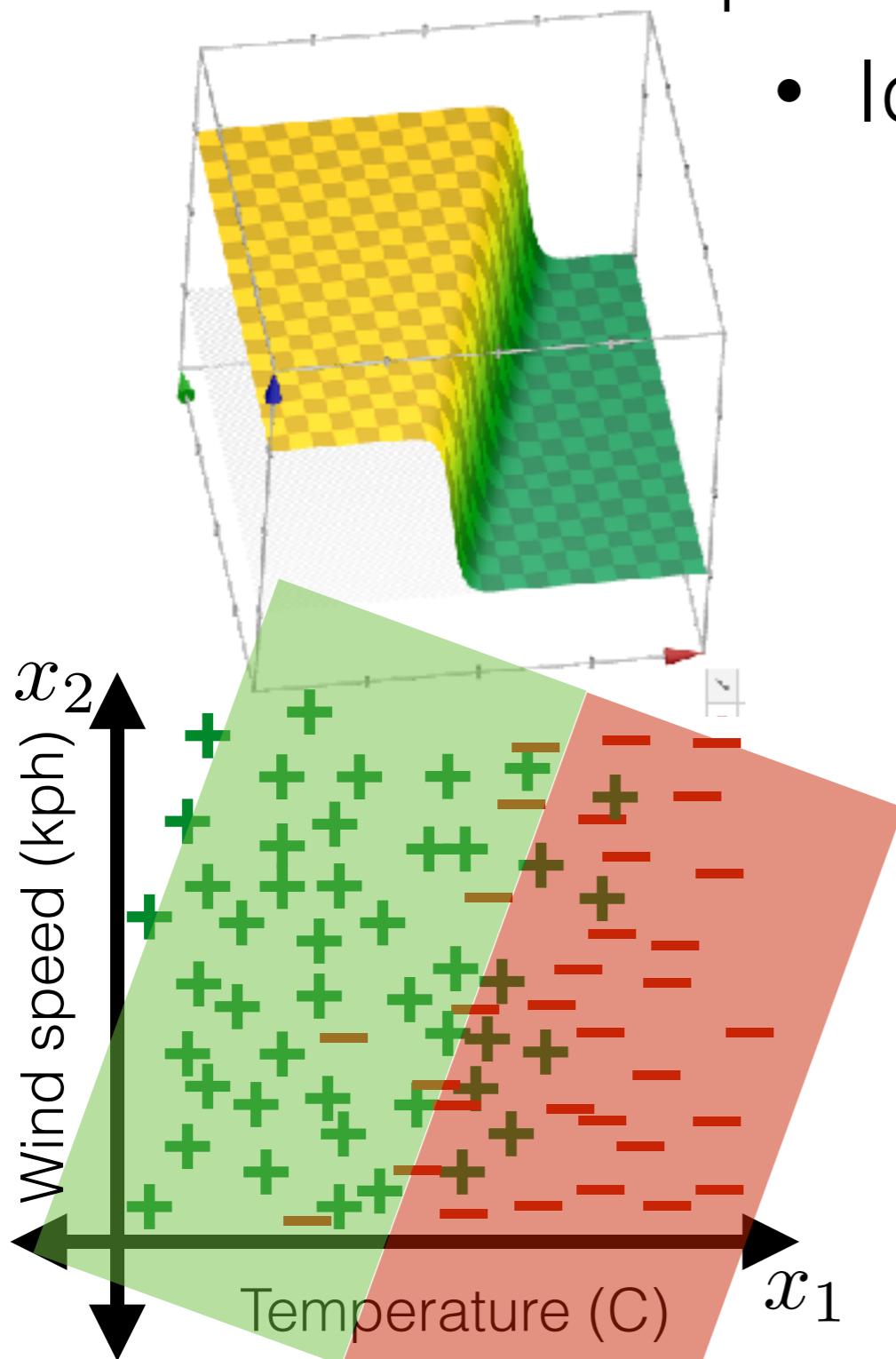


- Idea: predict +1 if: probability  $> 0.5$   
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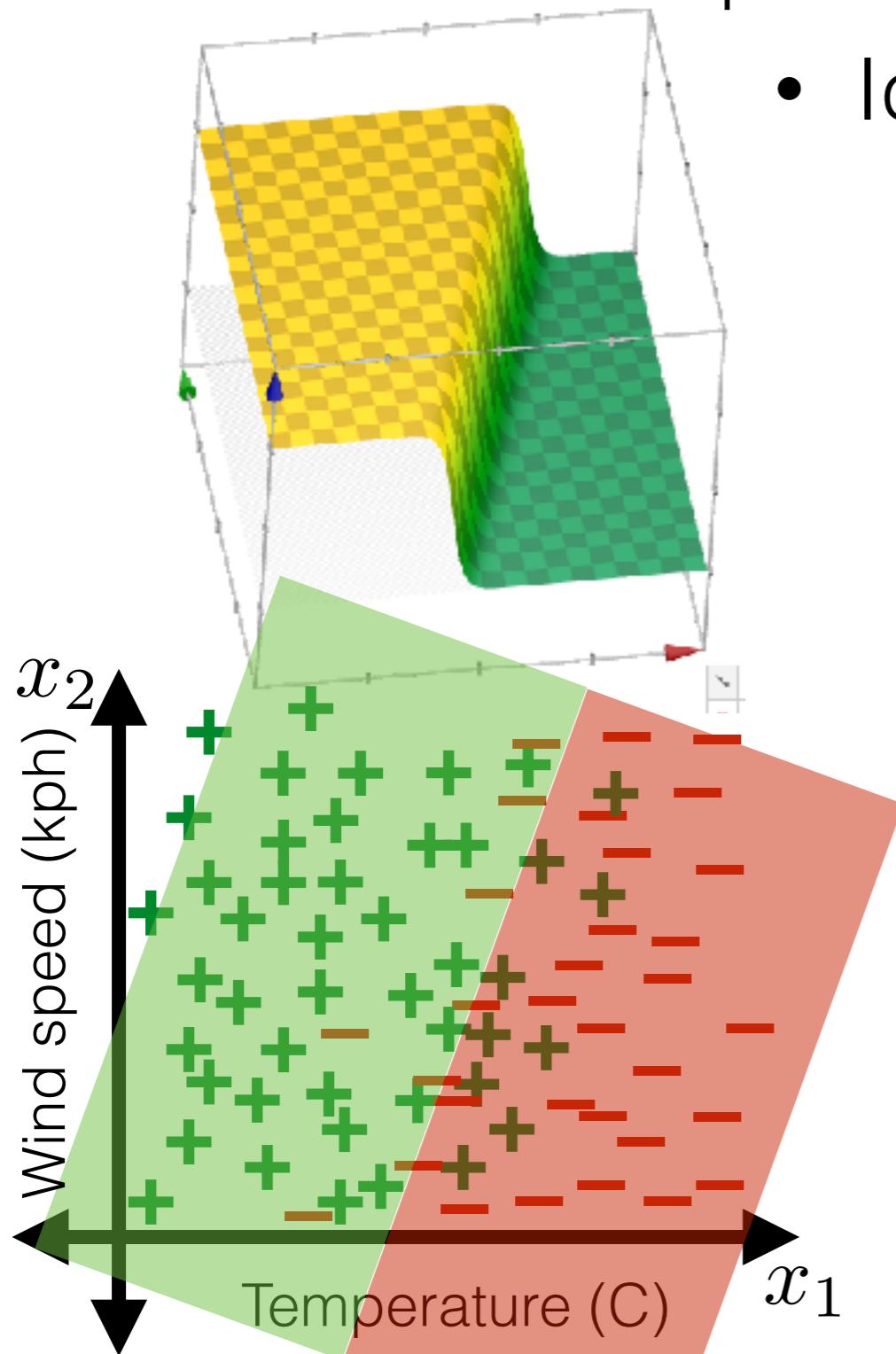


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- Same hypothesis class as before! But we will get:
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  - Quality guarantees when data not linearly separable

# Linear logistic classification

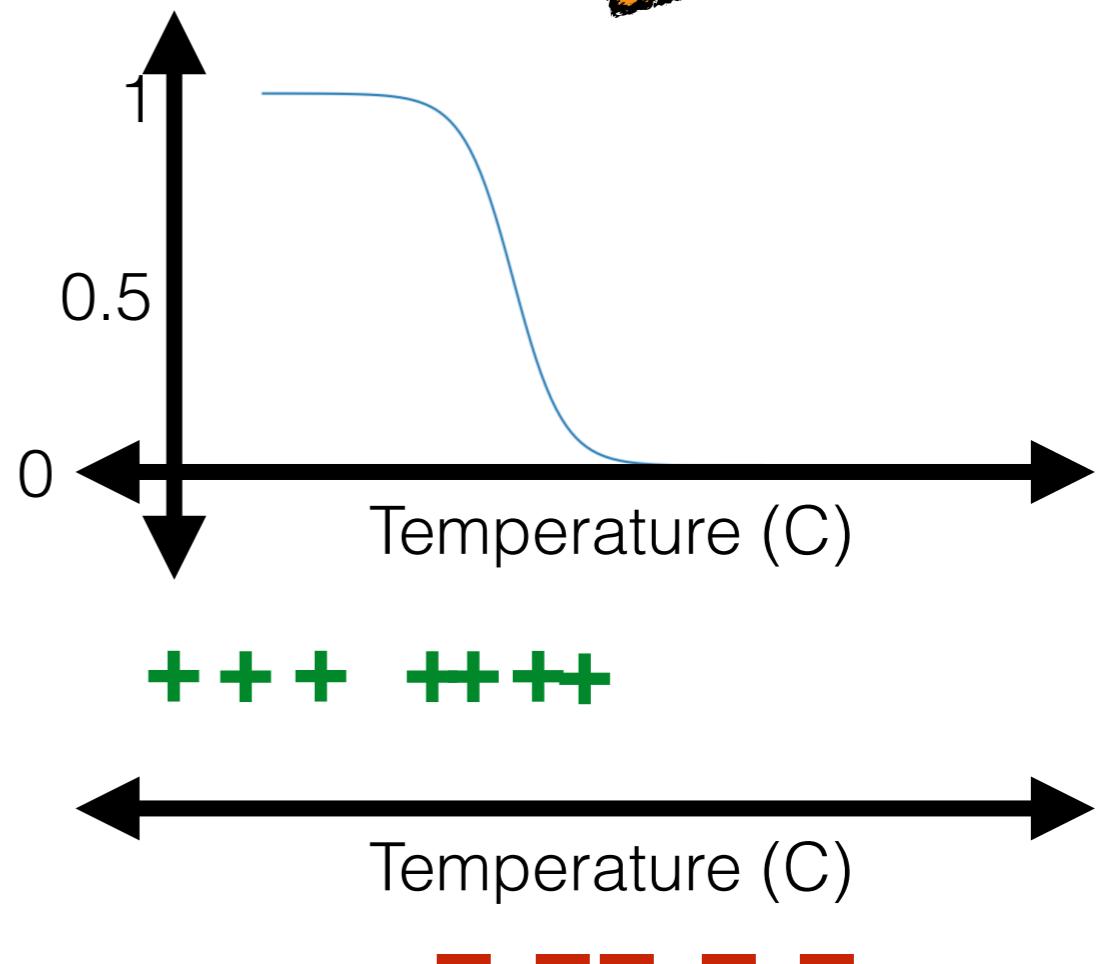
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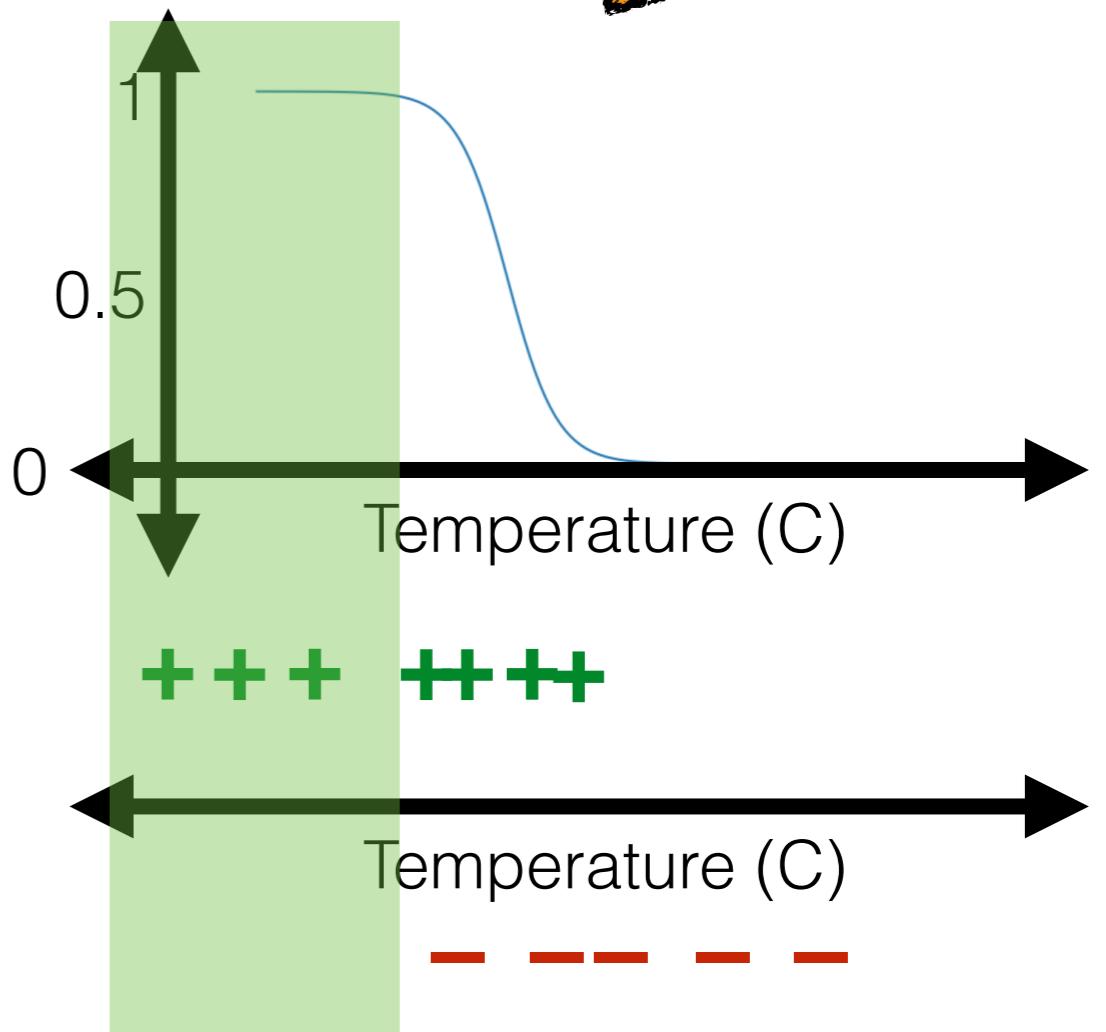
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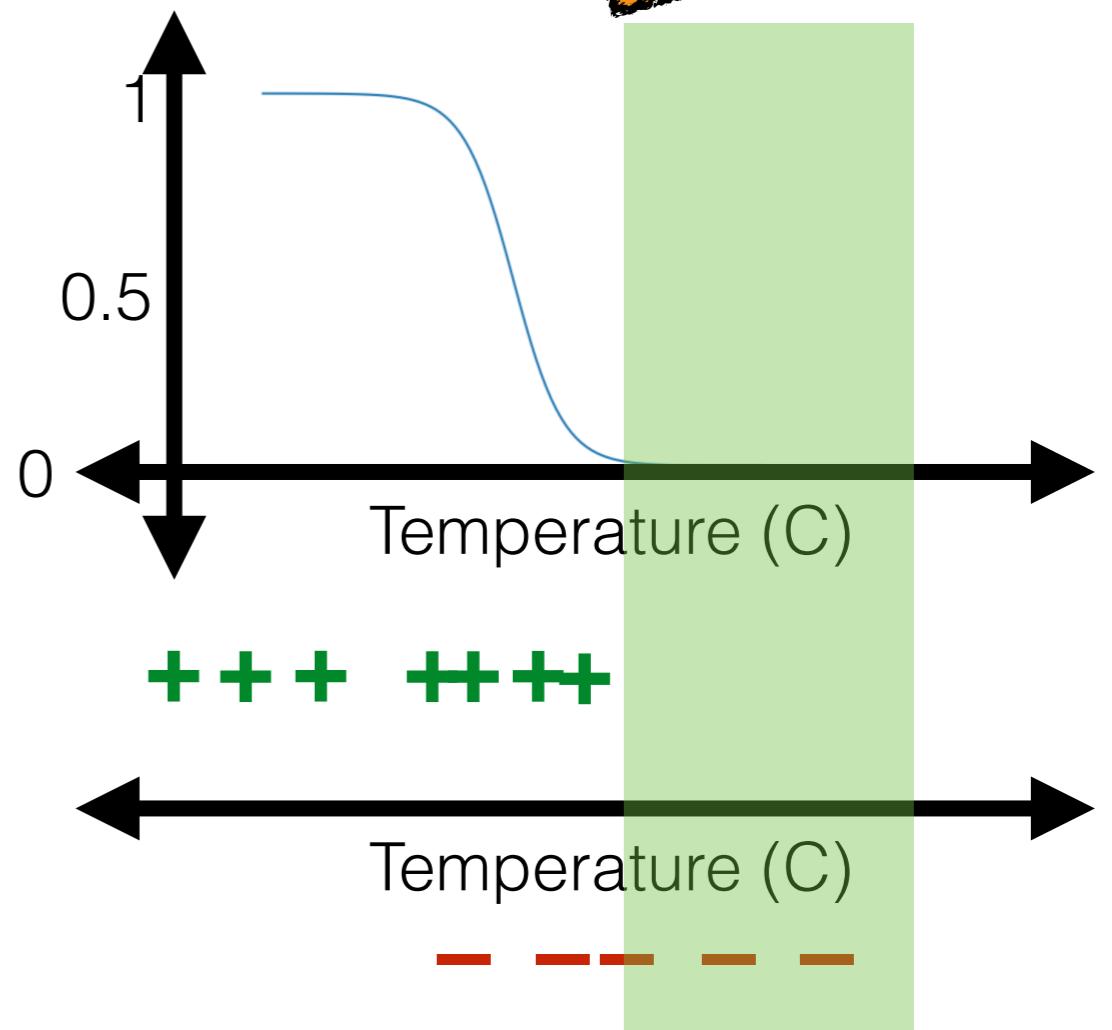
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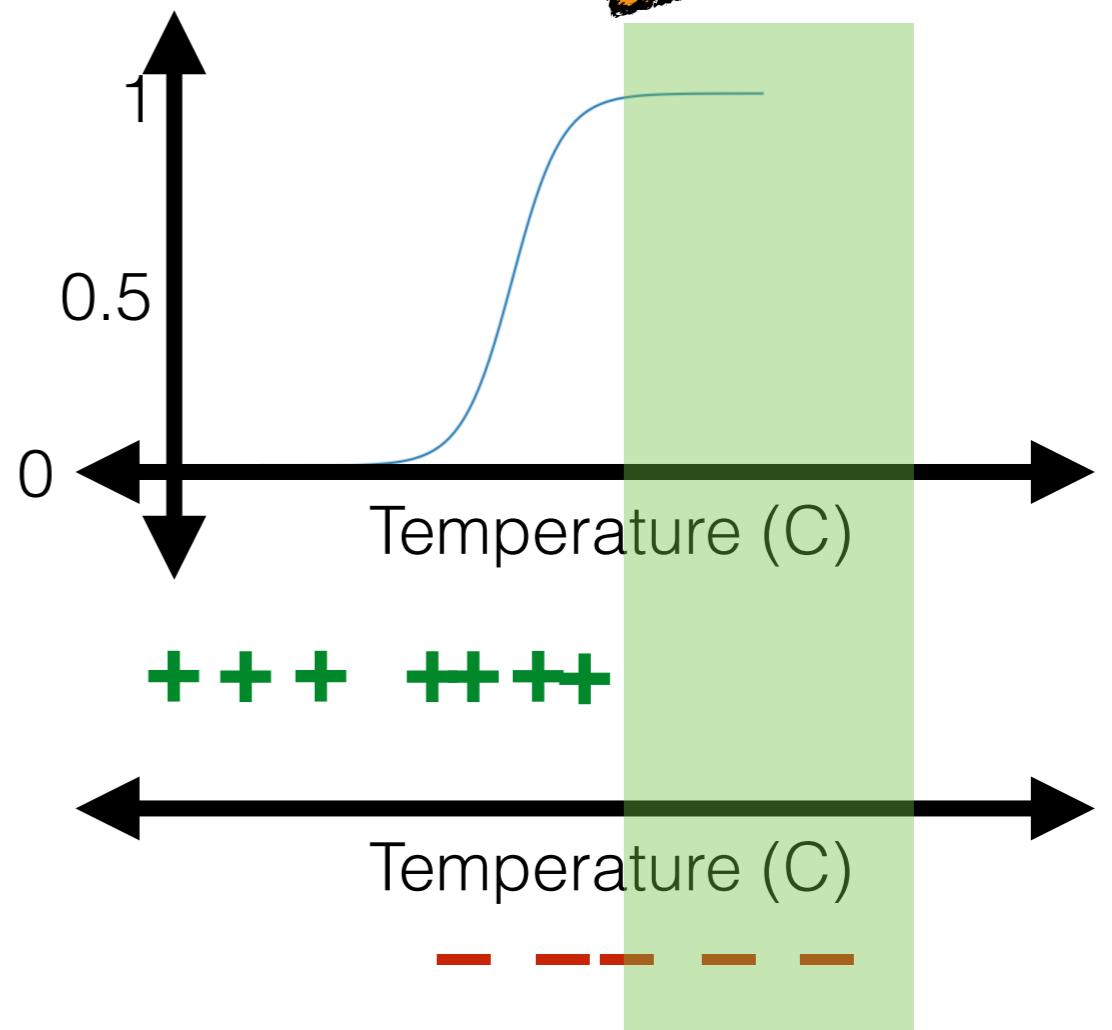
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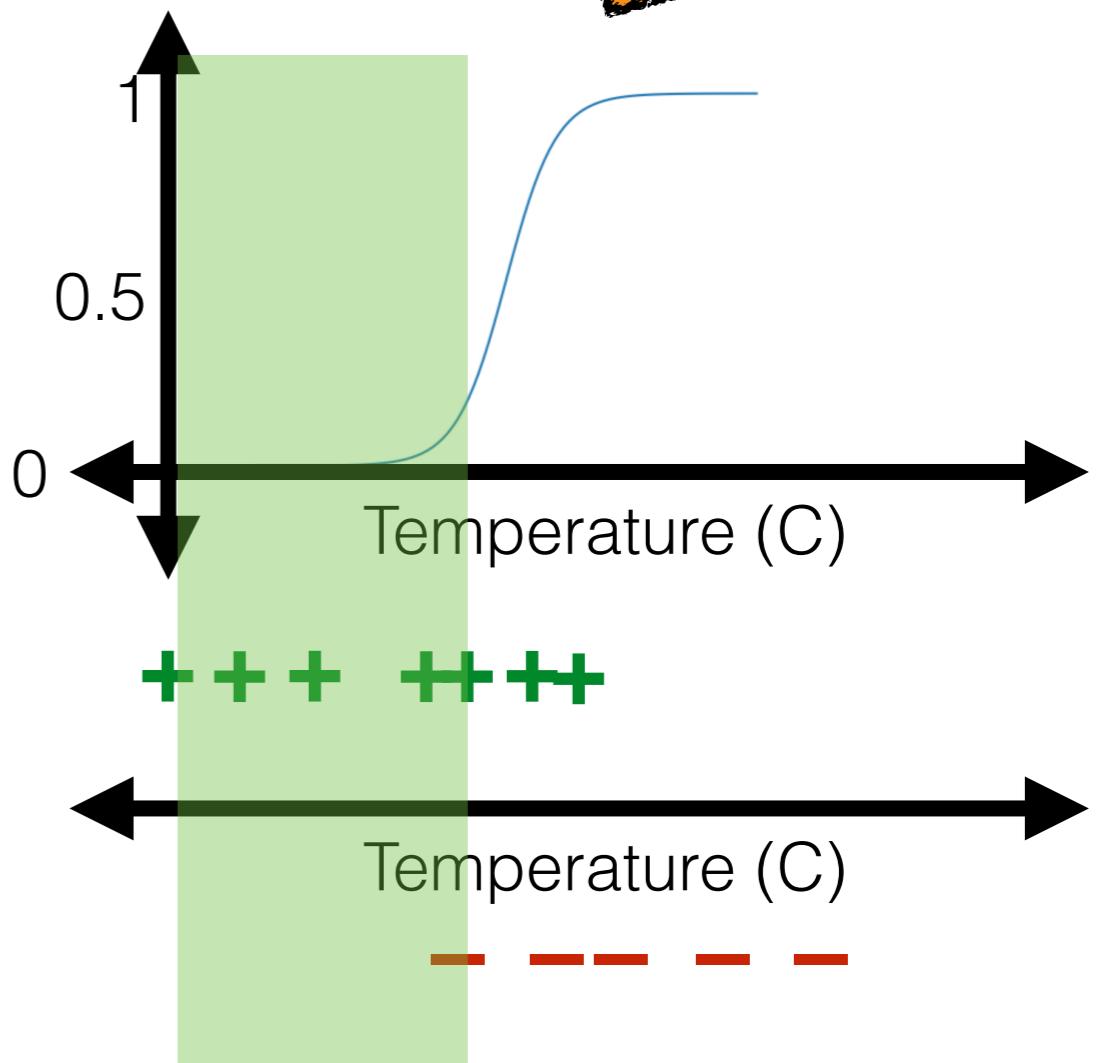
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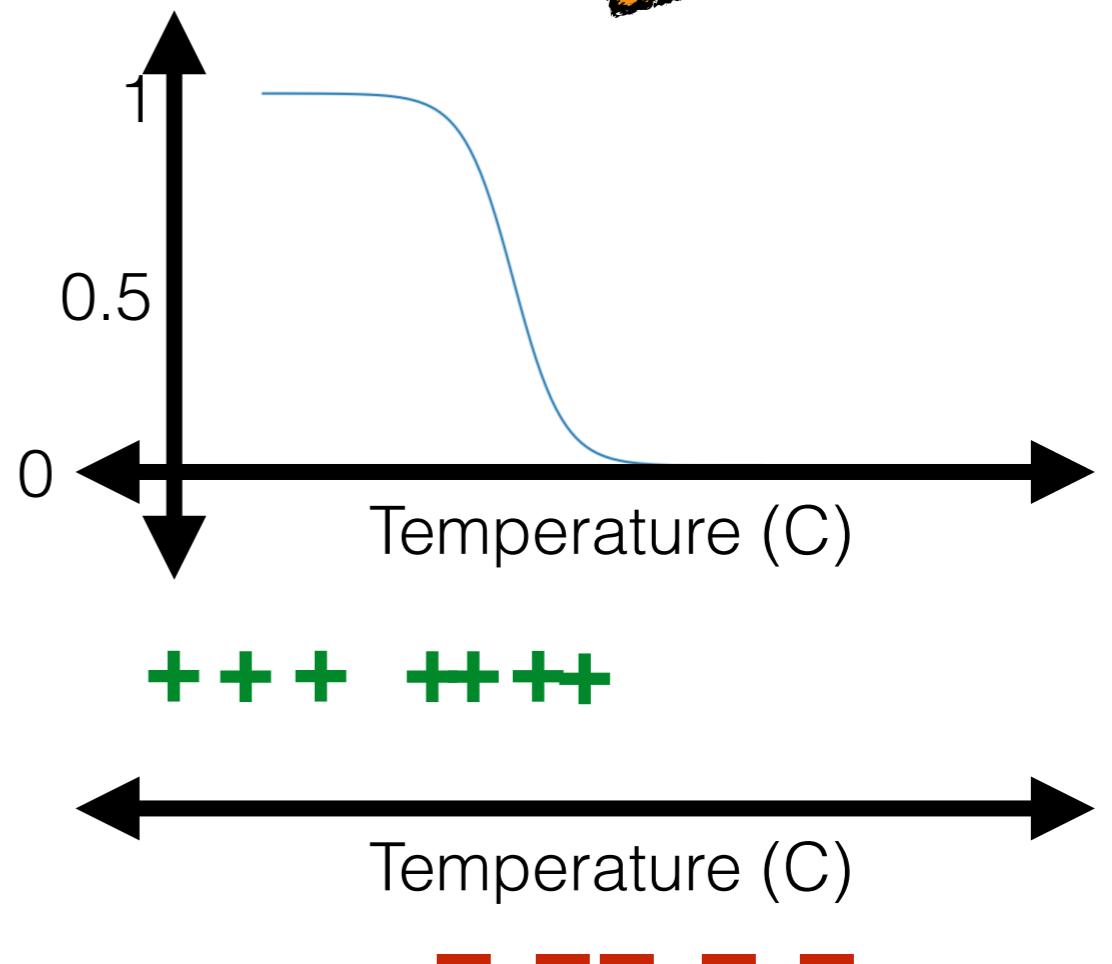
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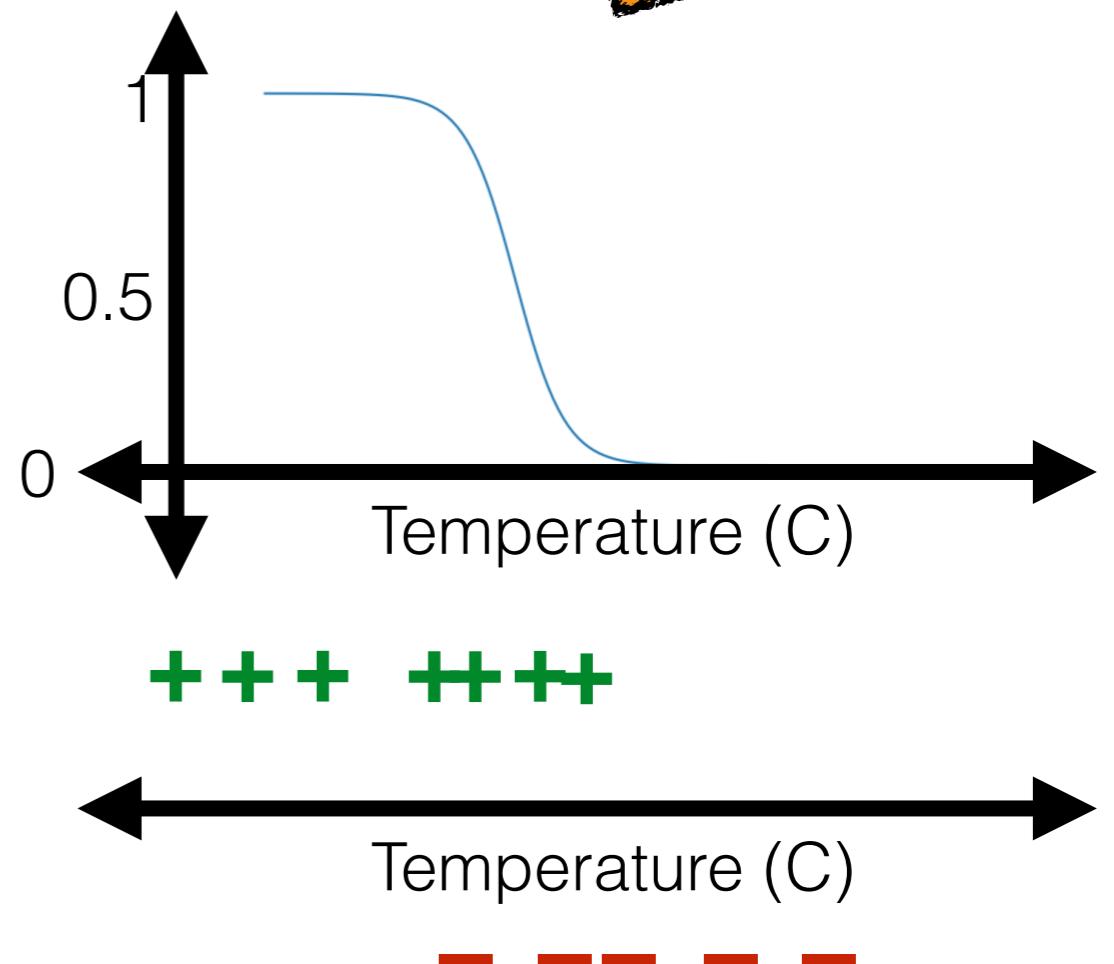


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aka logistic regression

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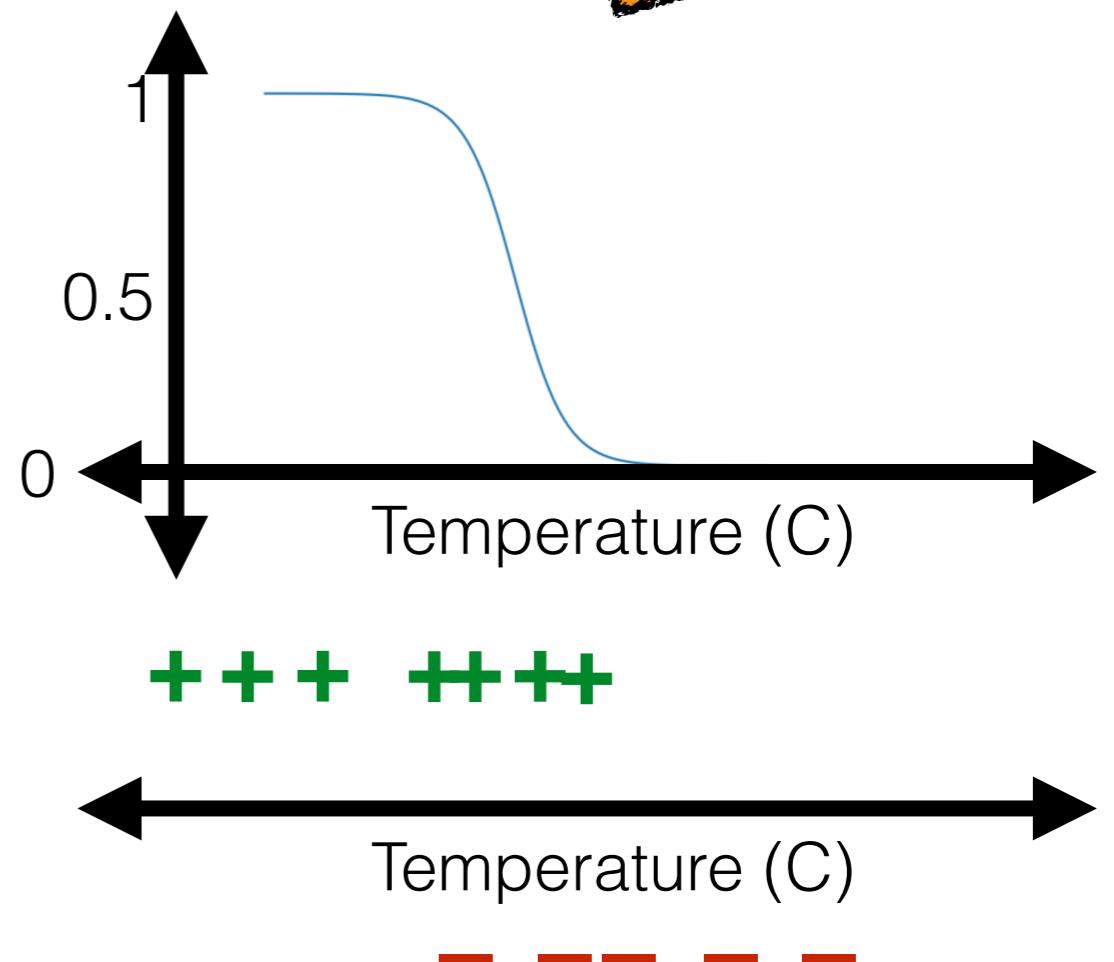
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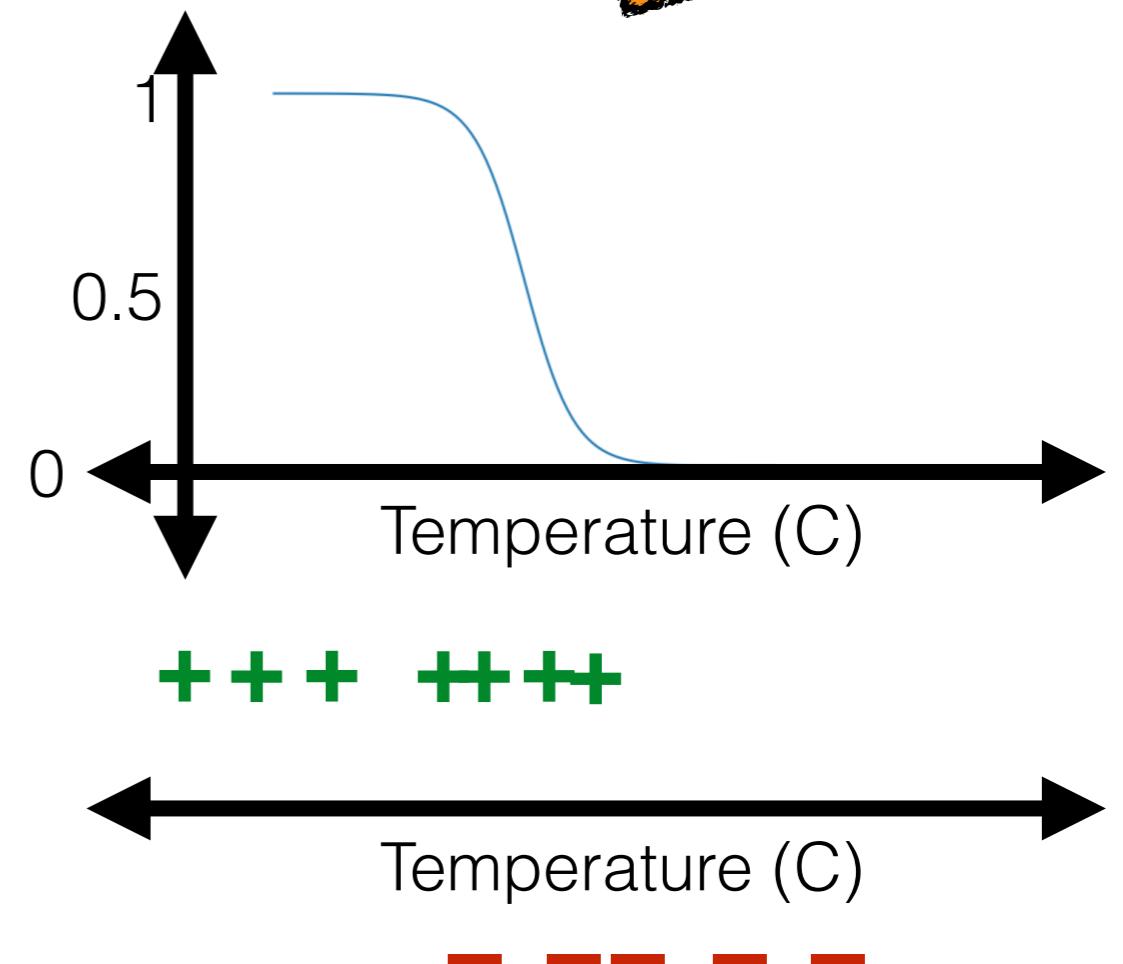
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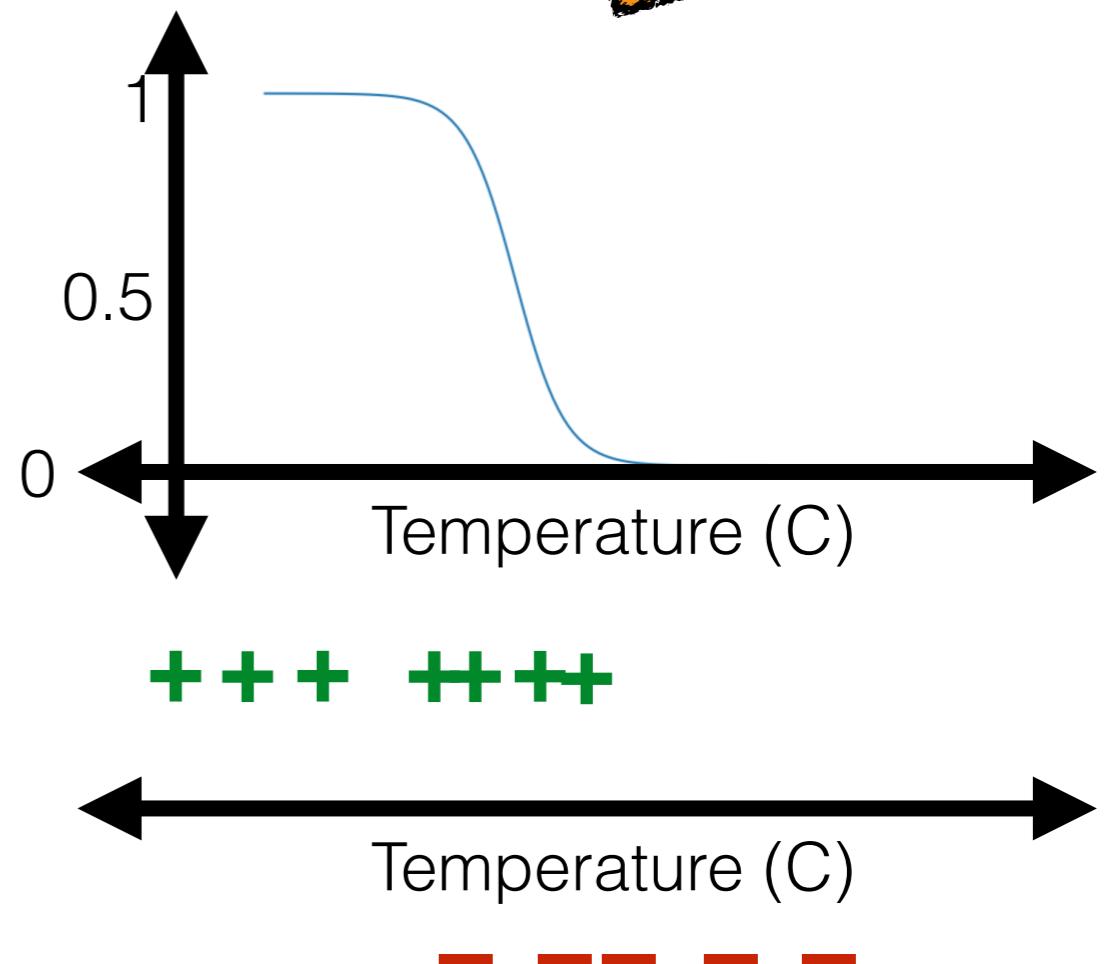
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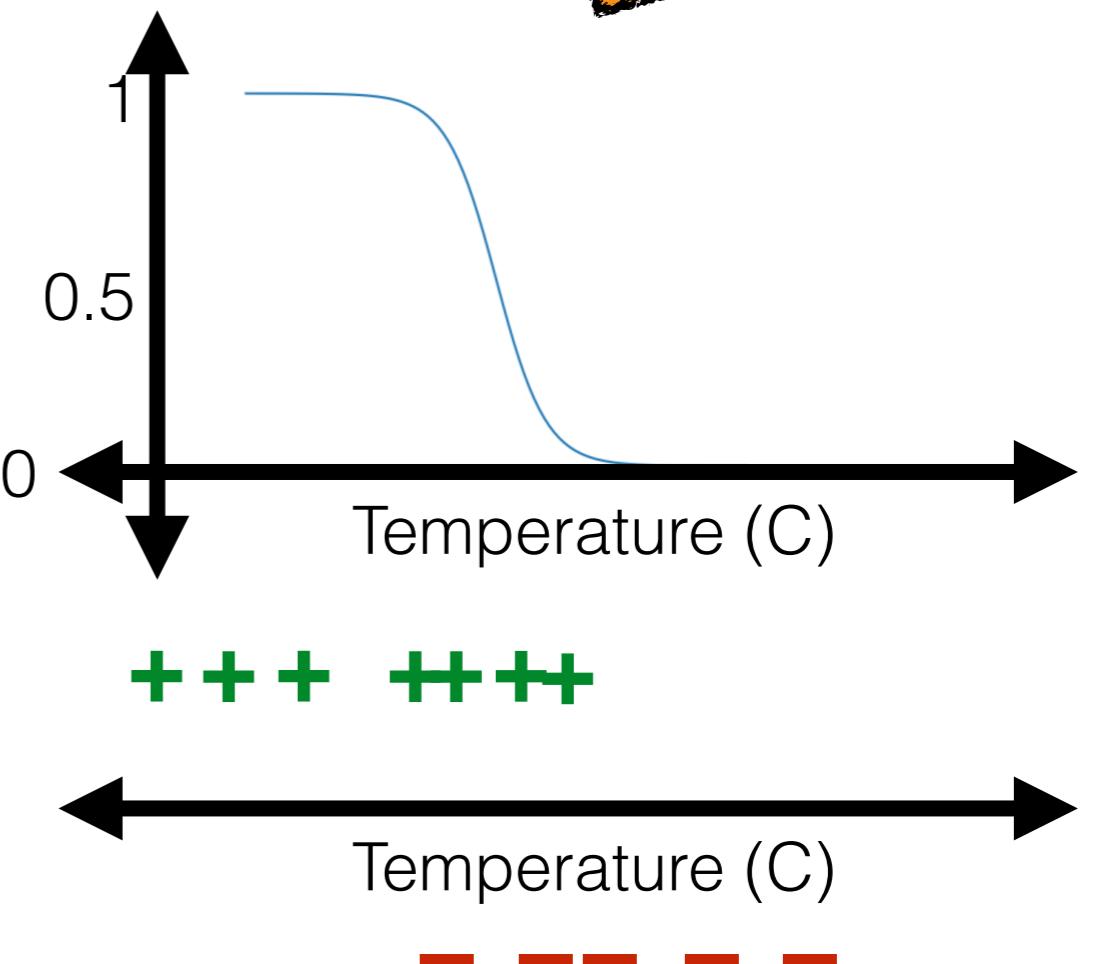
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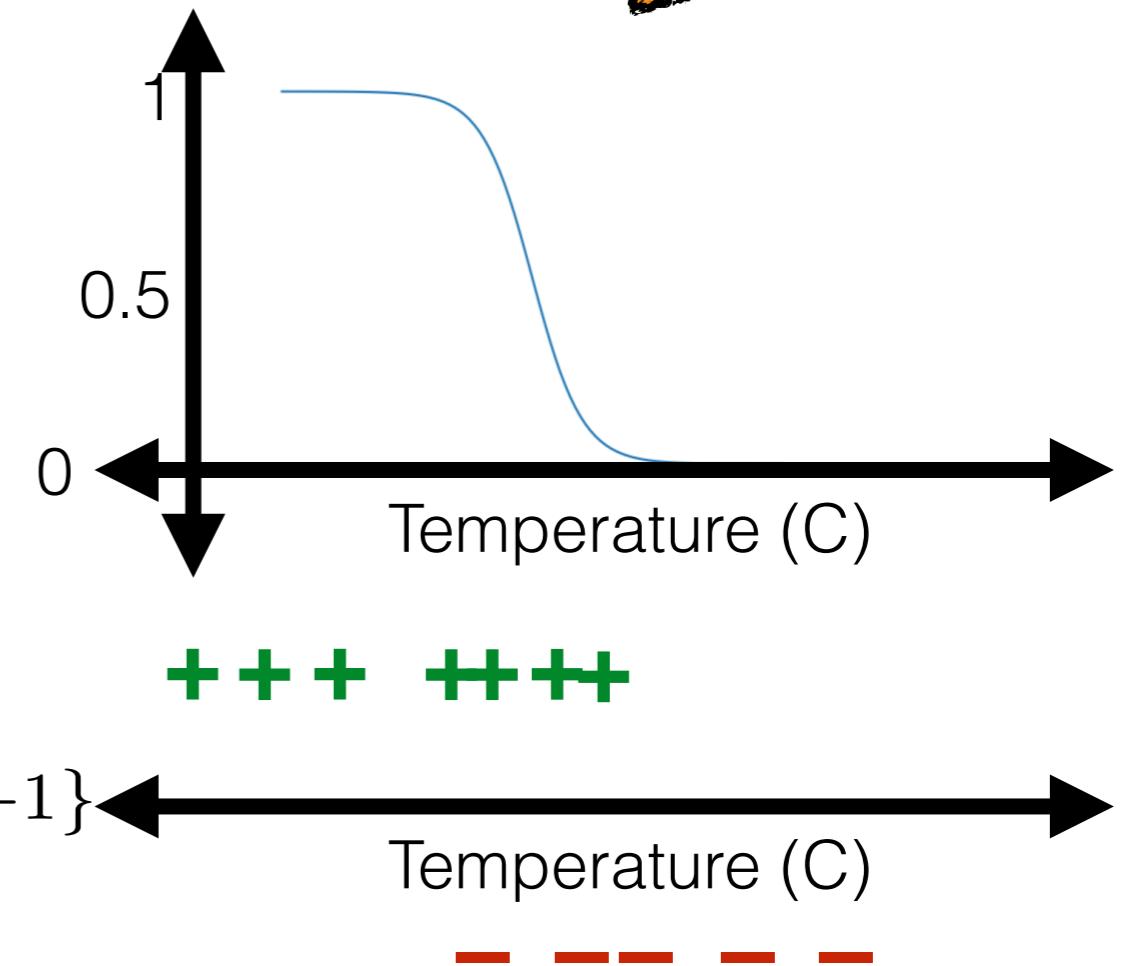
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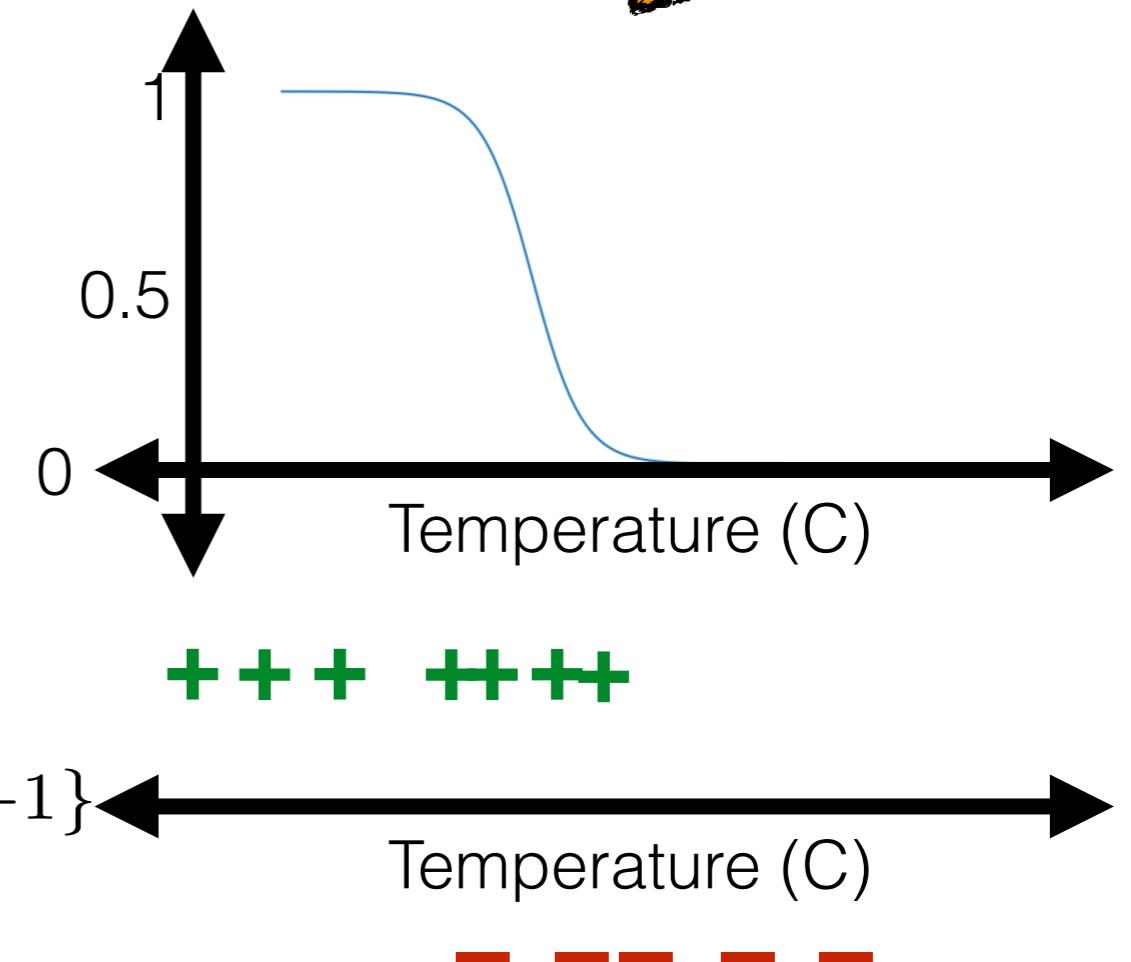
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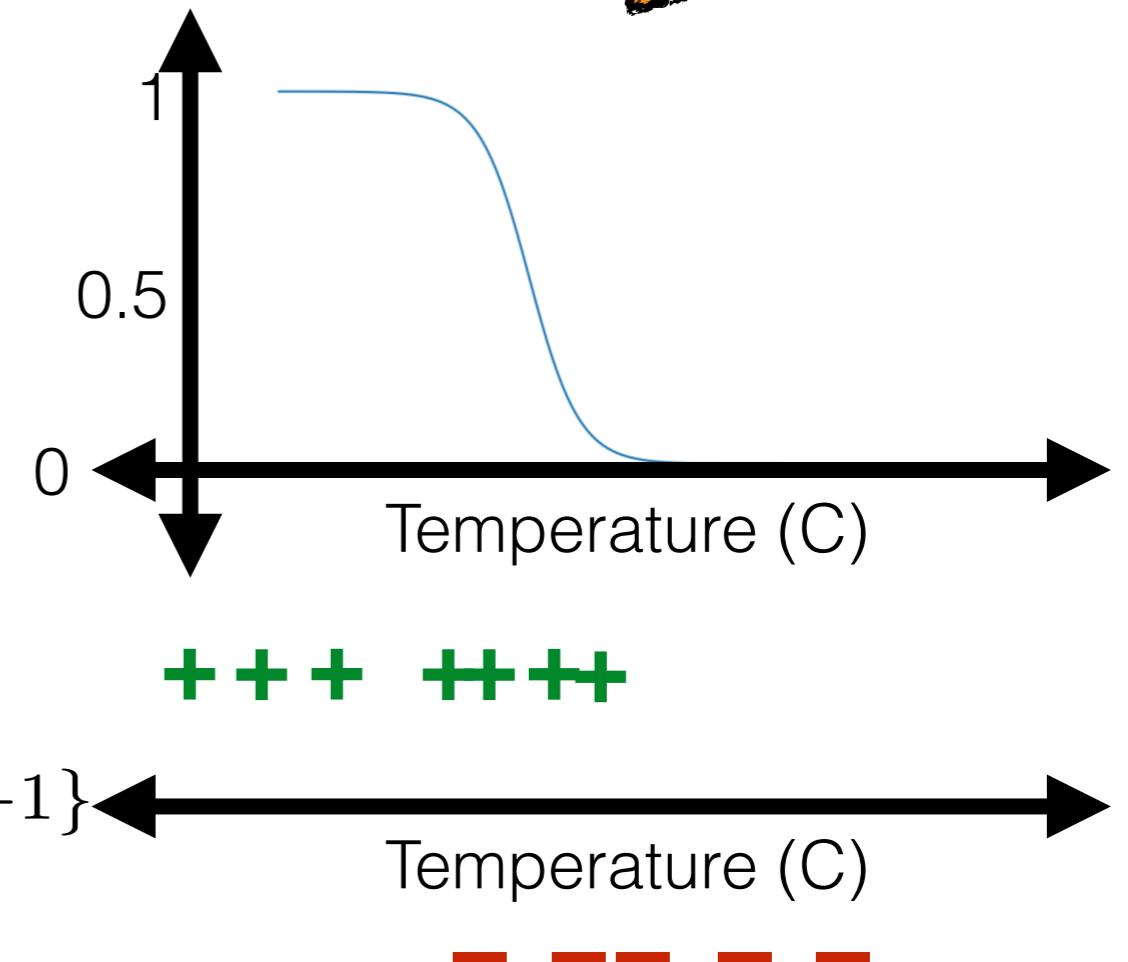
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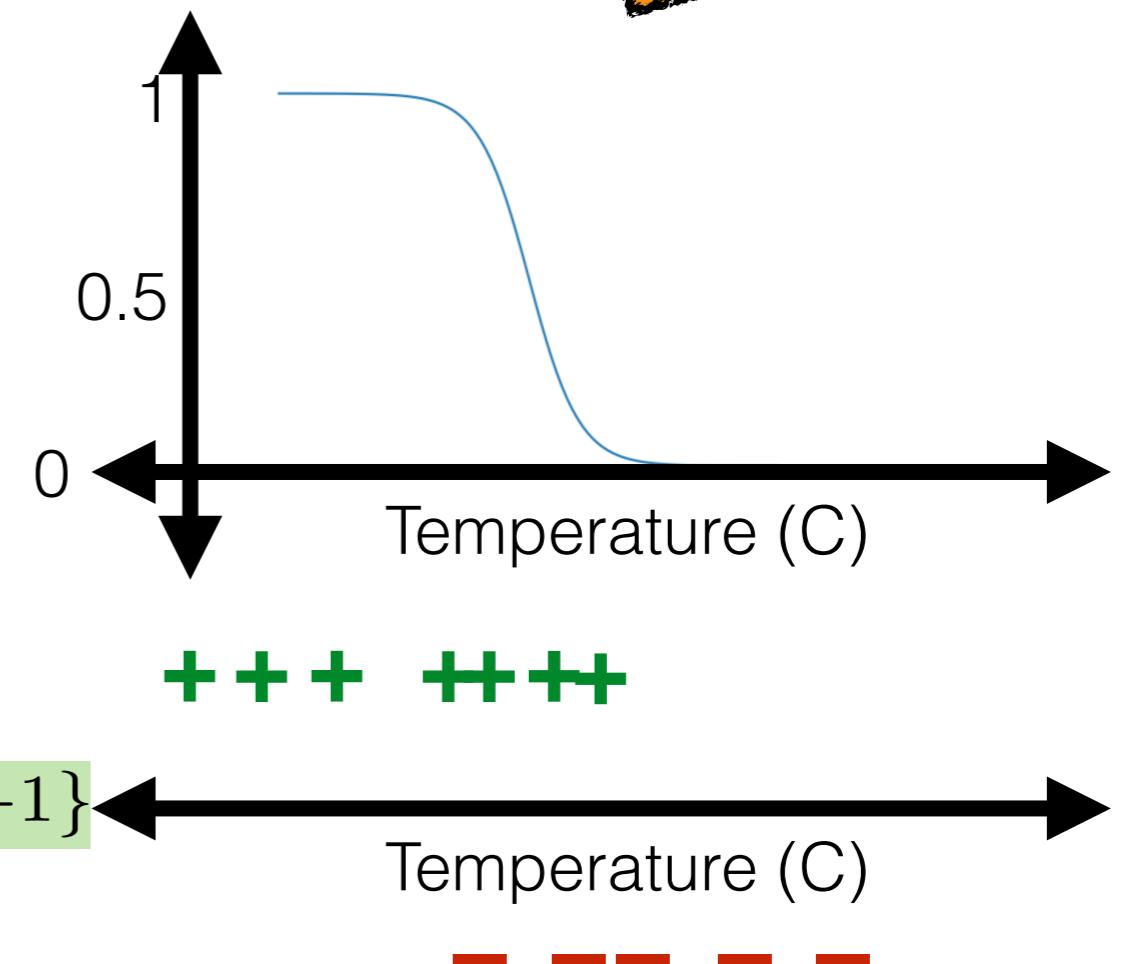
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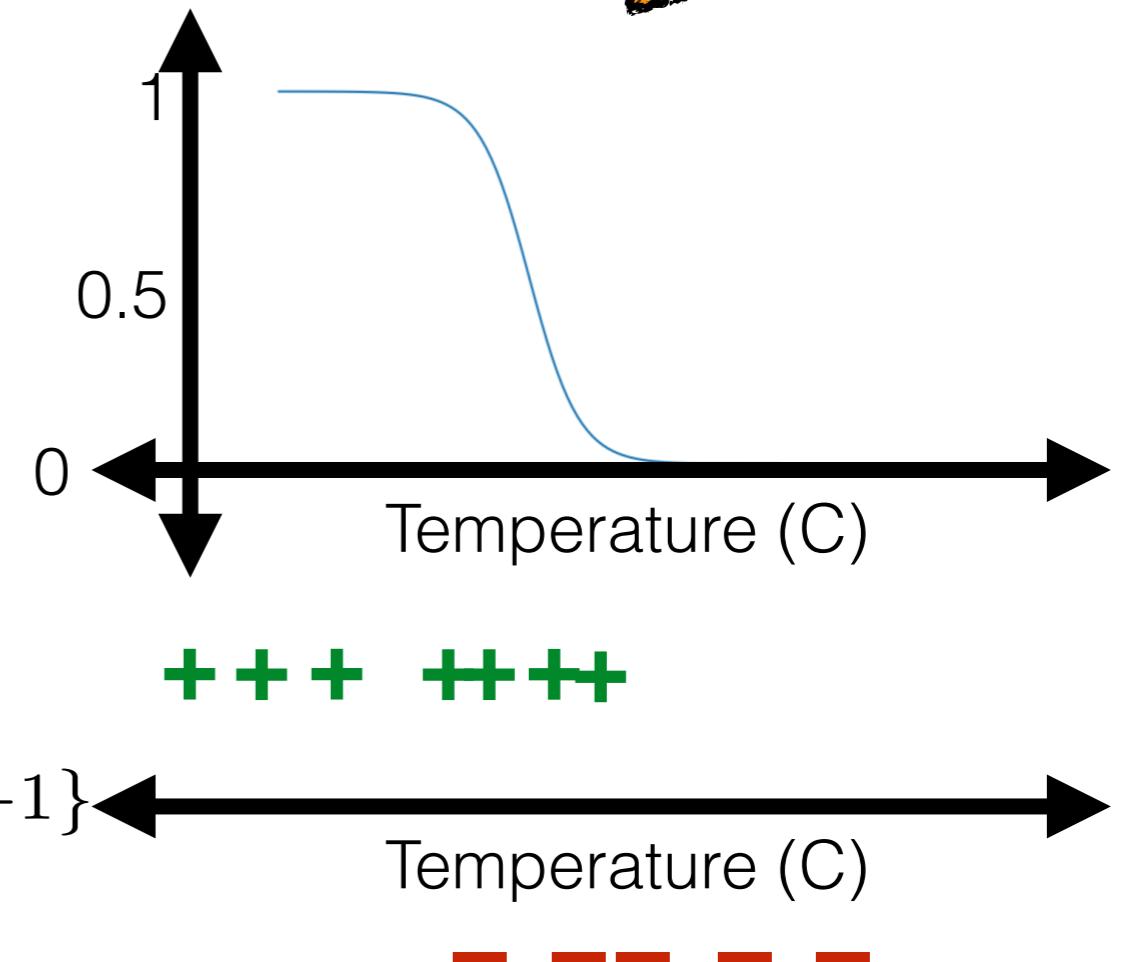
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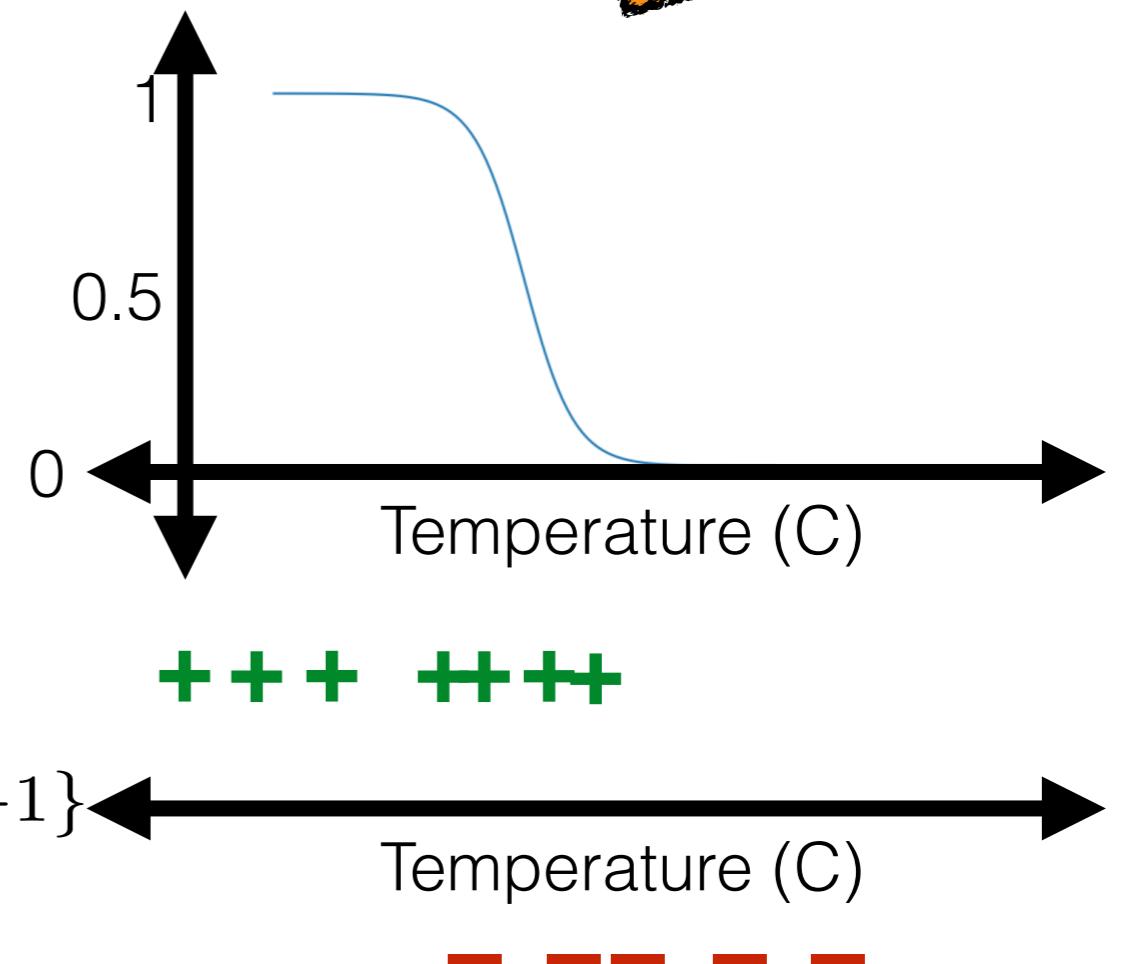
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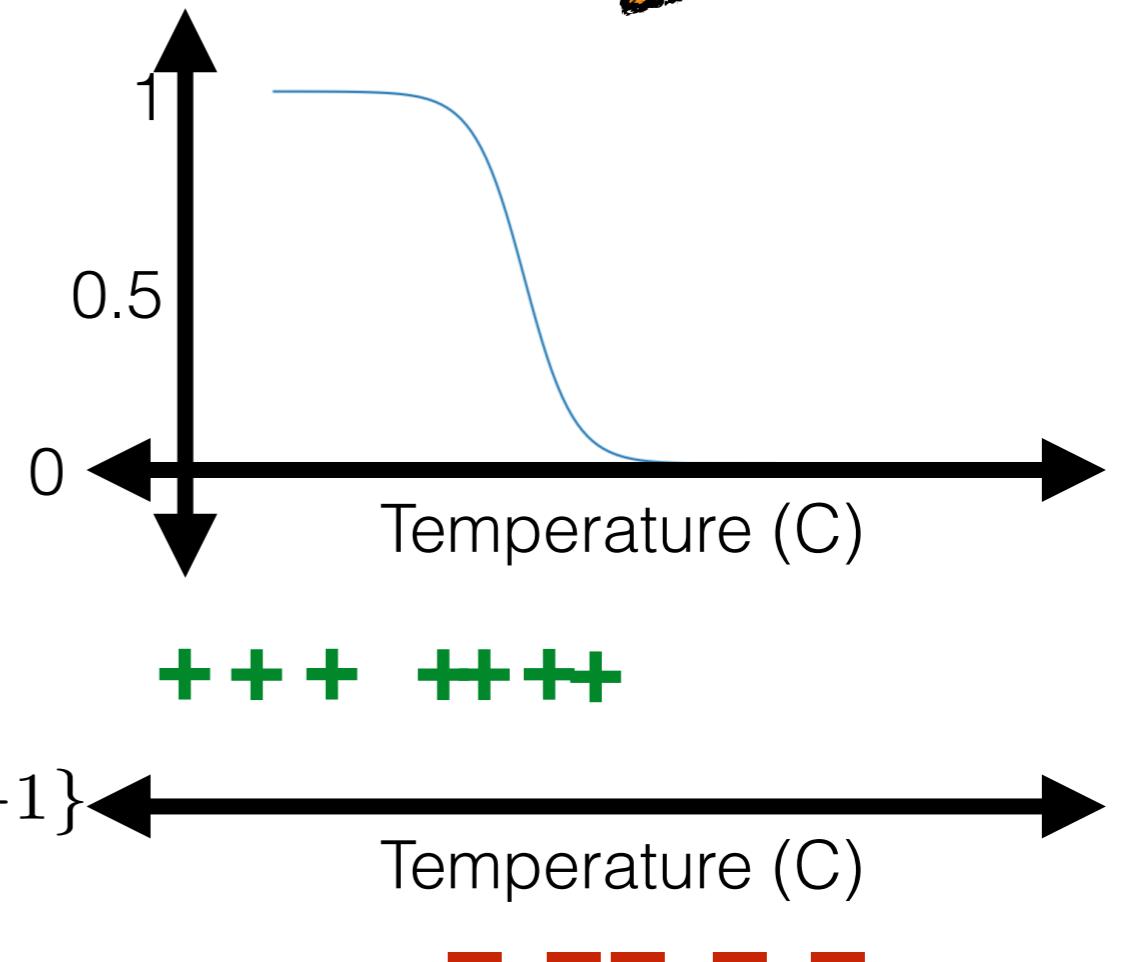
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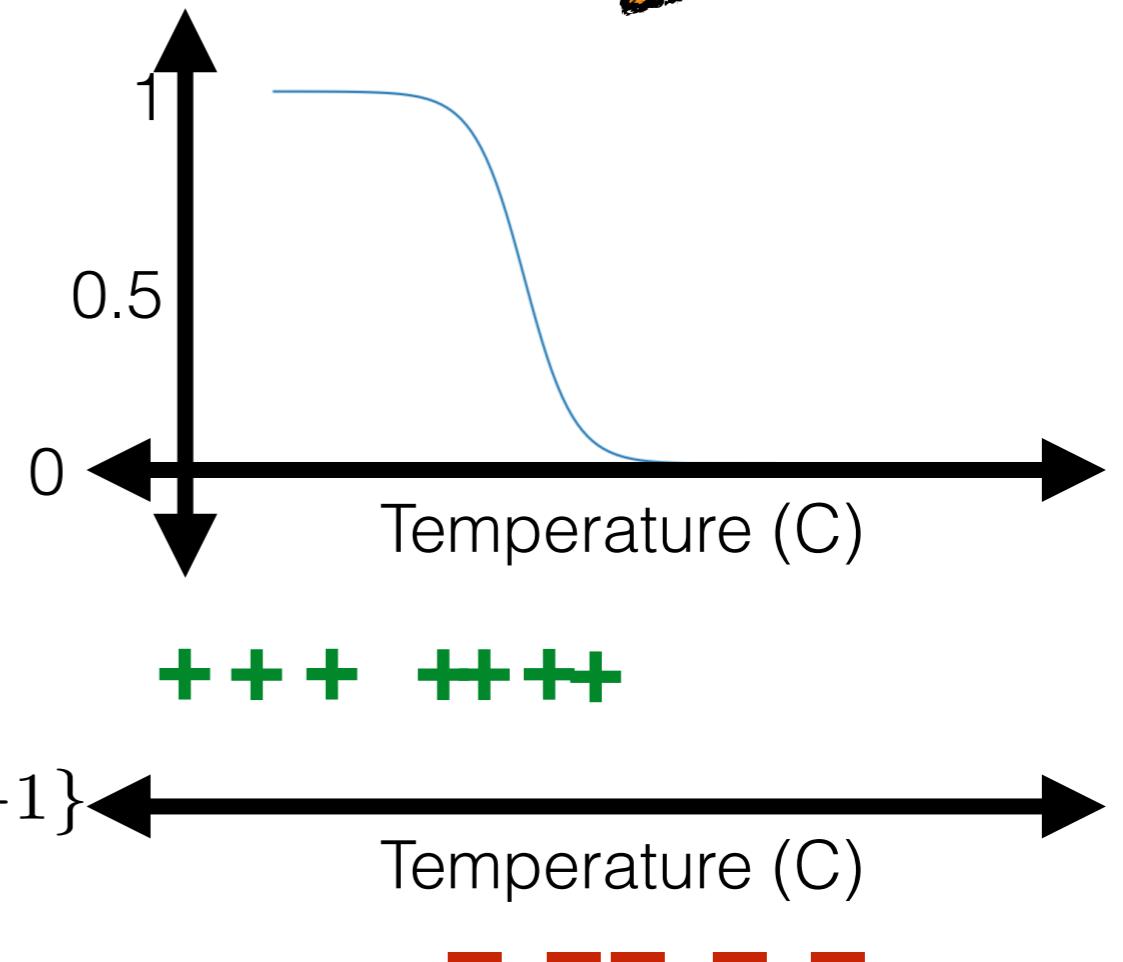
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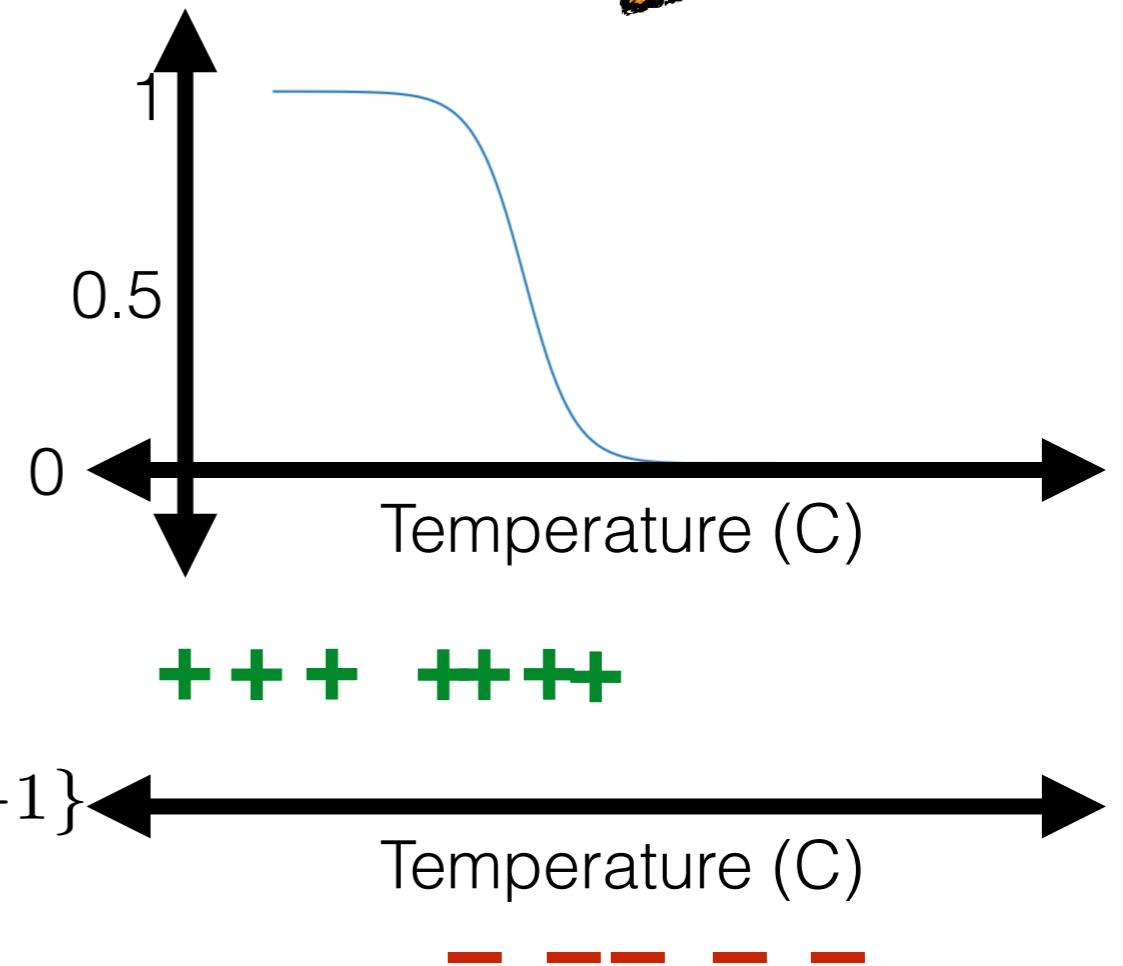
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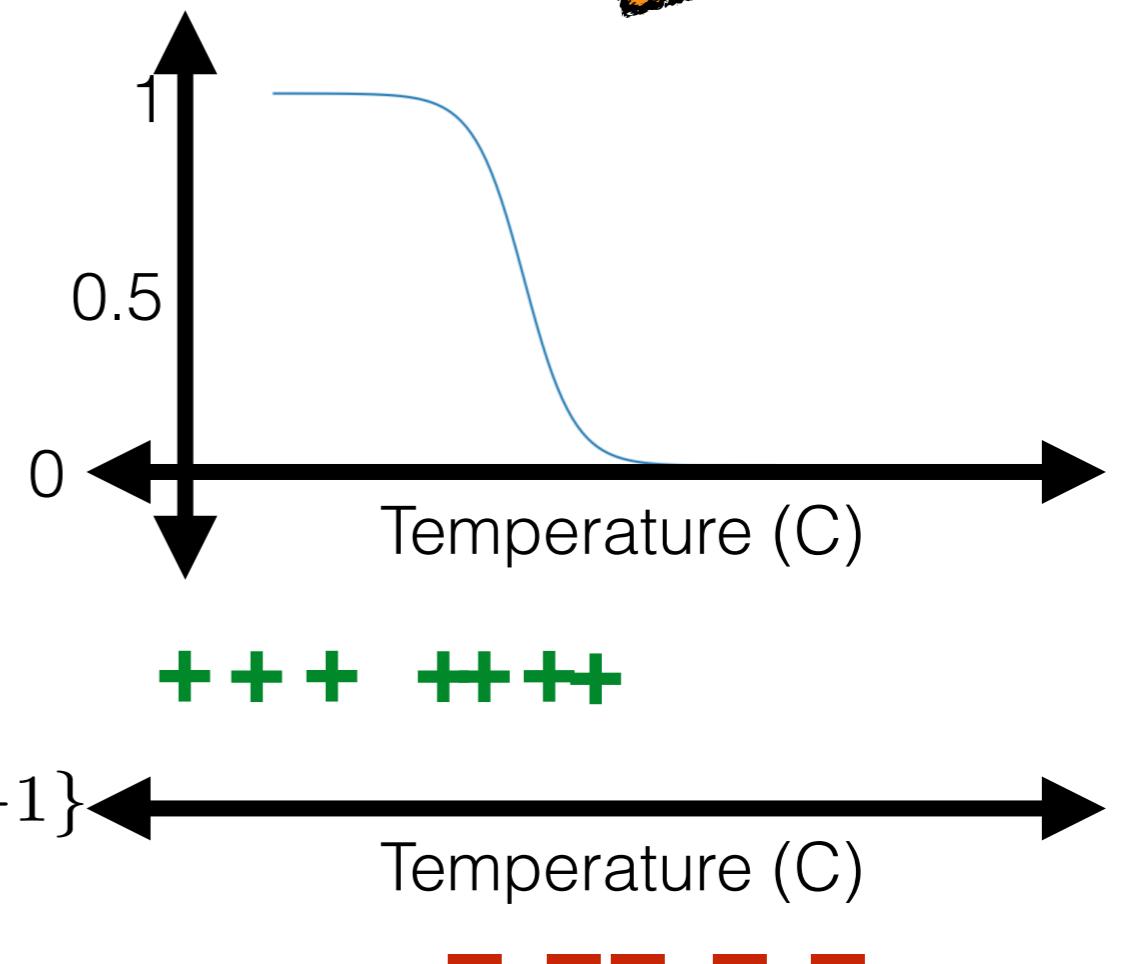
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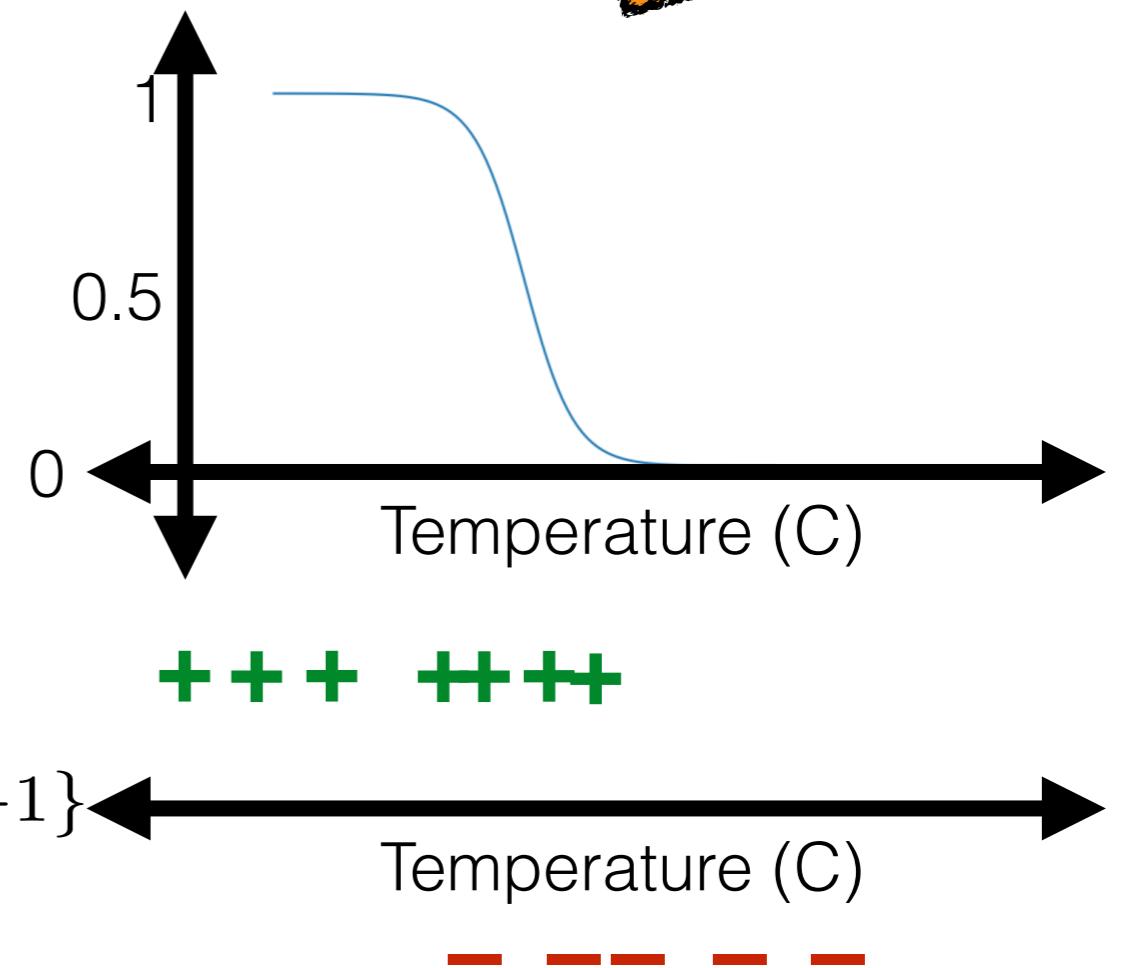
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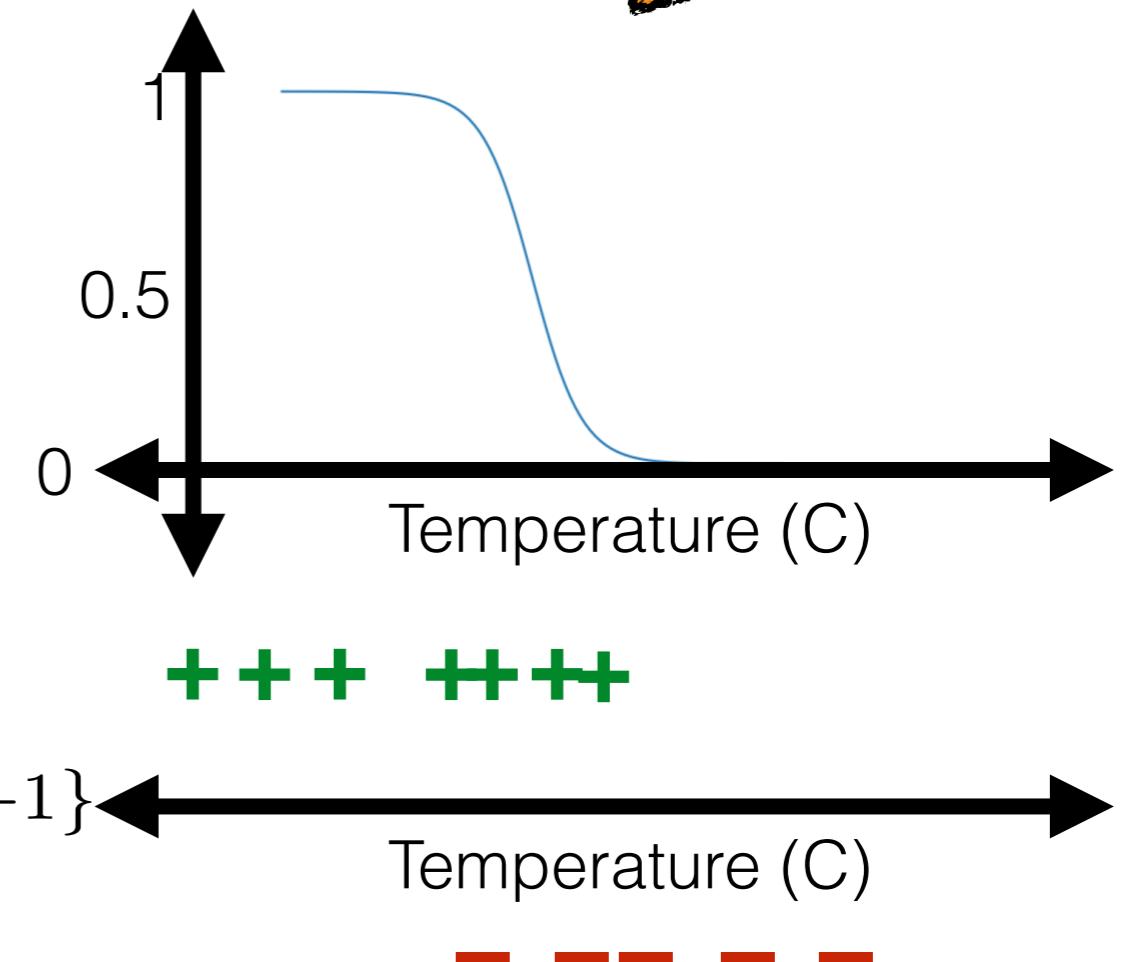
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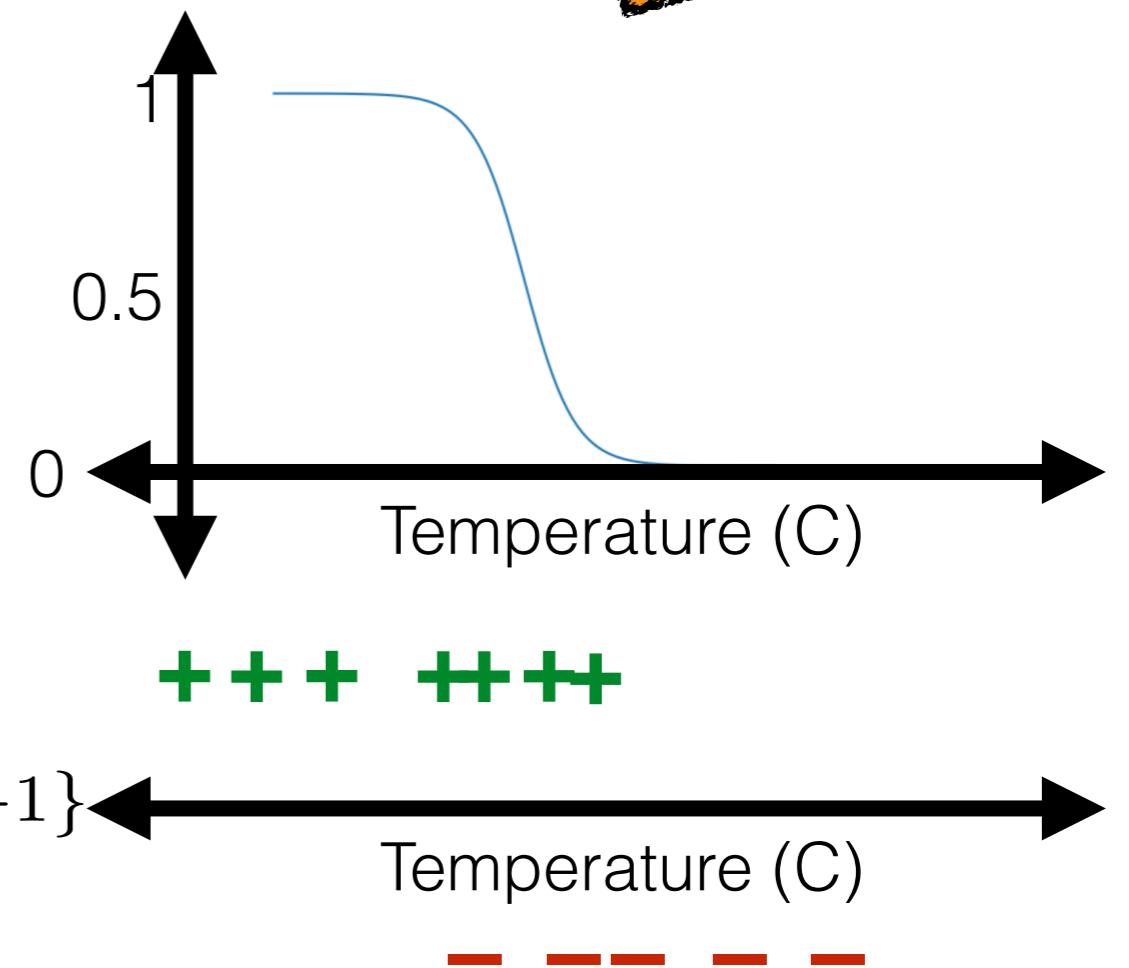
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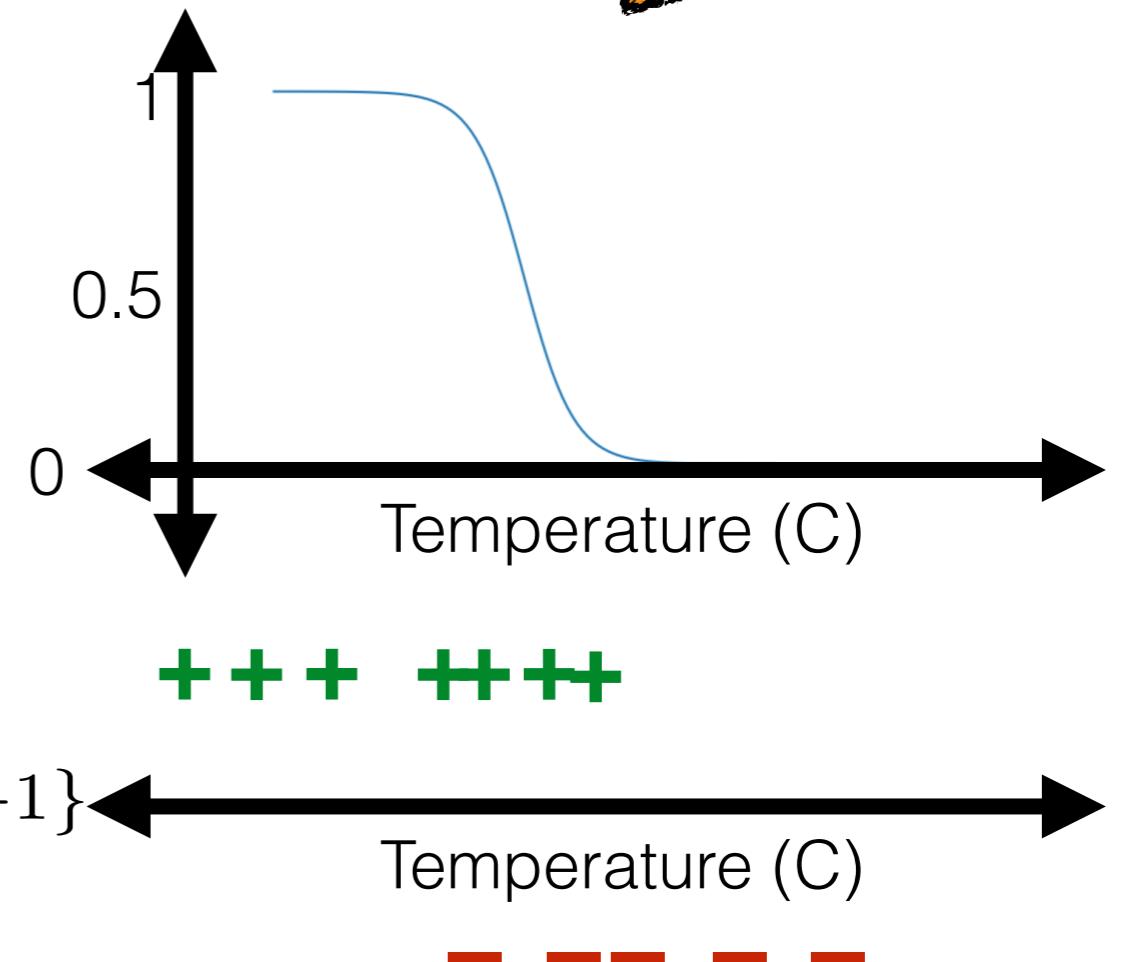
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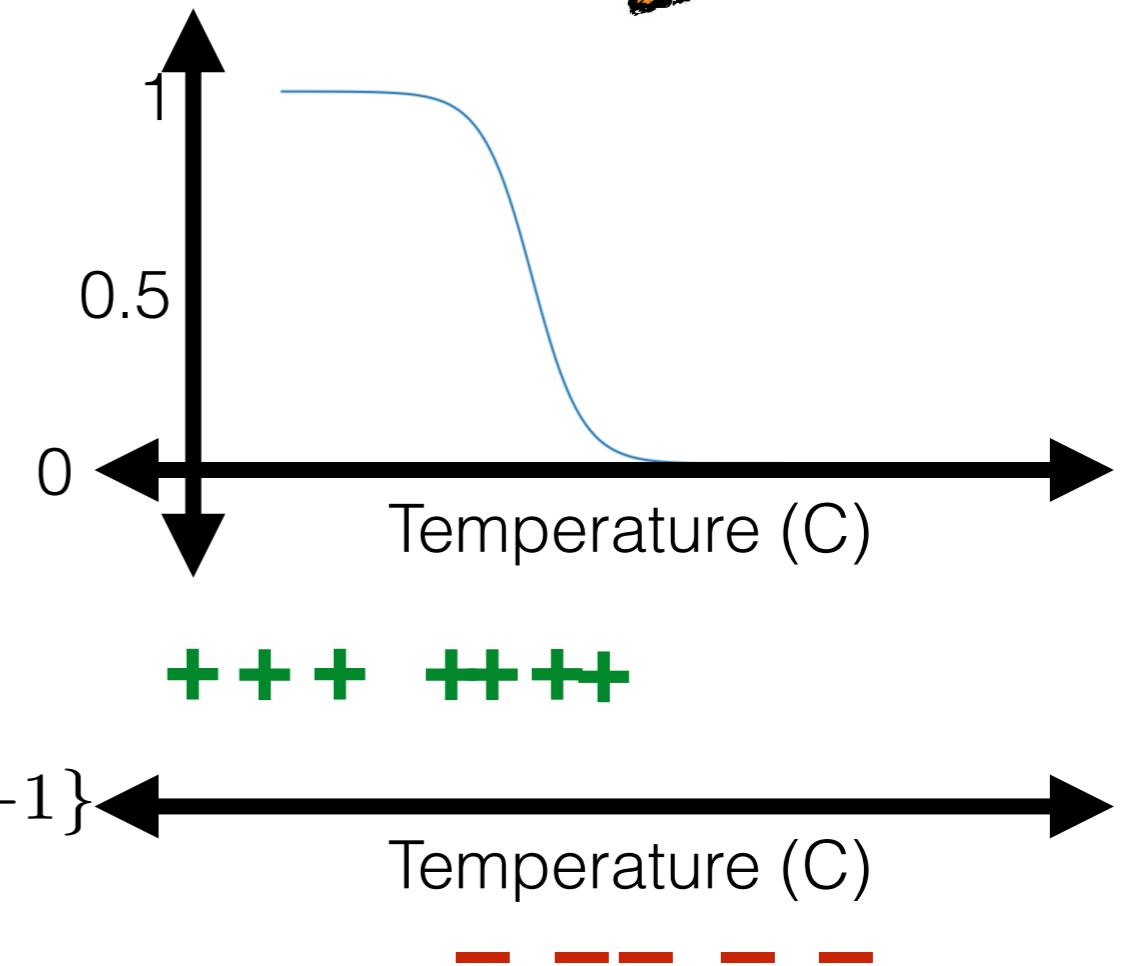
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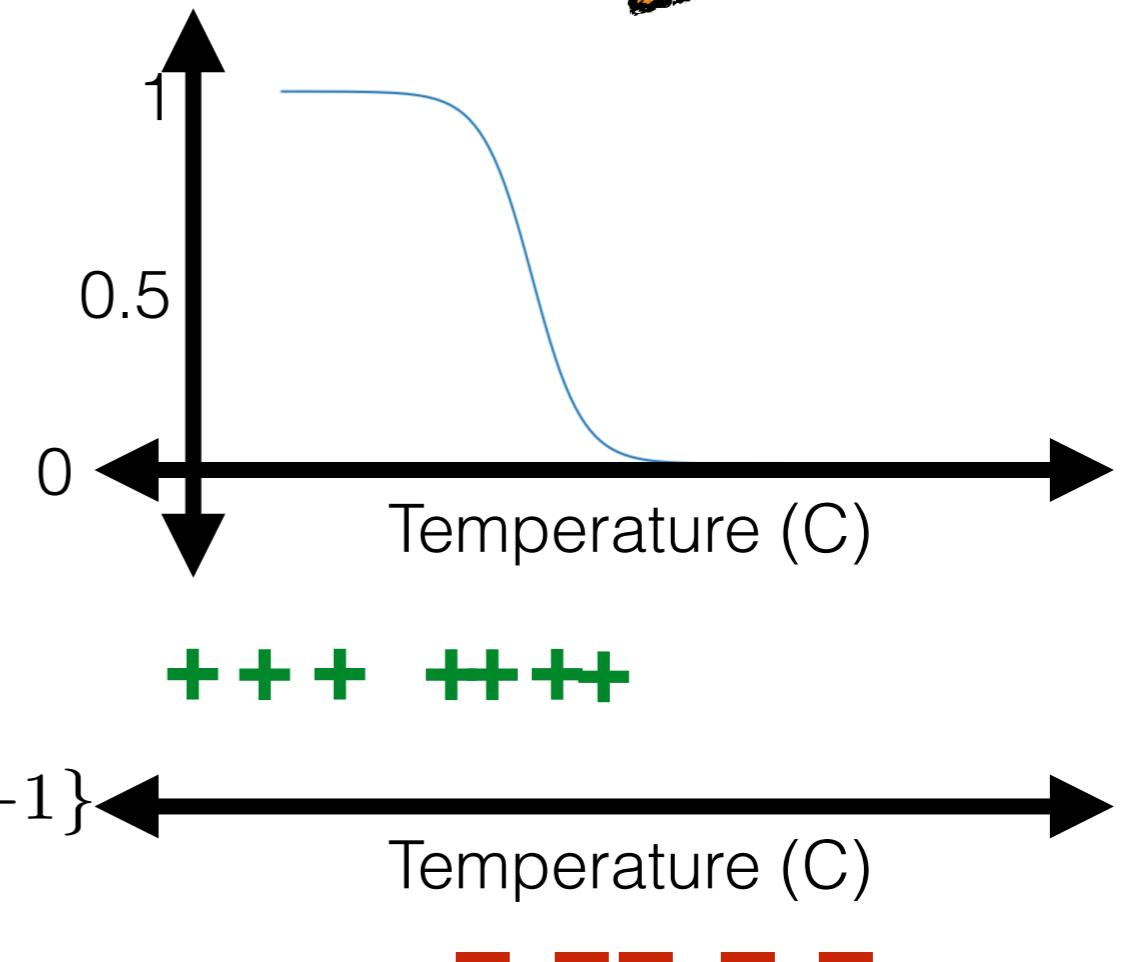
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Negative log likelihood loss ( $g$  for guess,  $a$  for actual):

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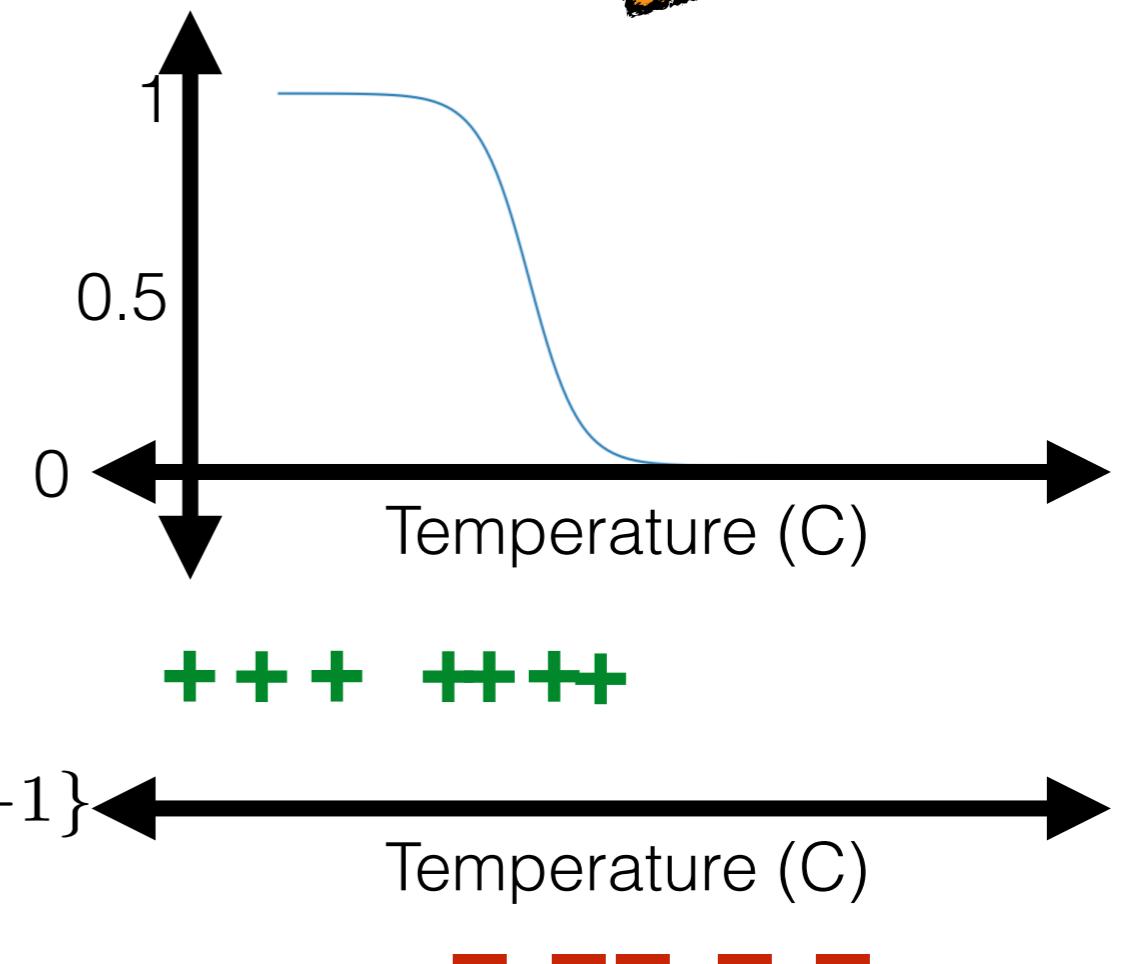
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Loss(data) =  $-(1/n) * \log \text{probability(data)}$

$$= \frac{1}{n} \sum_{i=1}^n - \left( \mathbf{1}\{y^{(i)} = +1\} \log g^{(i)} + \mathbf{1}\{y^{(i)} \neq +1\} \log(1 - g^{(i)}) \right)$$

Negative log likelihood loss ( $g$  for guess,  $a$  for actual):

$$-L_{\text{nll}}(g, a) = (\mathbf{1}\{a = +1\} \log g + \mathbf{1}\{a \neq +1\} \log(1 - g))$$

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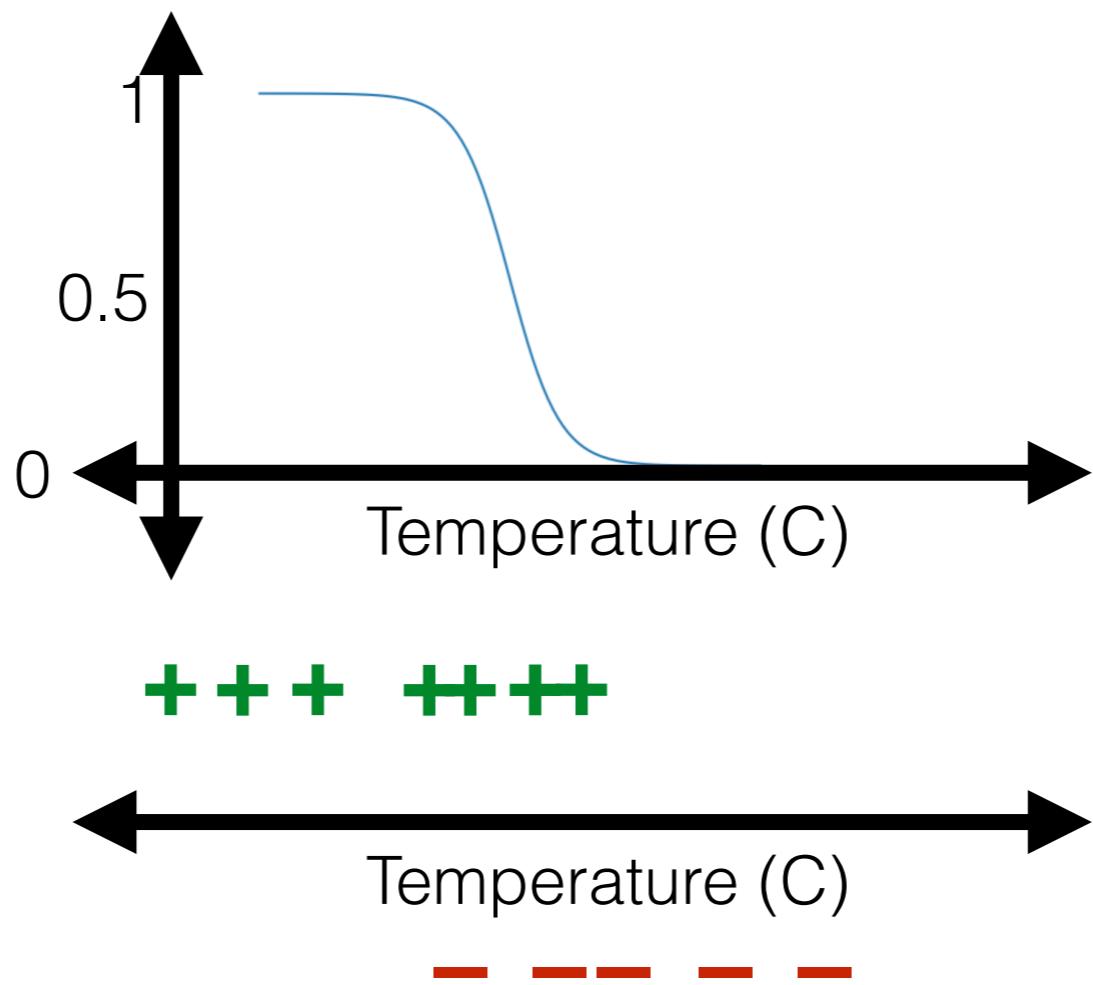
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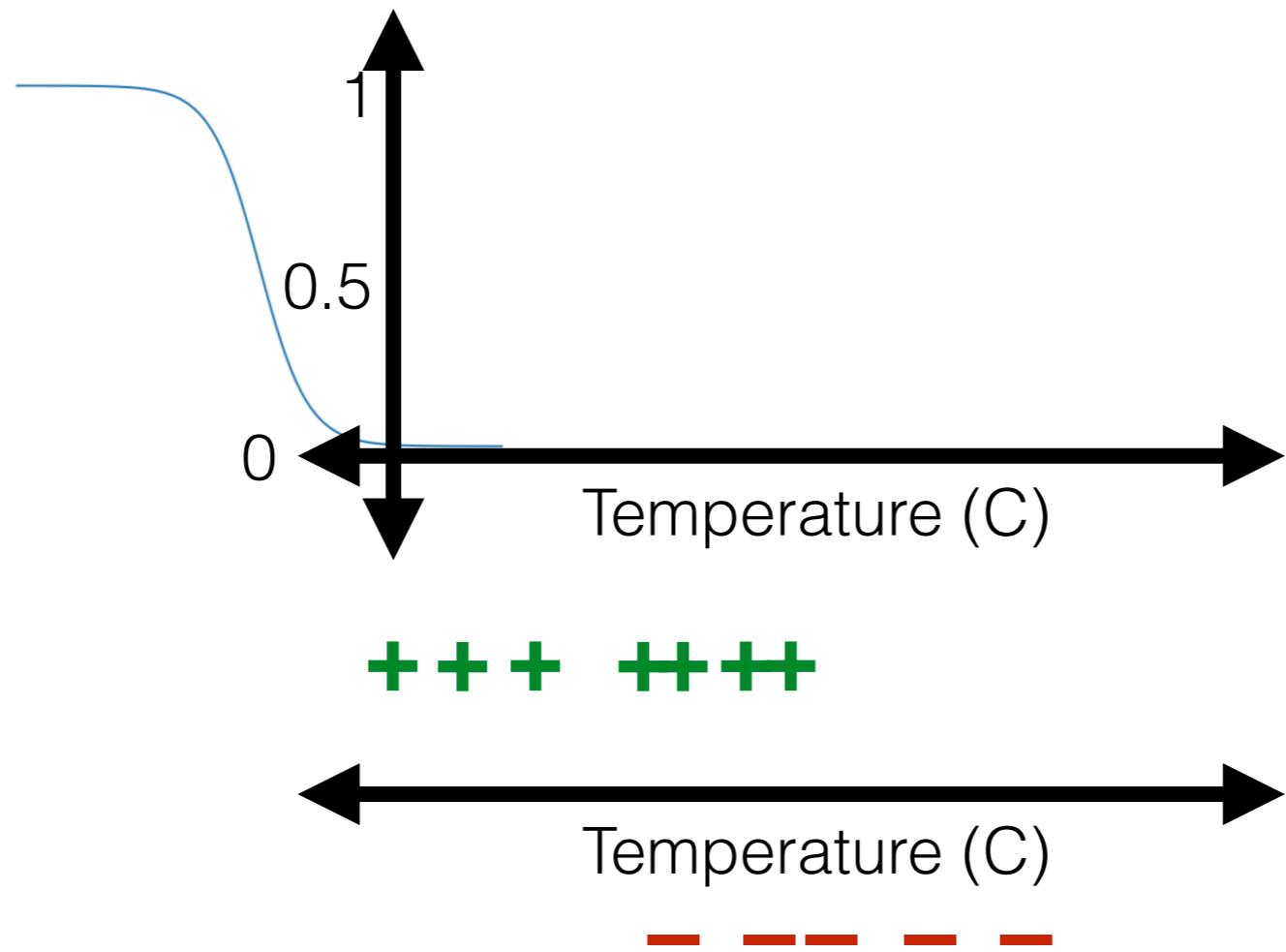


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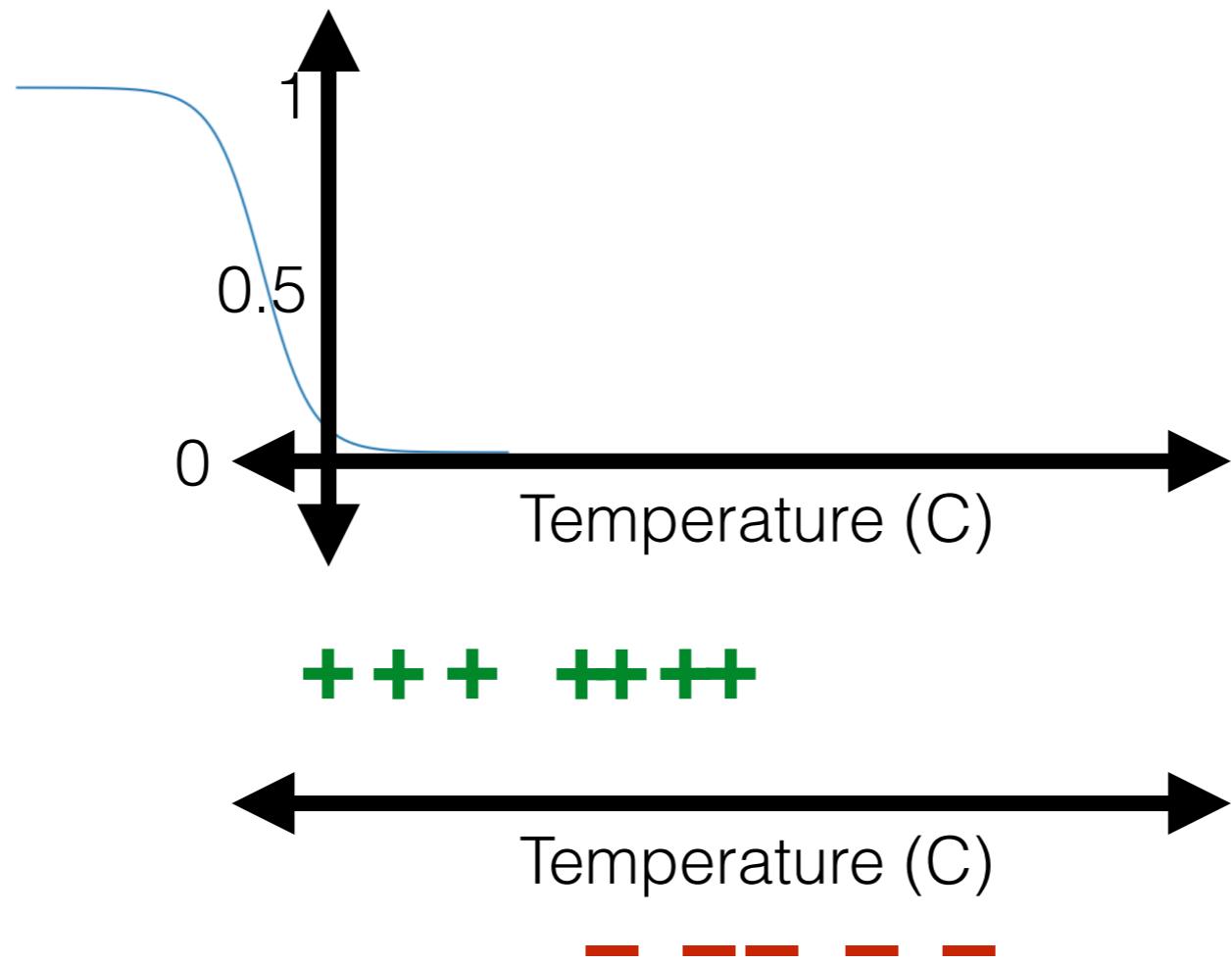


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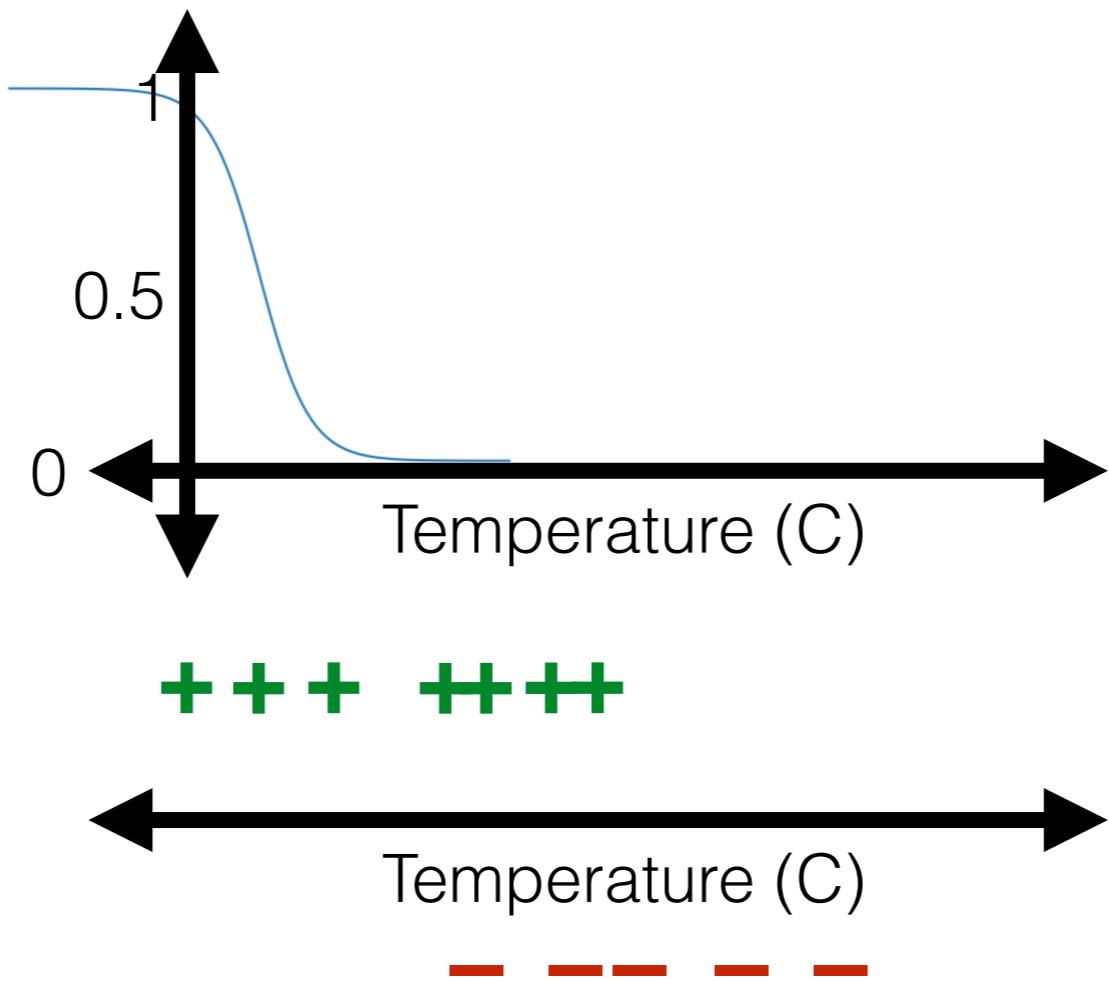


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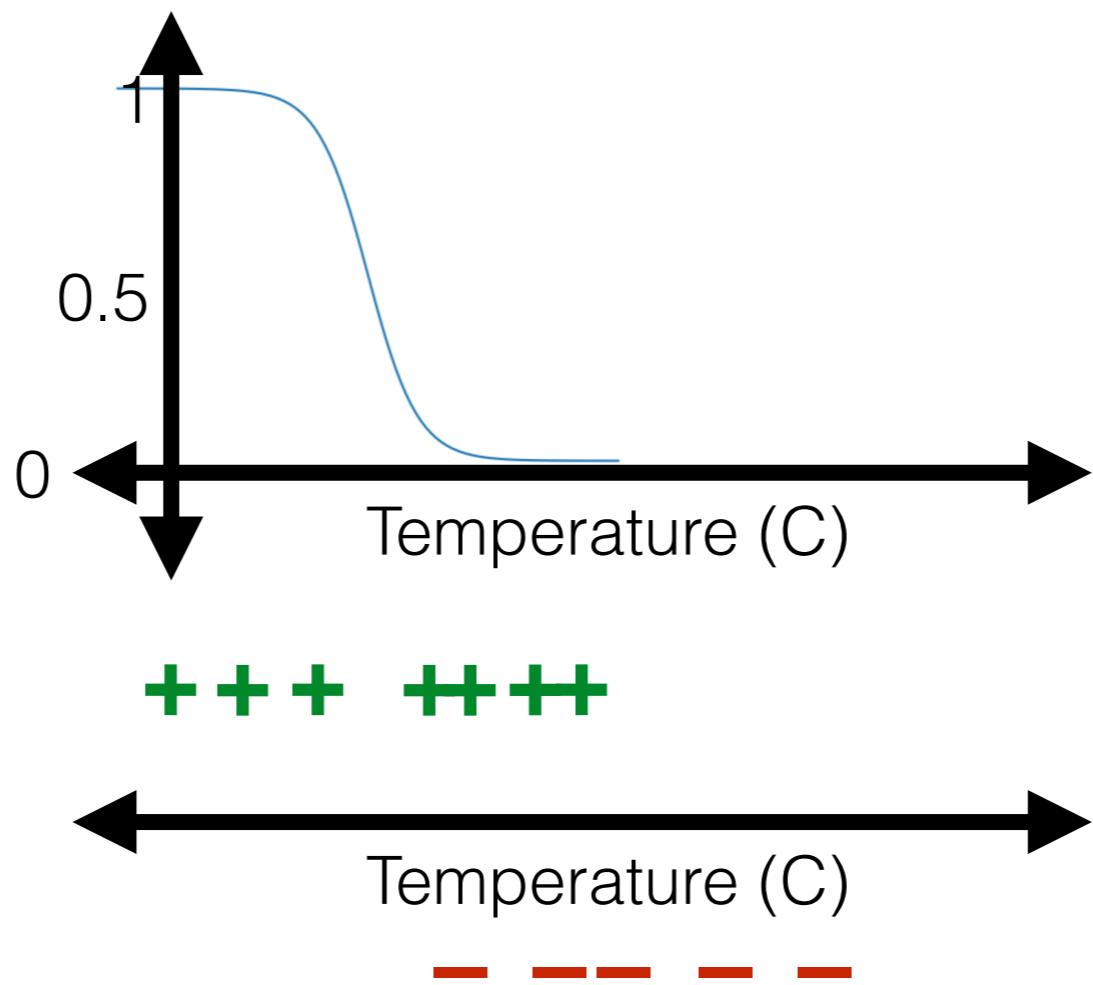


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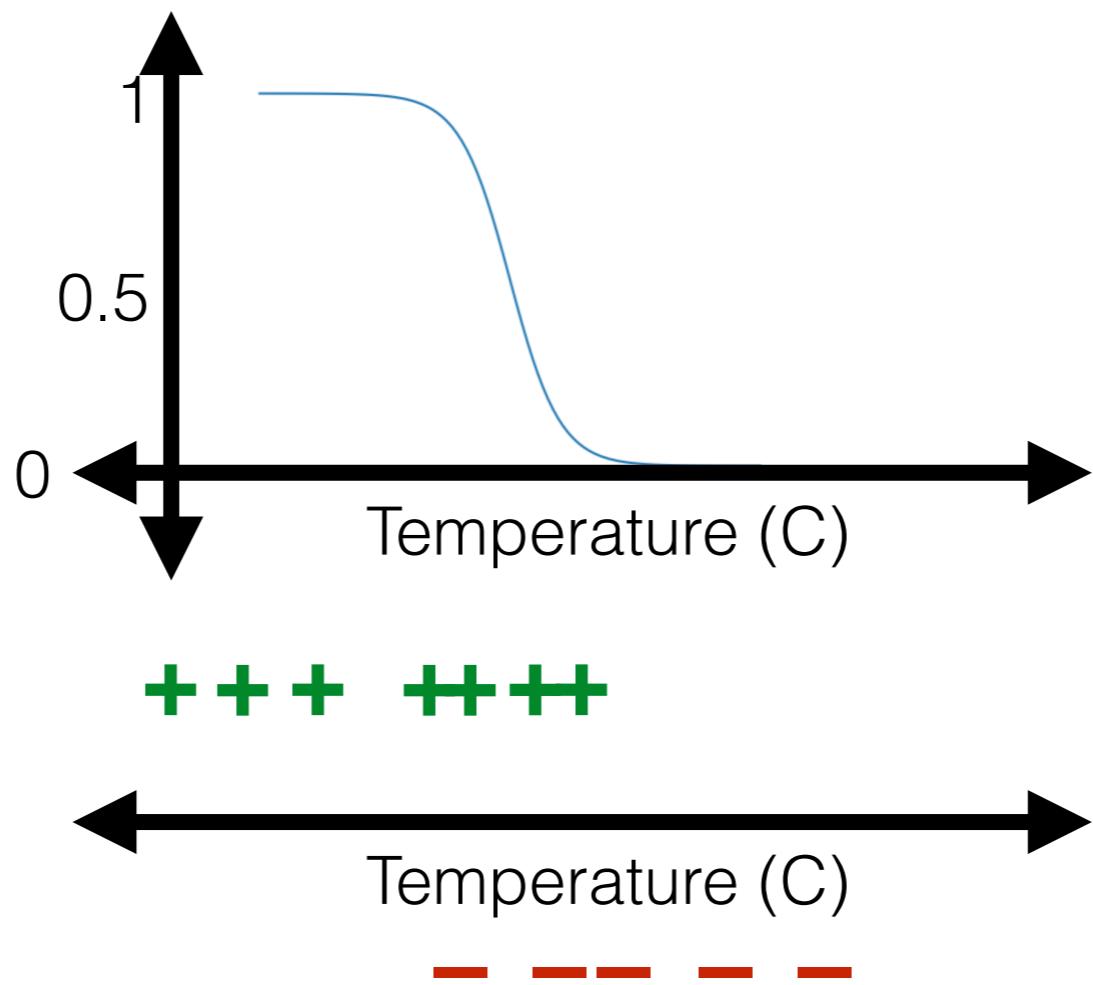


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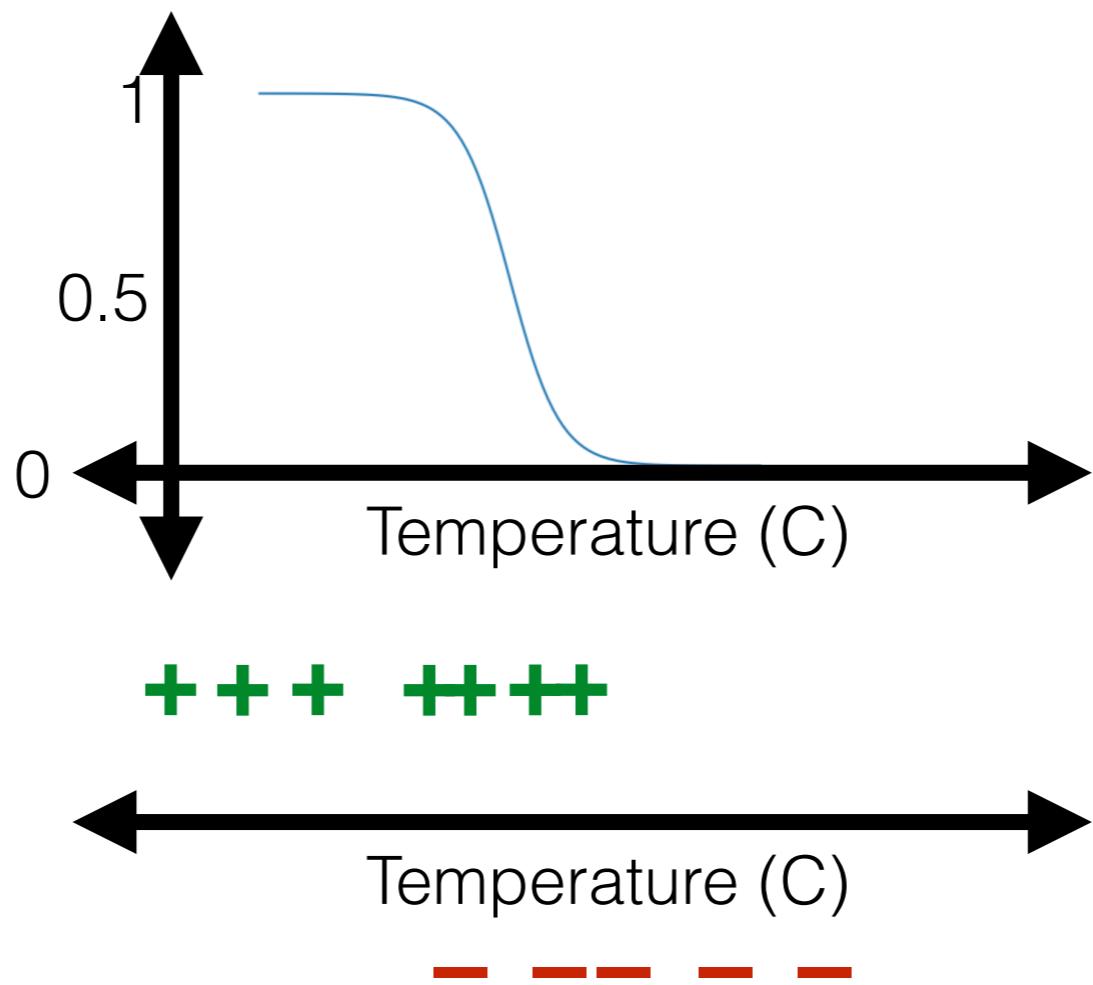


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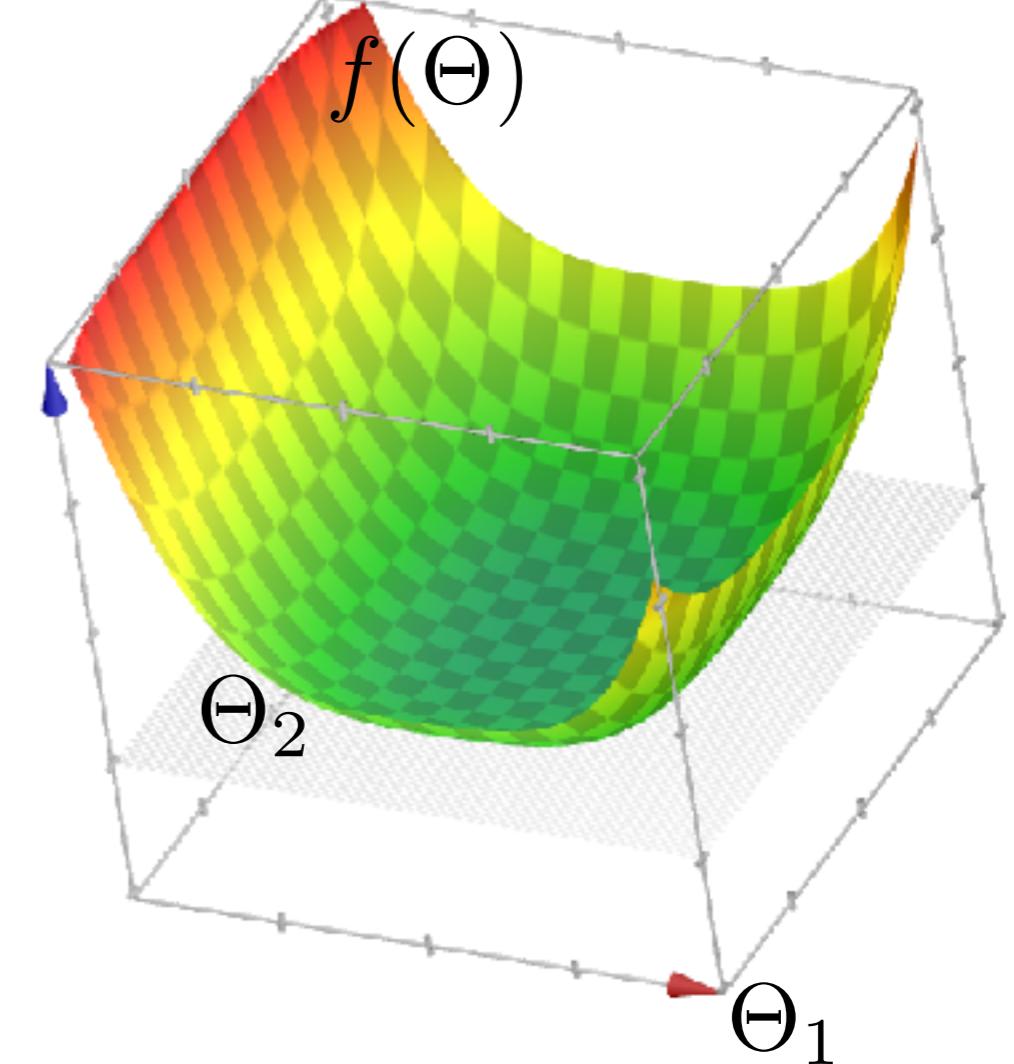
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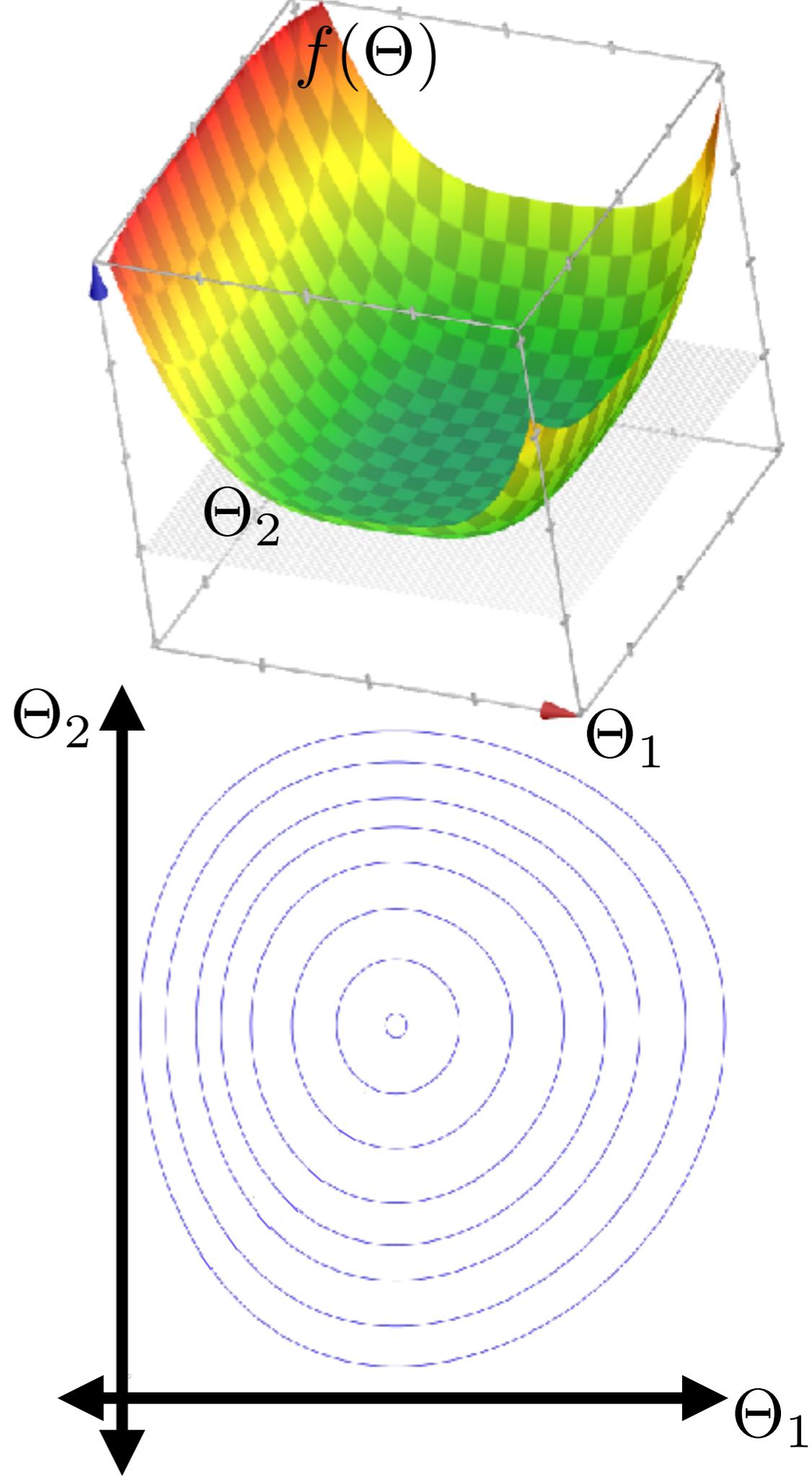


# Gradient descent

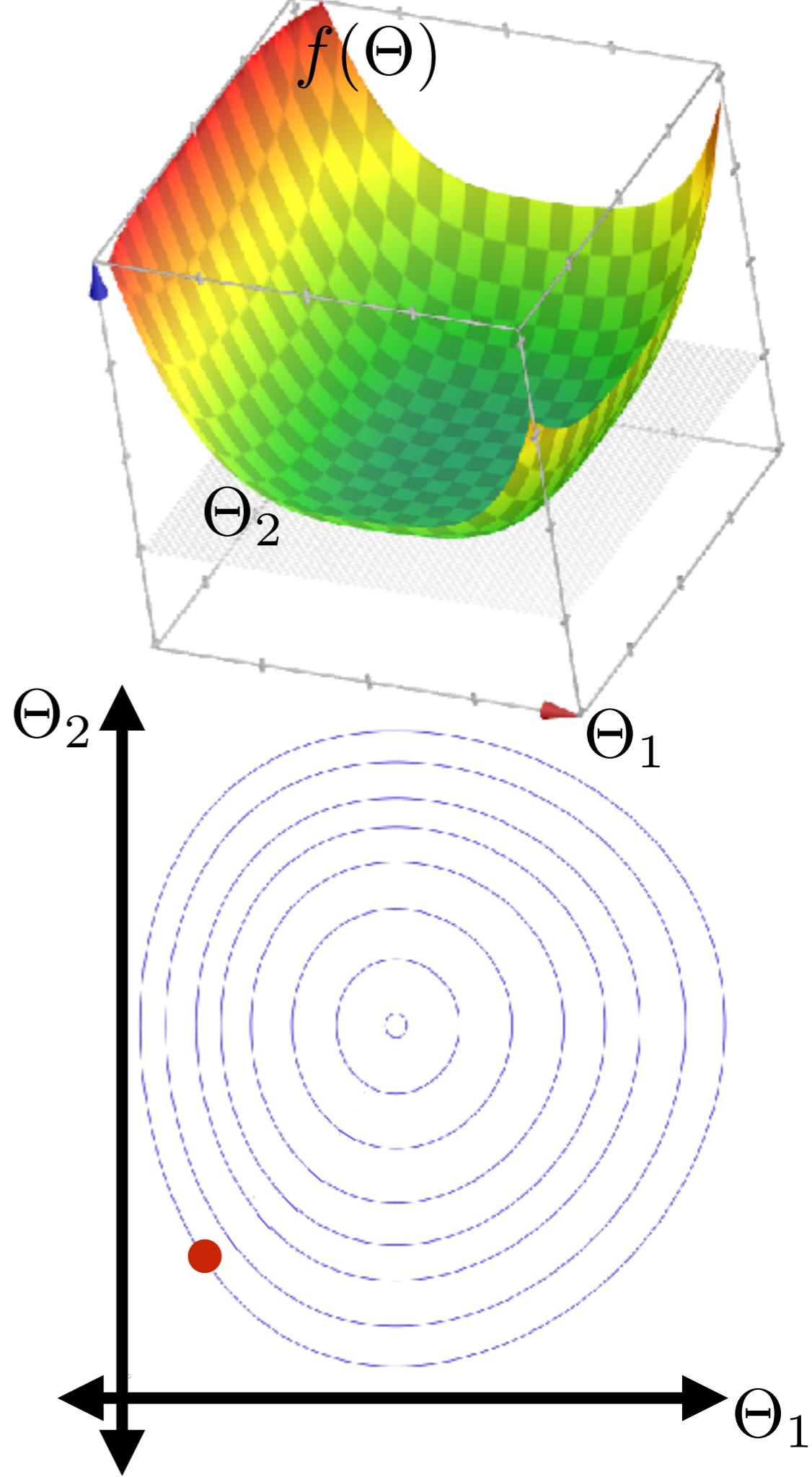
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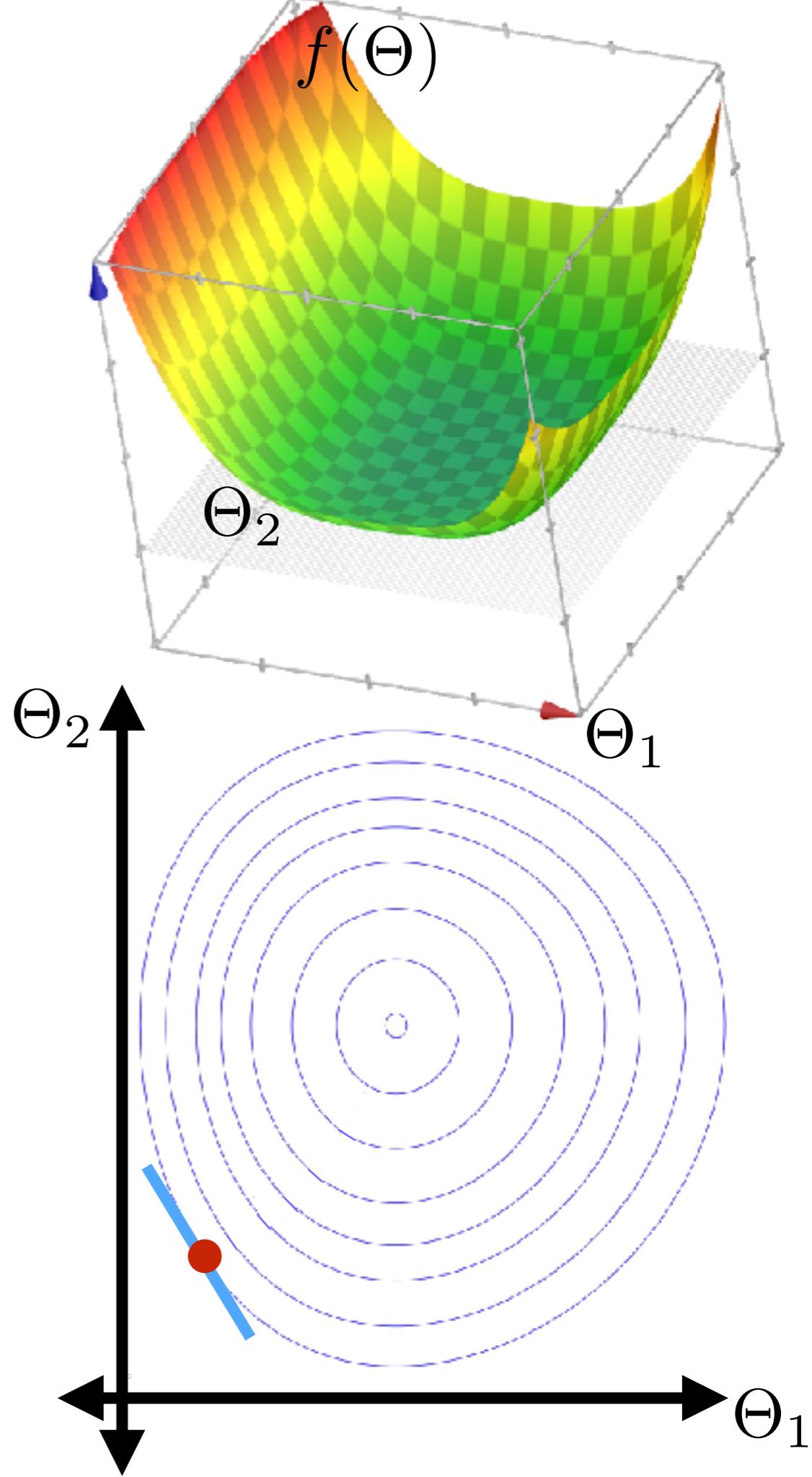
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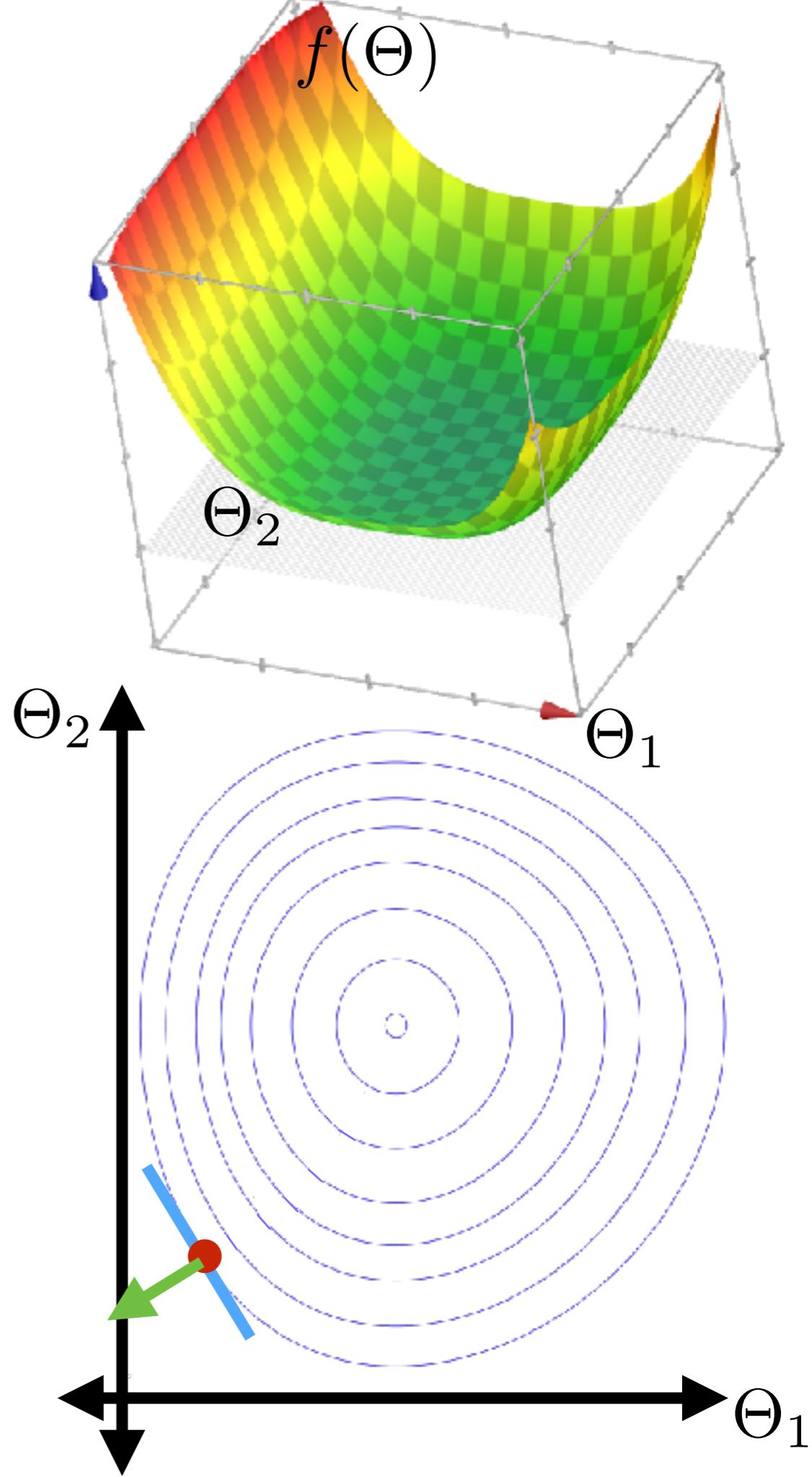
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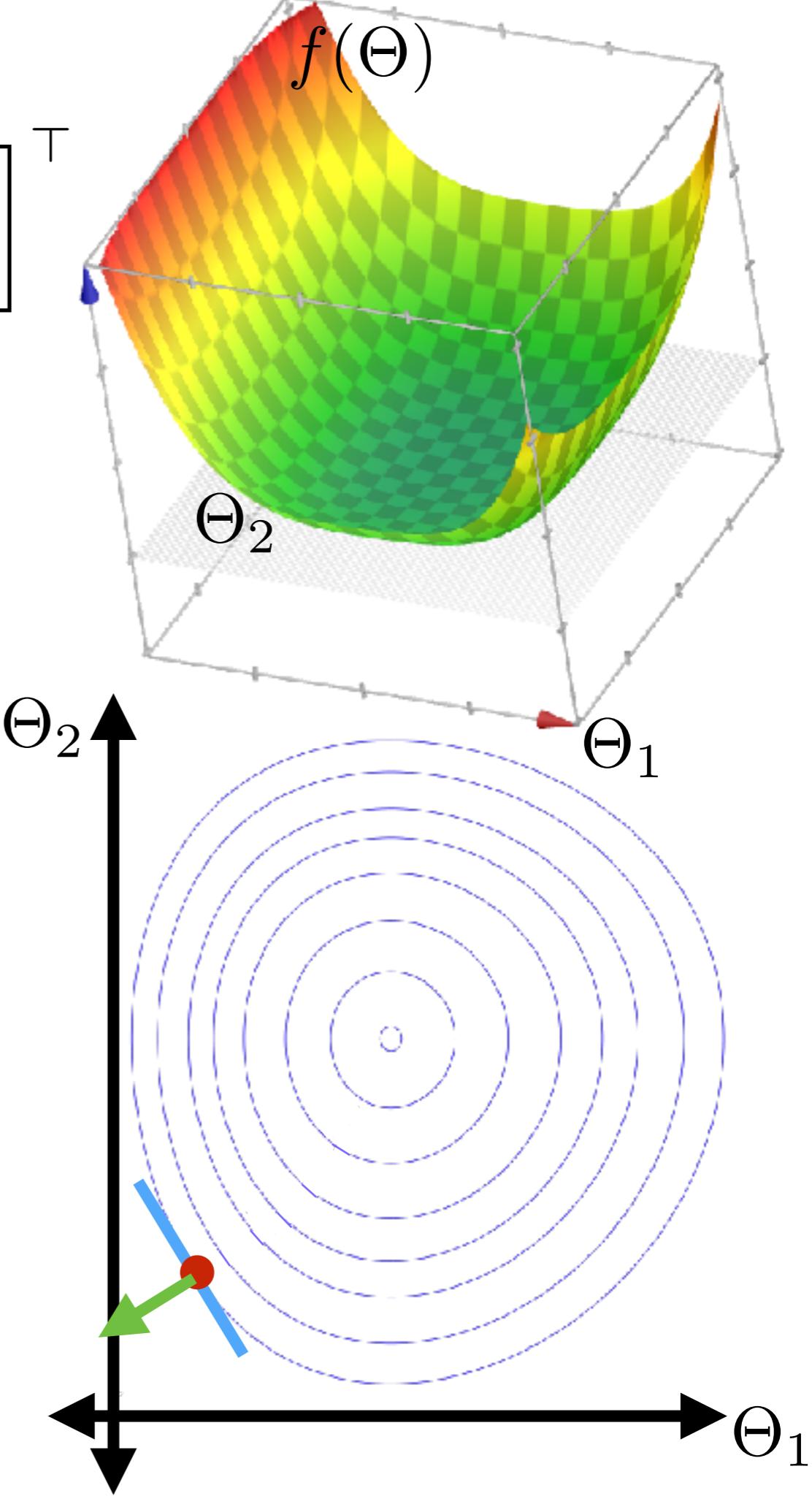


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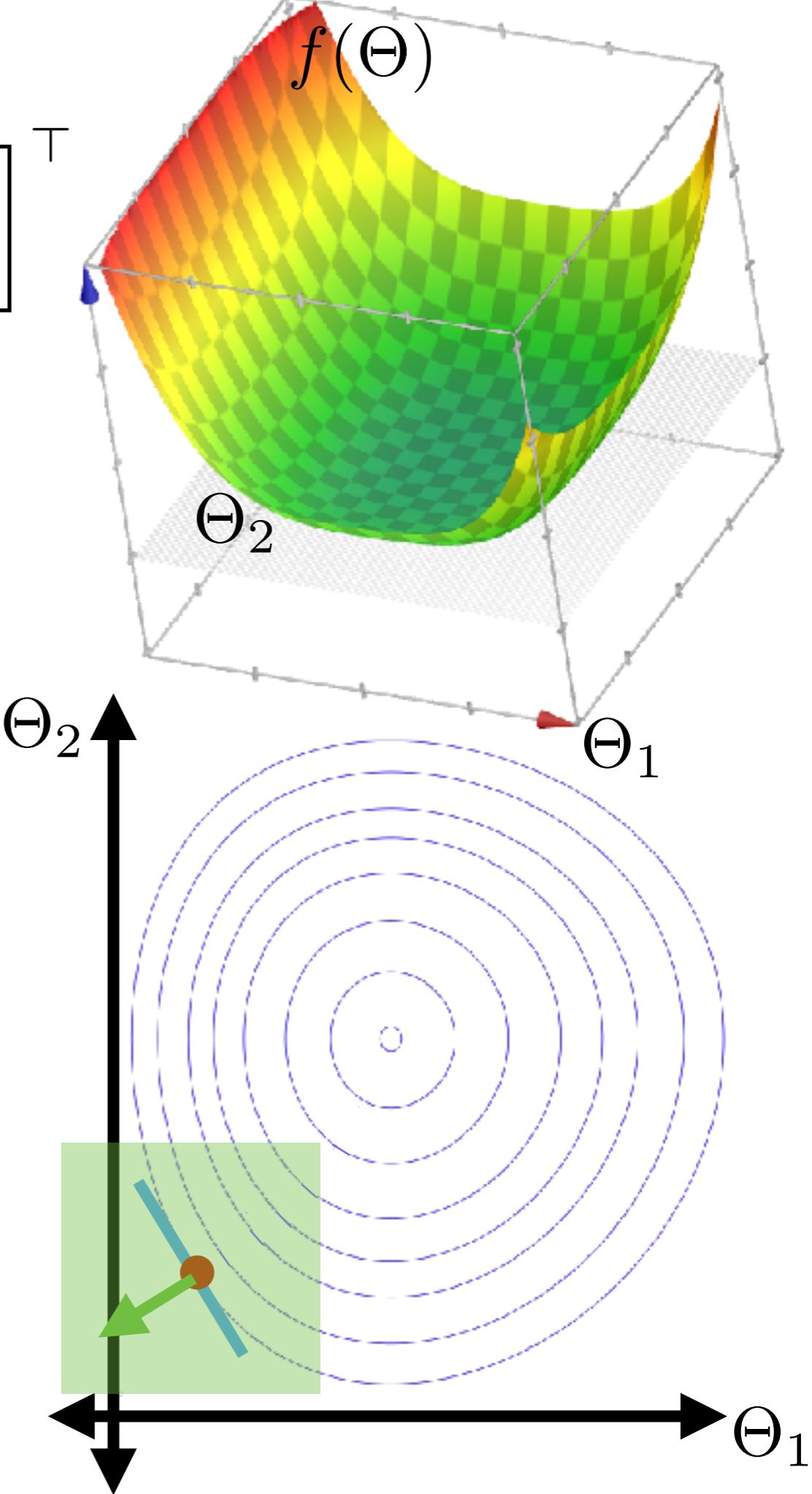
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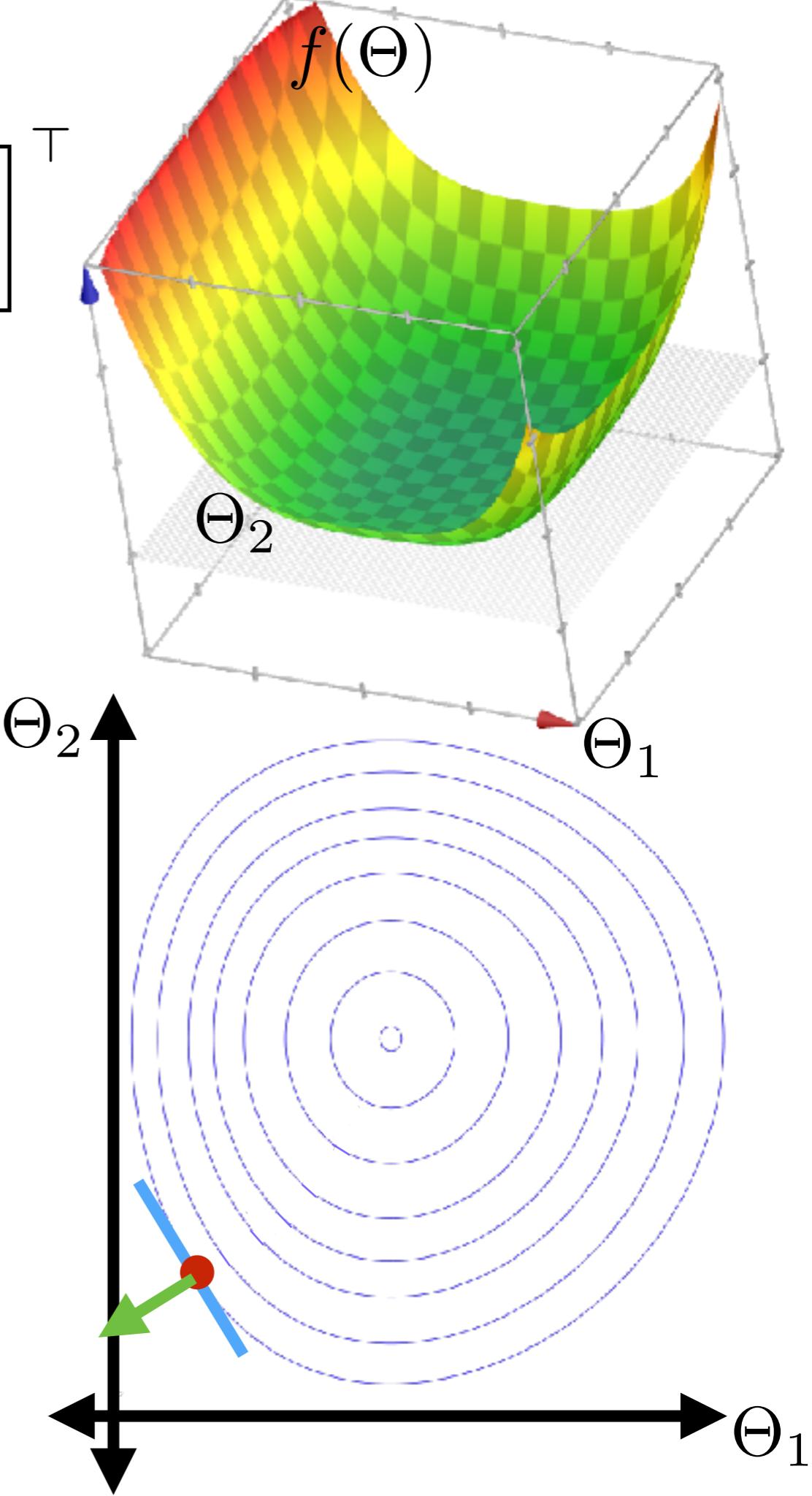
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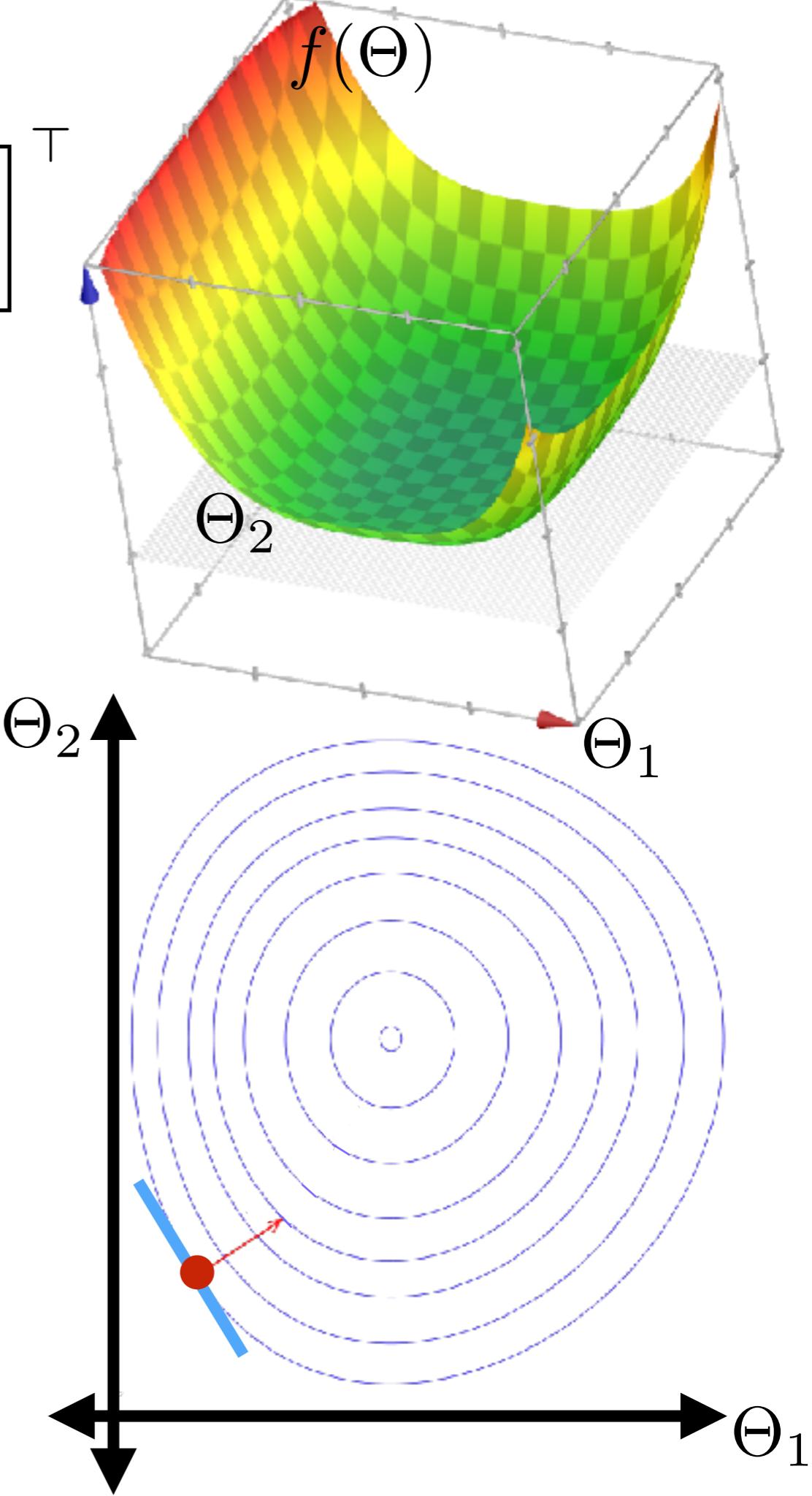
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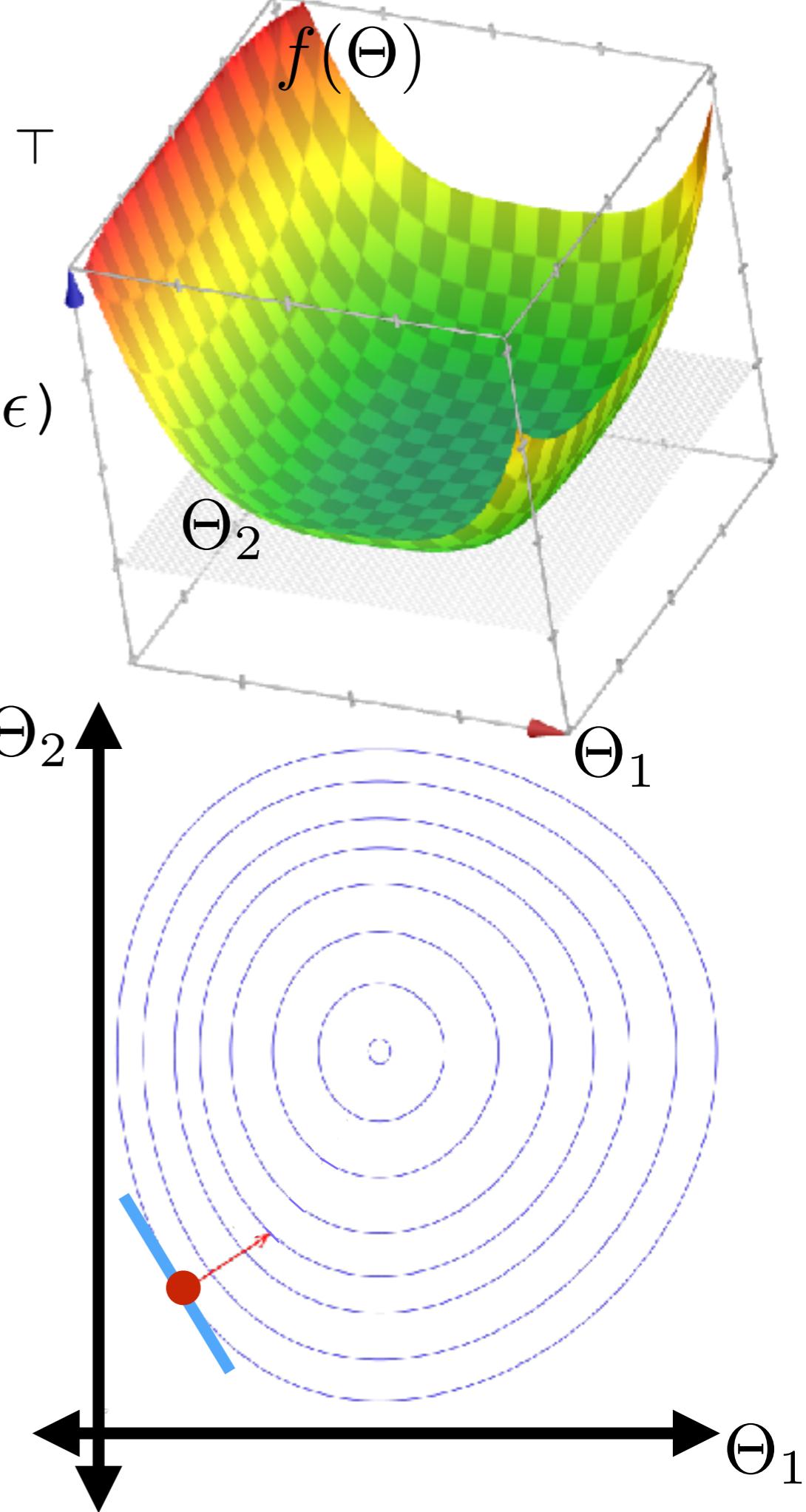
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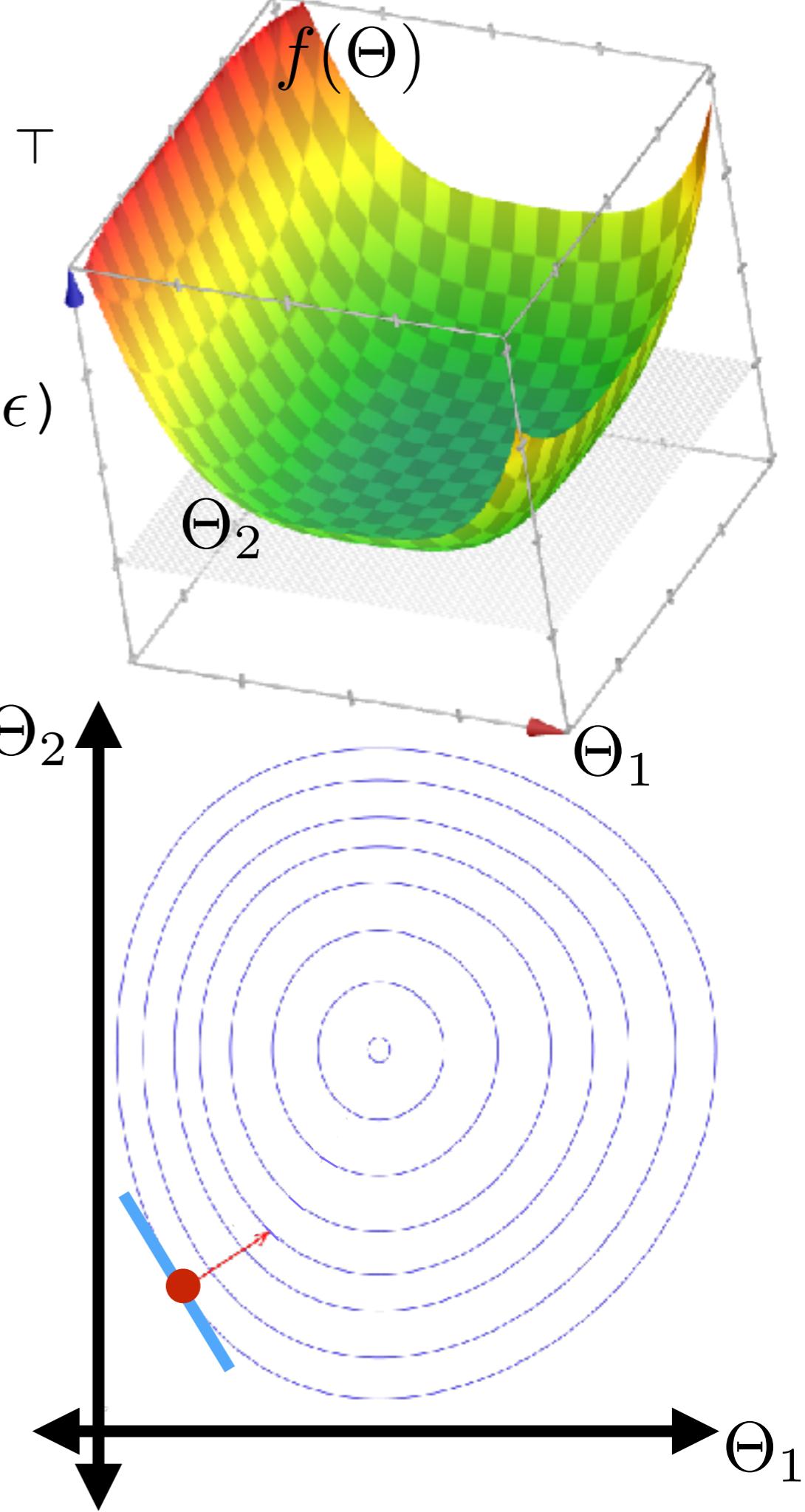


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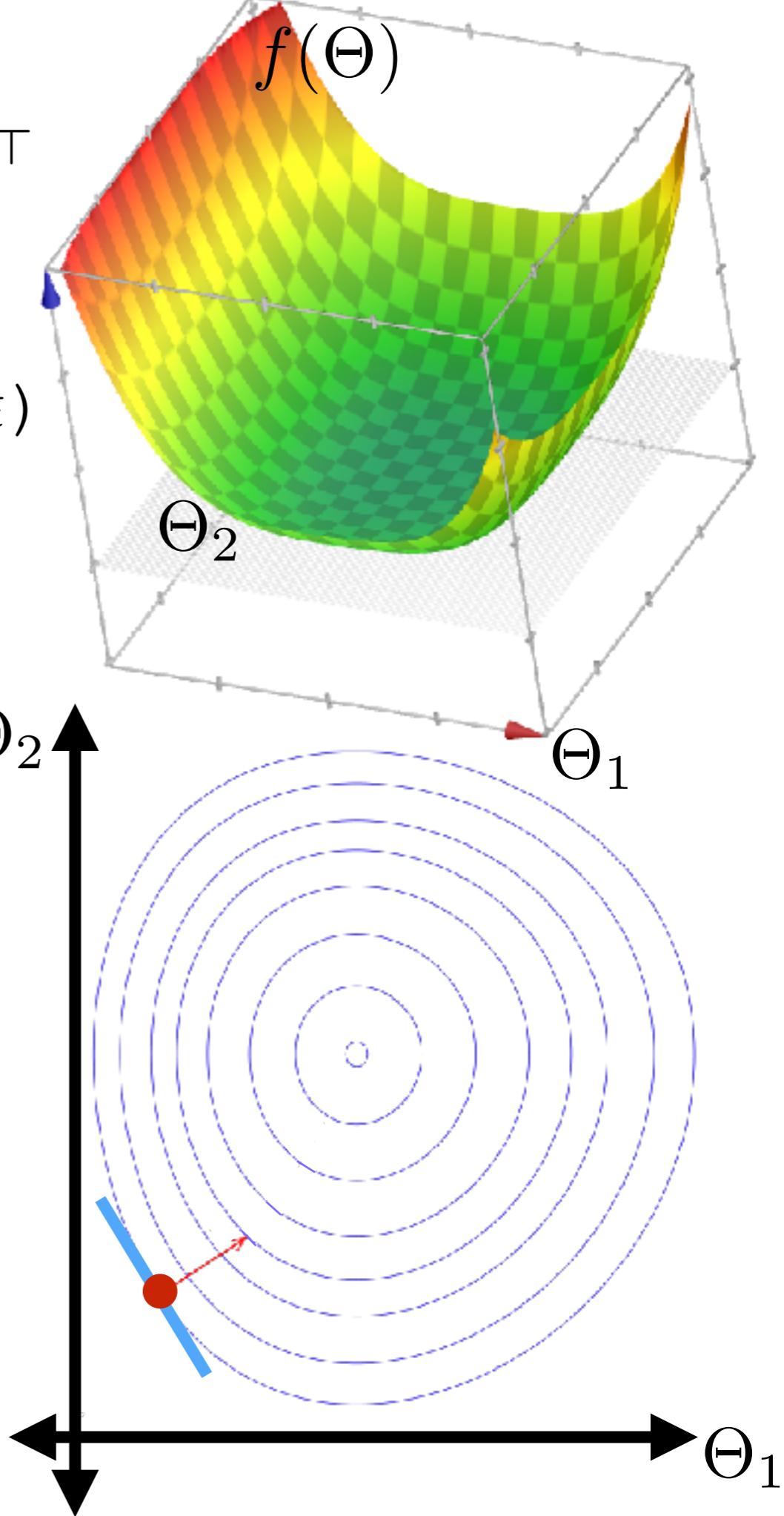
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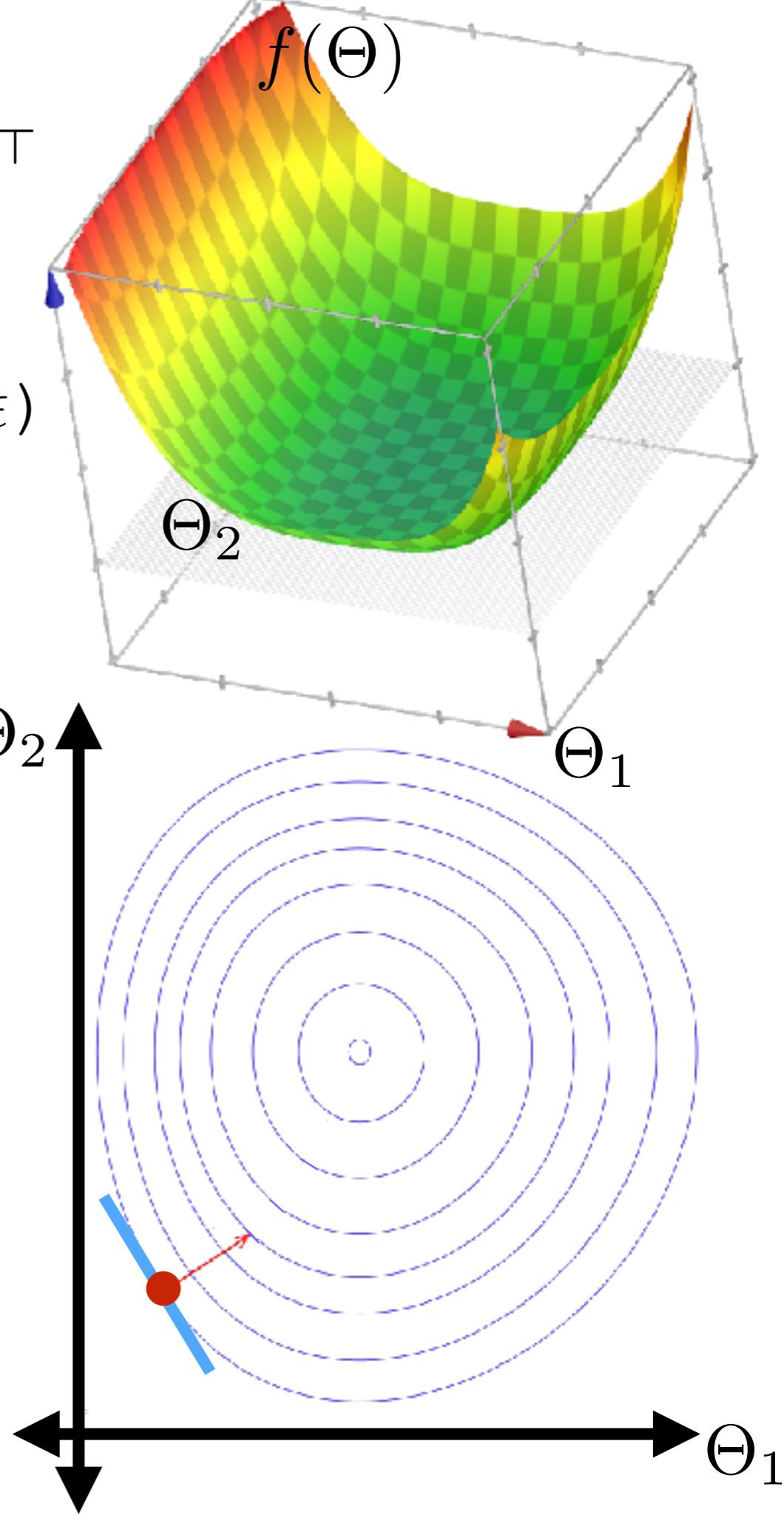
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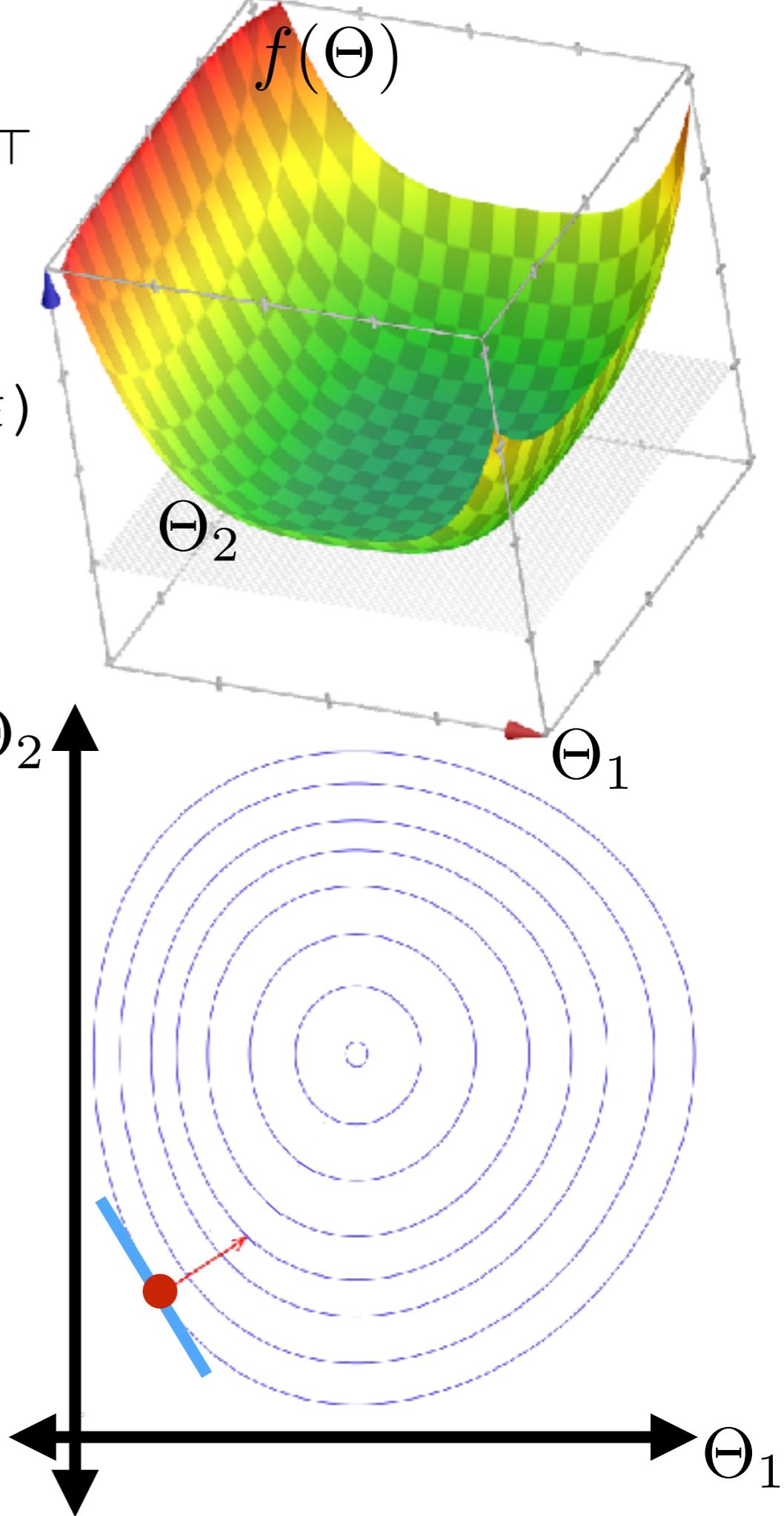
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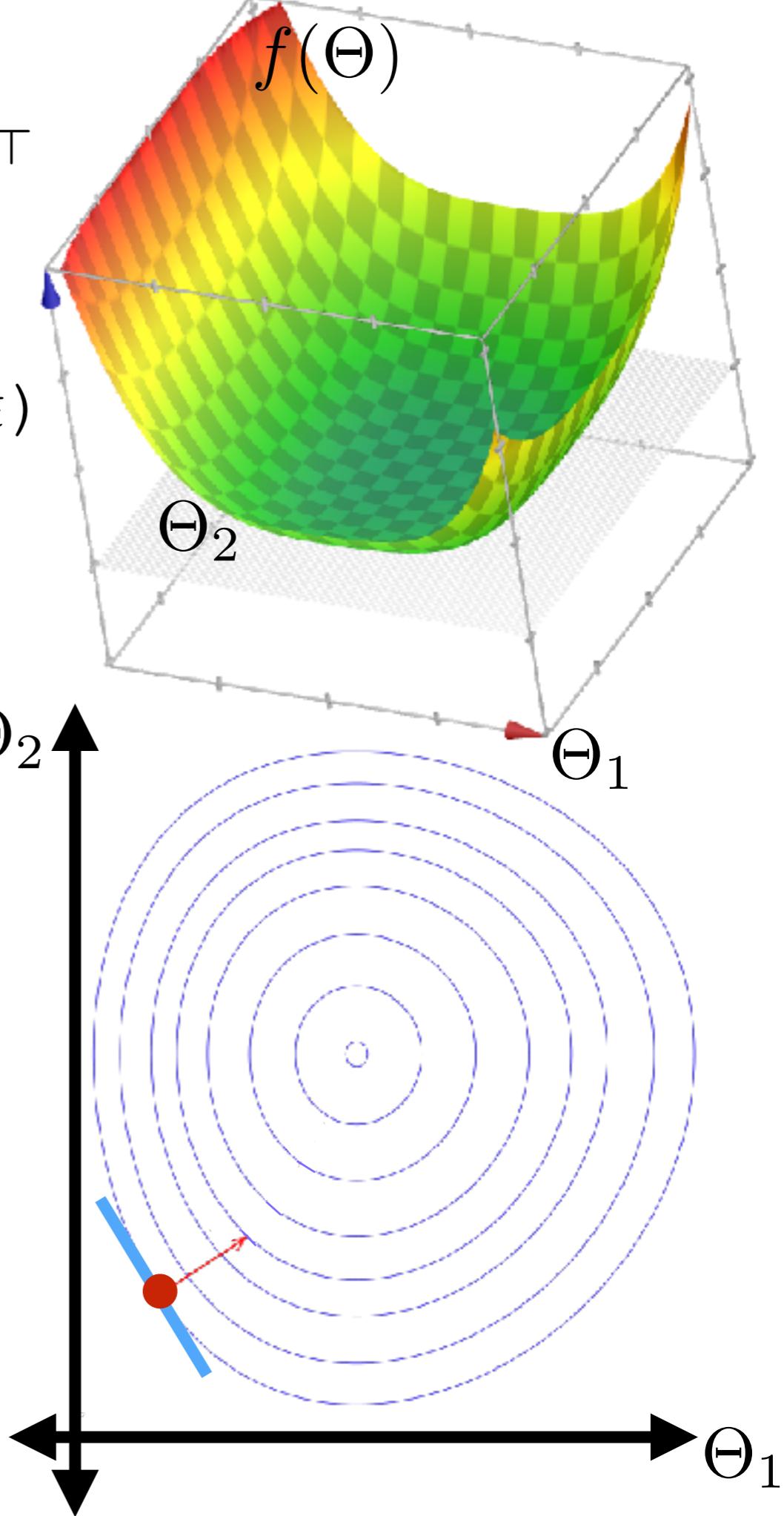
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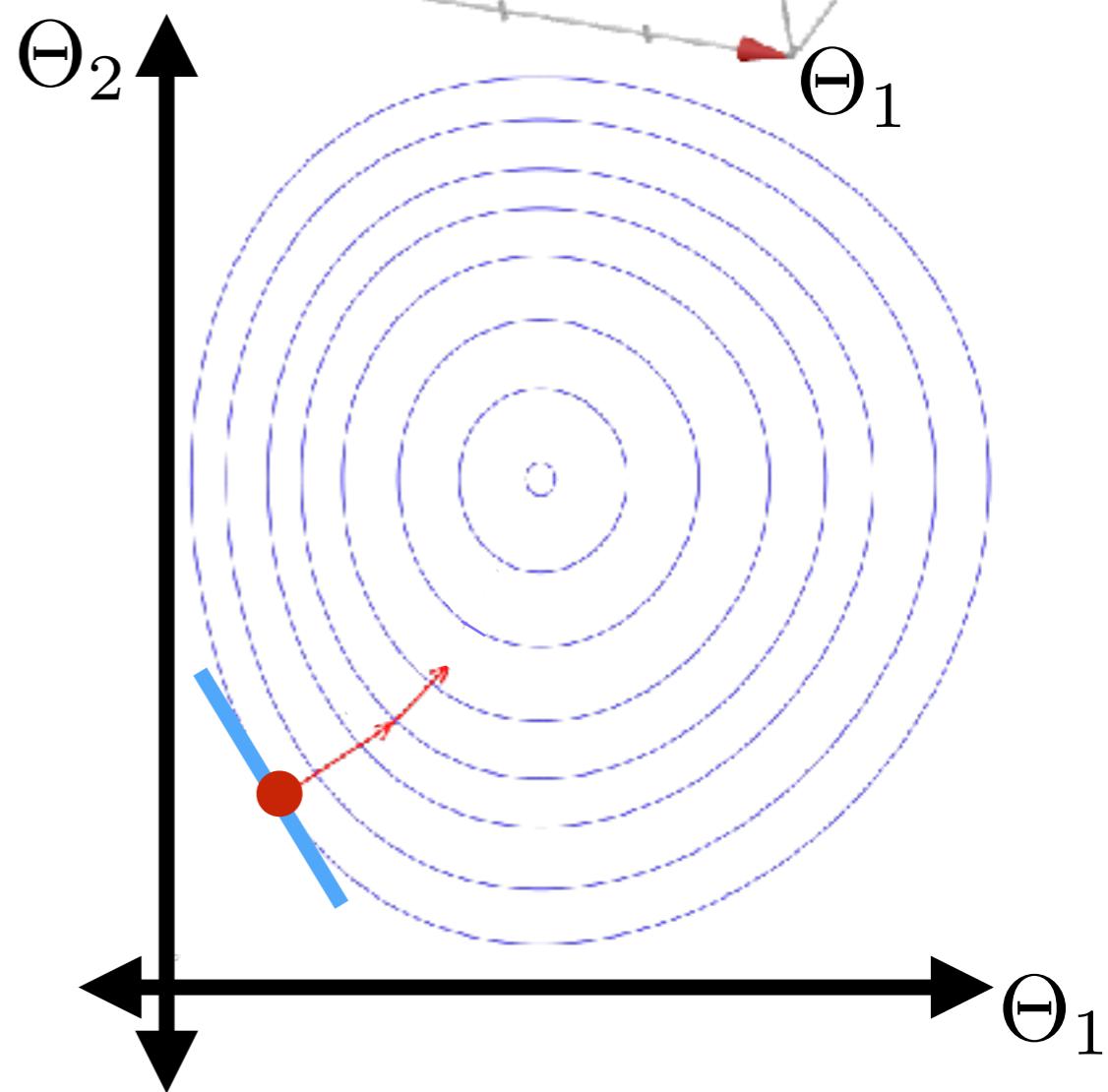
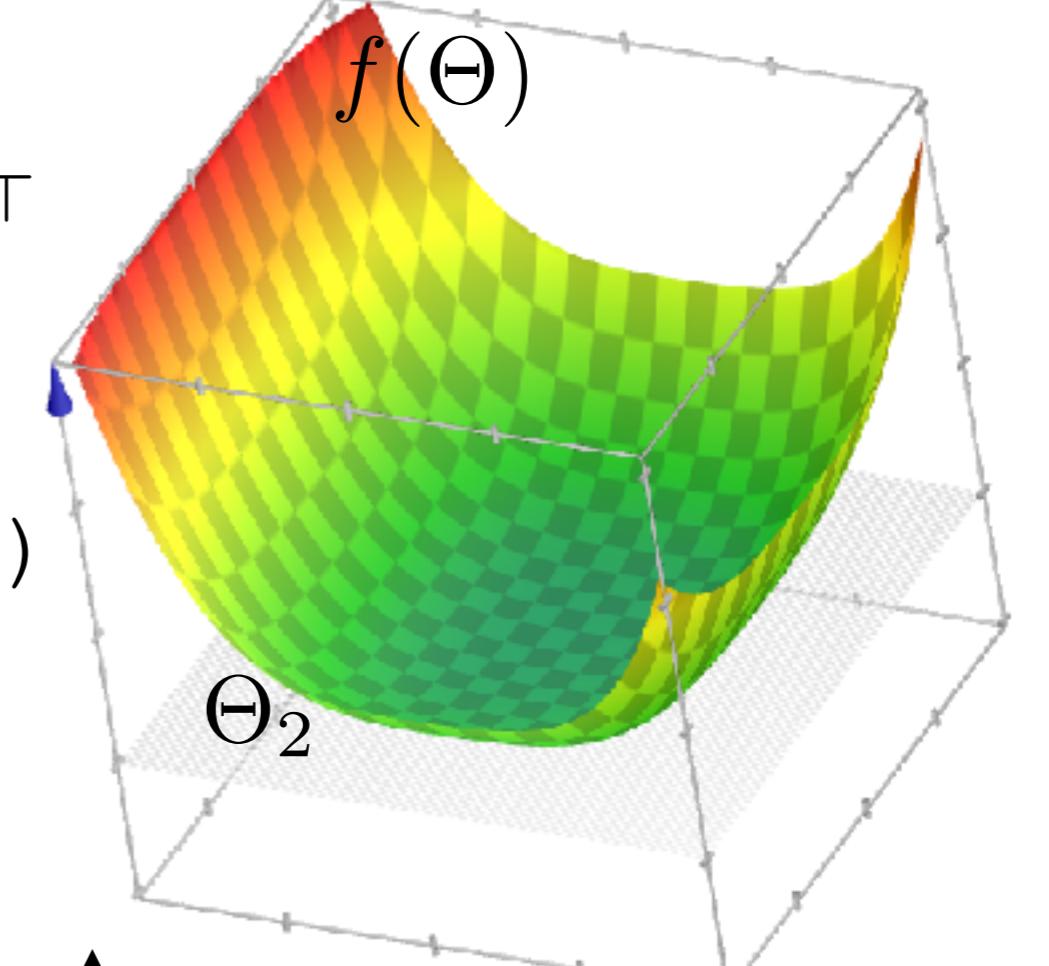
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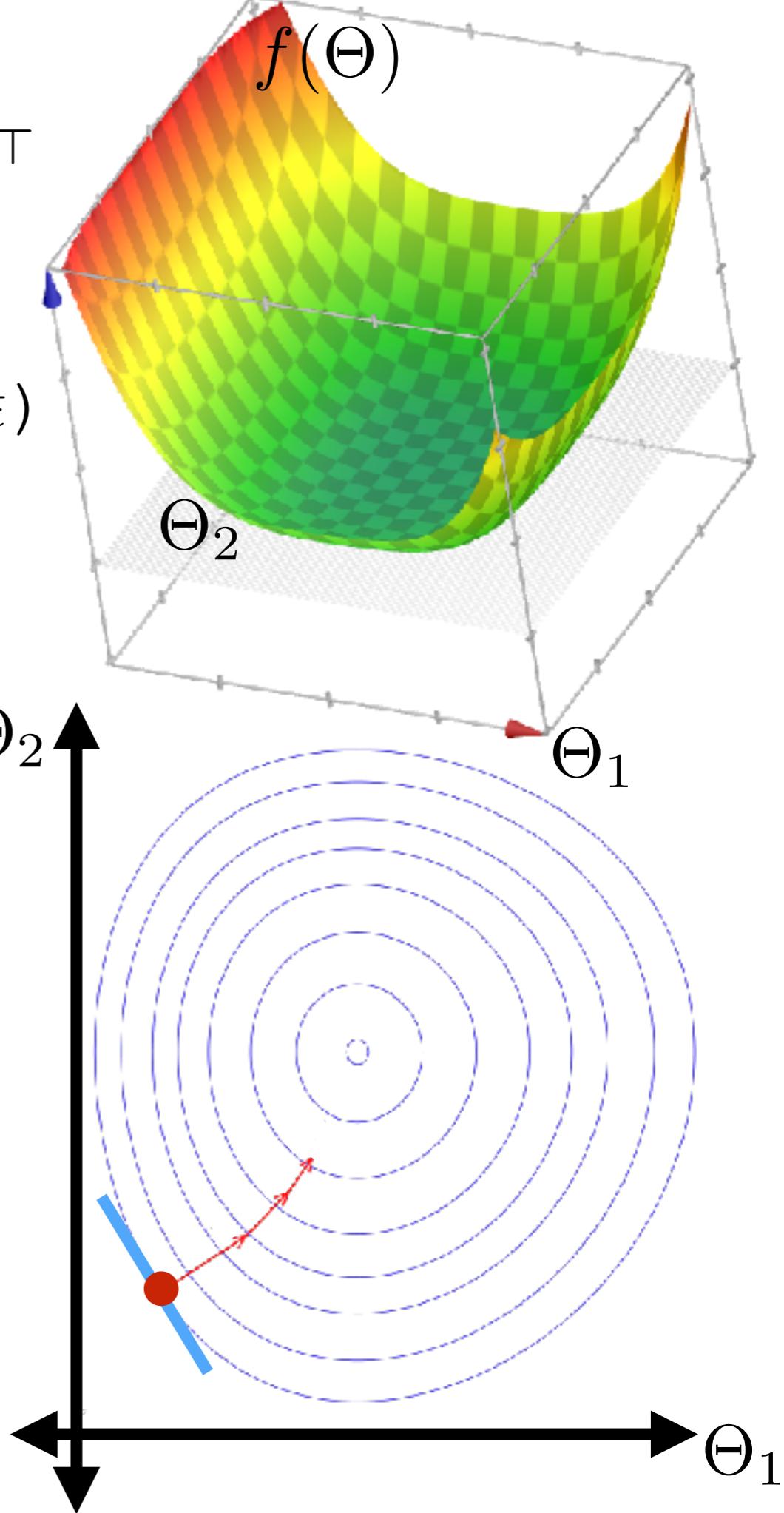
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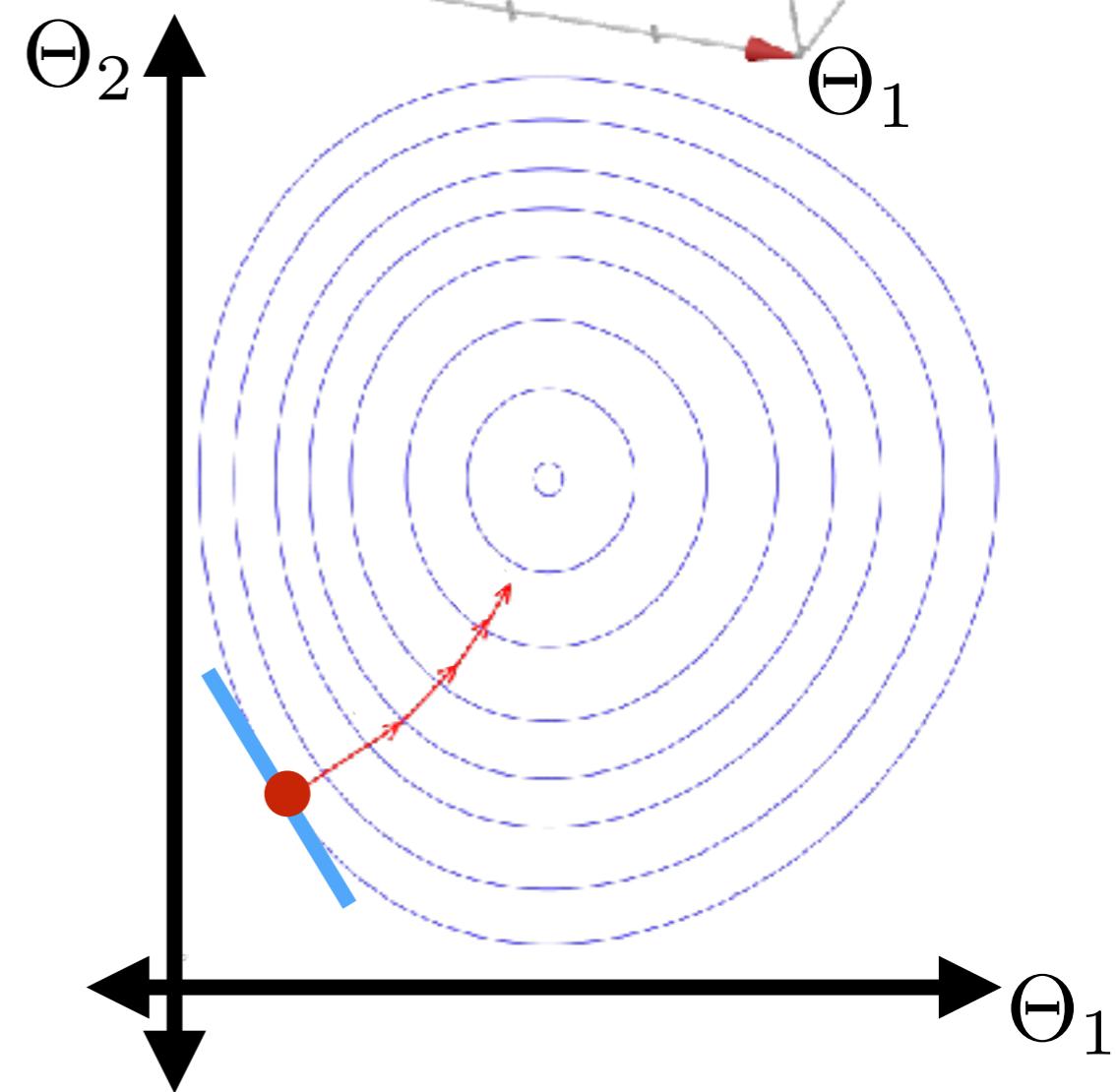
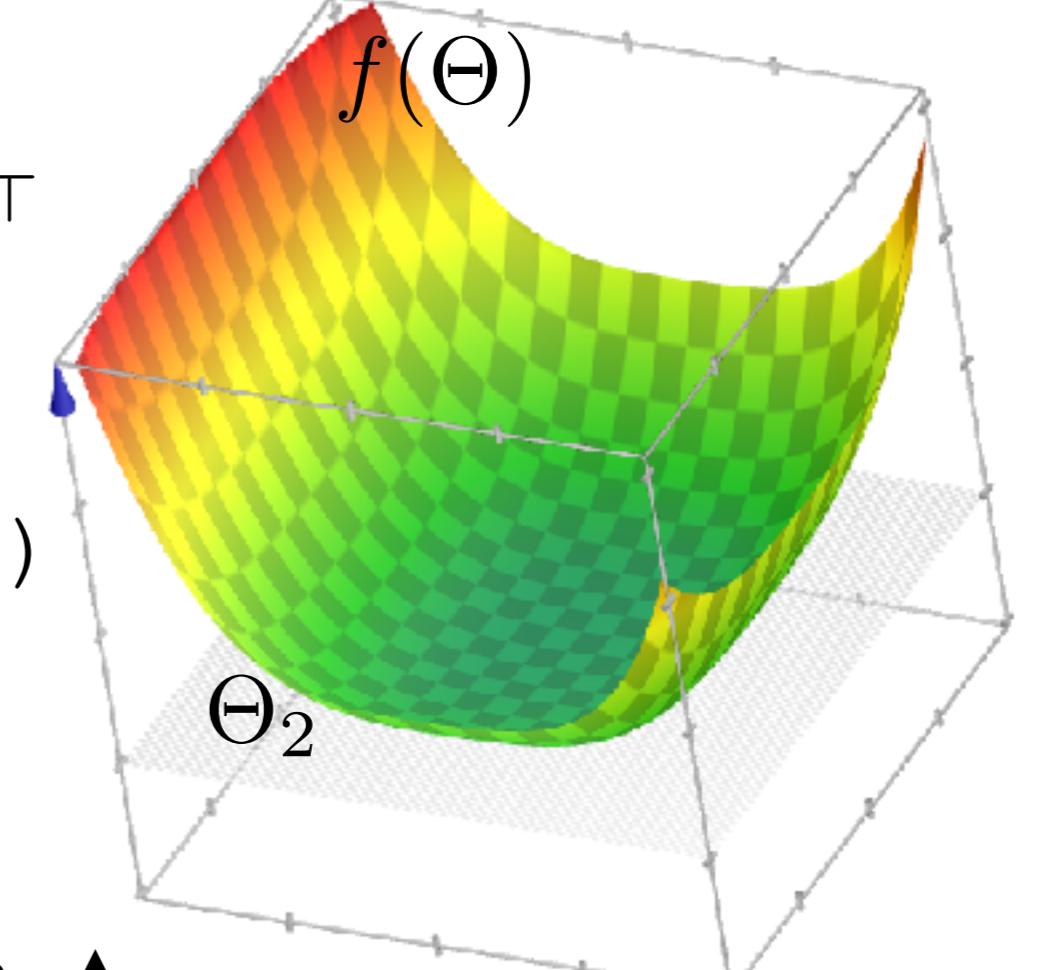
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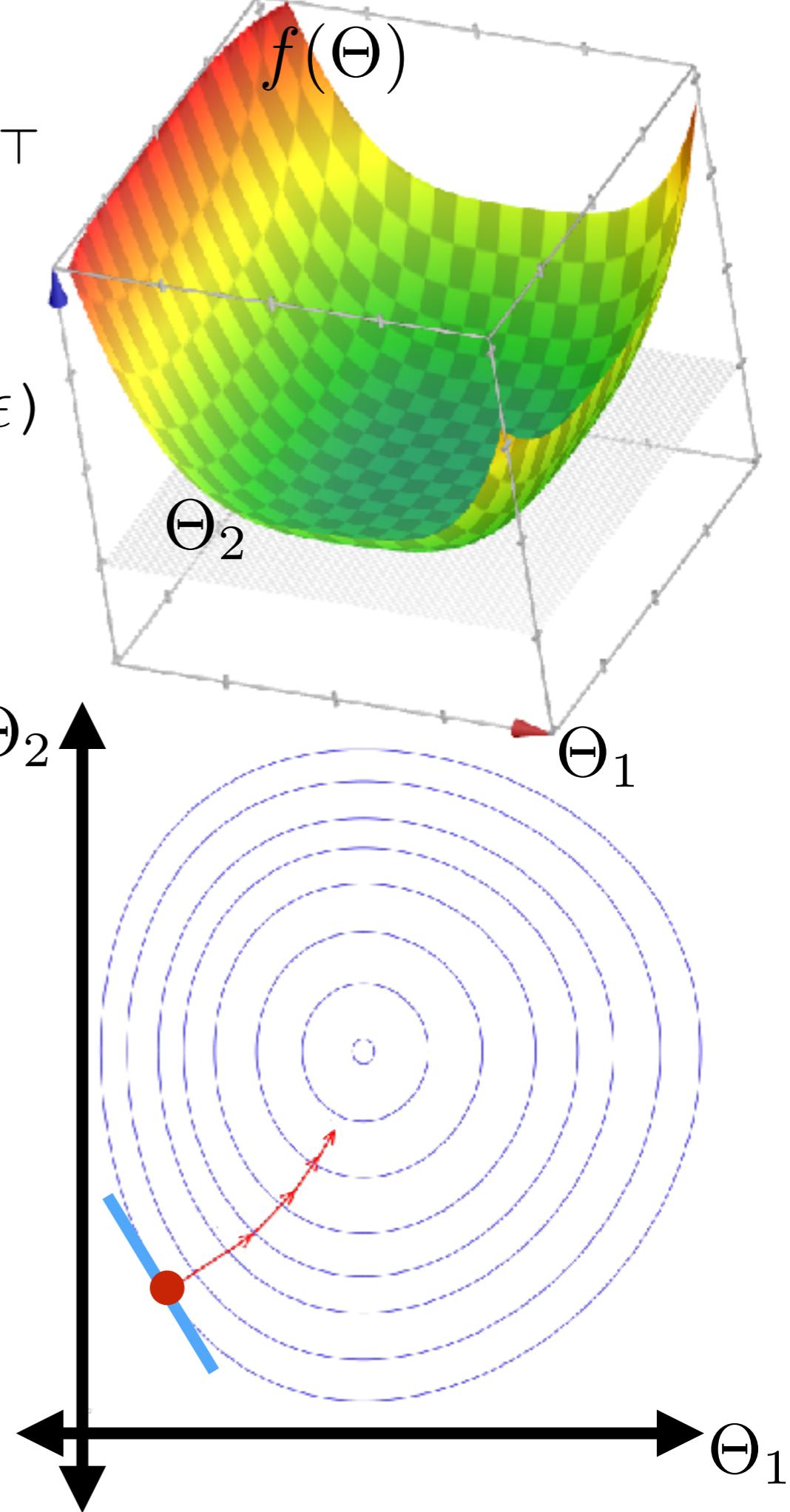
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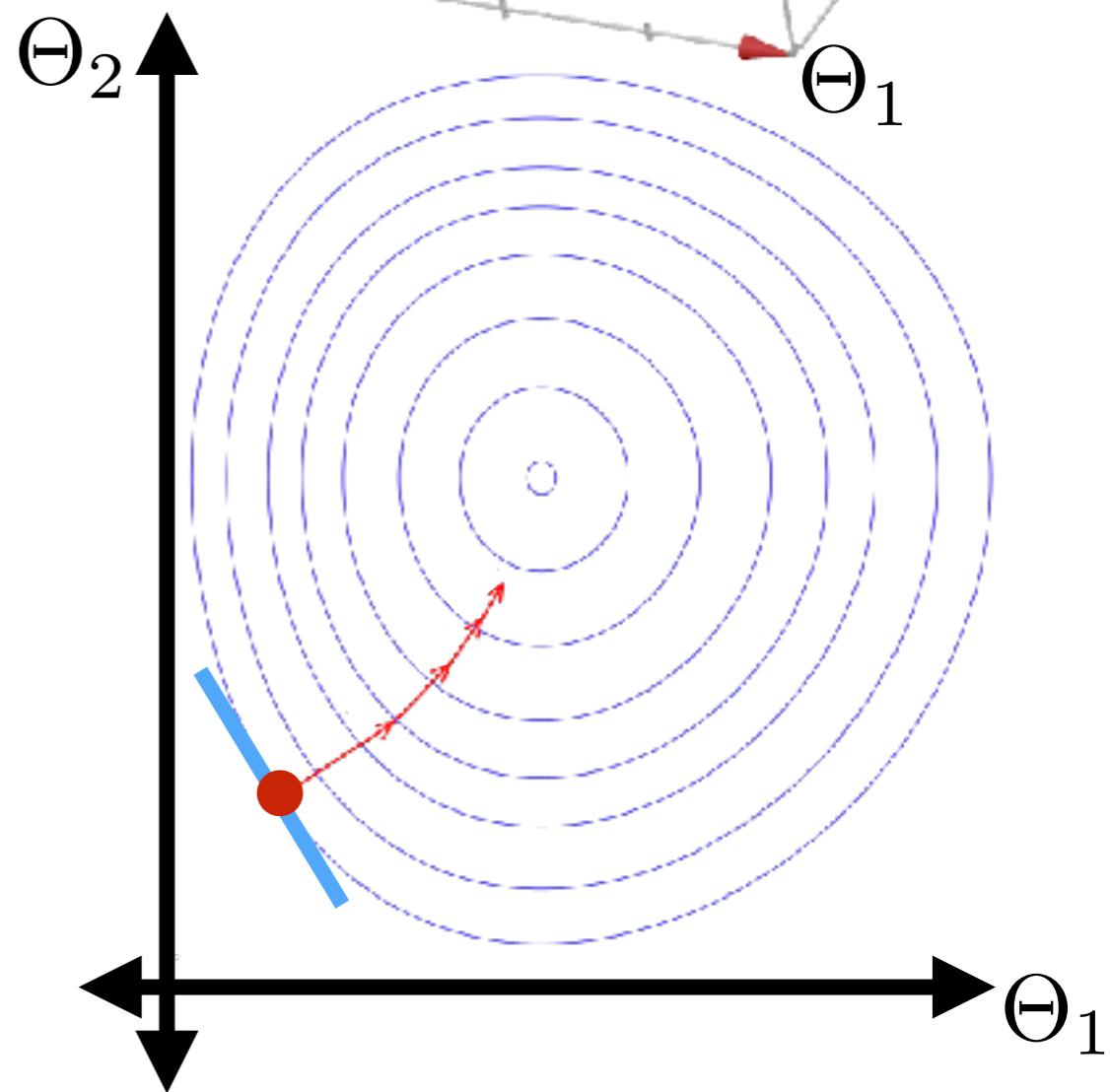
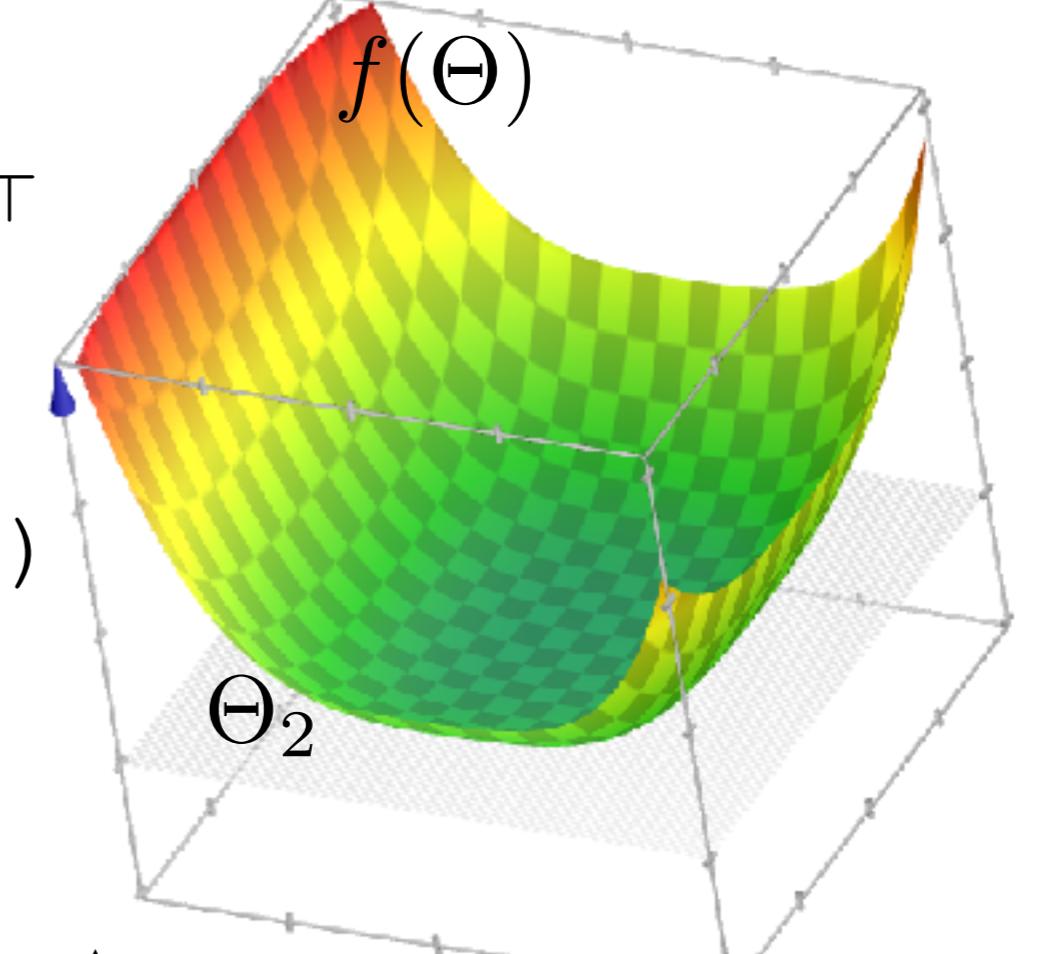
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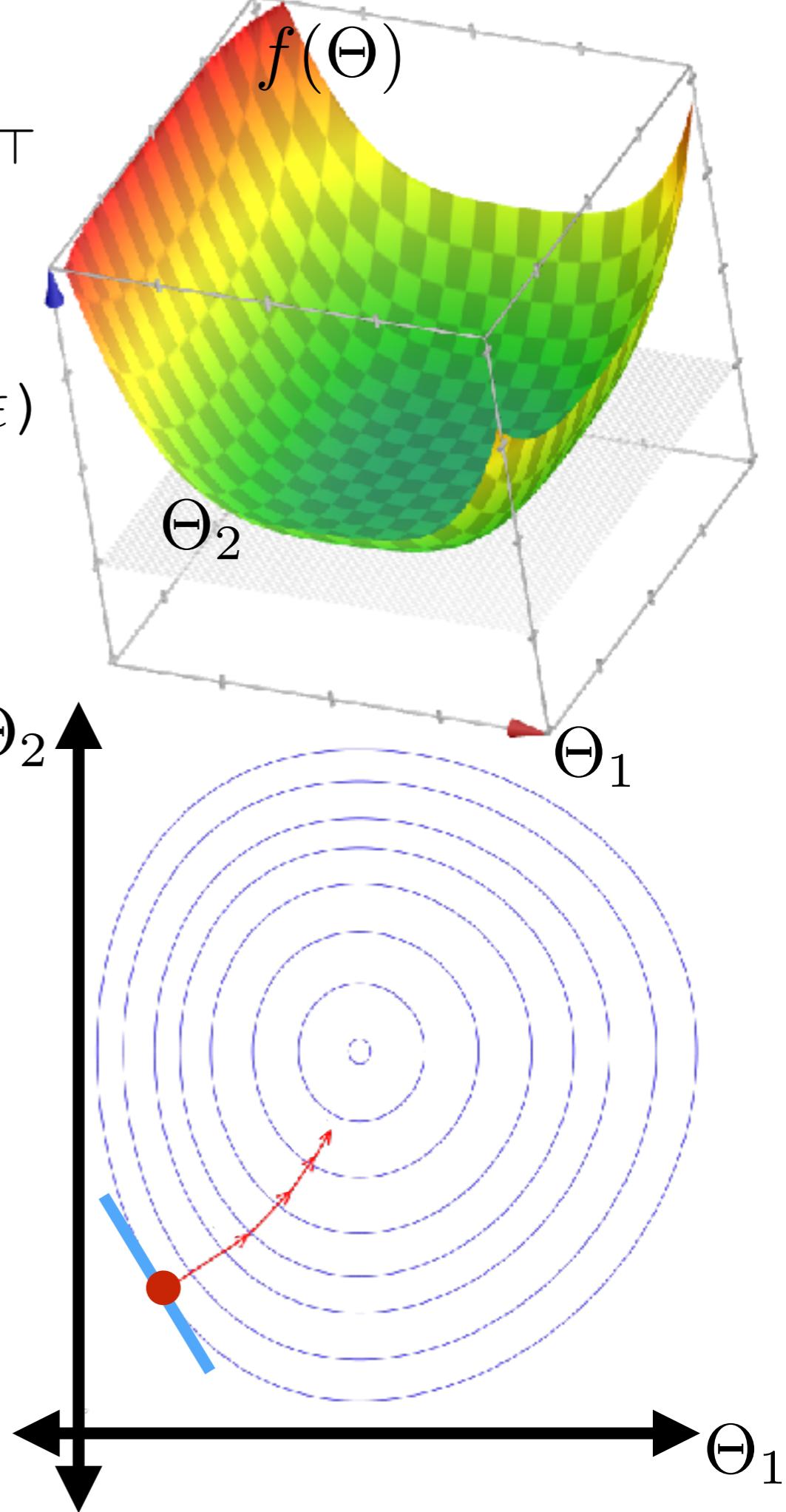
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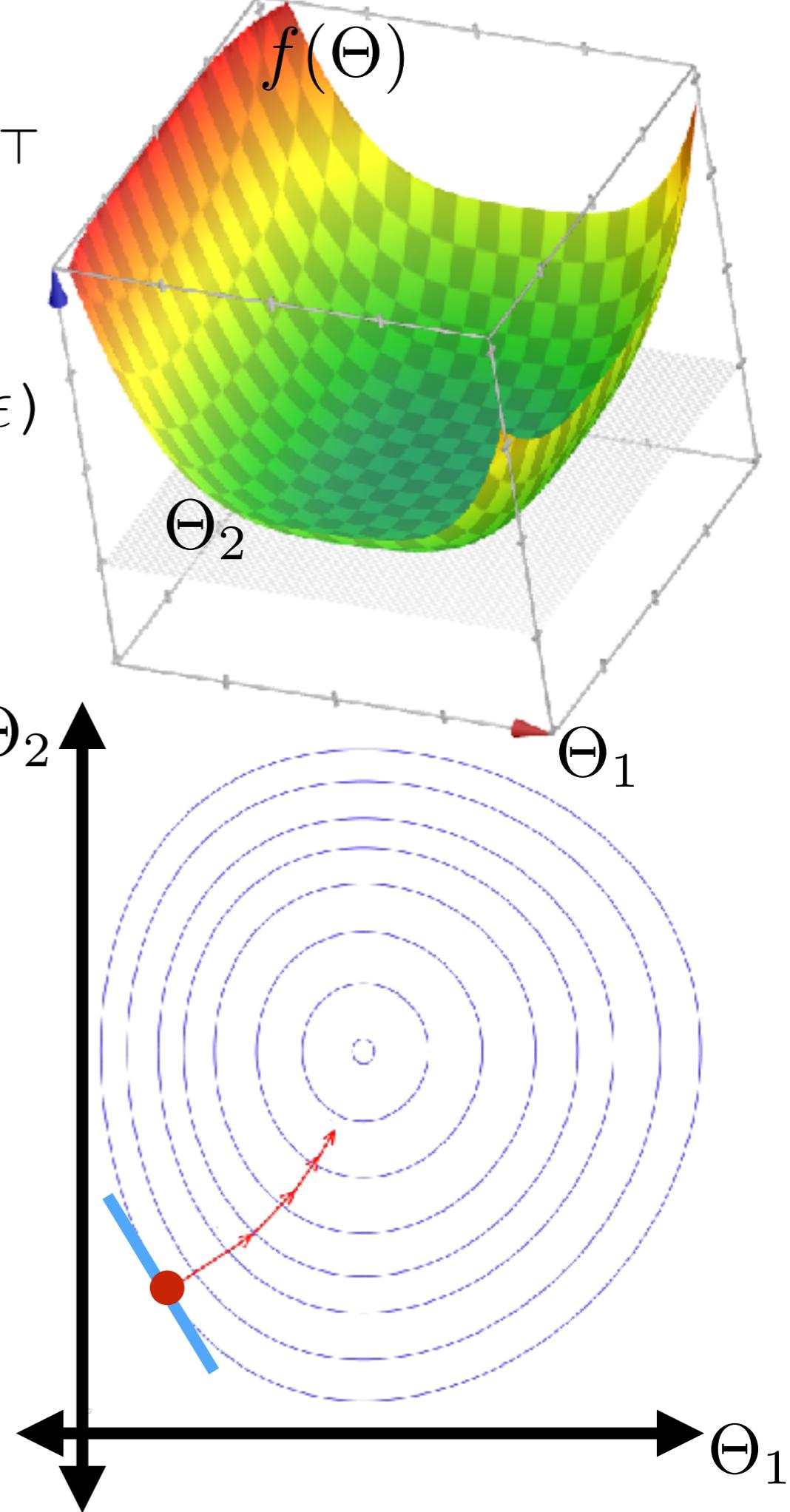
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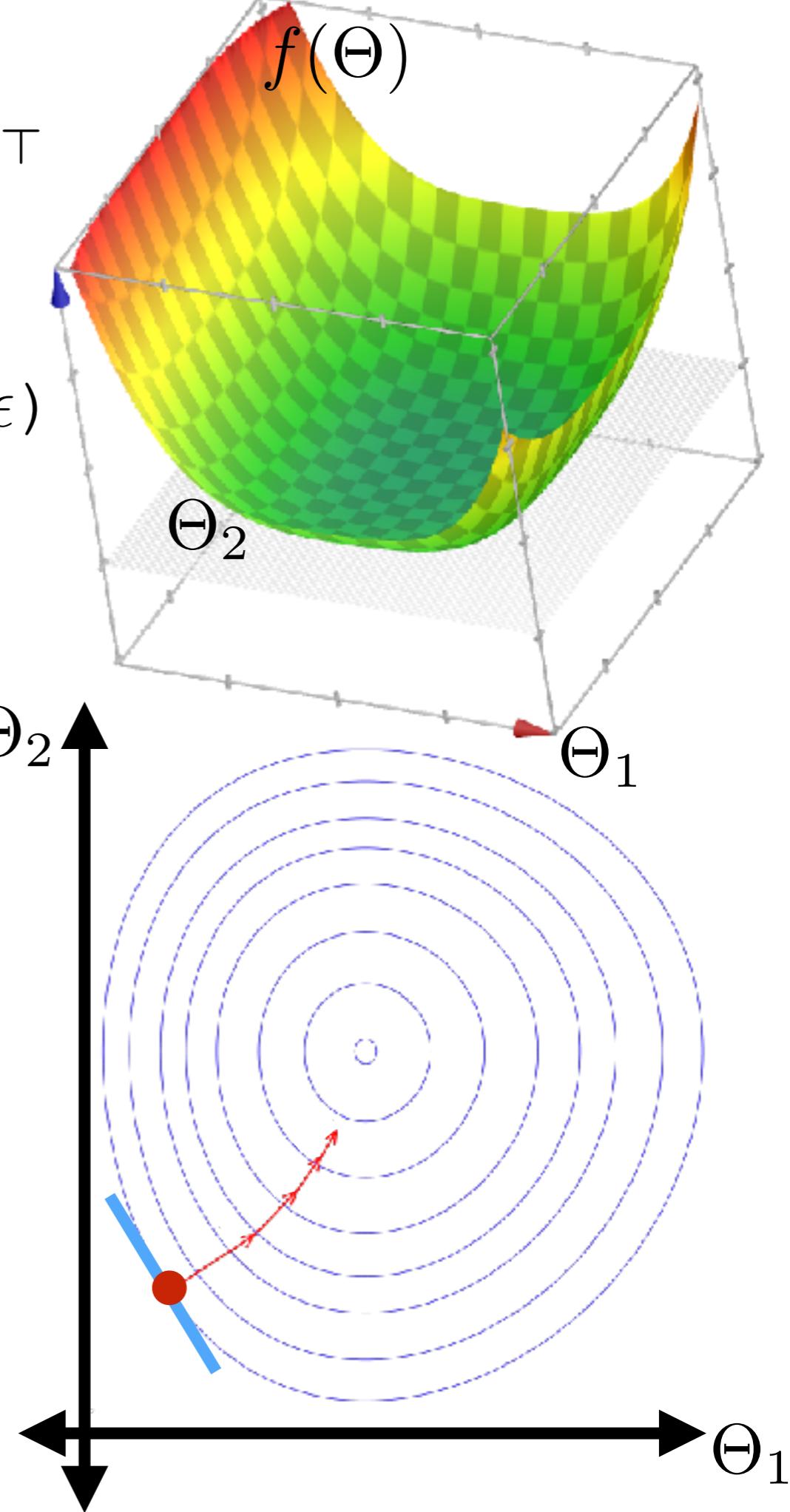
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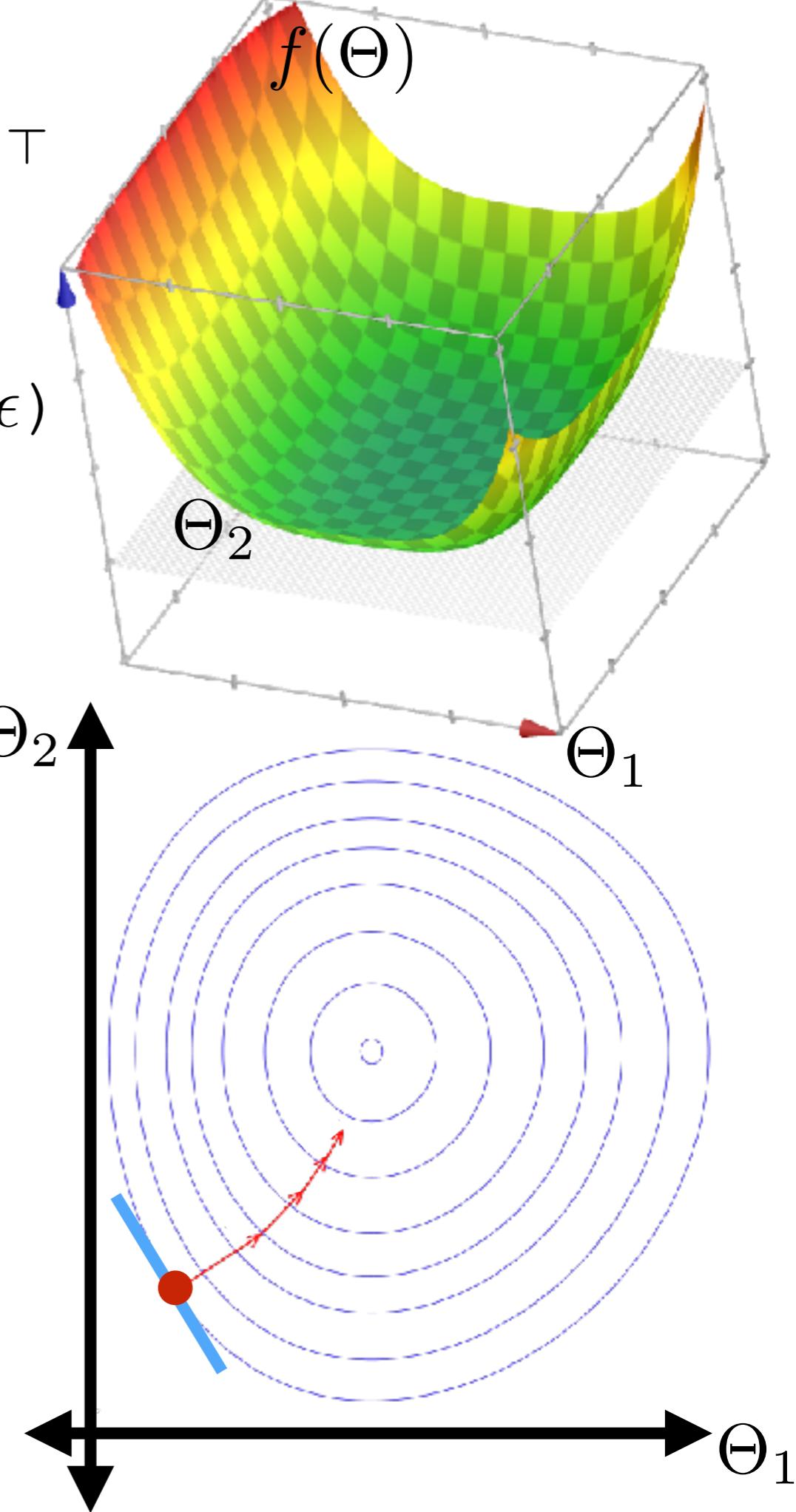
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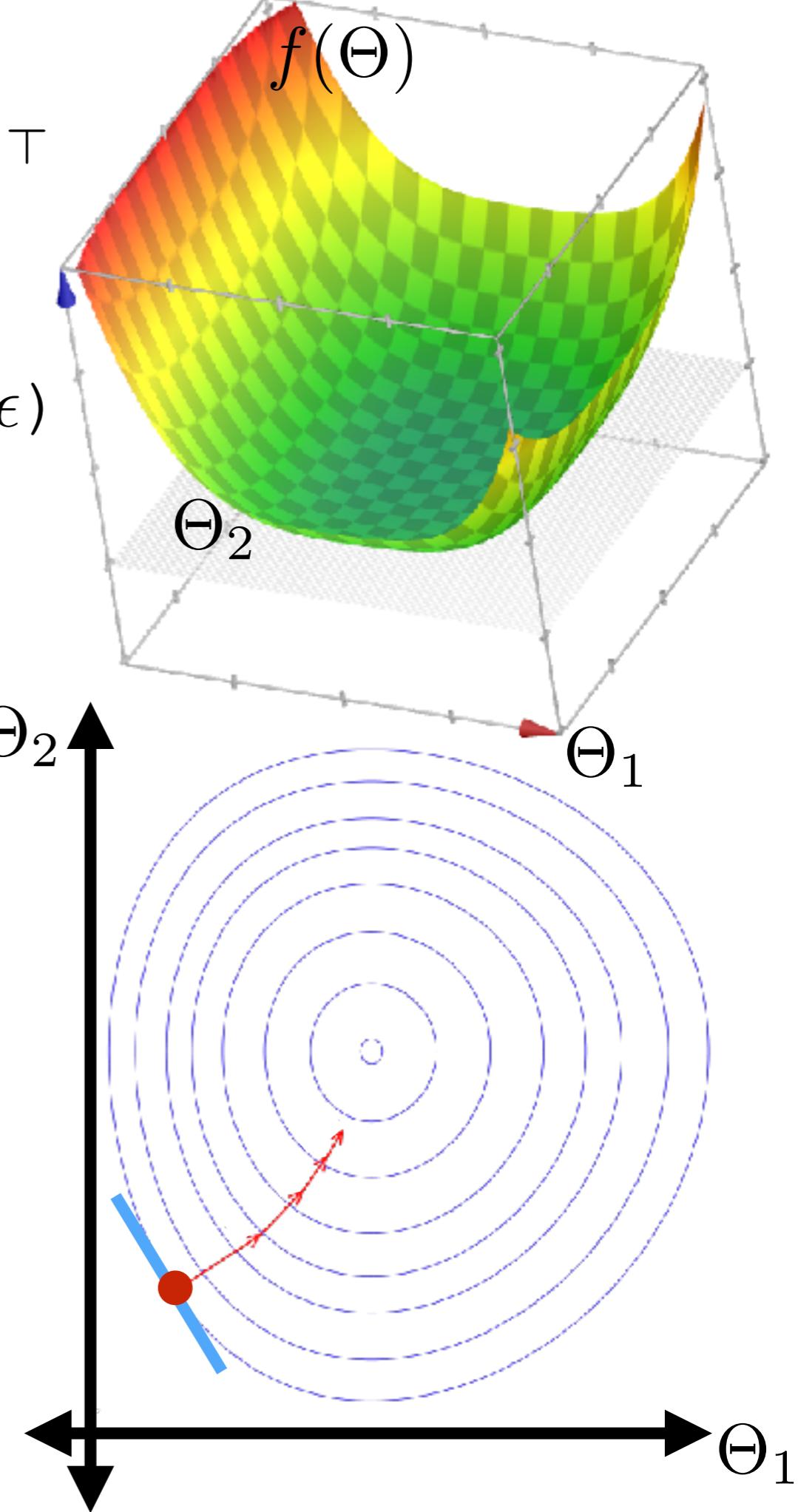
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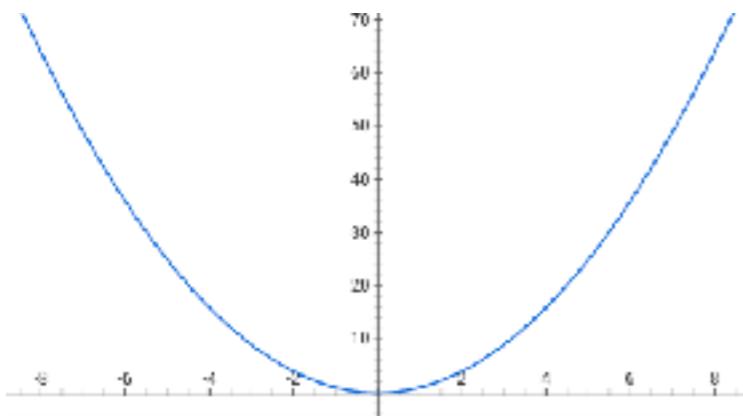


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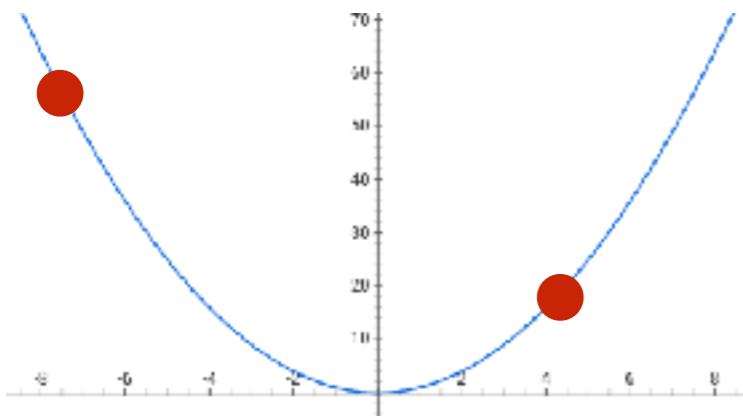
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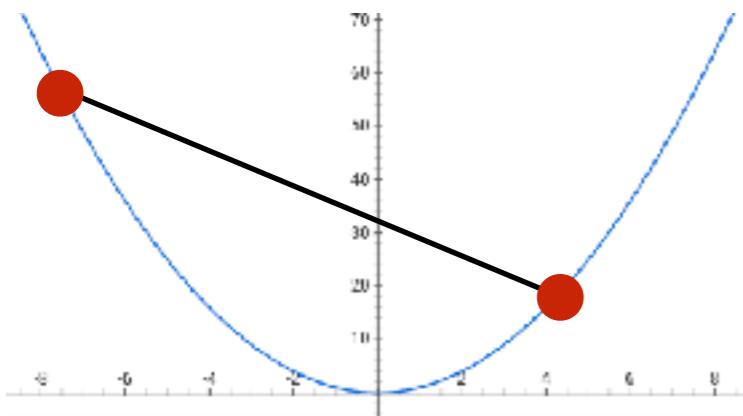
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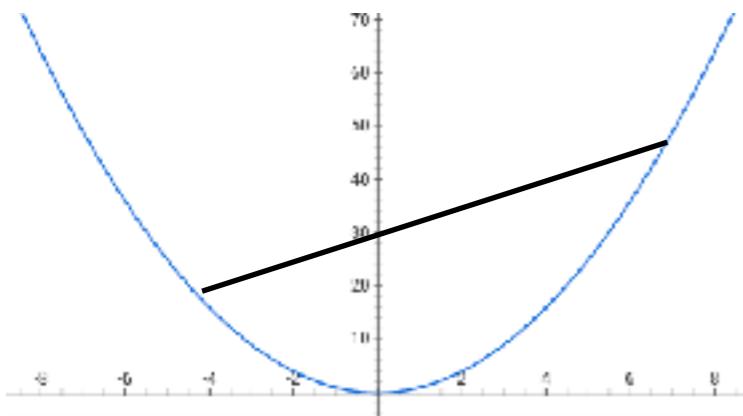
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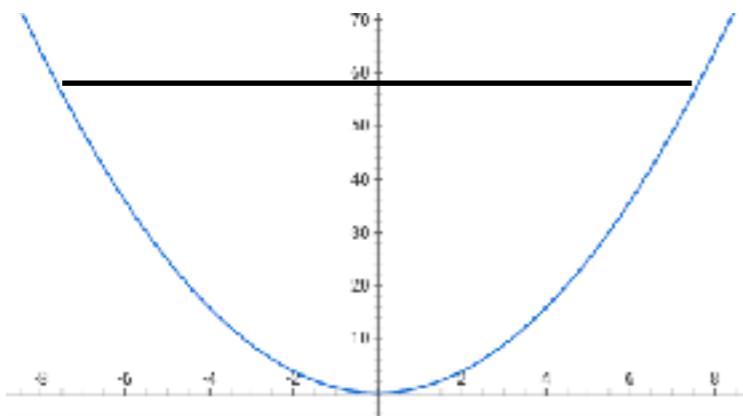
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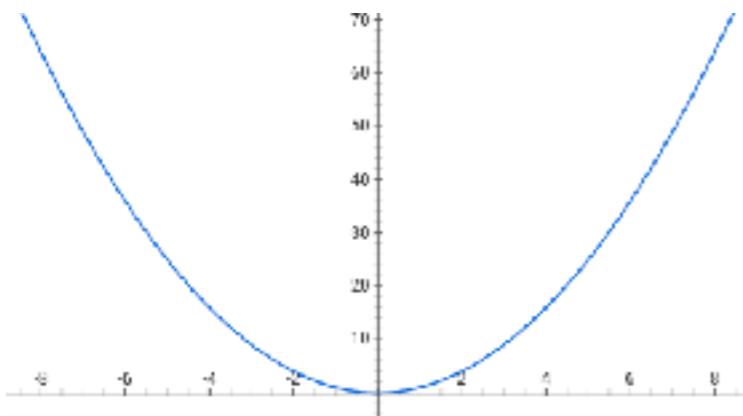
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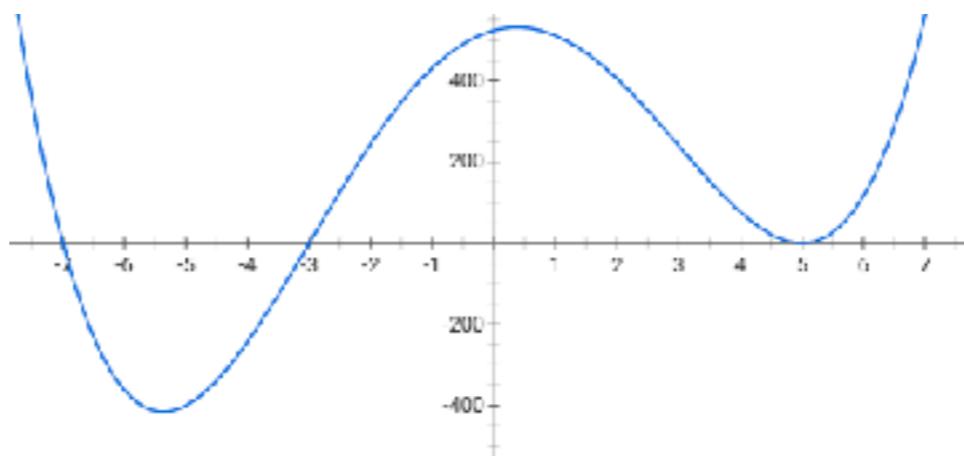
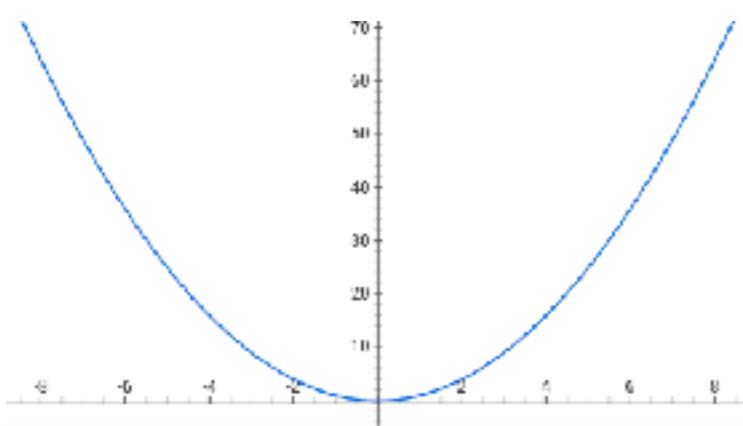
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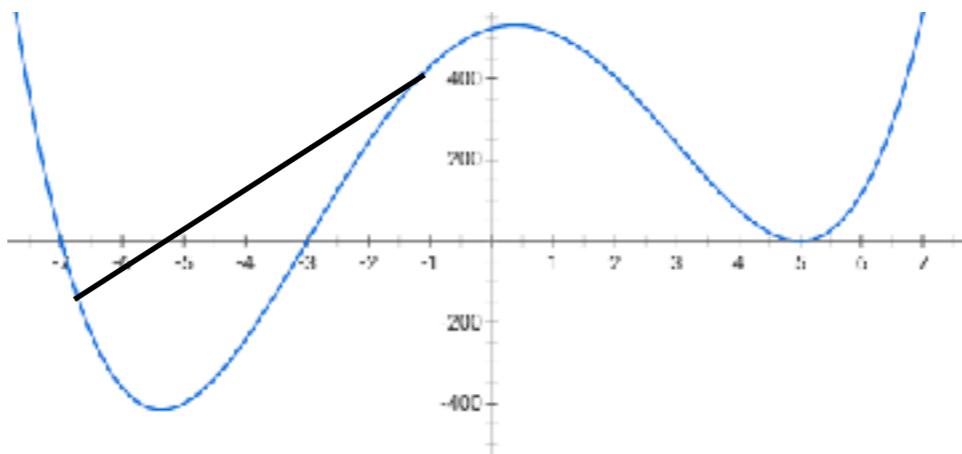
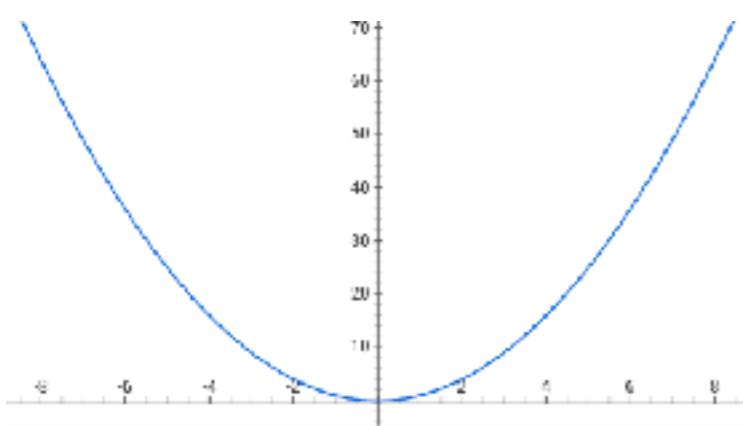
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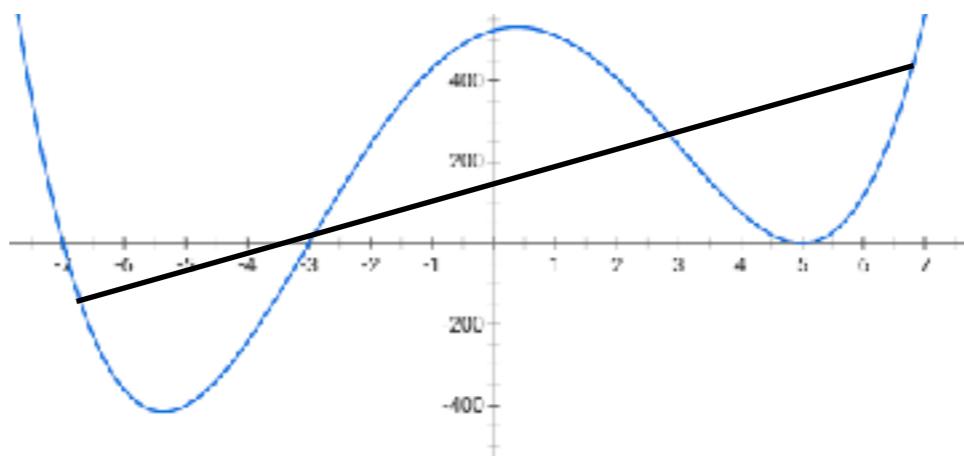
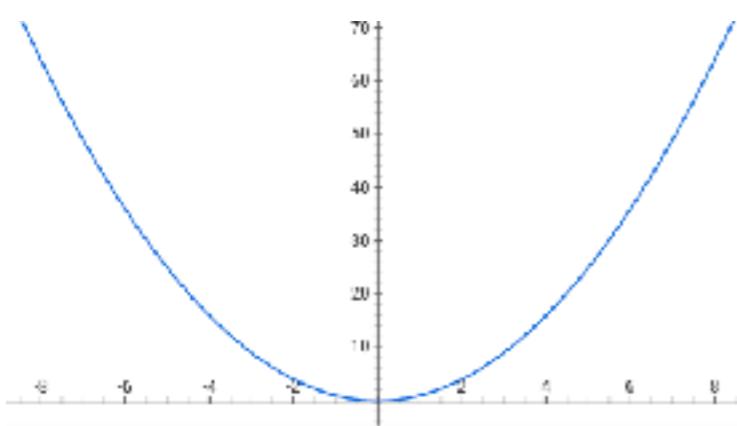
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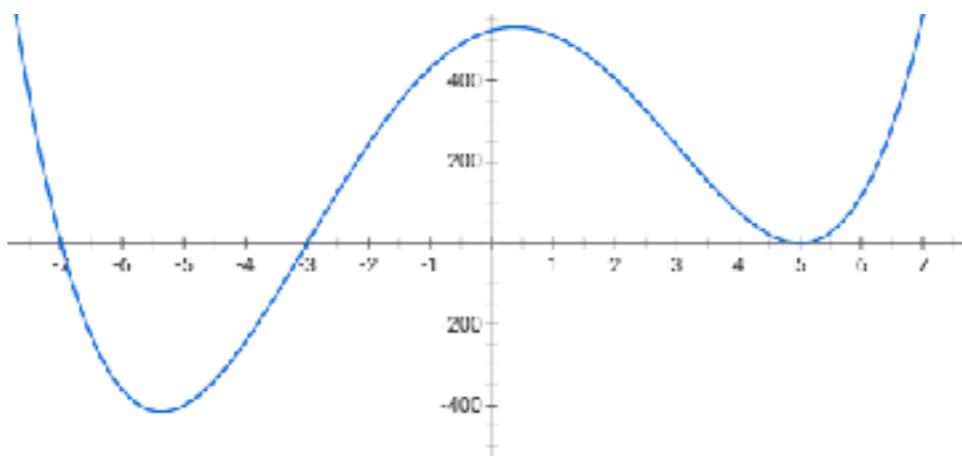
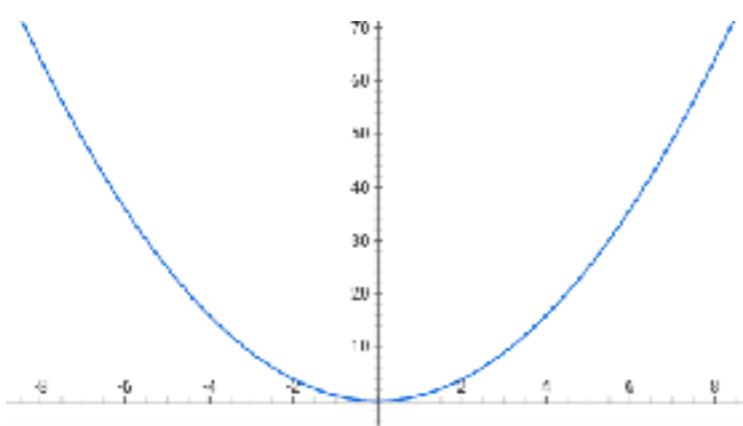
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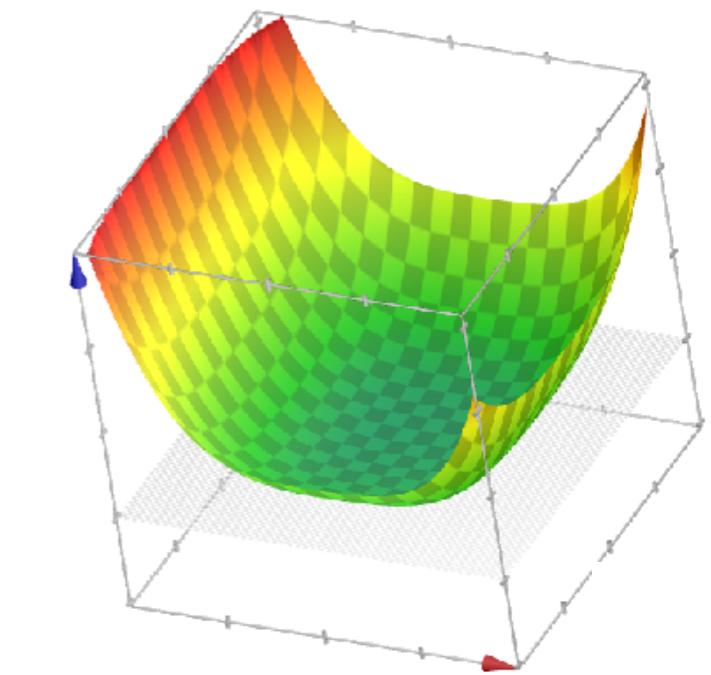
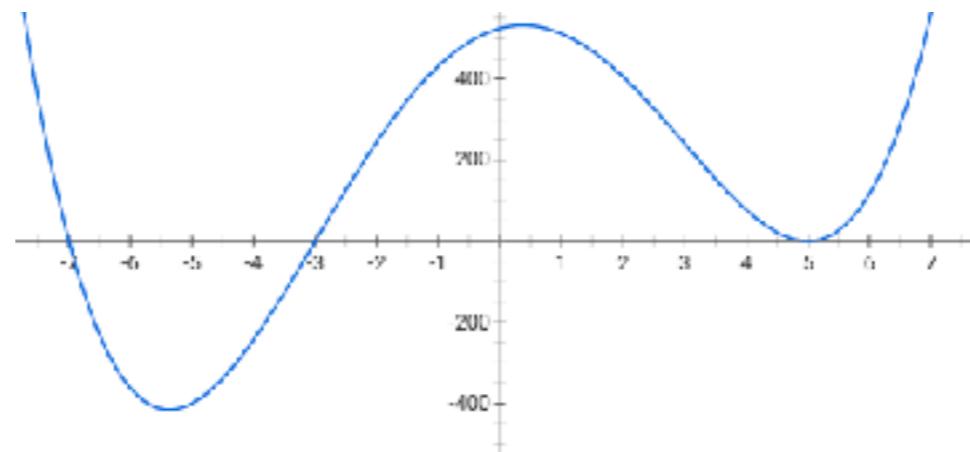
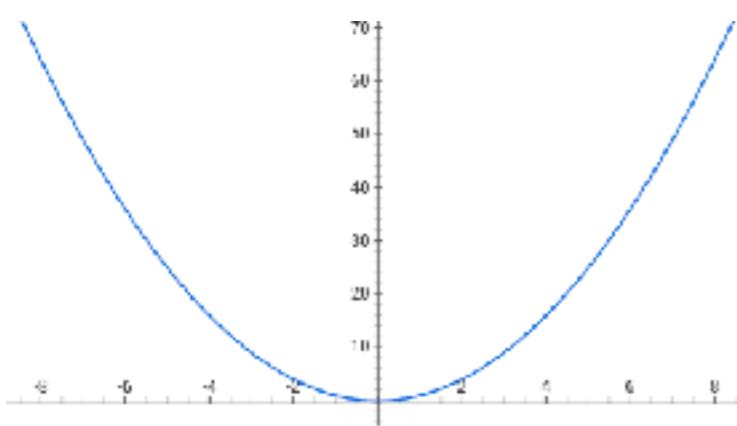
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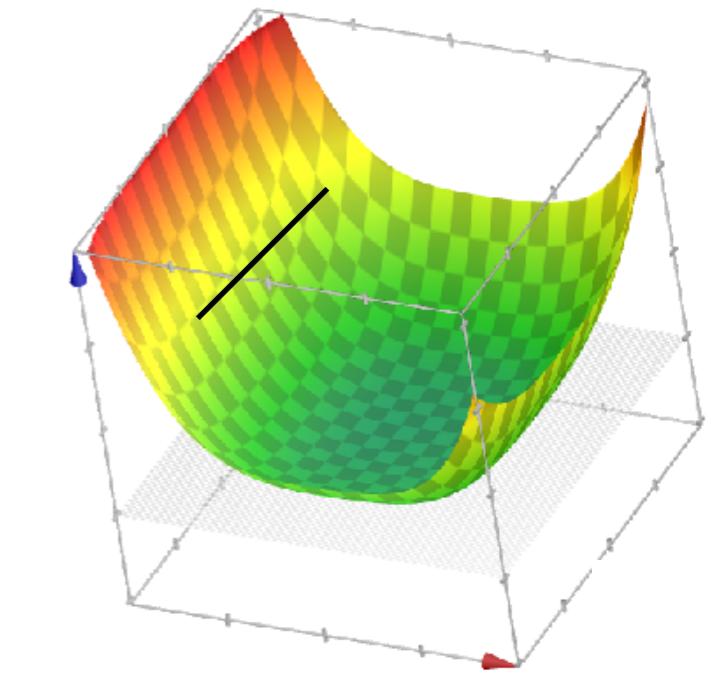
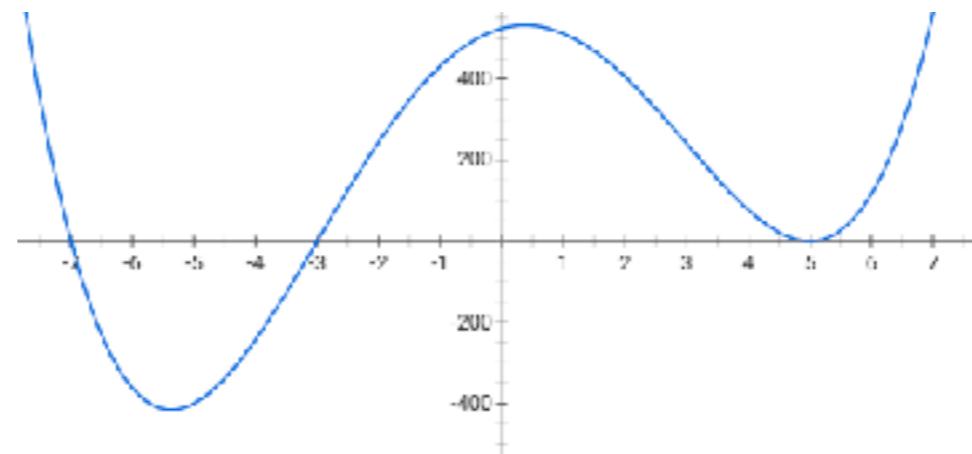
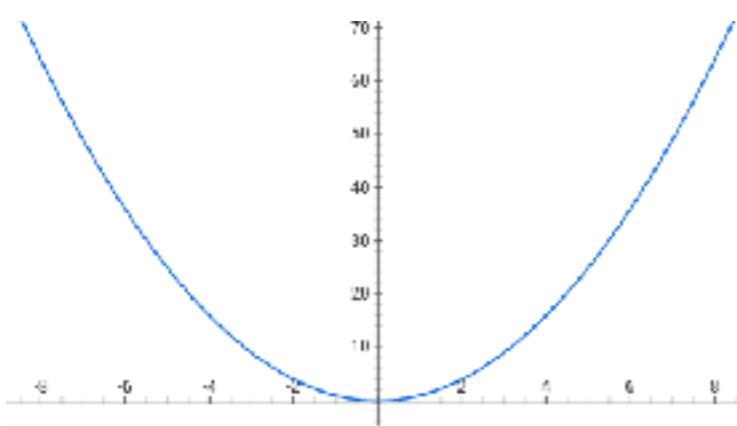
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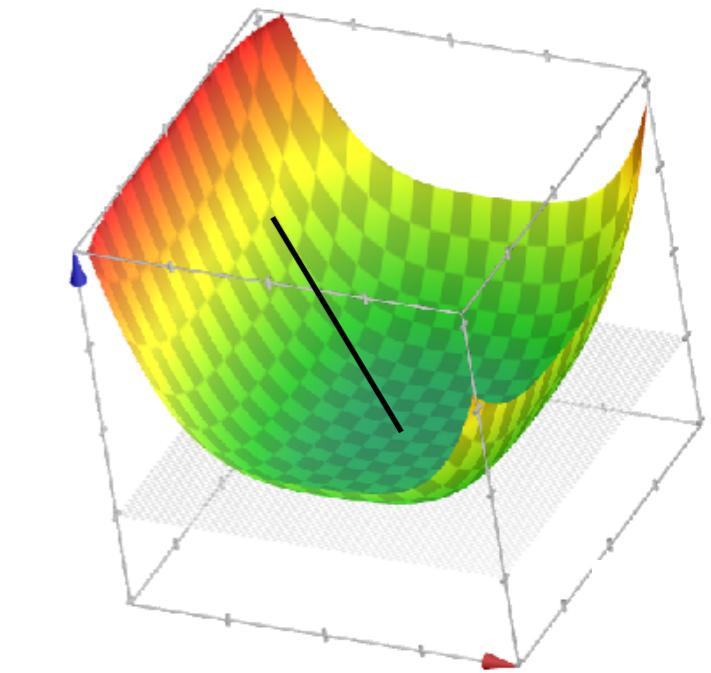
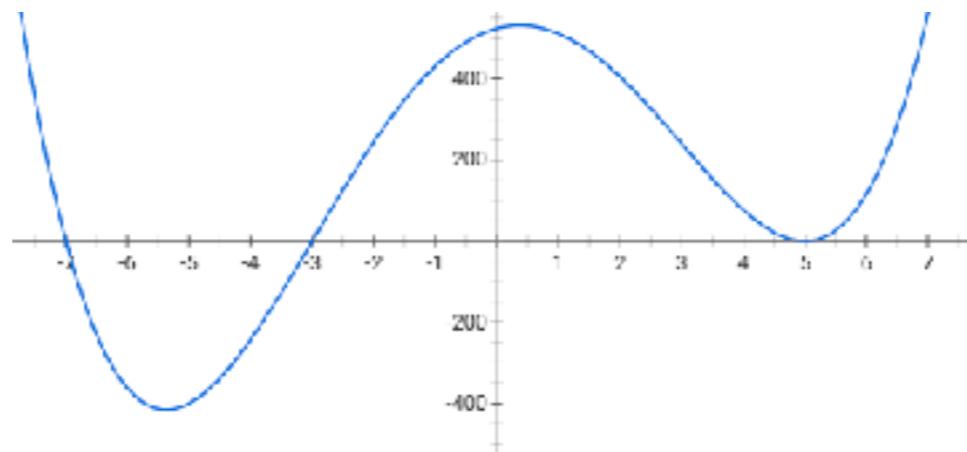
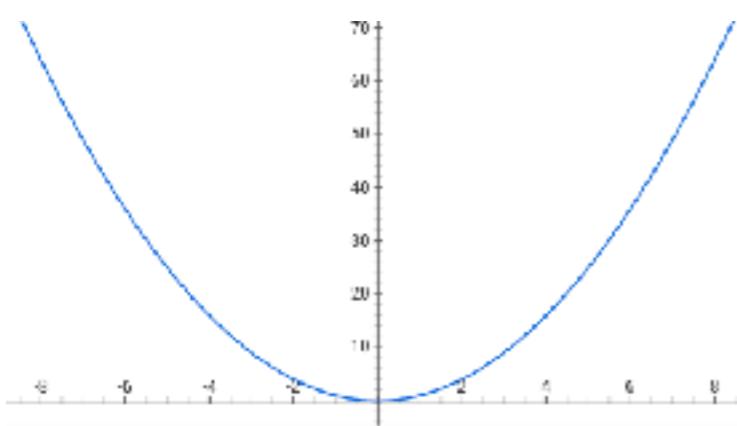
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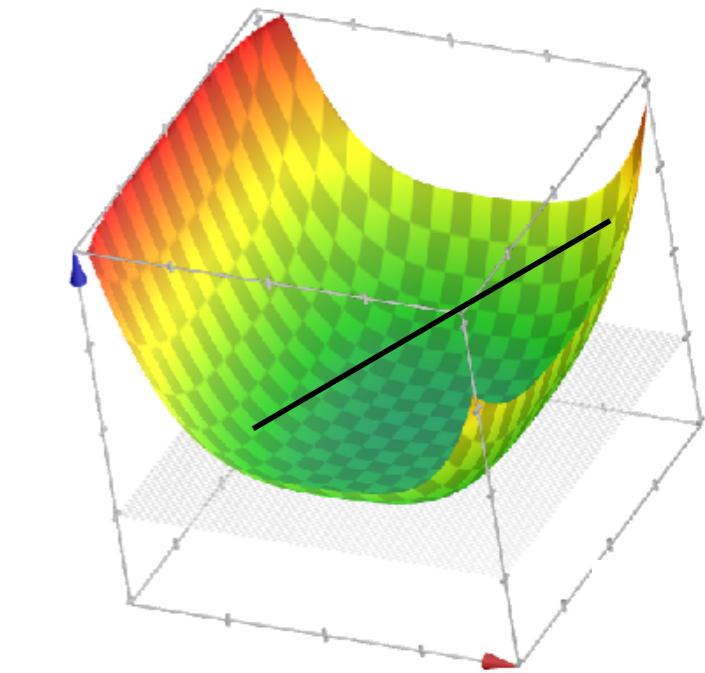
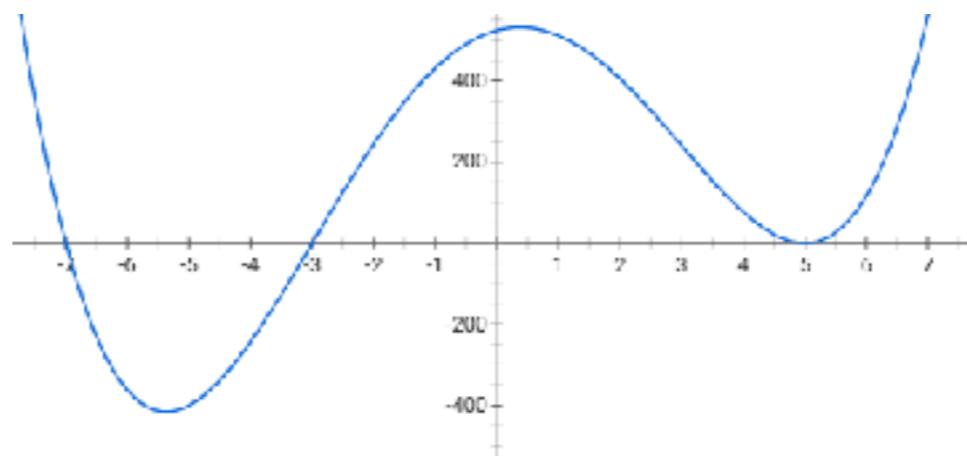
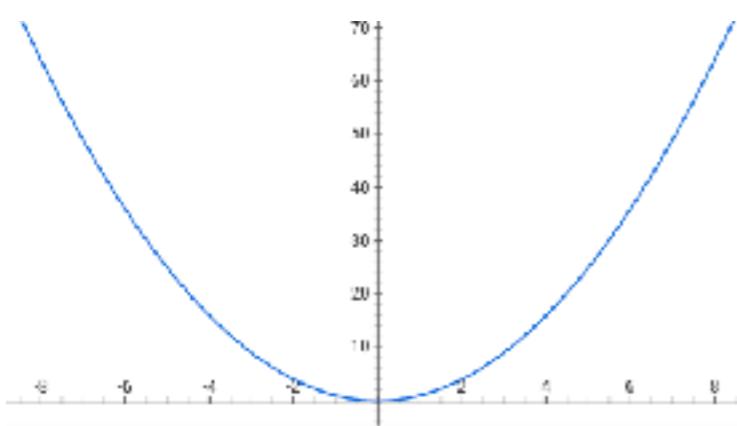
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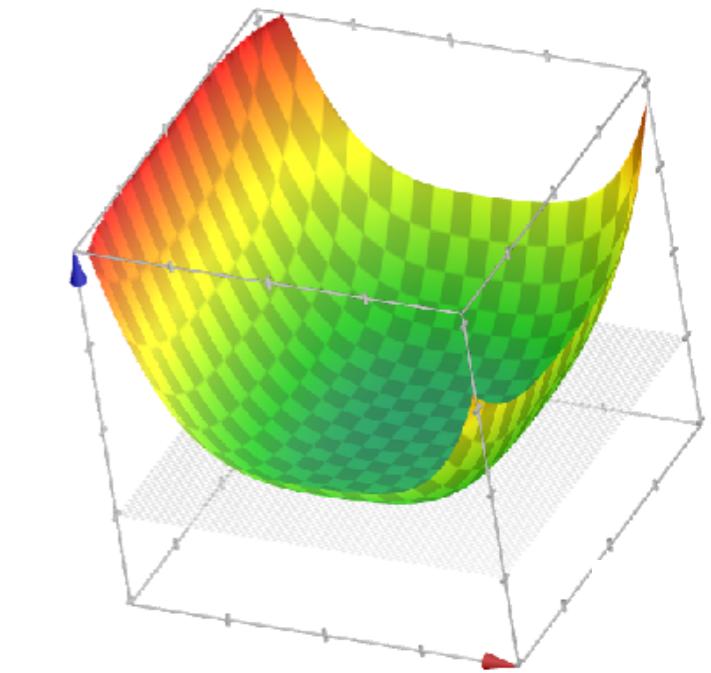
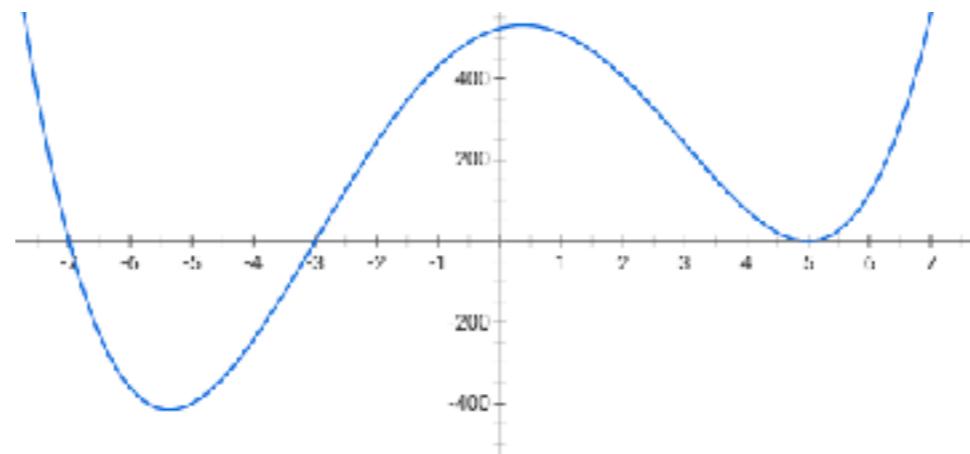
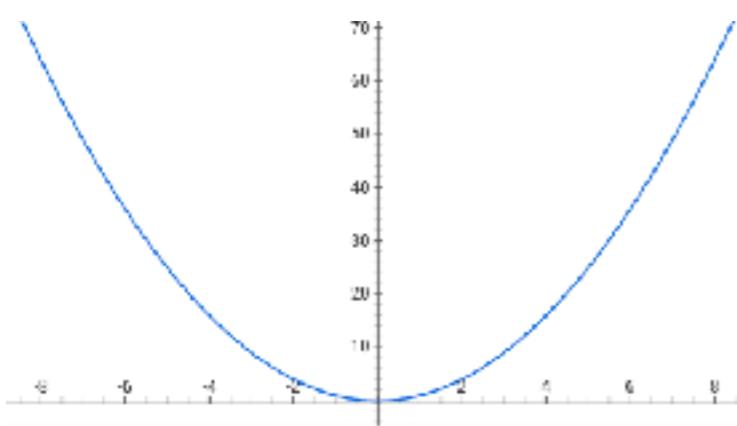
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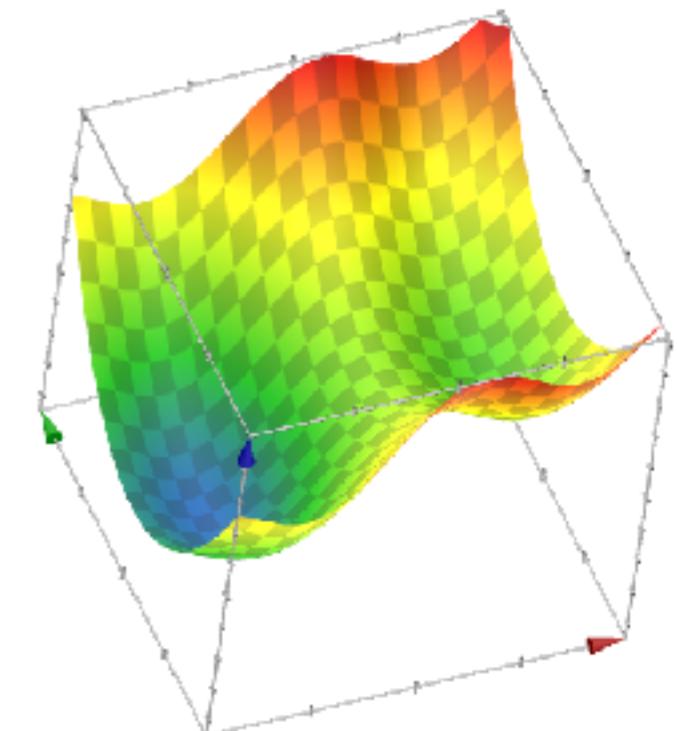
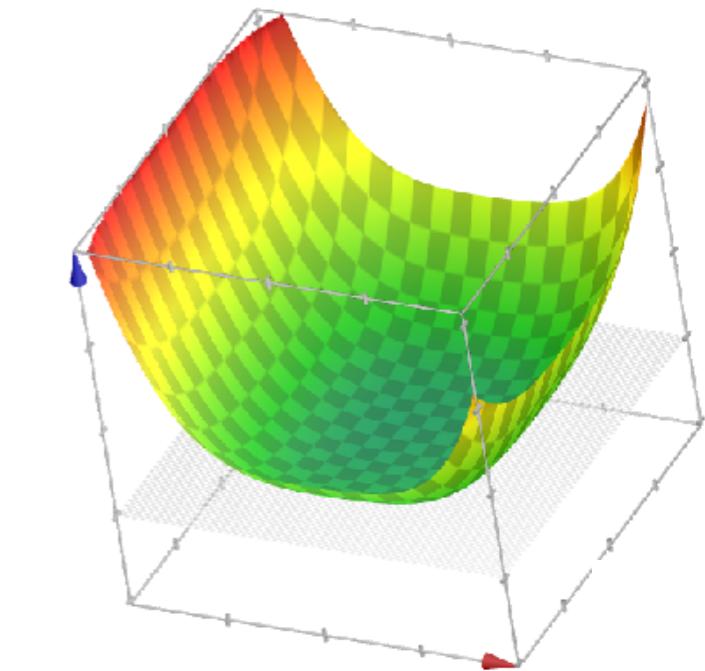
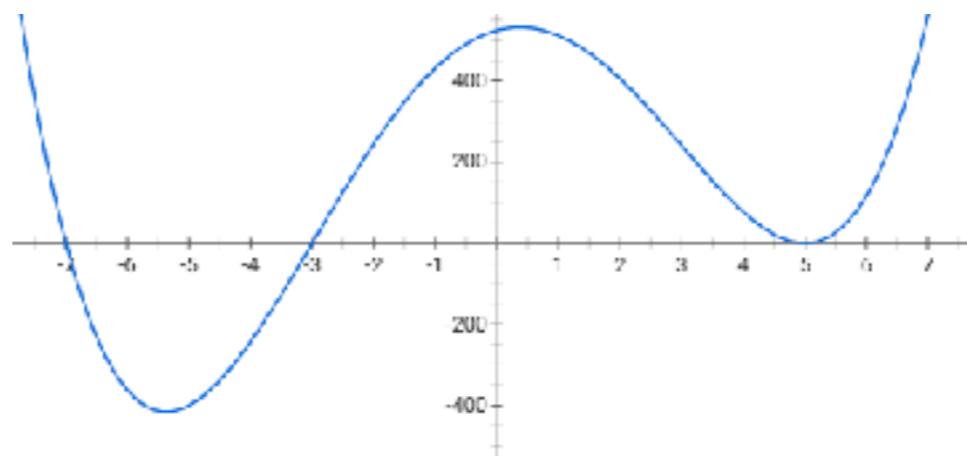
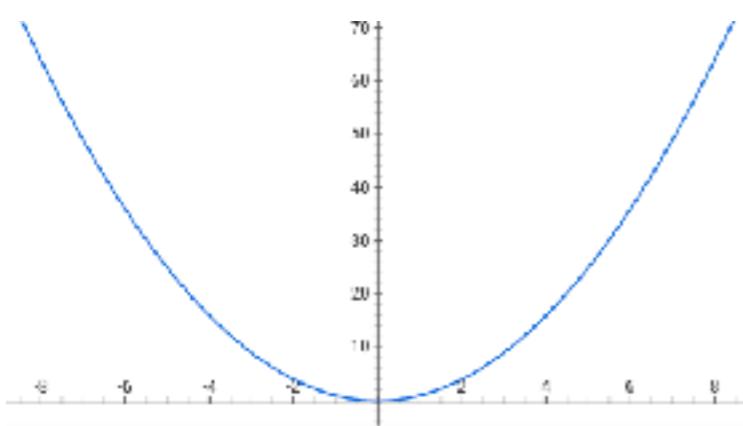
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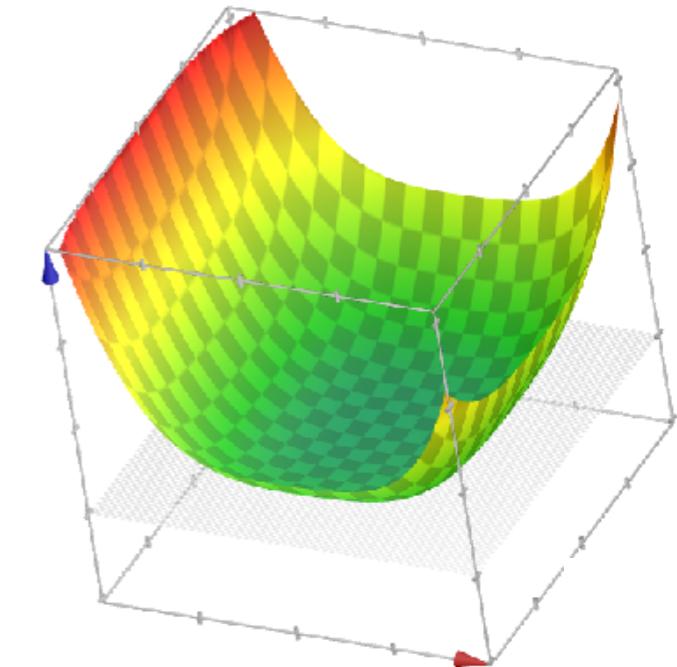
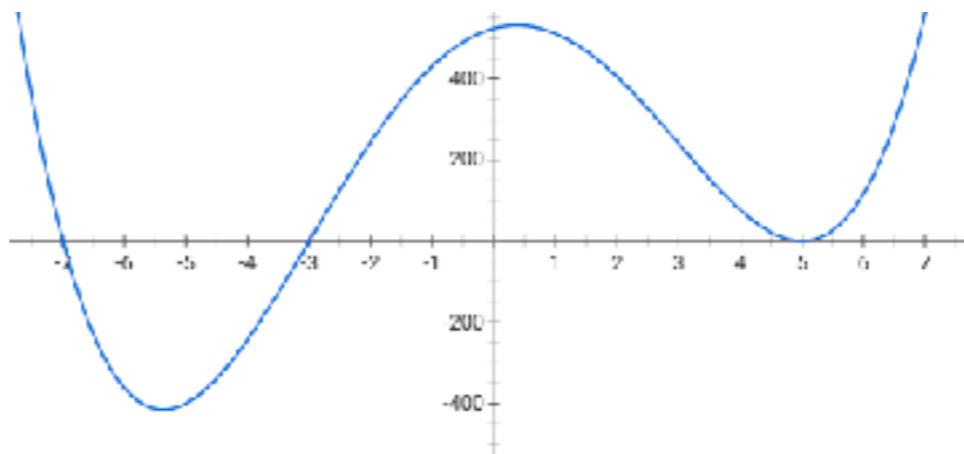
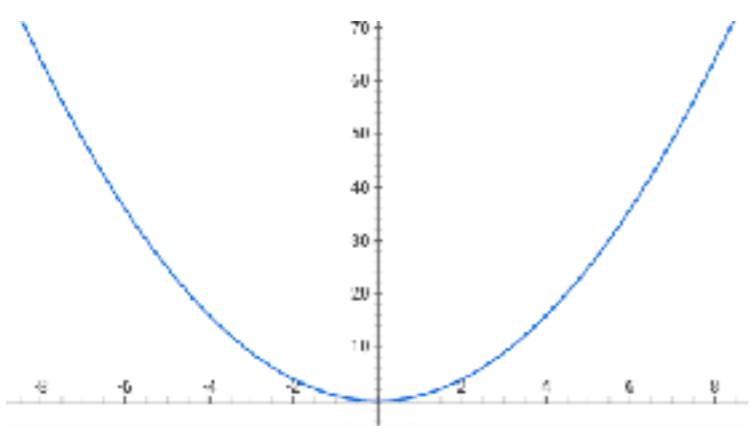
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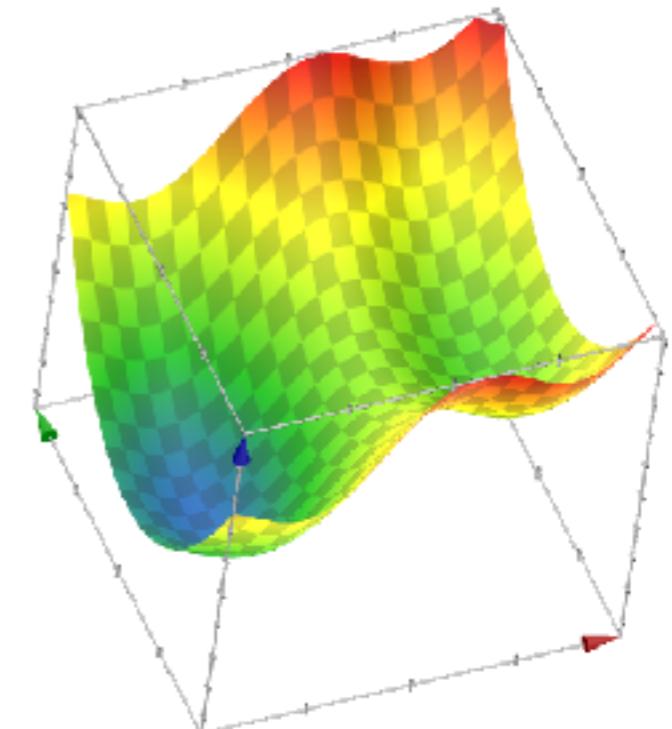


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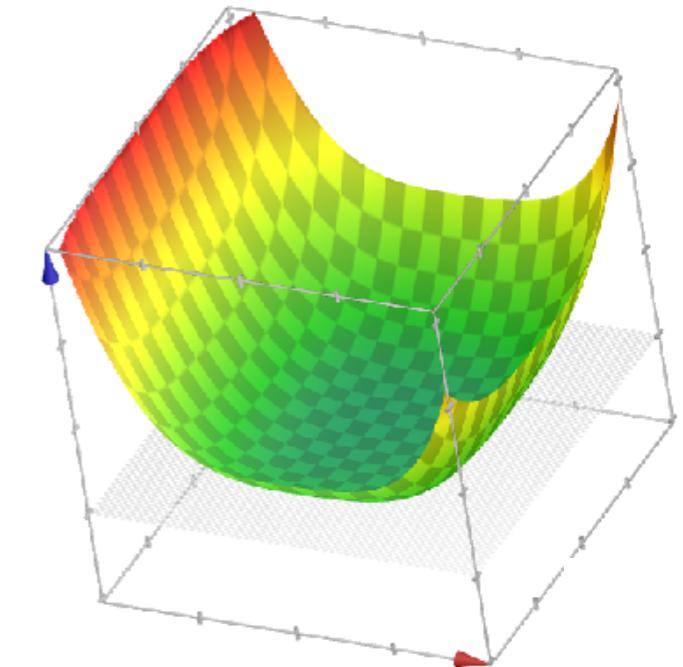
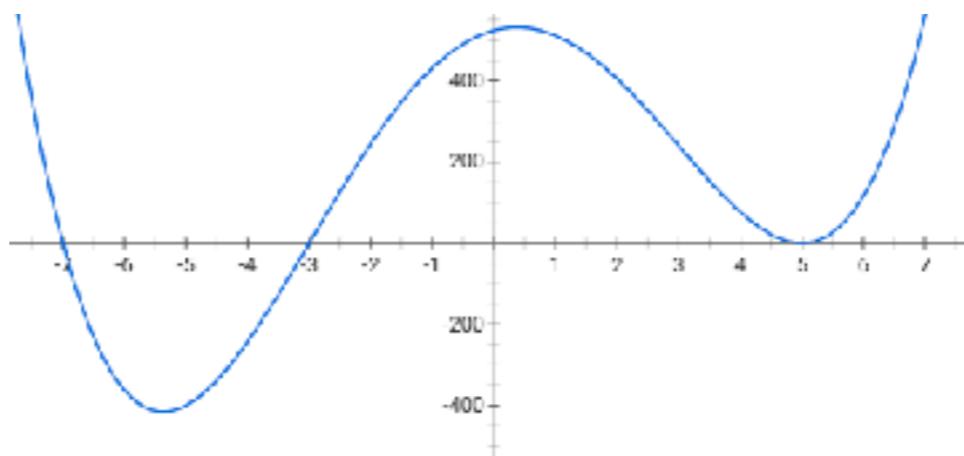
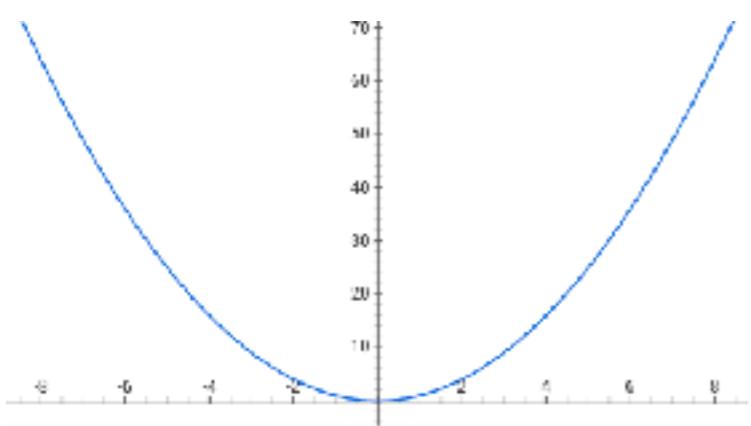


- **Theorem:** Gradient descent performance

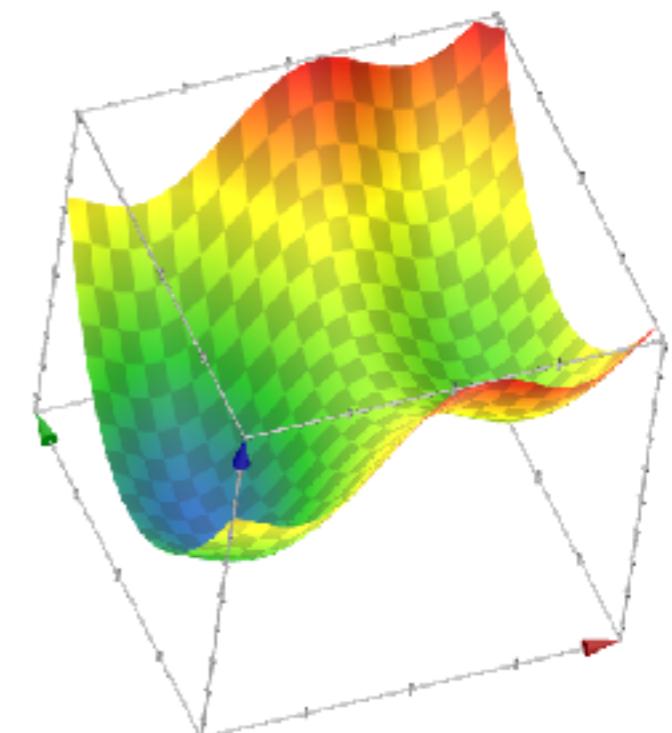


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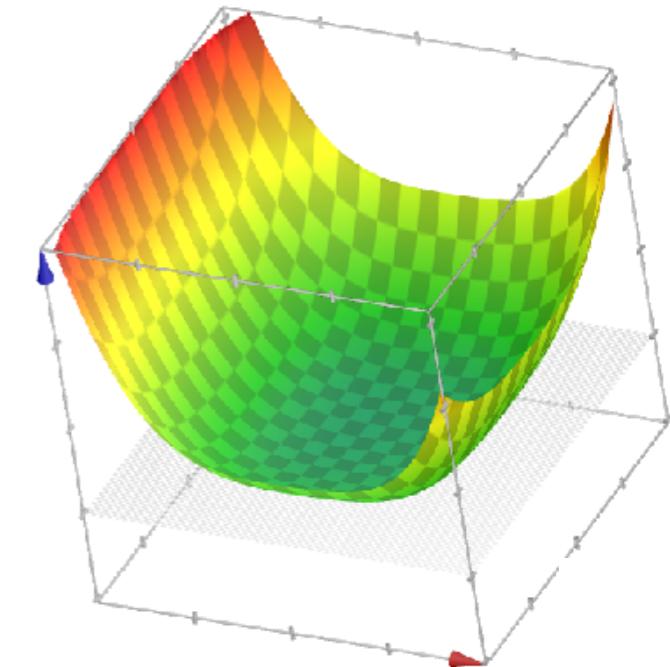
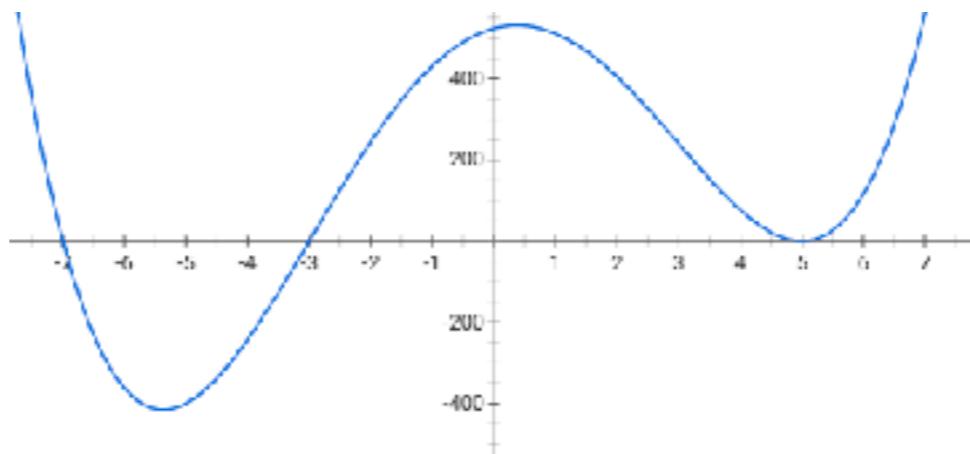
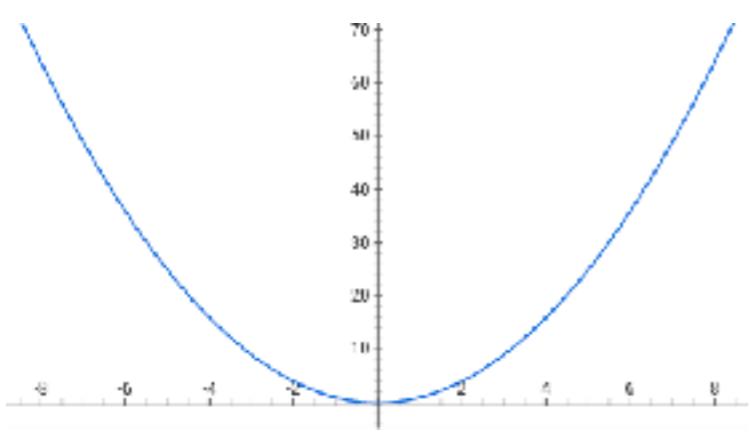


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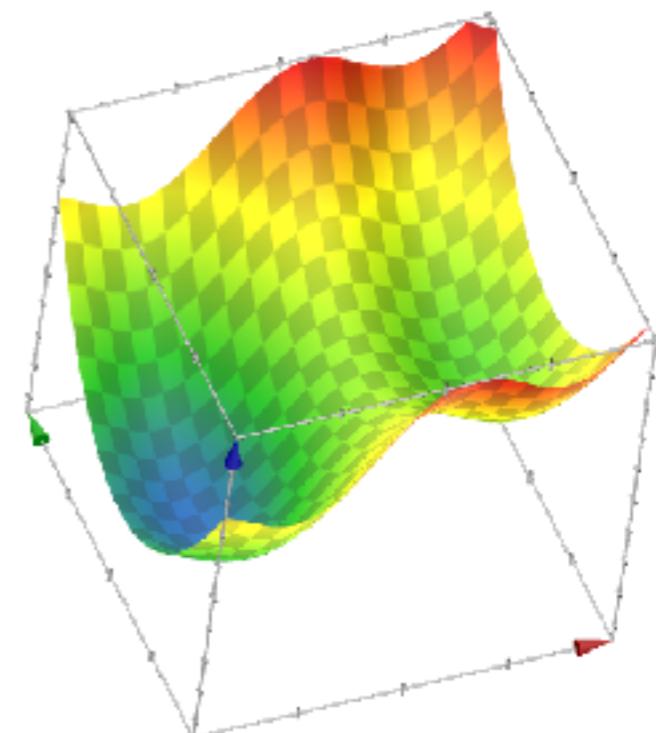


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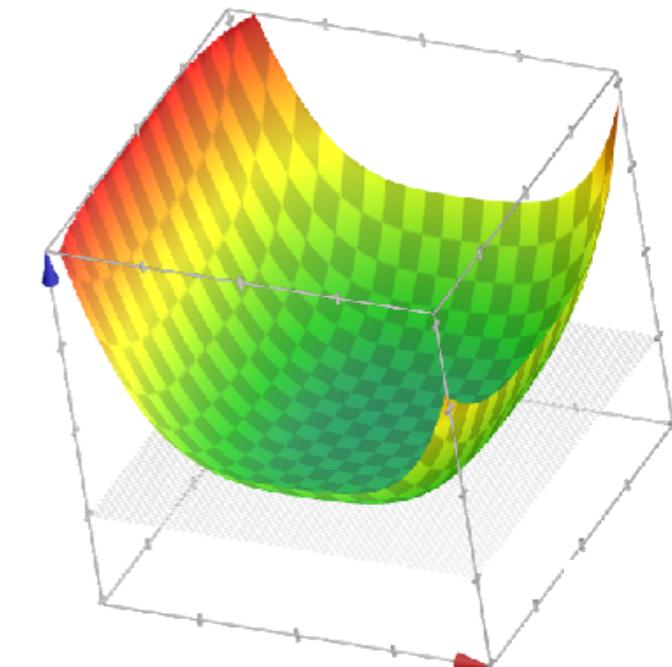
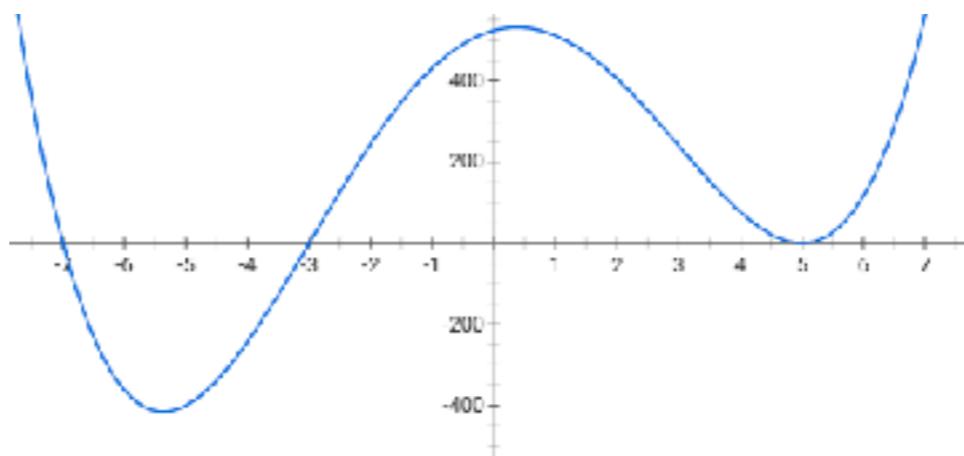
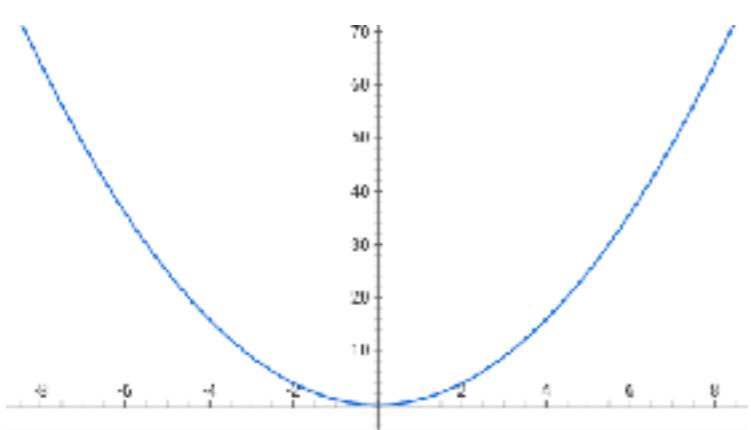


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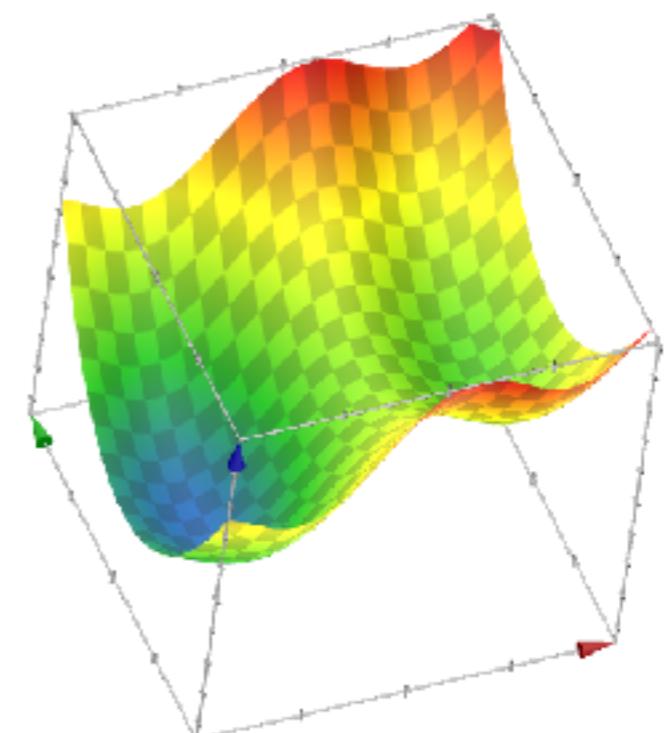


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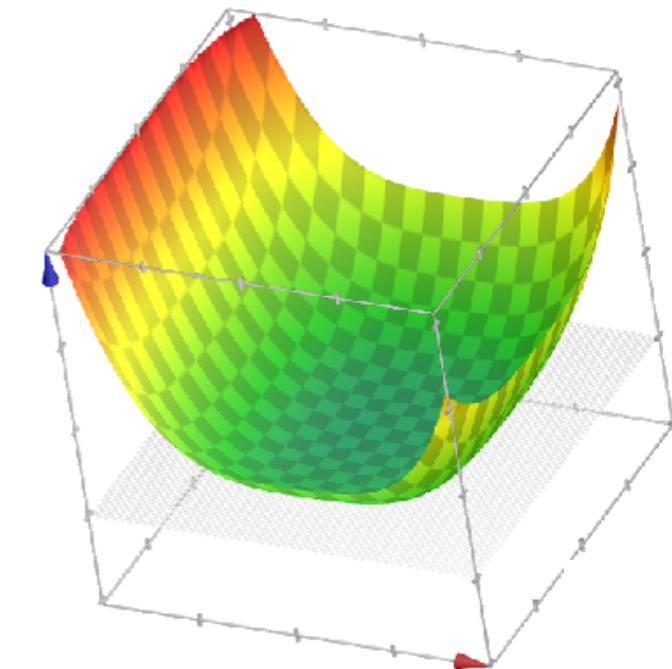
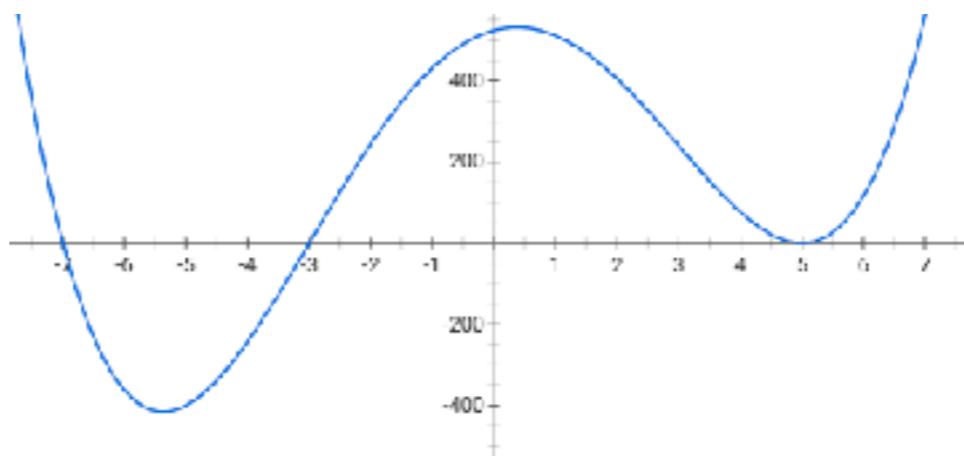
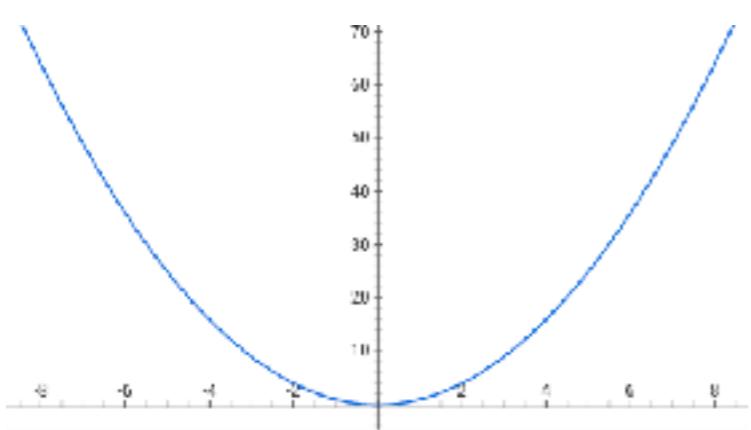


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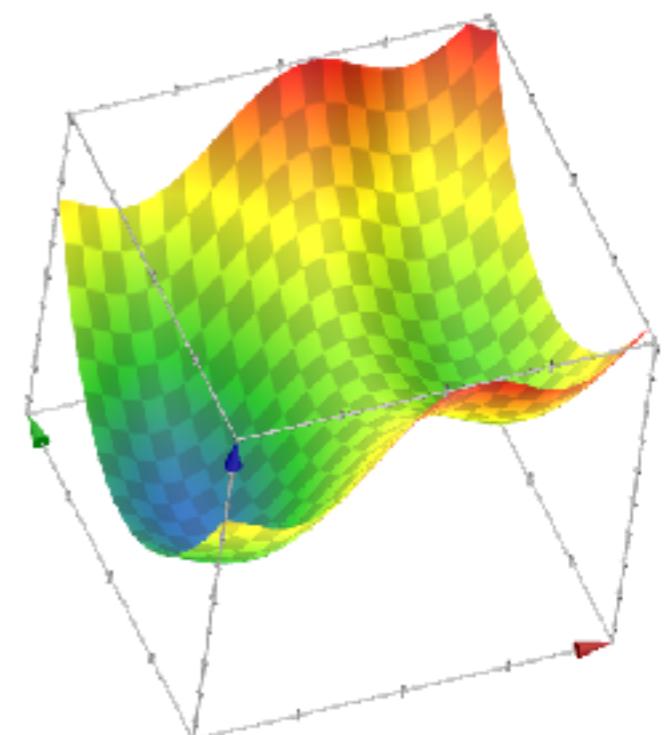


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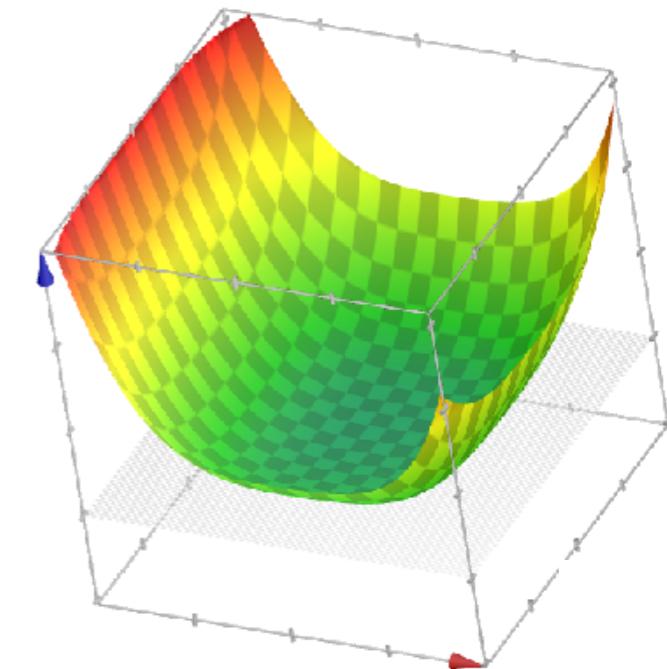
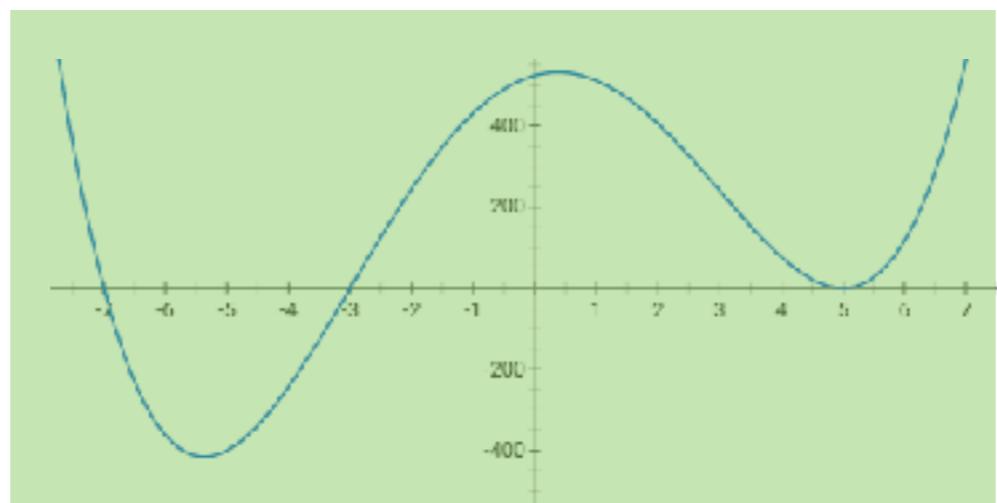
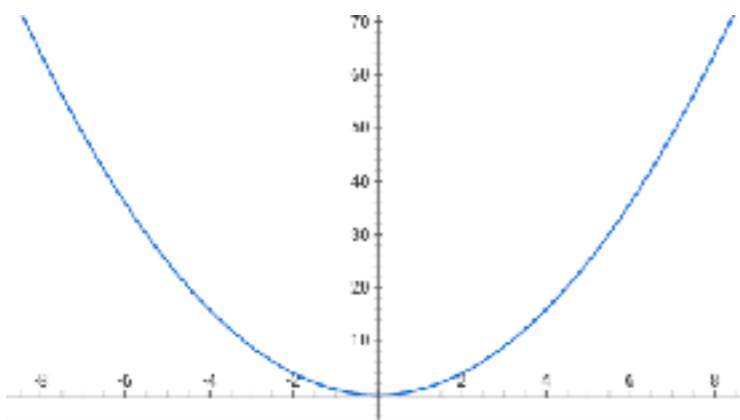


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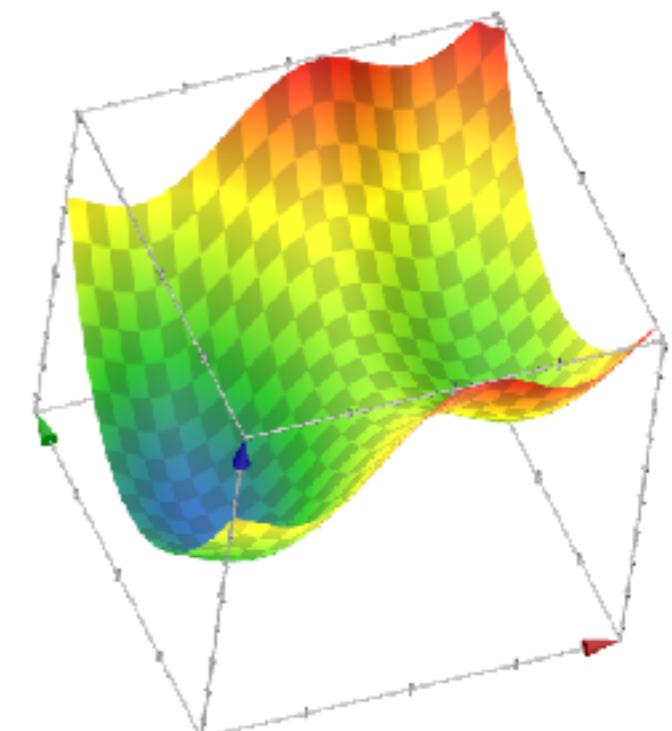
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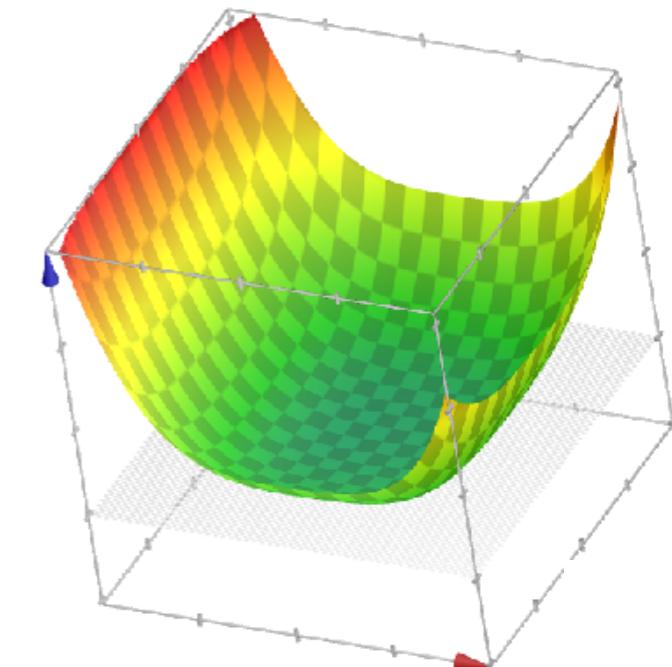
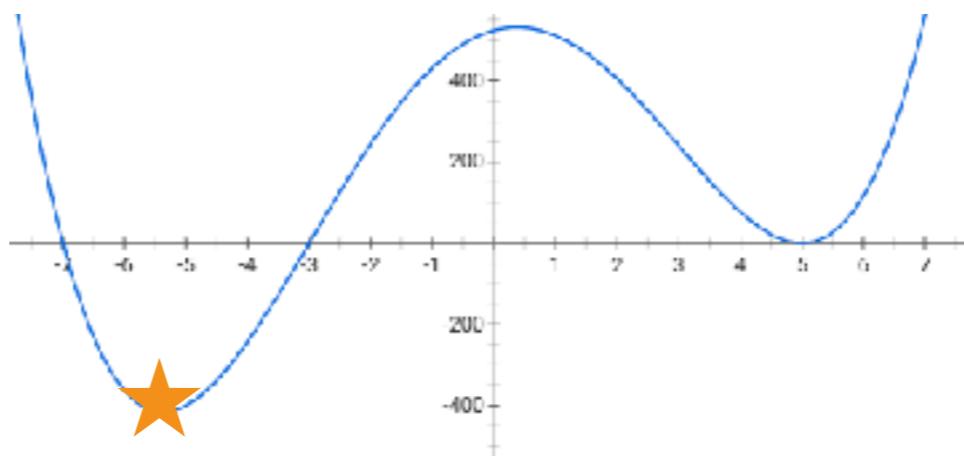
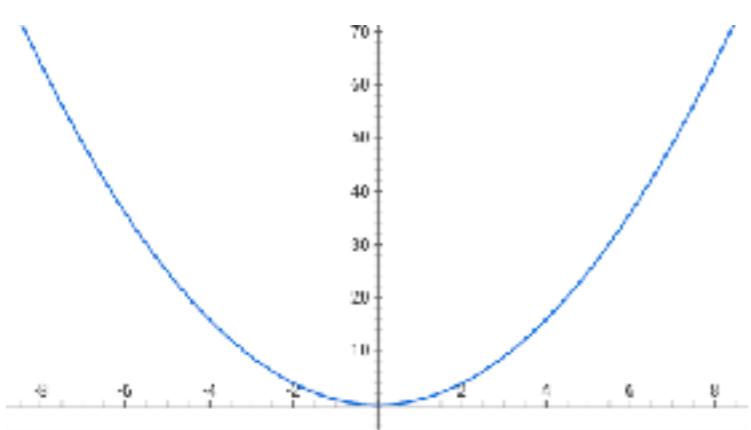
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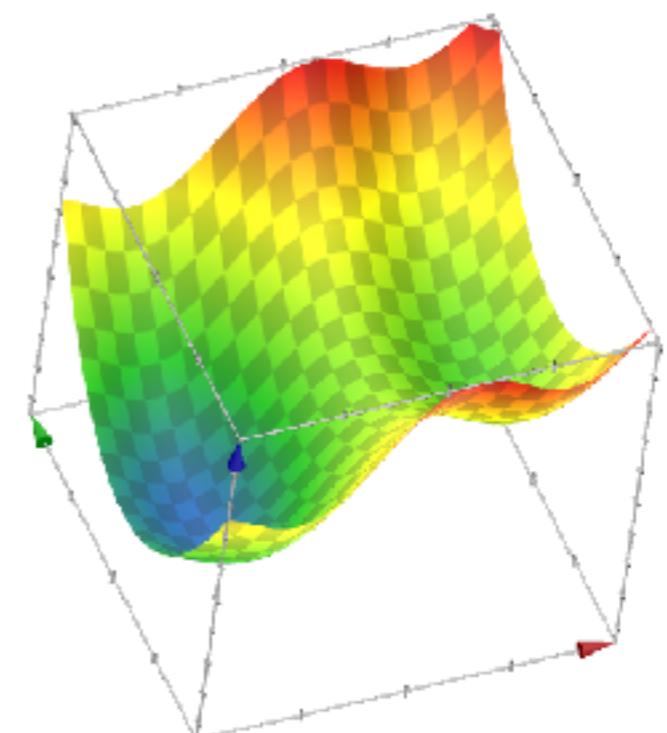


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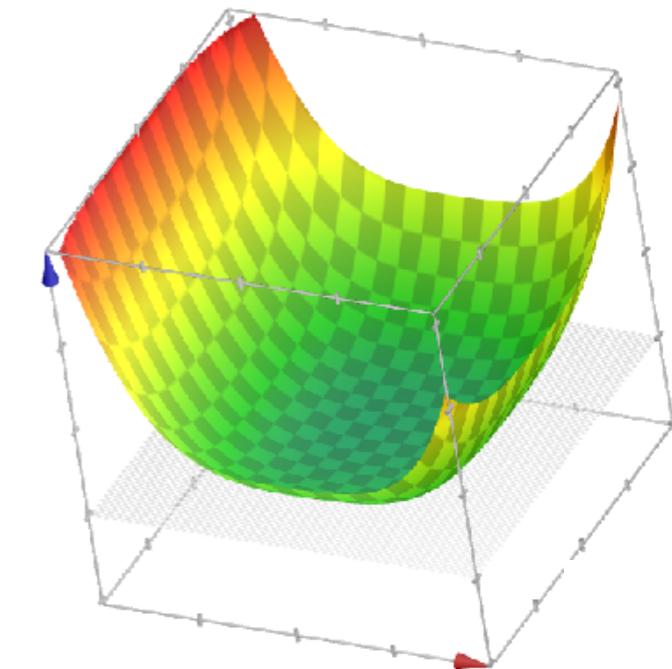
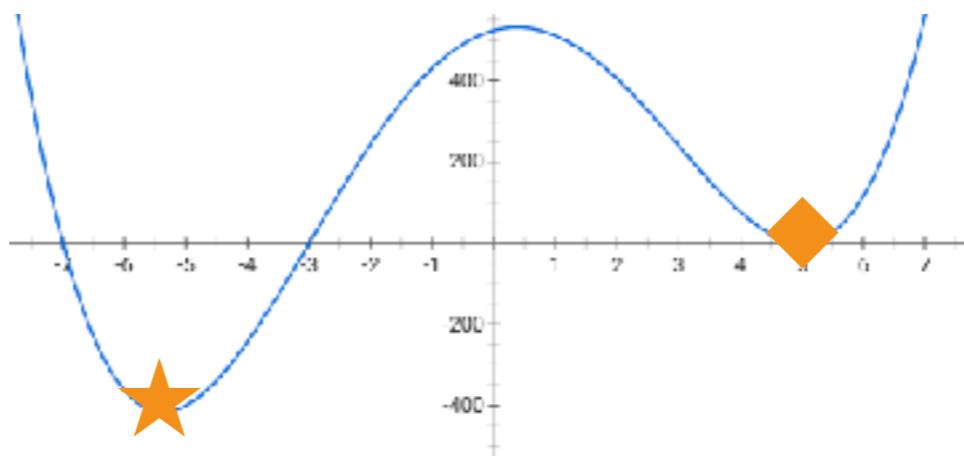
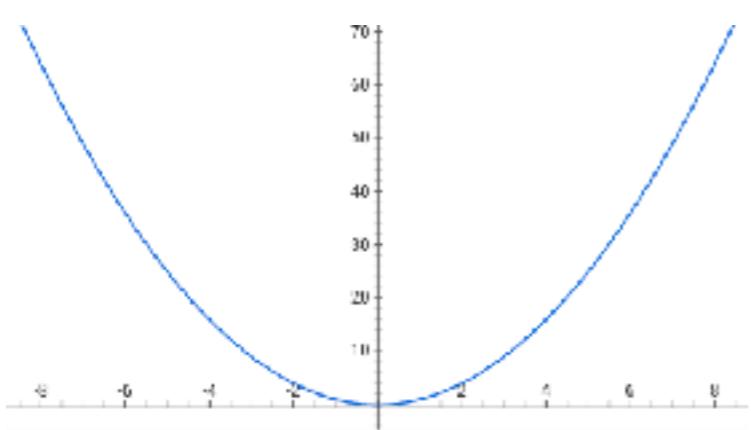


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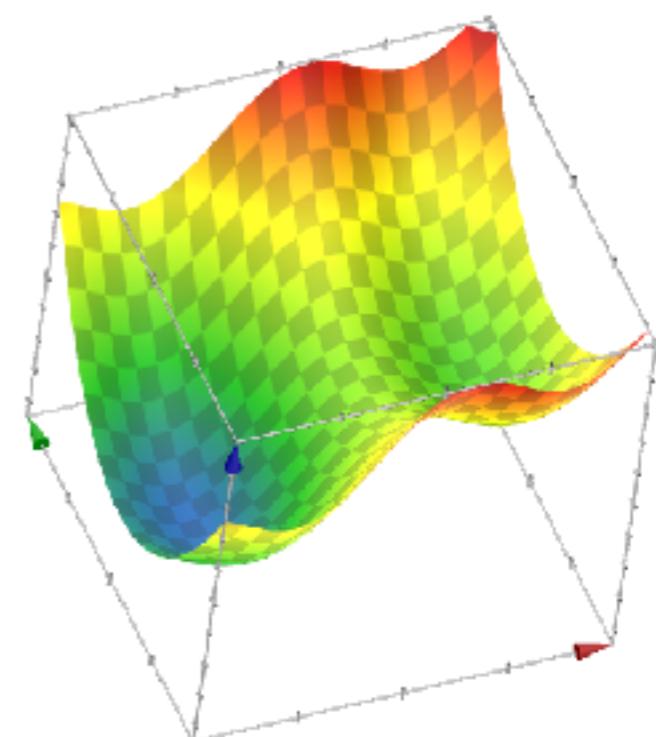


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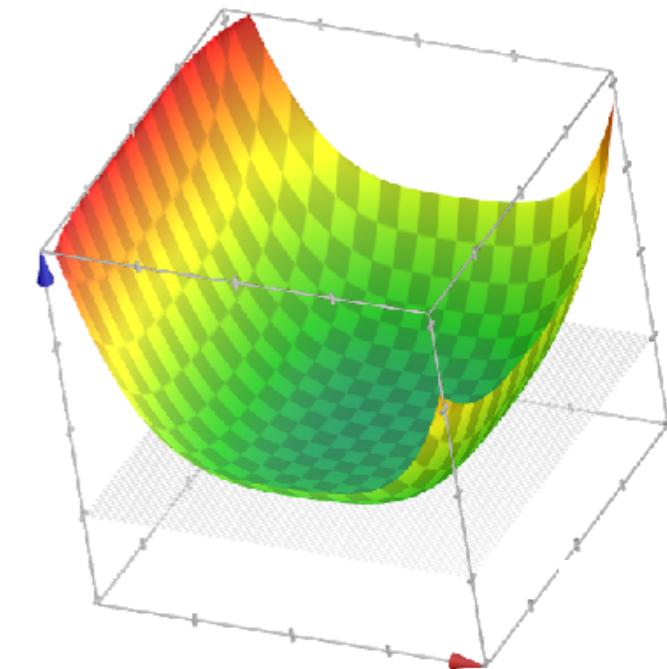
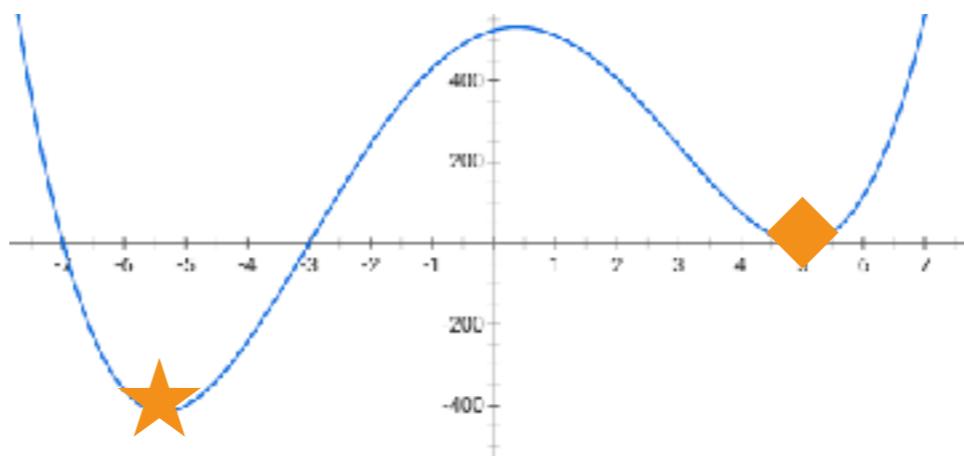
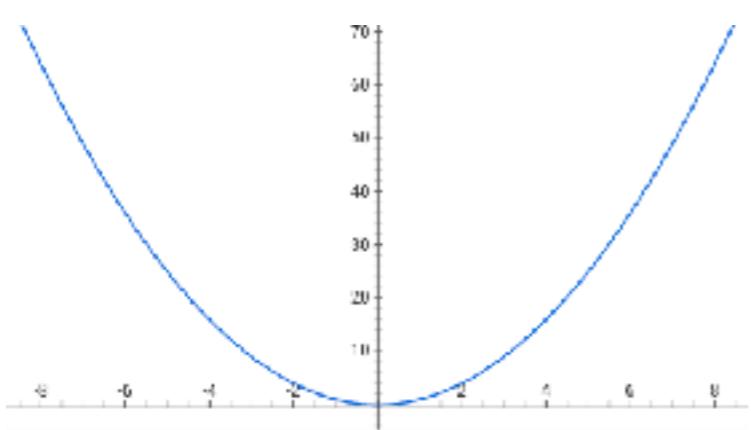


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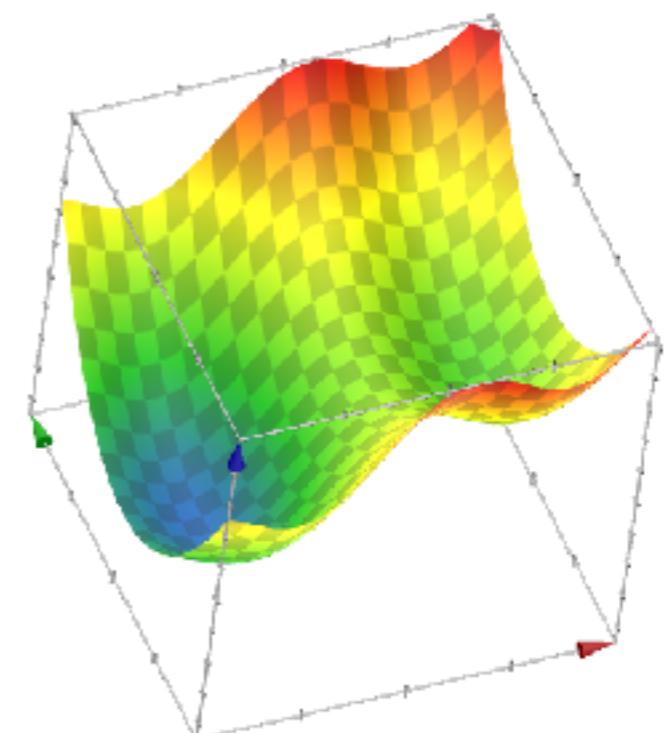


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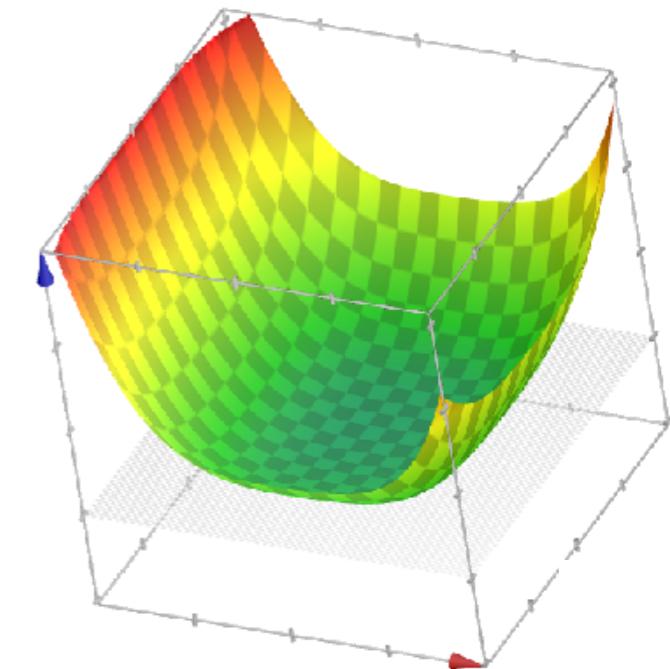
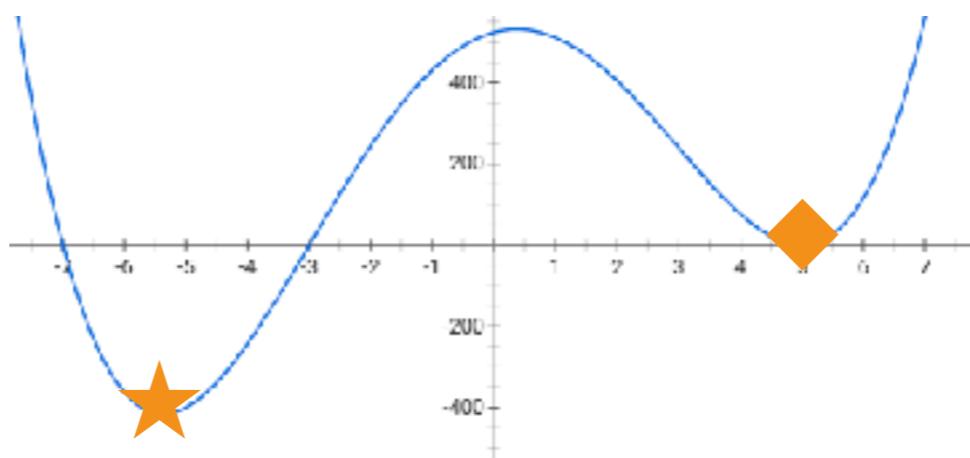
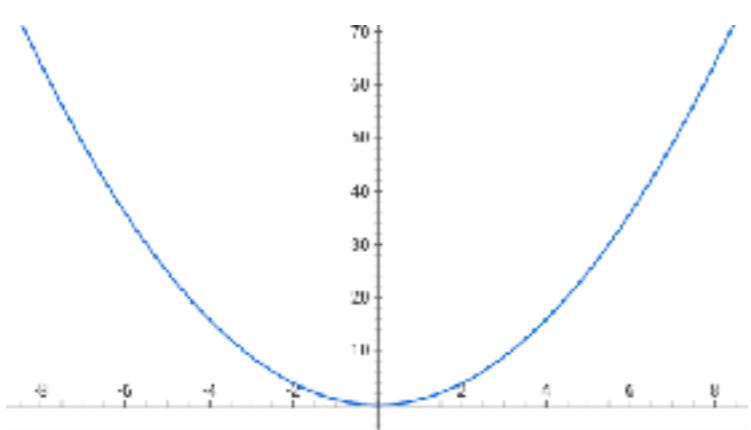


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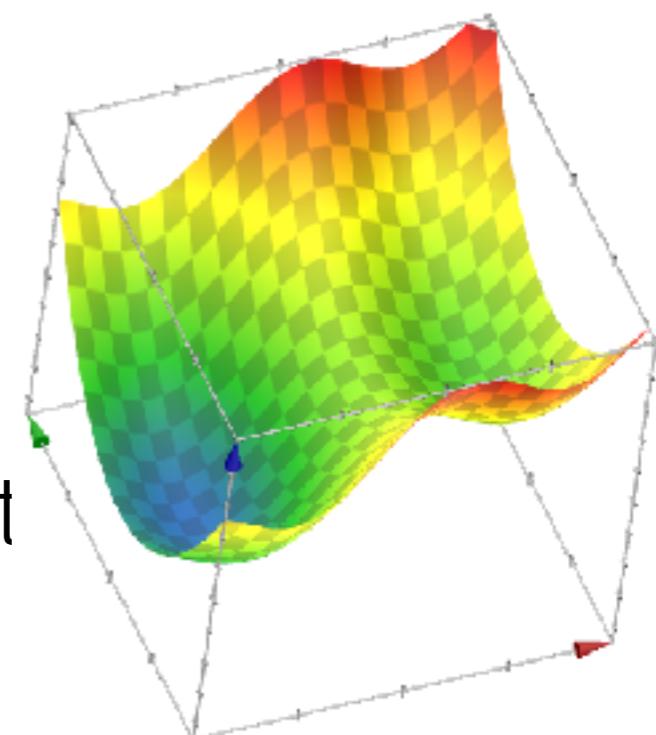


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  - **Conclusion:** If run long enough, gradient descent will return a value within  $\tilde{\epsilon}$  of a global optimum  $\Theta$



# Gradient descent for logistic regression

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- Loss  $J_{\text{lr}}(\Theta) = J_{\text{lr}}(\theta, \theta_0)$  is differentiable

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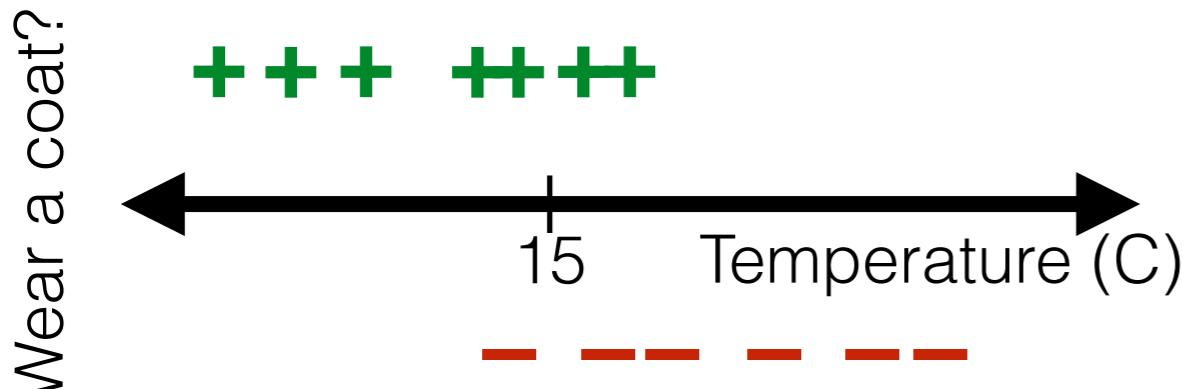
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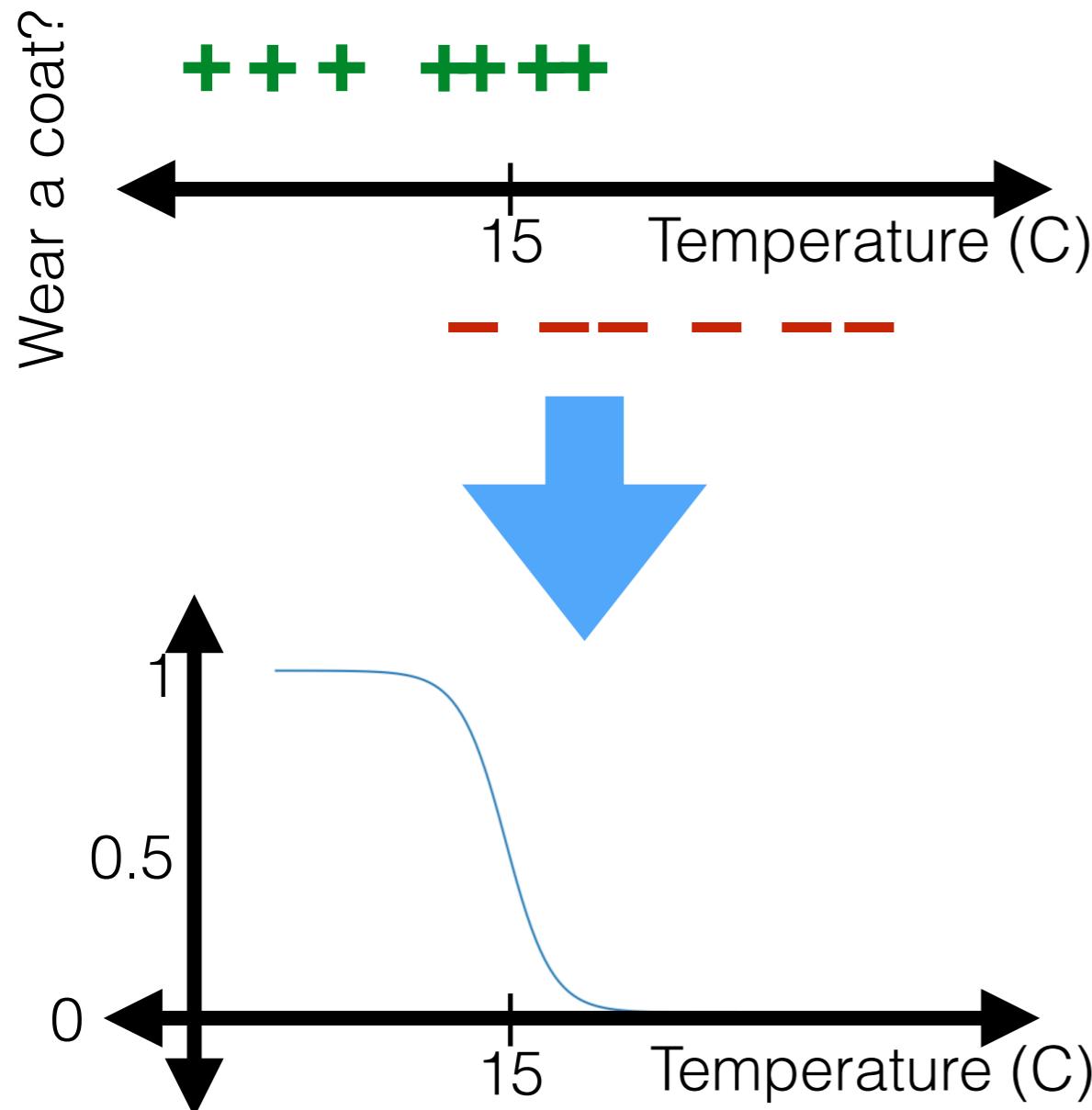
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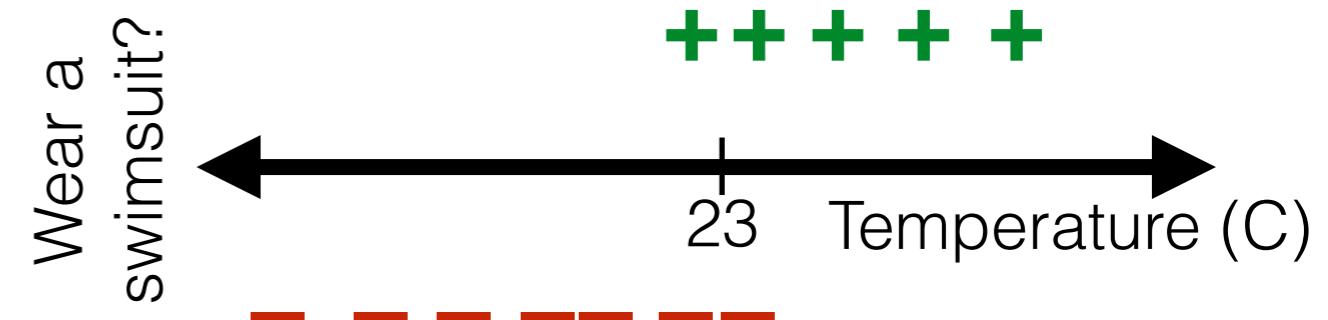
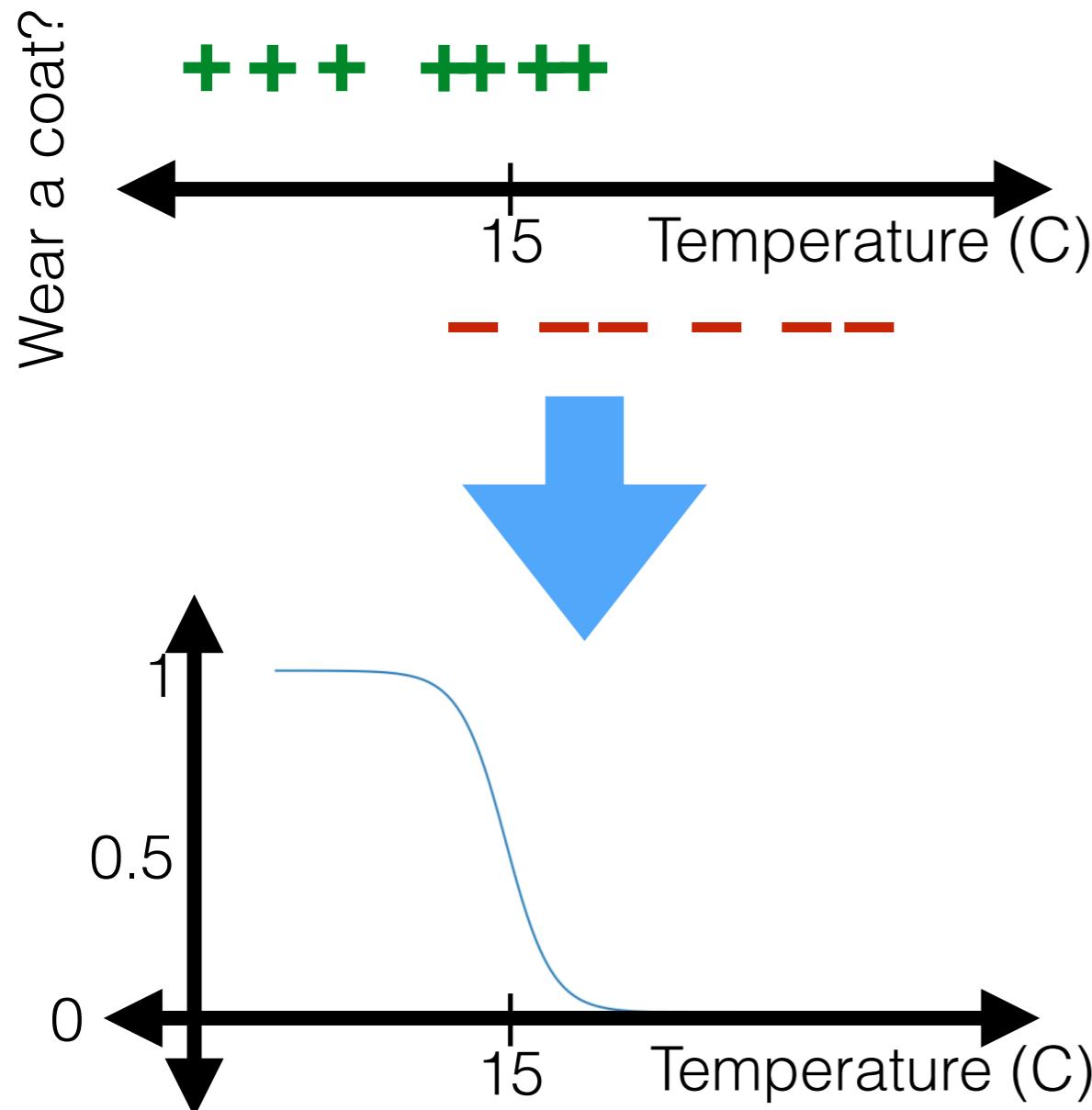
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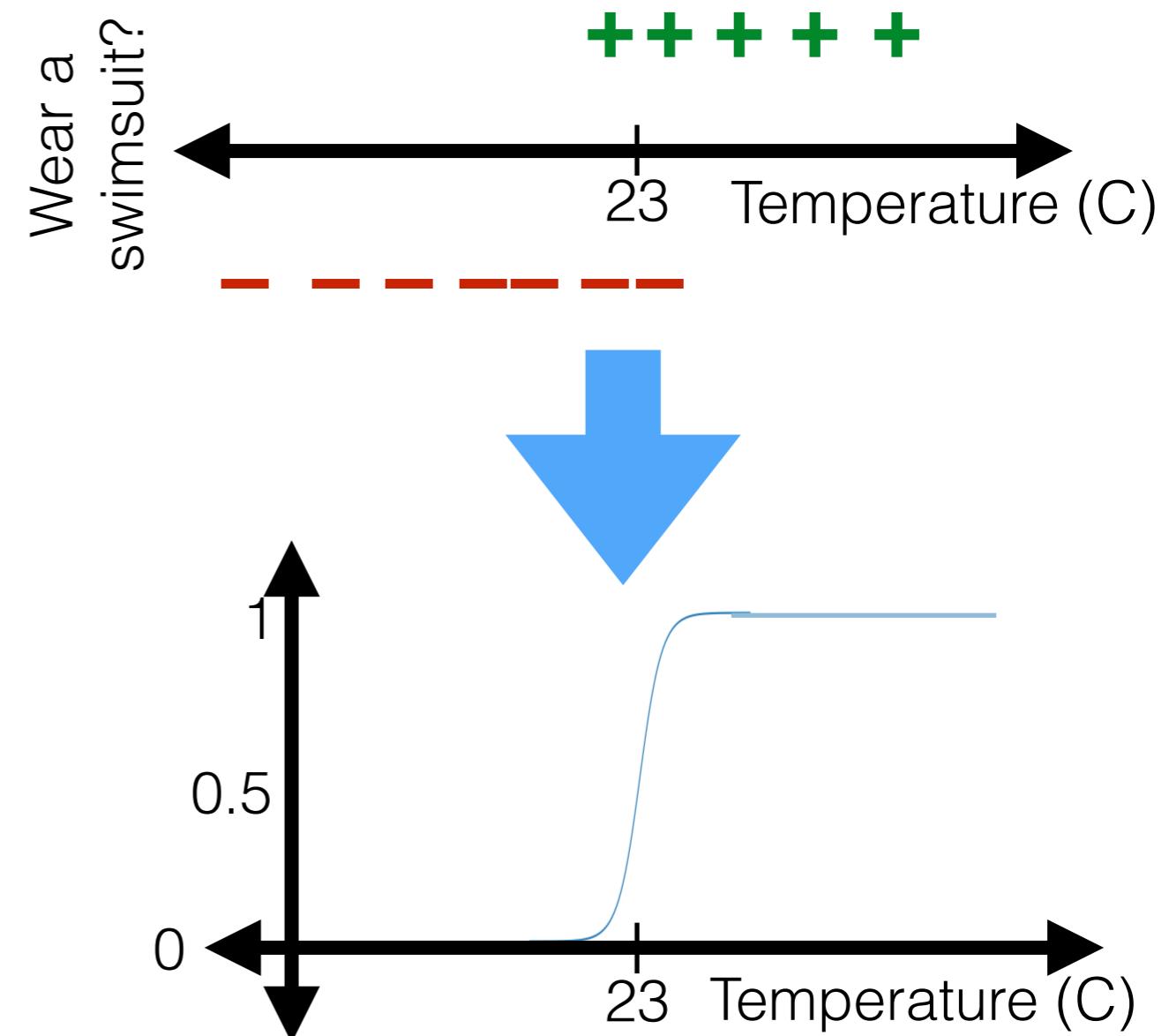
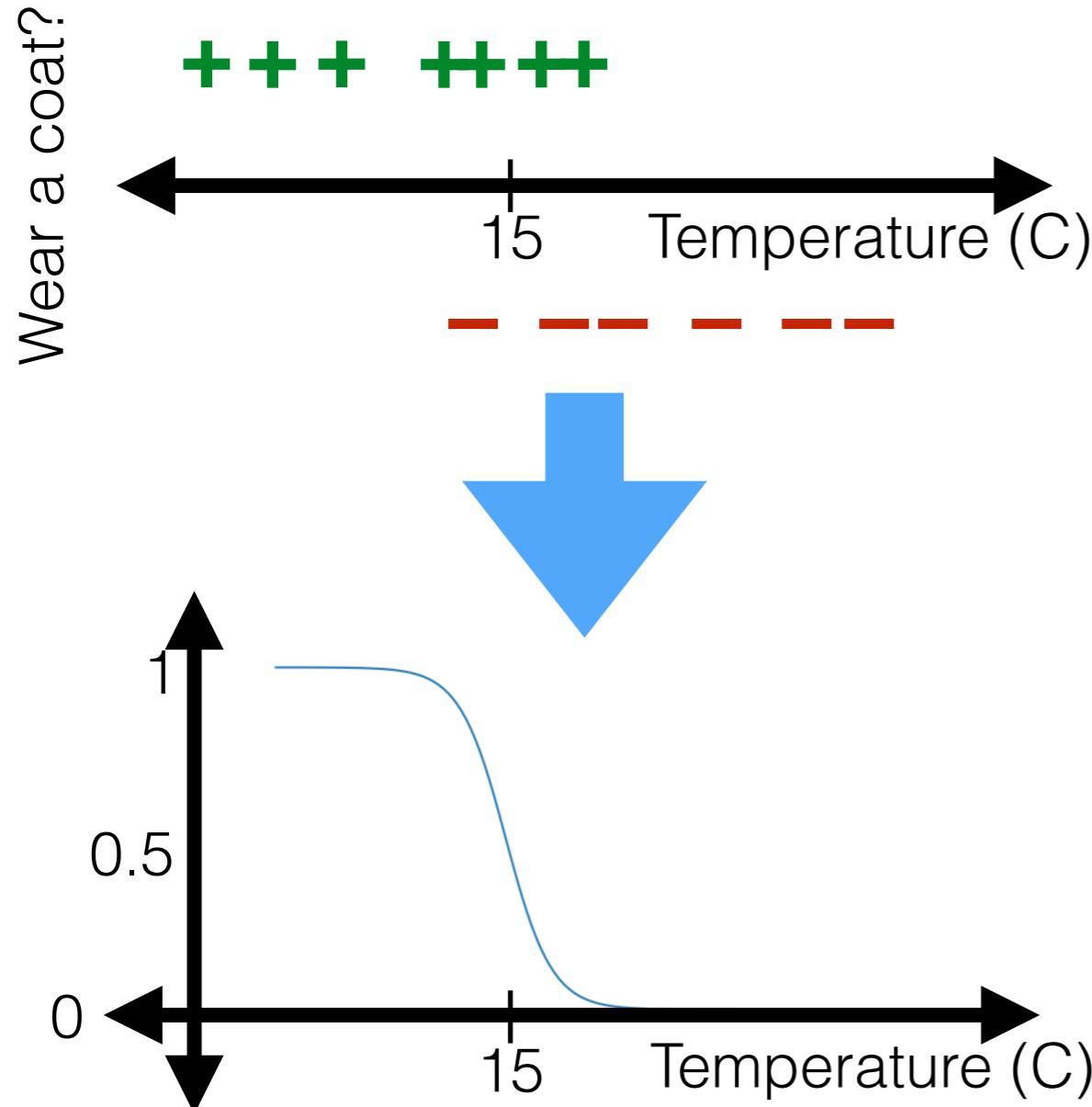
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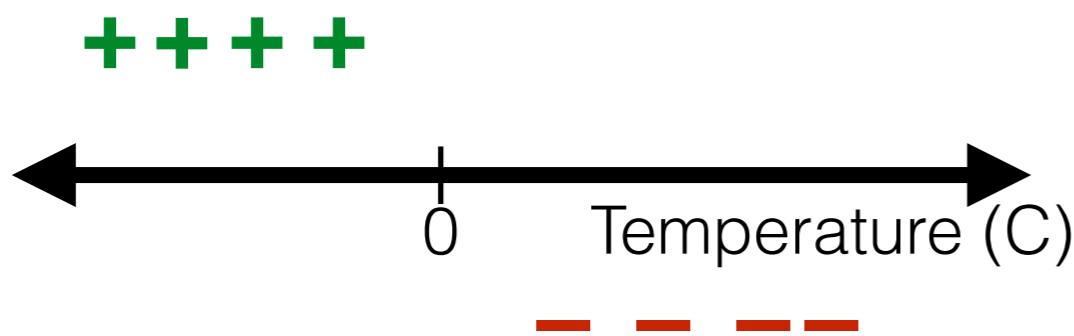
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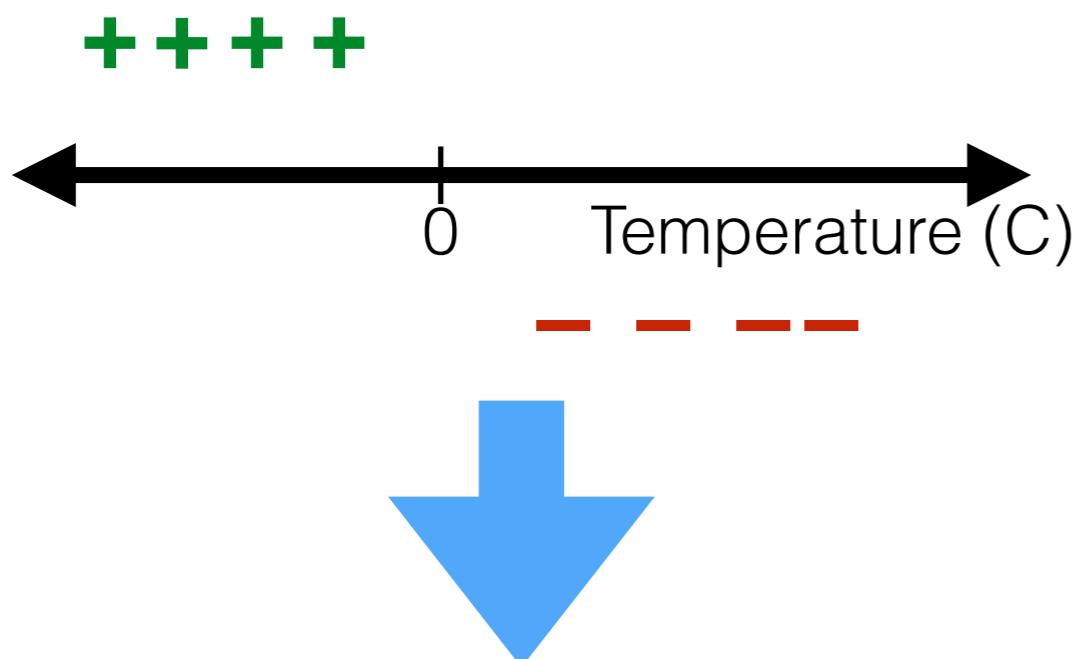
Wear base layer?



# Gradient descent for logistic regression

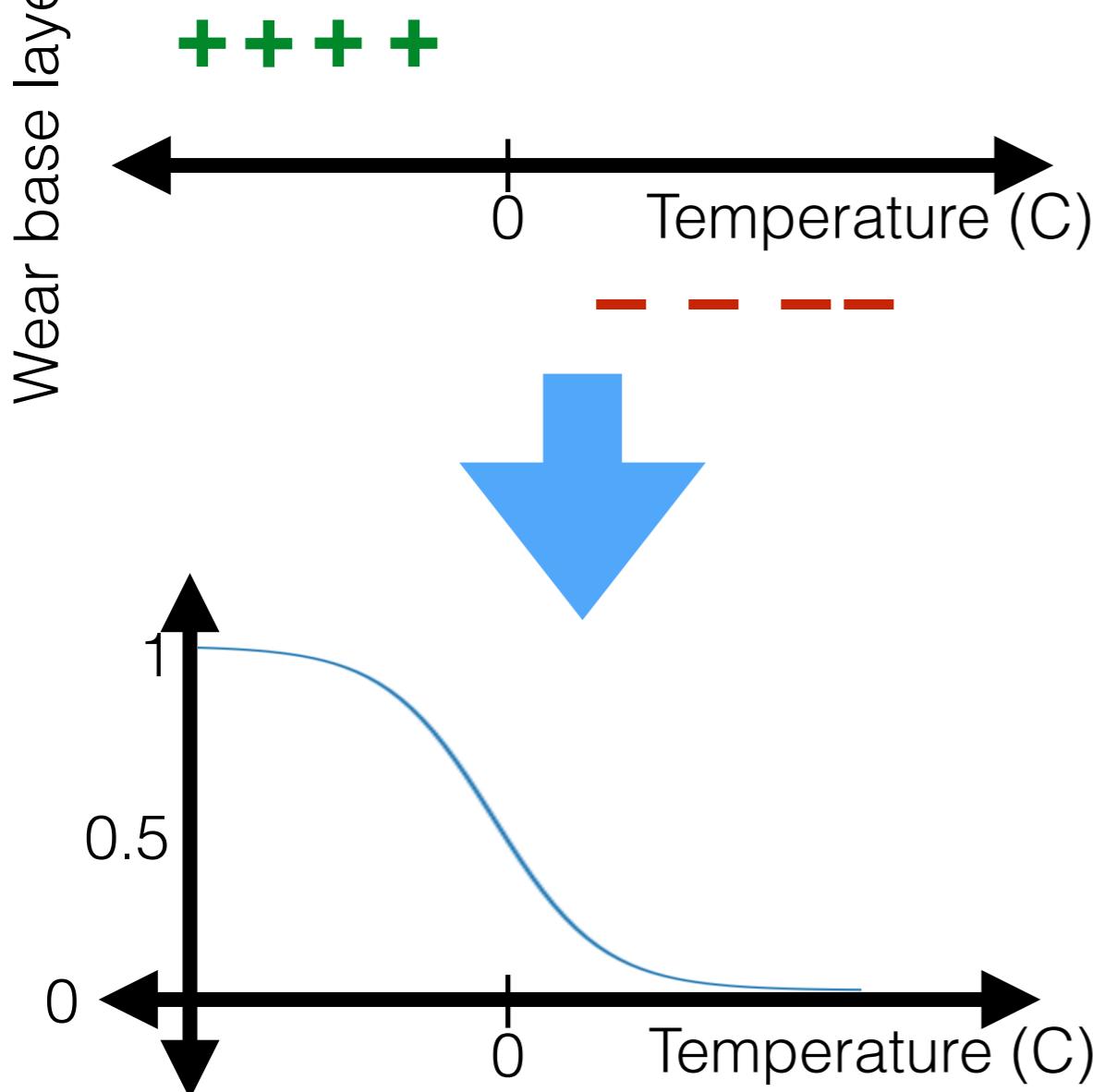
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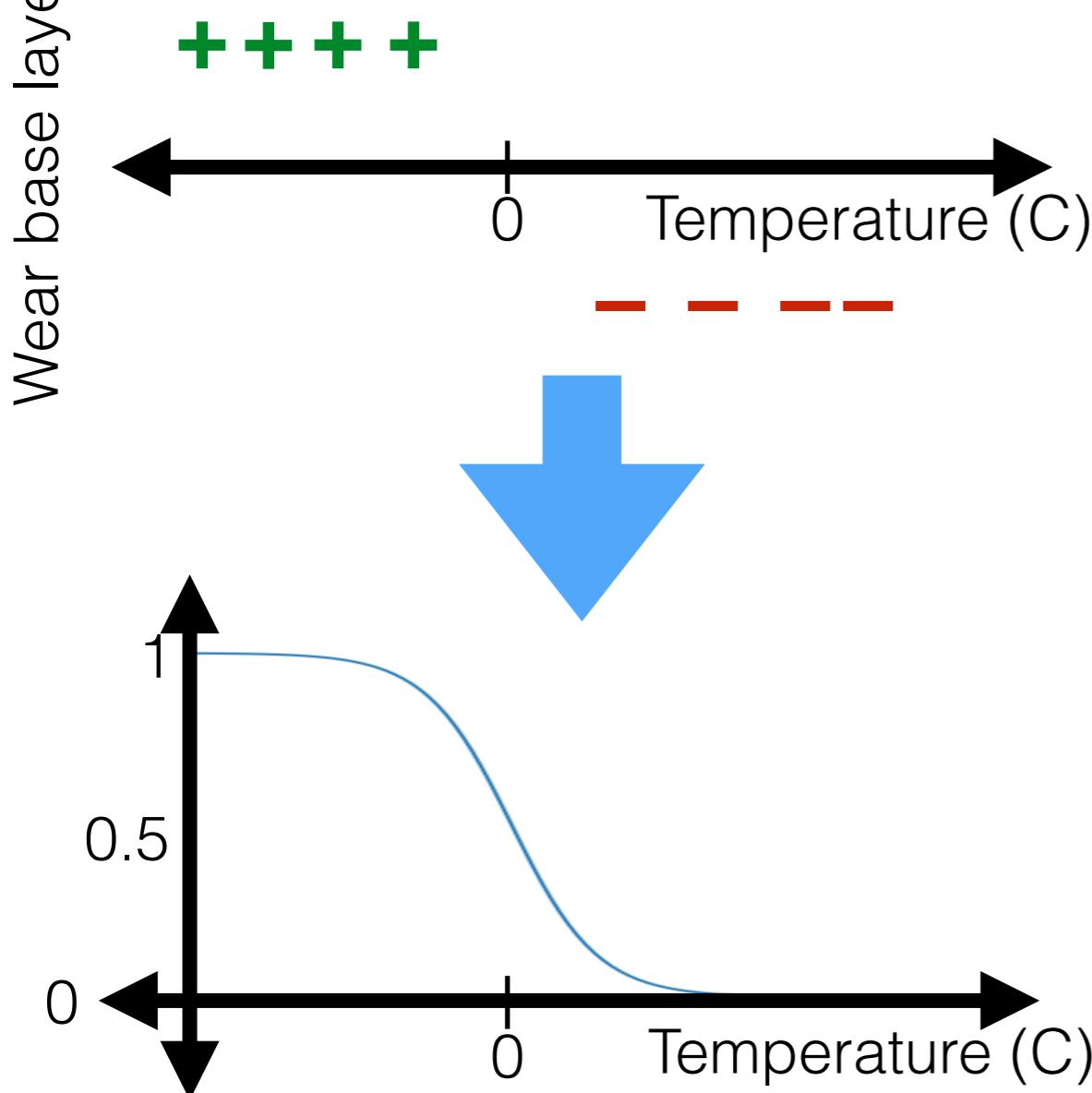
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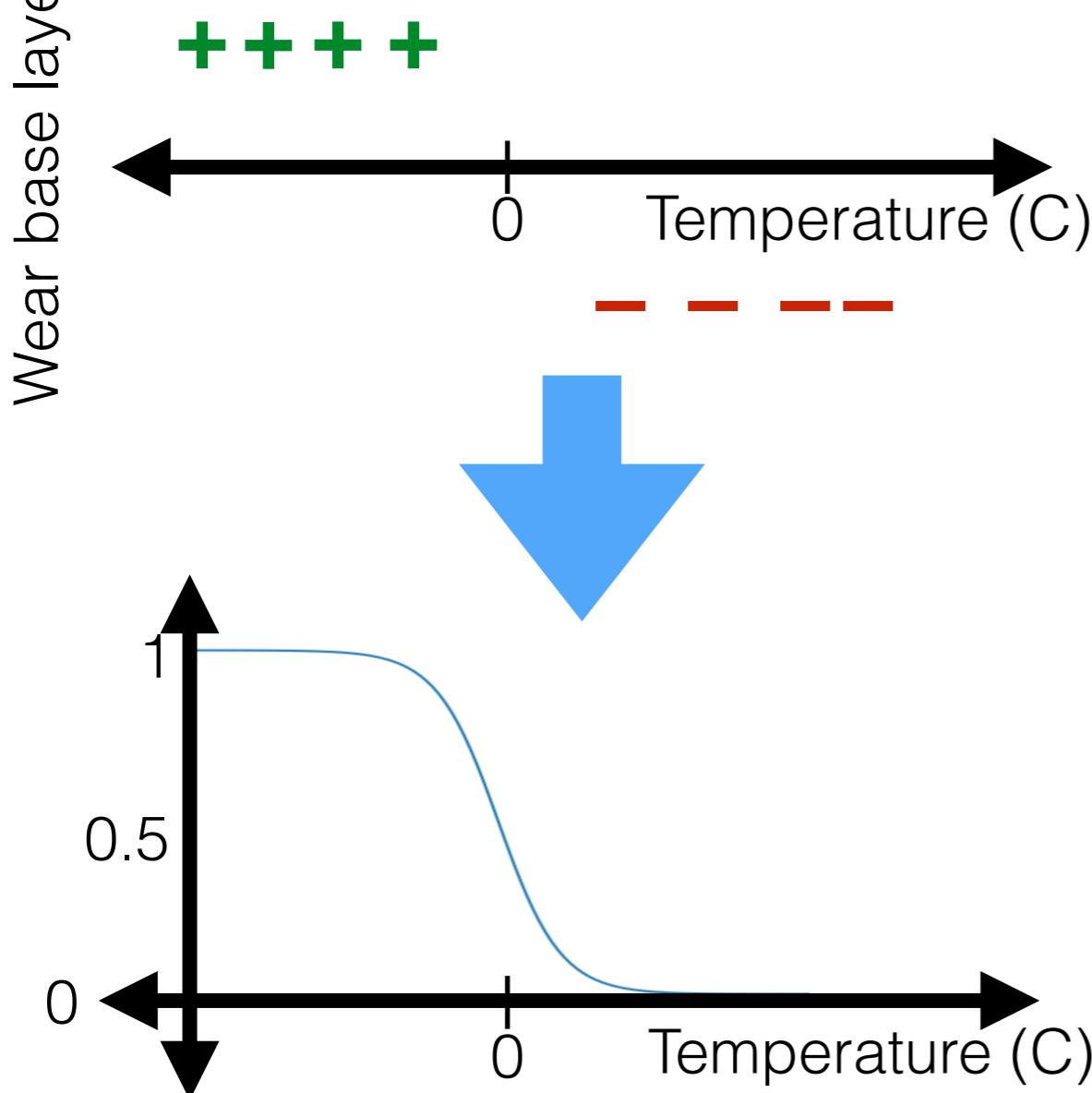
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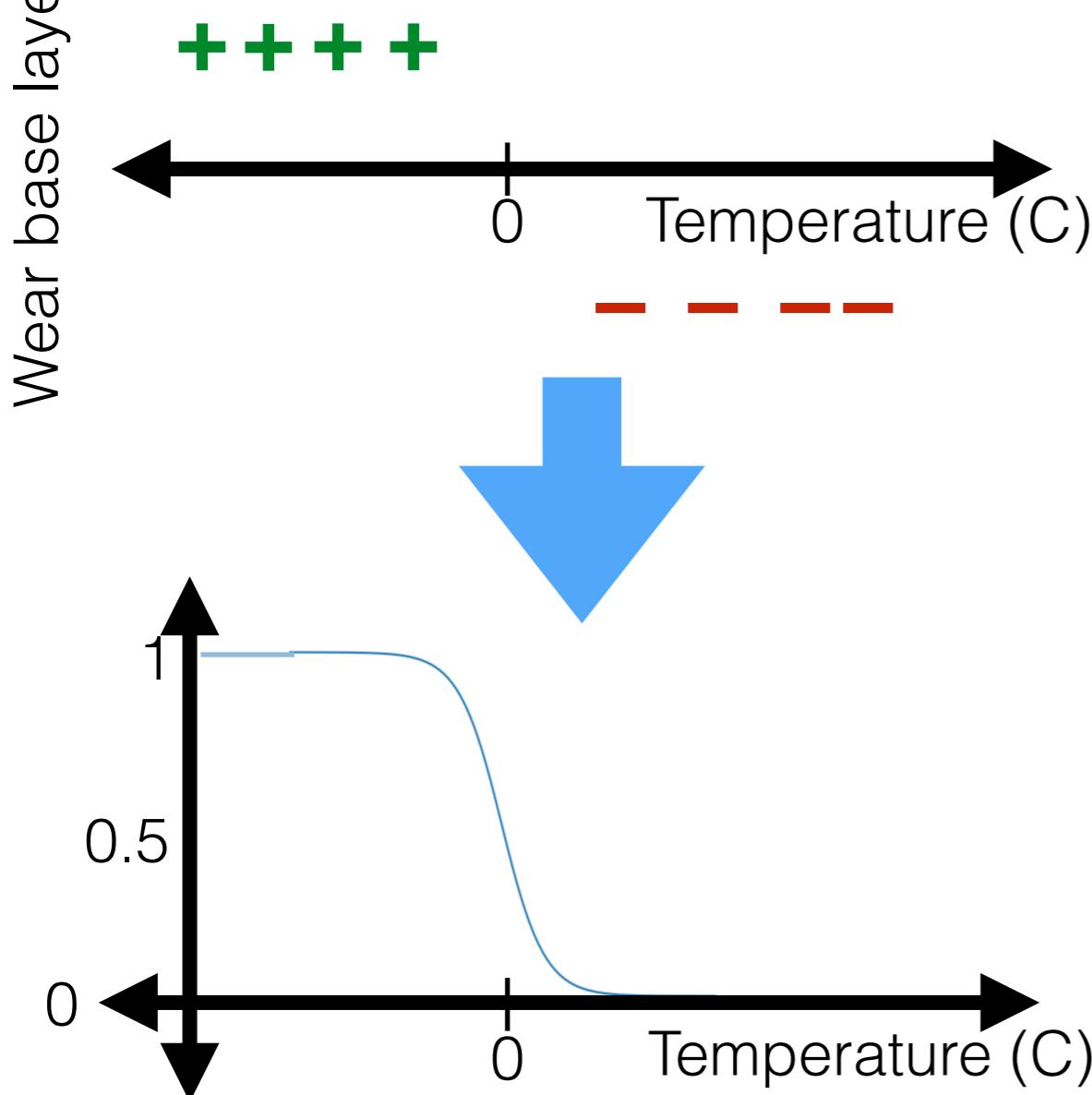
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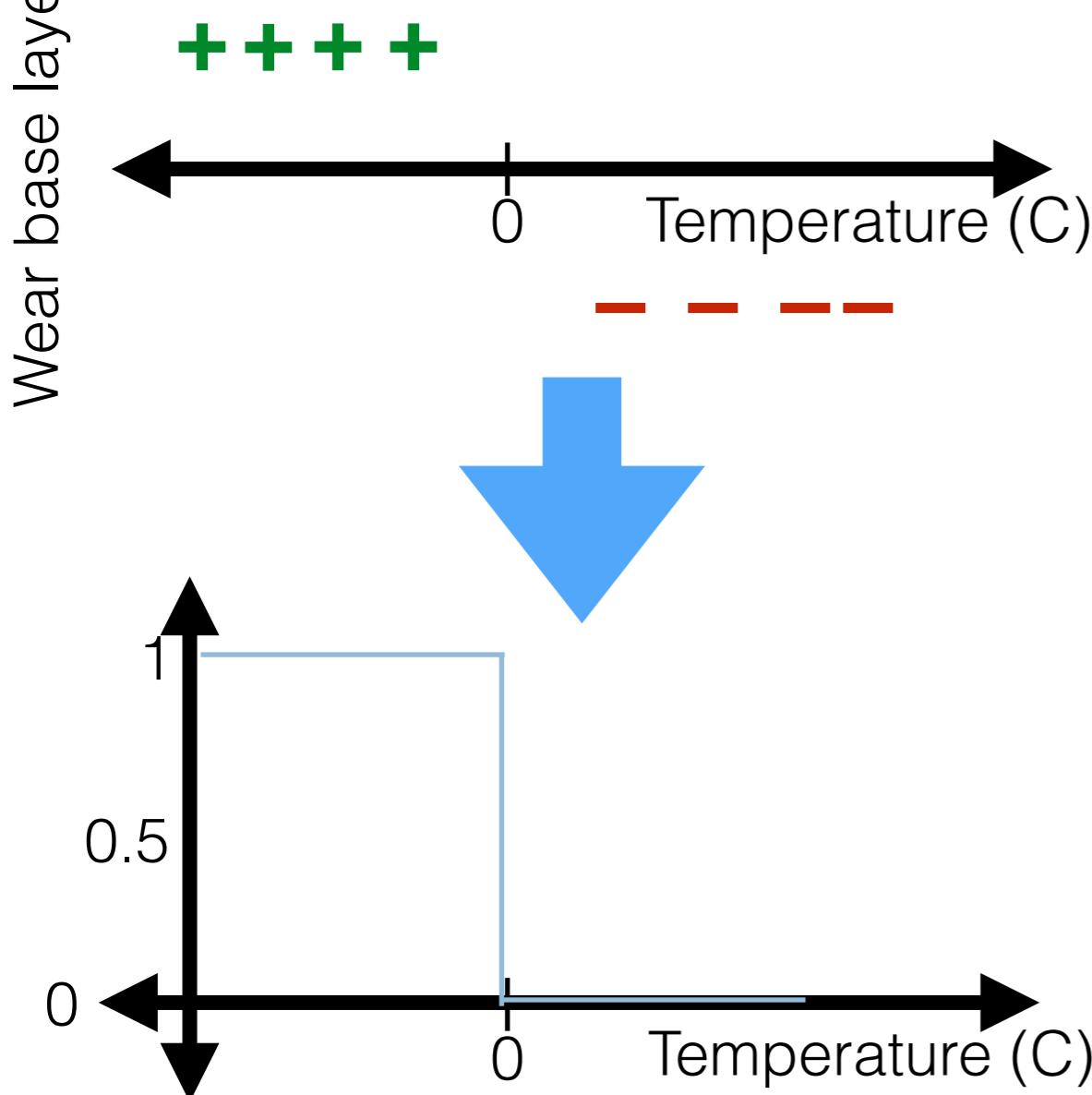
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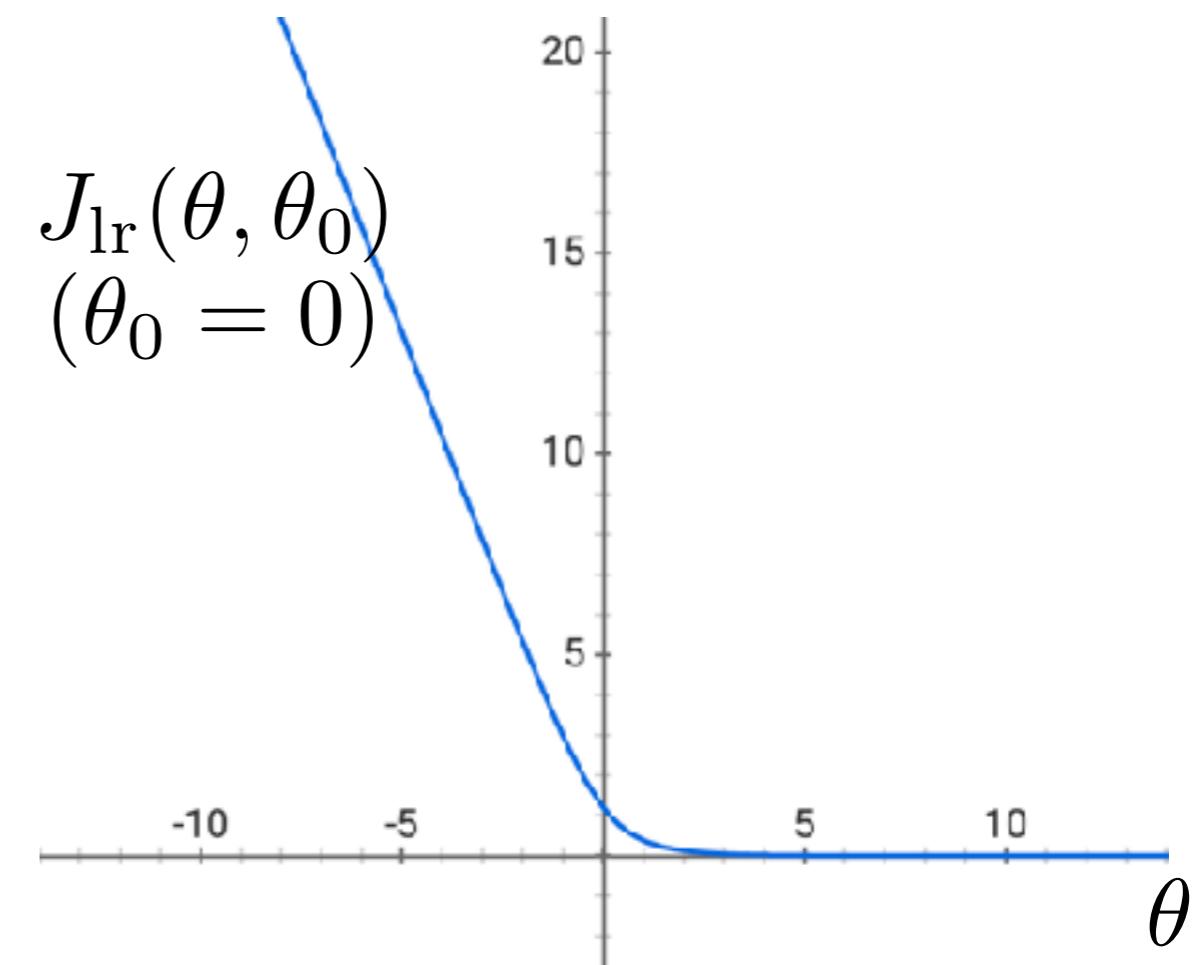
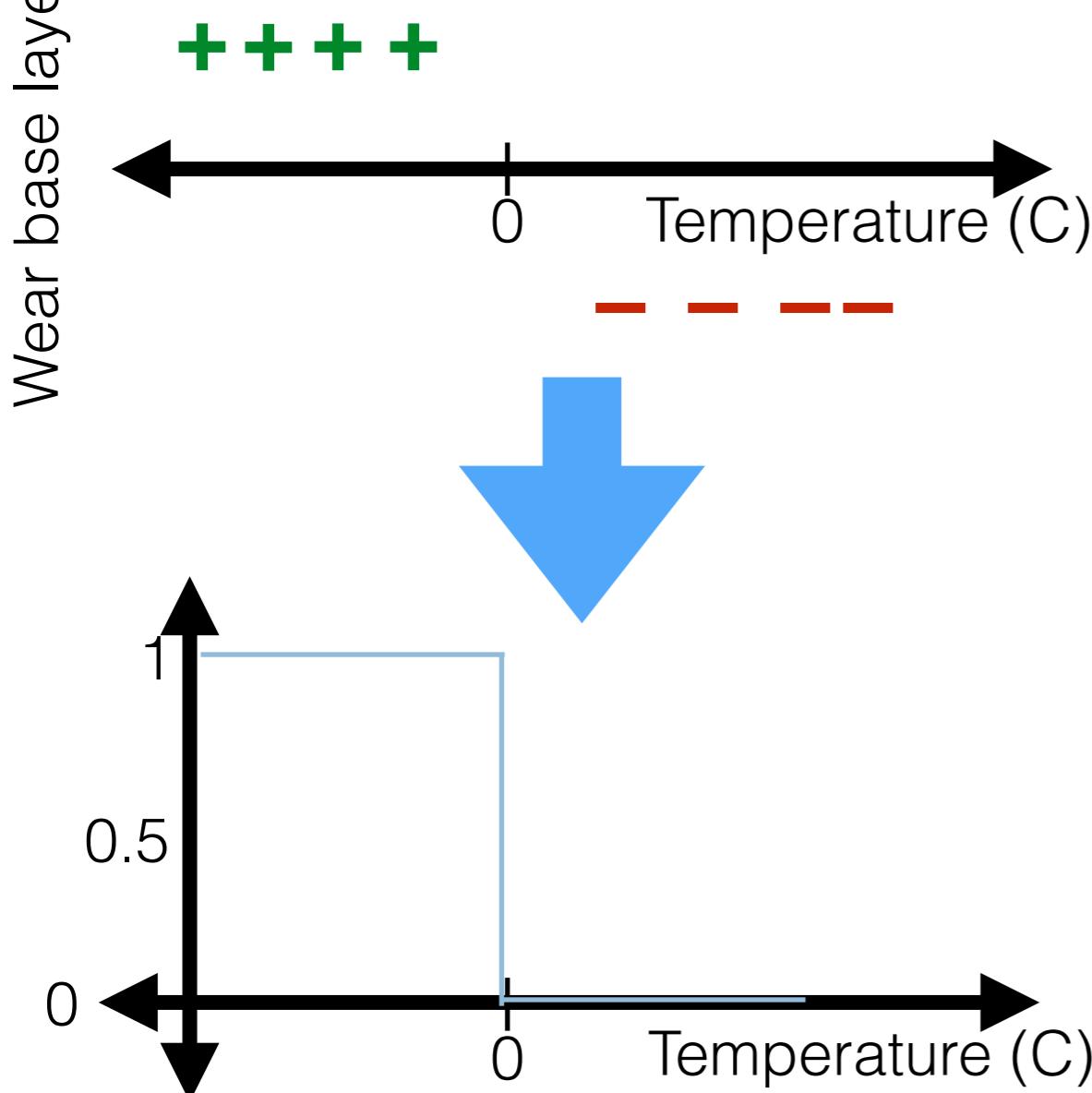
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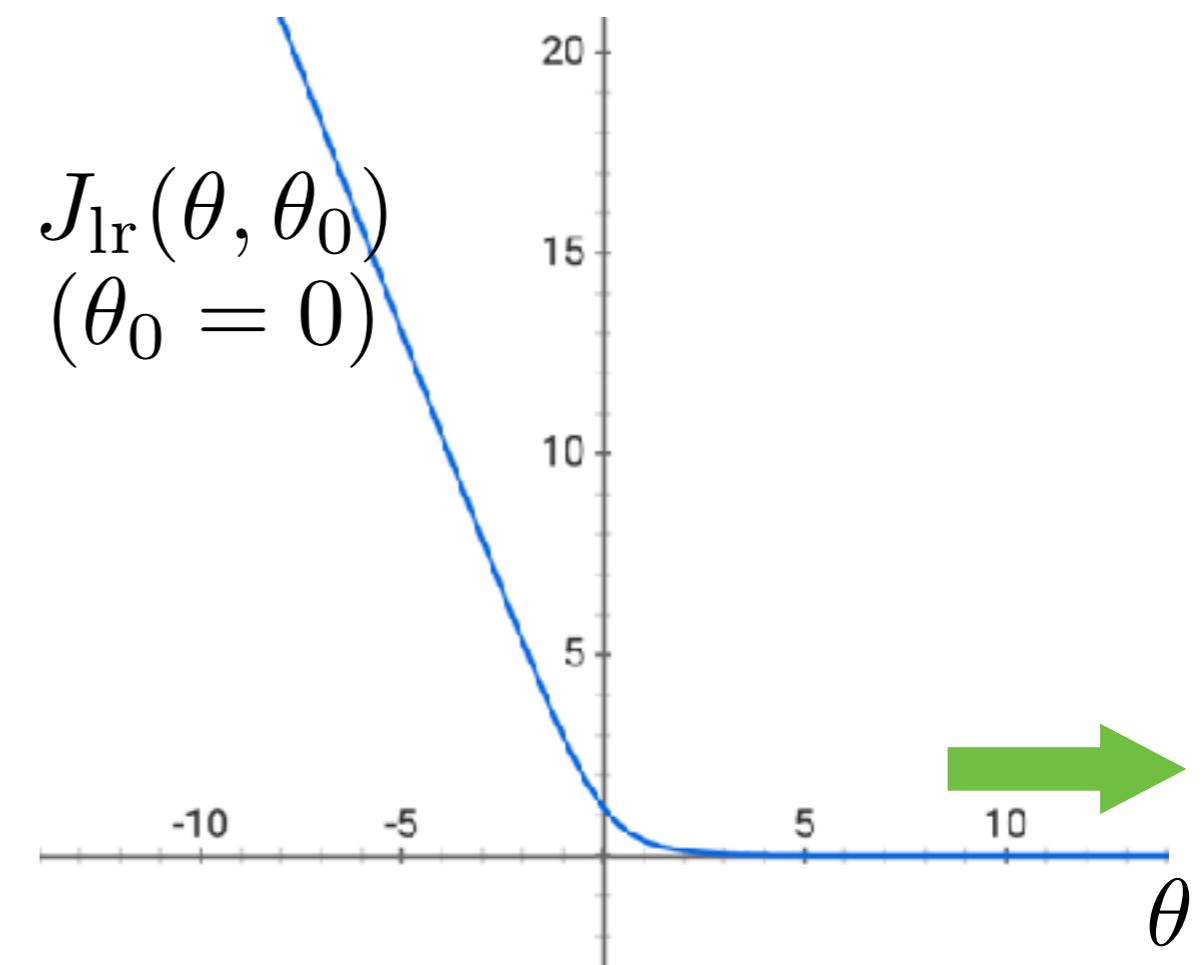
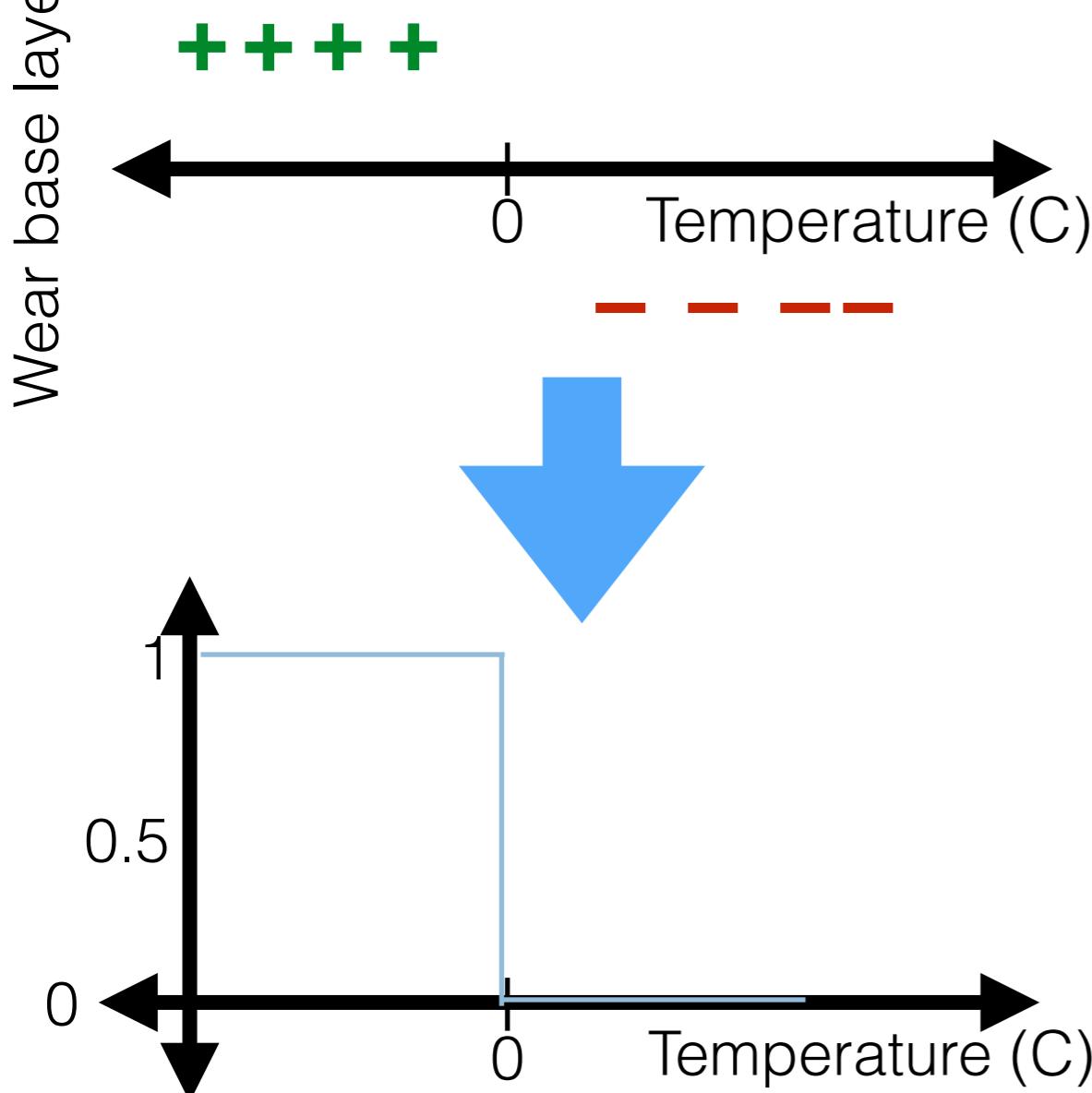
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# Logistic regression loss revisited

$$\begin{aligned} J_{\text{lr}}(\Theta) &= J_{\text{lr}}(\theta, \theta_0) \\ &= \frac{1}{n} \sum_{i=1}^n L_{\text{nll}}(\sigma(\theta^\top x^{(i)} + \theta_0), y^{(i)}) \end{aligned}$$

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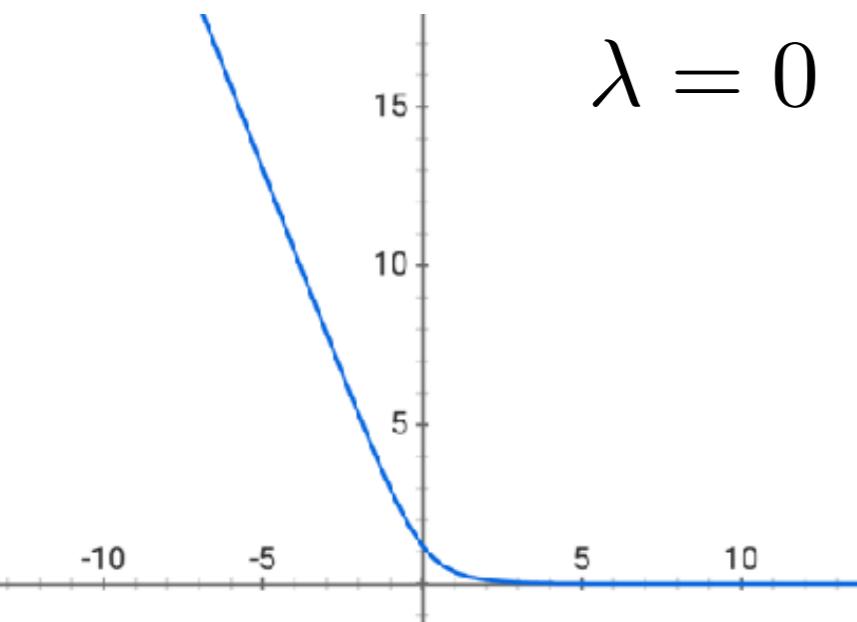
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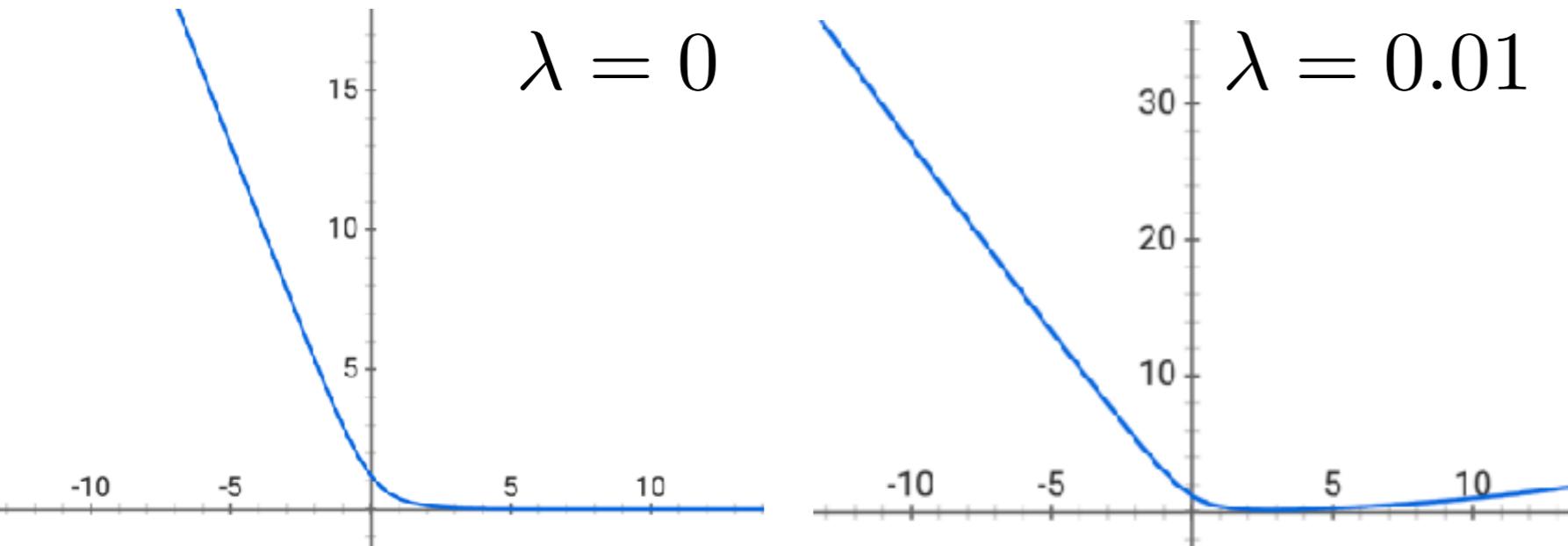
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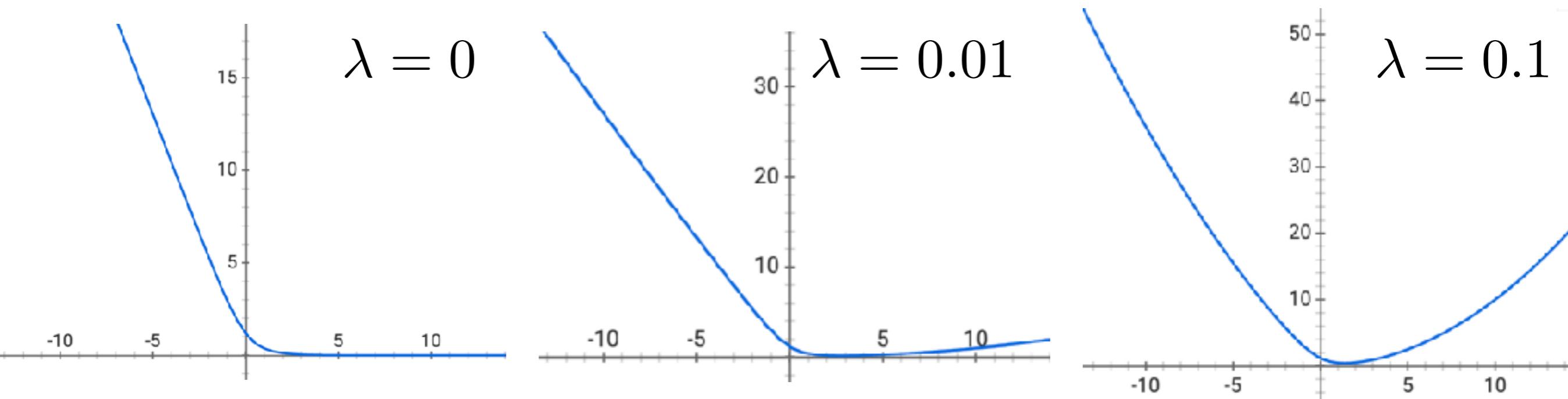
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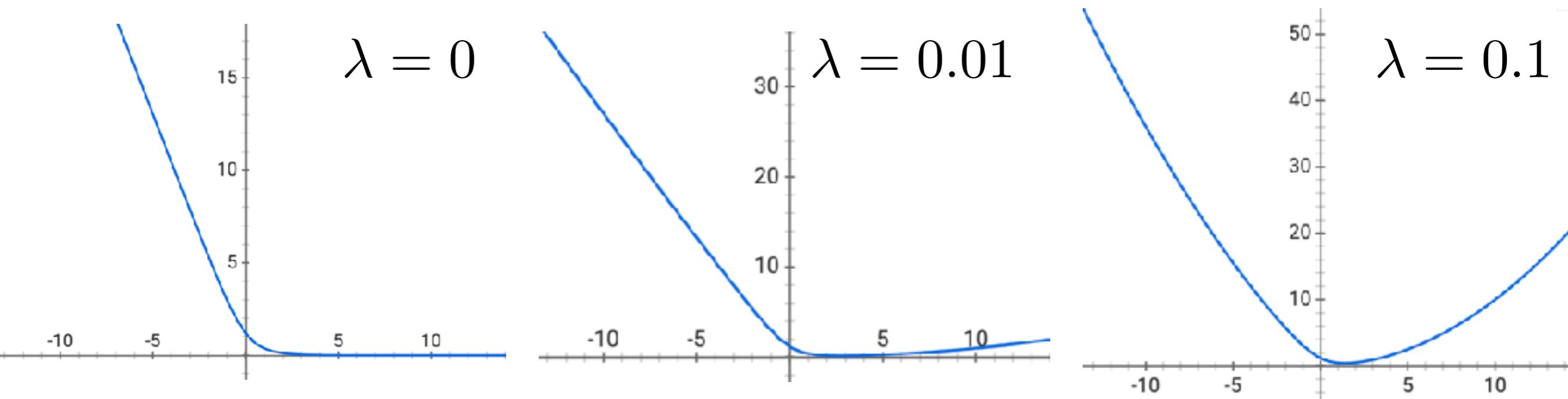
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- How to choose hyperparameters? One option: consider a handful of possible values and compare via CV

# Logistic regression learning algorithm

Exactly gradient descent  
with  $f$  given by logistic  
regression objective

# Logistic regression learning algorithm

LR-Gradient-Descent ( $\theta_{\text{init}}, \theta_{0,\text{init}}, \eta, \epsilon$ )

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**until**  $|J_{\text{lr}}(\theta^{(t)}, \theta_0^{(t)}) - J_{\text{lr}}(\theta^{(t-1)}, \theta_0^{(t-1)})| < \epsilon$

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**Return**  $\theta^{(t)}, \theta_0^{(t)}$

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