DATA MINING 2
Support Vector Machine

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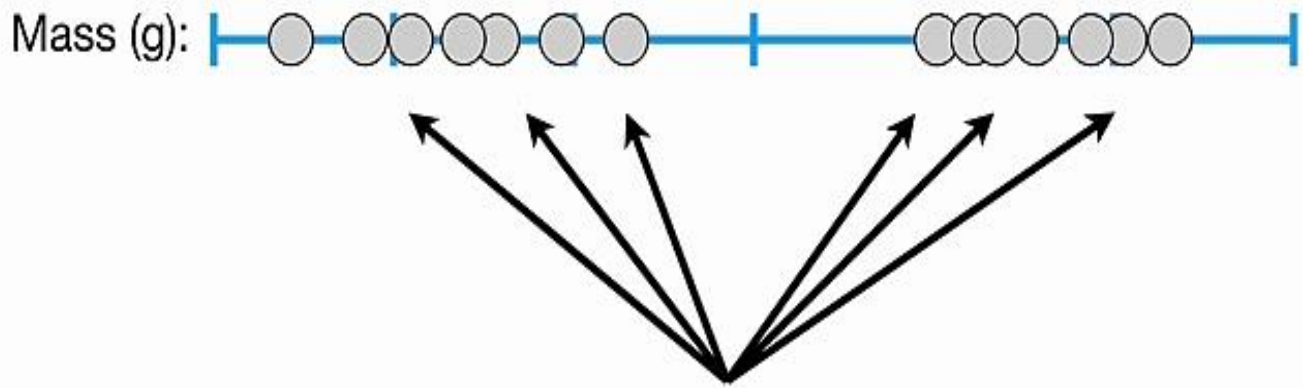
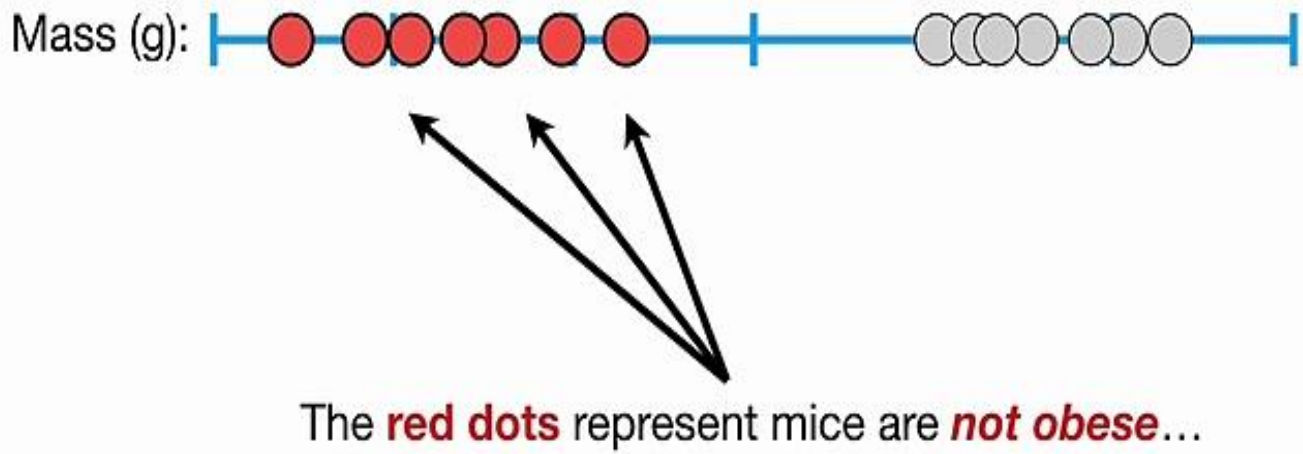
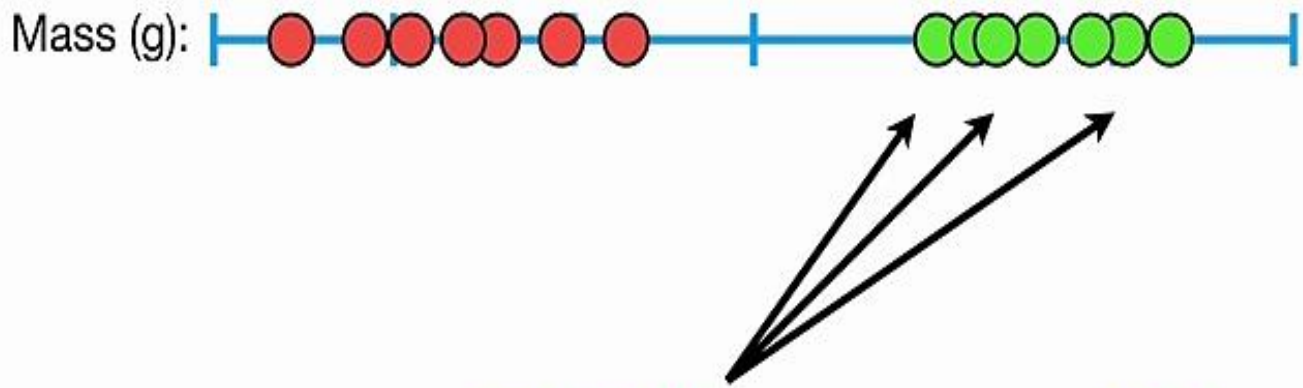
Slides edited from Tan, Steinbach, Kumar, Introduction to Data Mining
Contains slides integrated with StatQuest

UNIVERSITÀ DI PISA

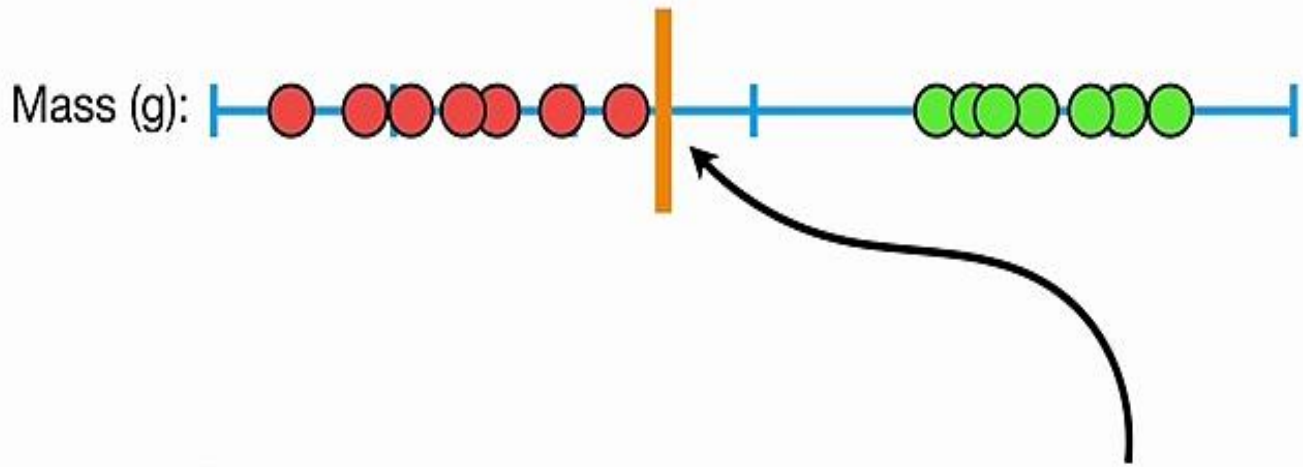


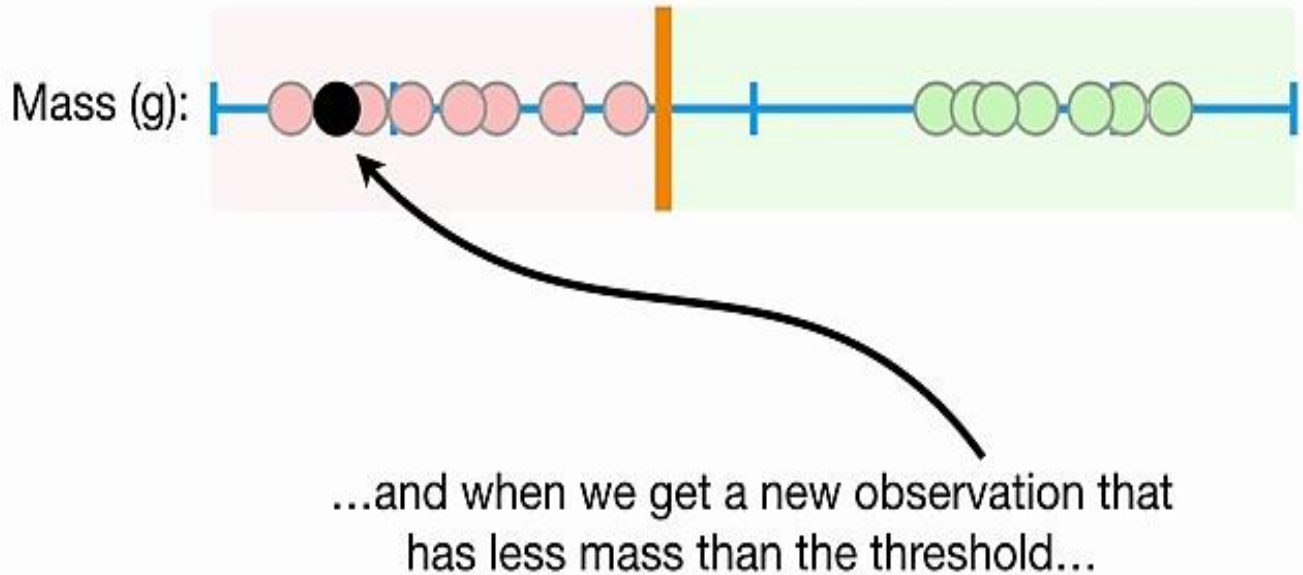
Let's start by imagining we measured the mass of a bunch of mice…

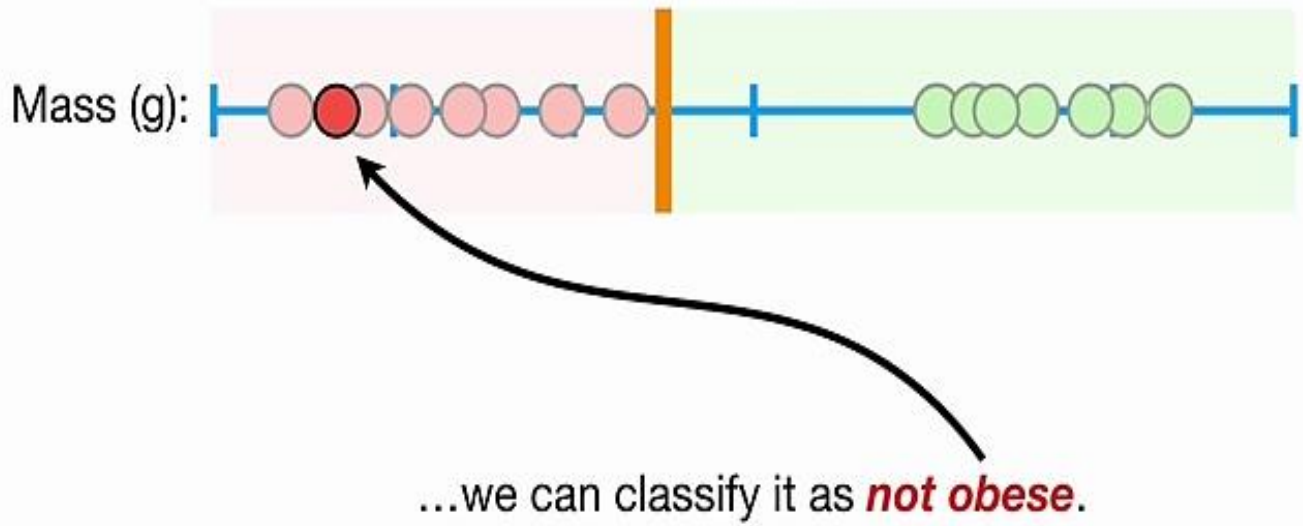

Mass (g):
The red dots represent mice are not obese…

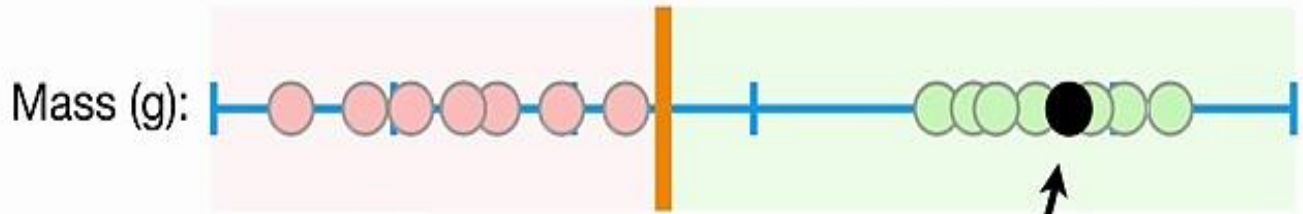


…and the **green dots** represent mice are ***obese***.

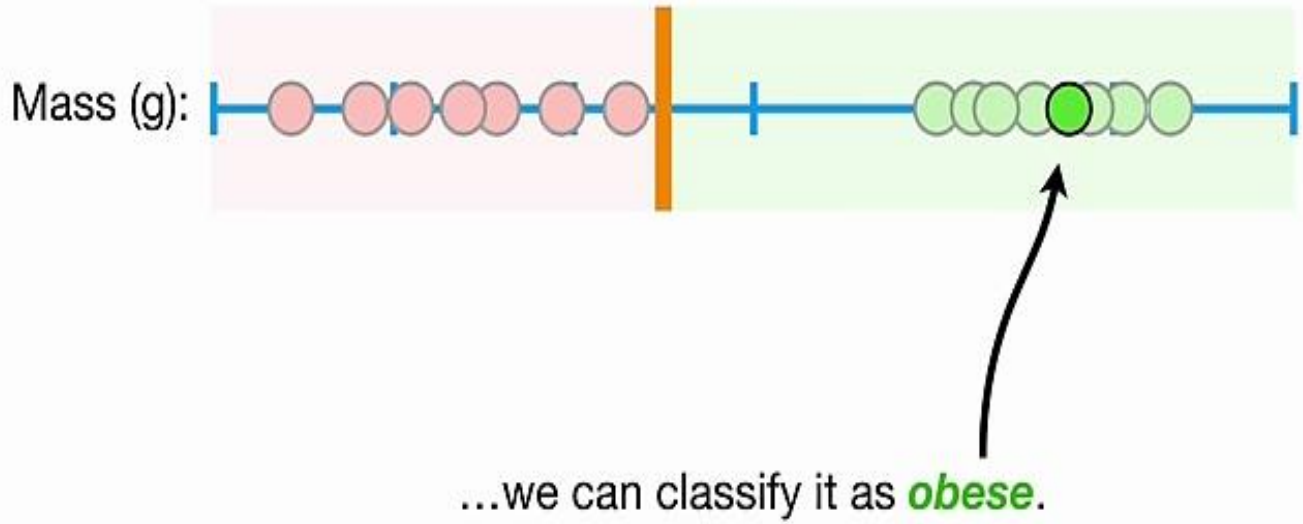

Mass (g):
Based on these observations, we can pick a threshold…

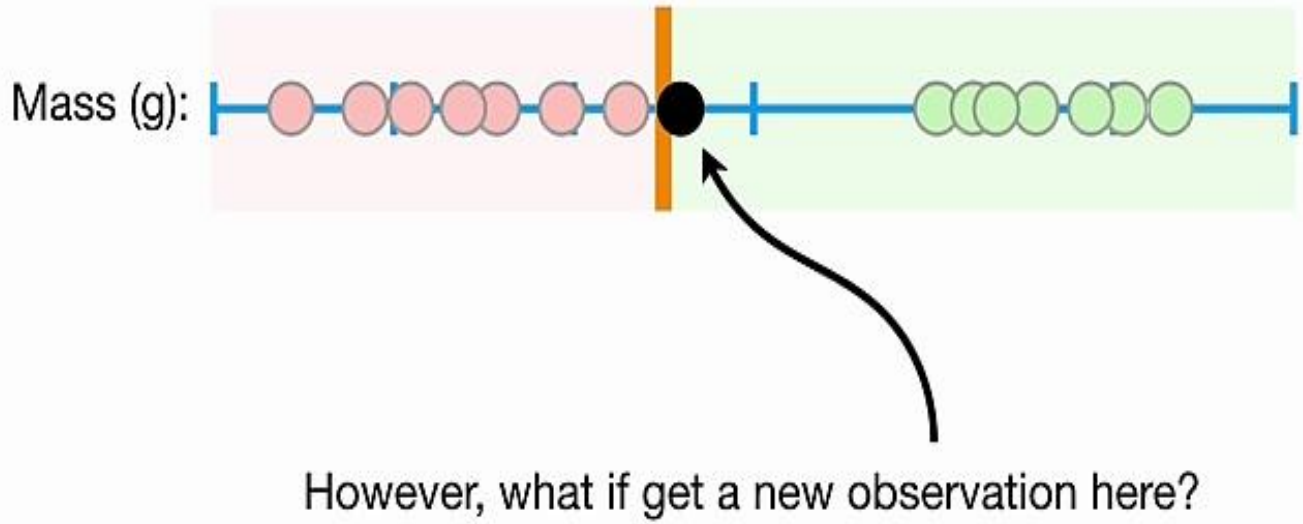

Mass (g):
…and when we get a new observation that
has less mass than the threshold…

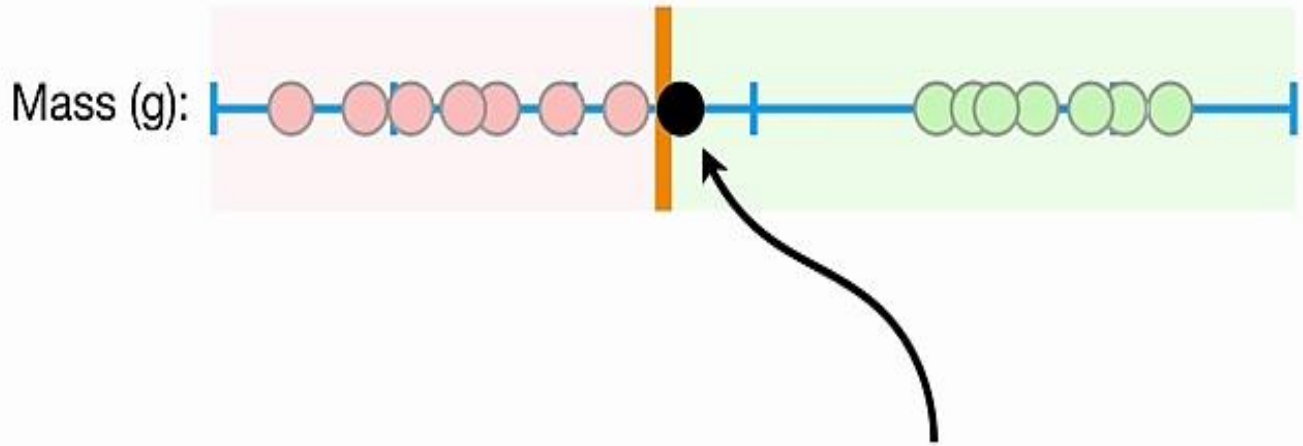

Mass (g):
…we can classify it as not obese.



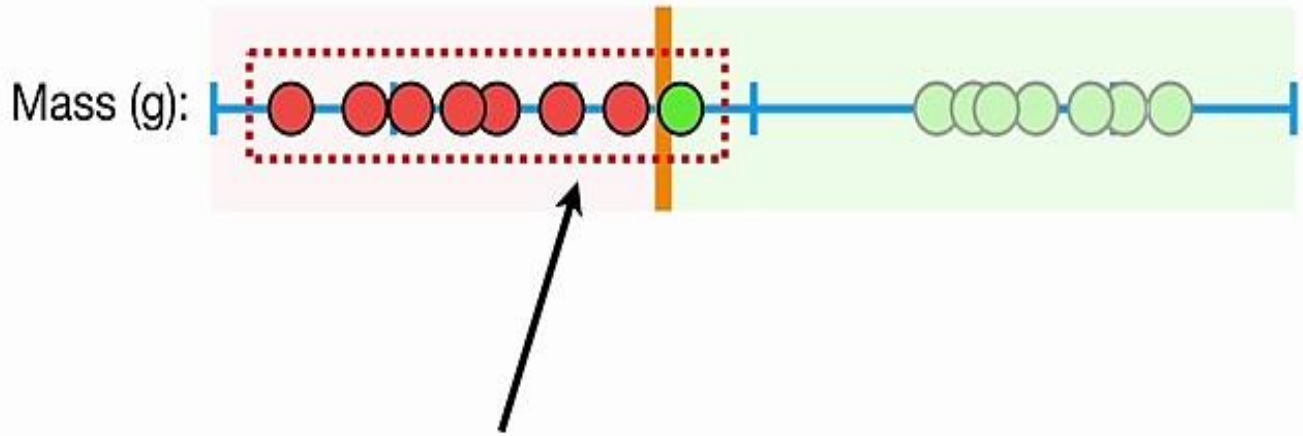
And when we get a new observation with more mass than the threshold…


Mass (g):
…we can classify it as obese.

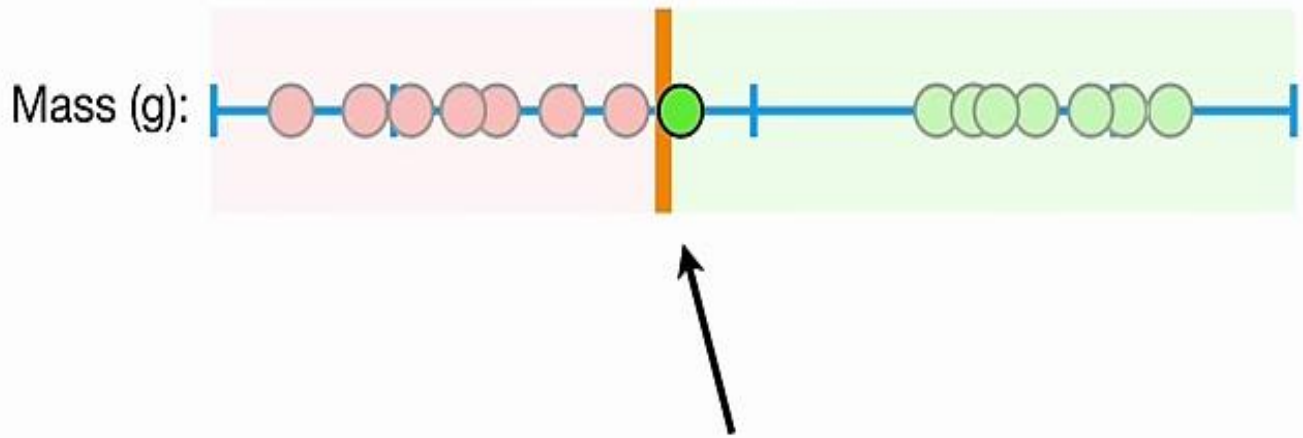

Mass (g):
However, what if get a new observation here?

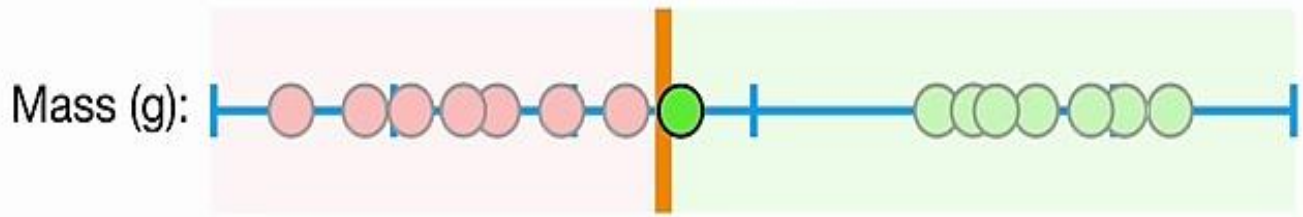


Because this observation has more mass than the threshold, we classify it as ***obese***.

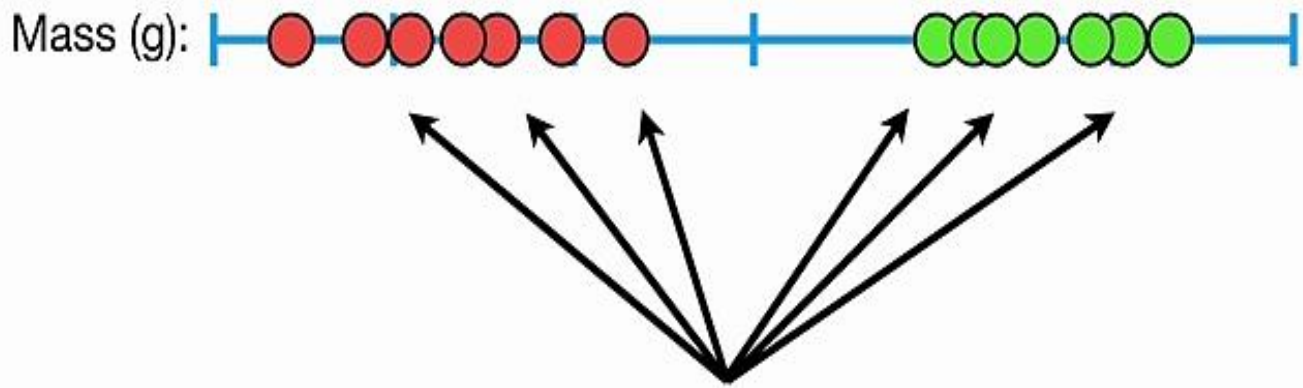


But that doesn't make sense, because it is much closer to the observations that are ***not obese***.

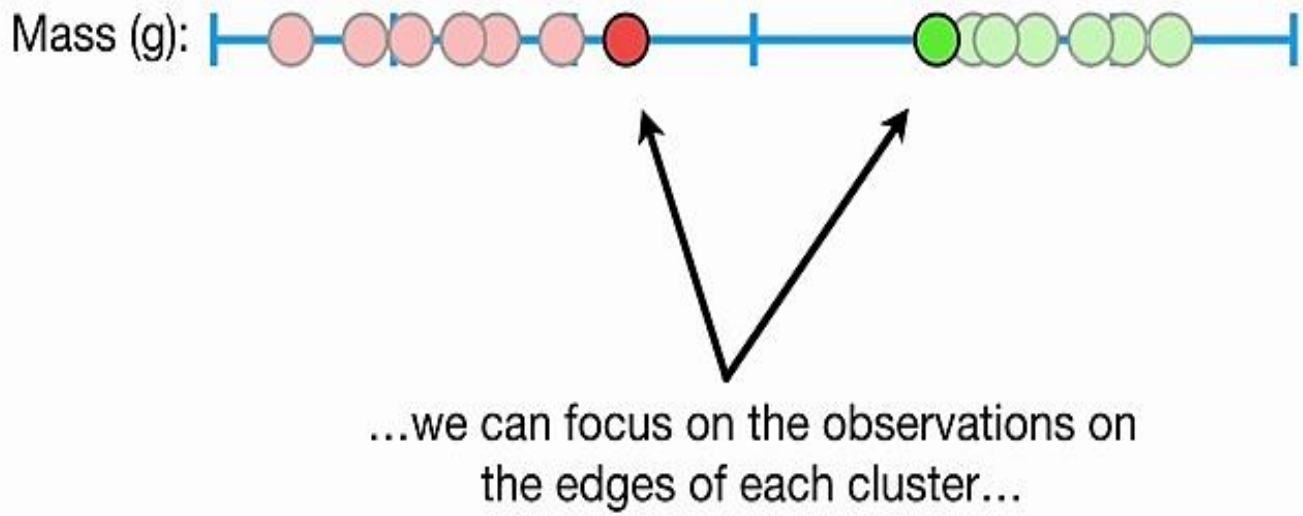

Mass (g):
So this threshold is pretty lame.

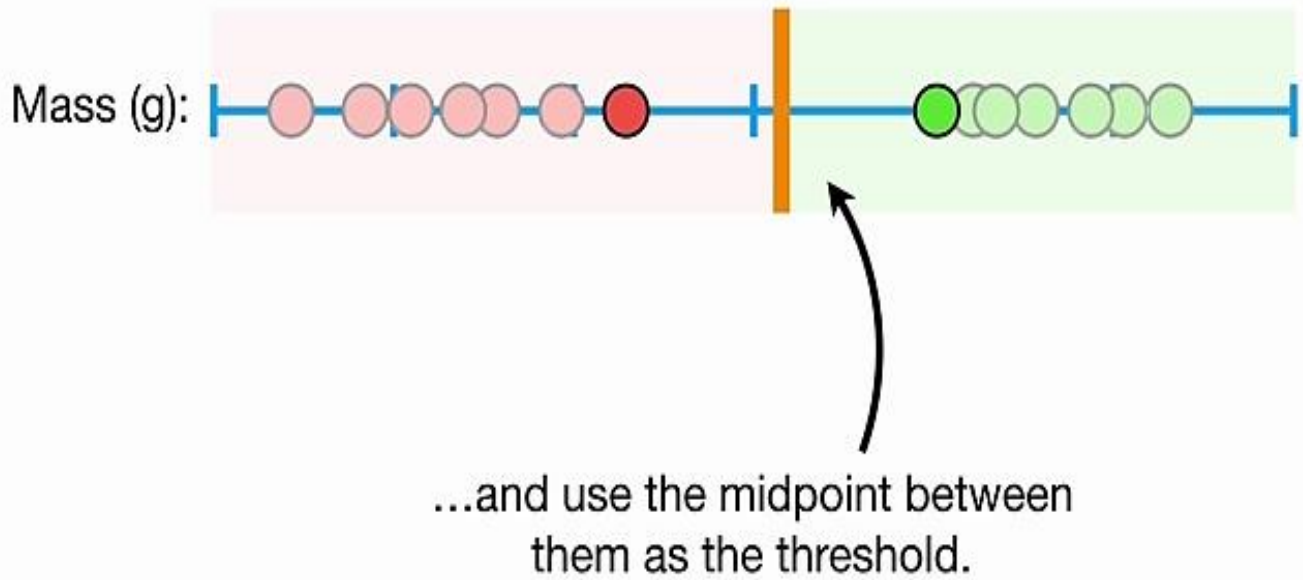


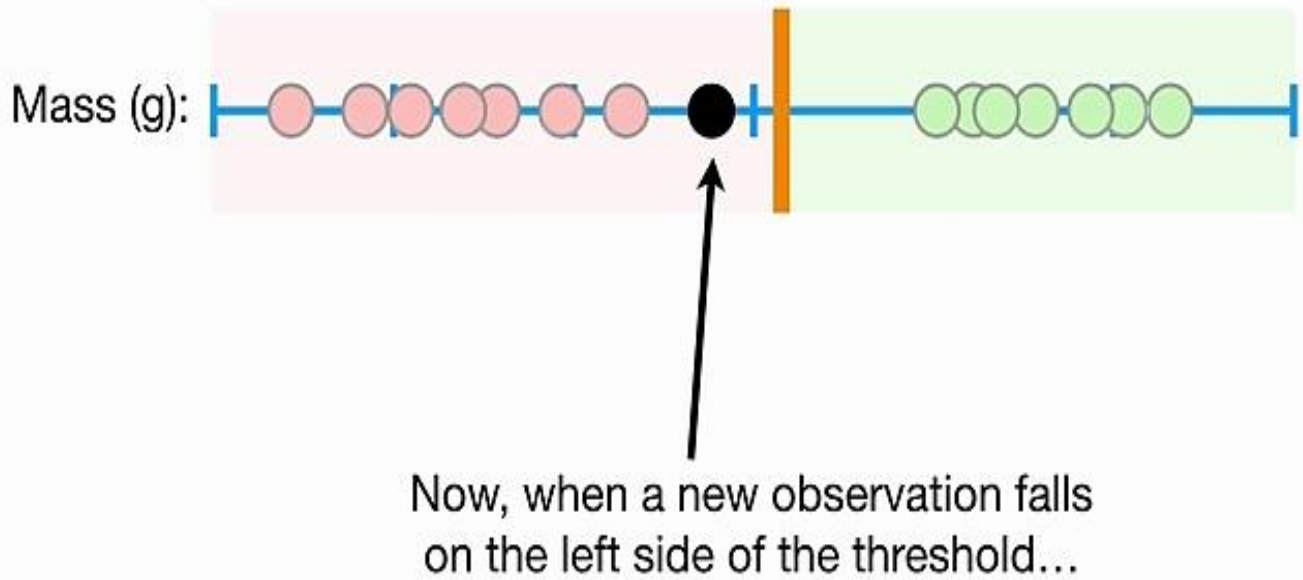
Can we do better?

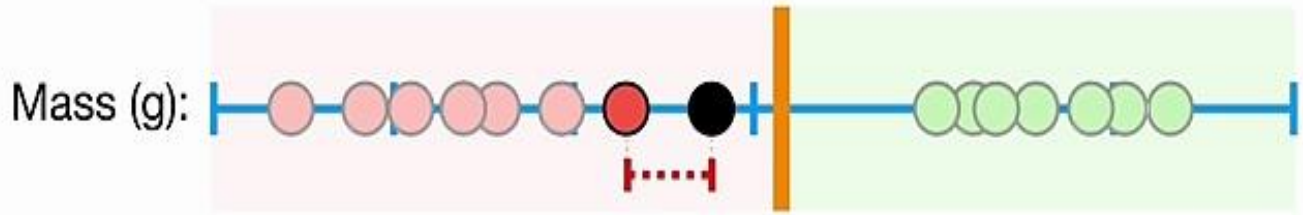


Going back to the original training dataset…

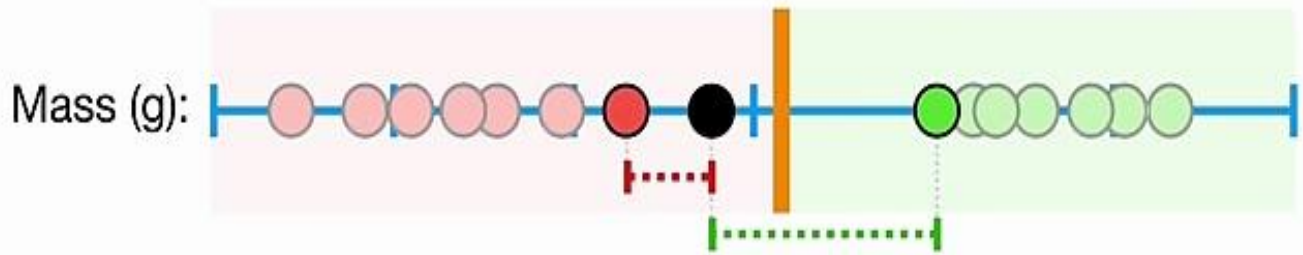

Mass (g):
…we can focus on the observations on
the edges of each cluster…


Mass (g):
...and use the midpoint between them as the threshold.

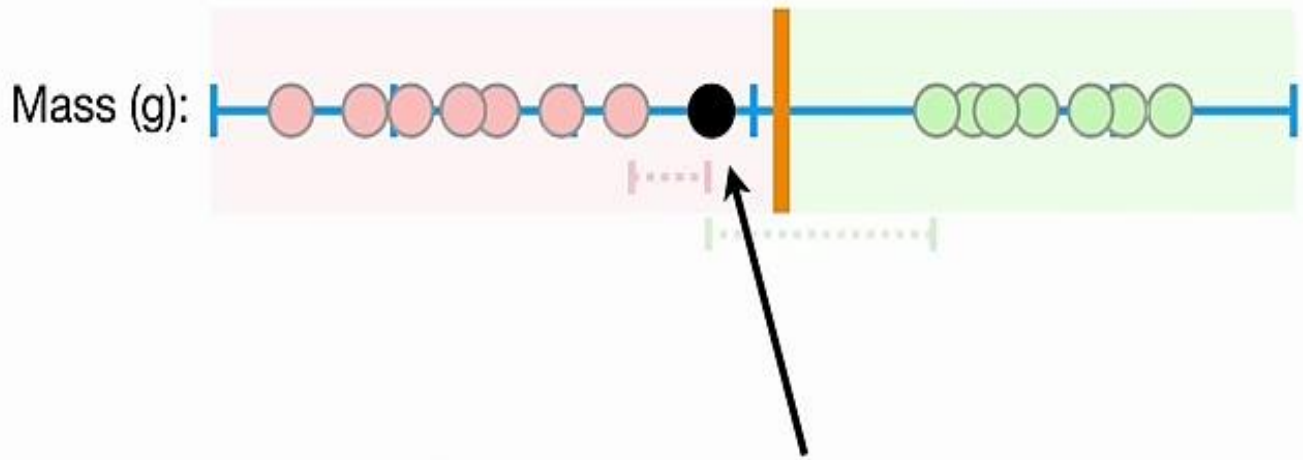

Mass (g):
Now, when a new observation falls
on the left side of the threshold…

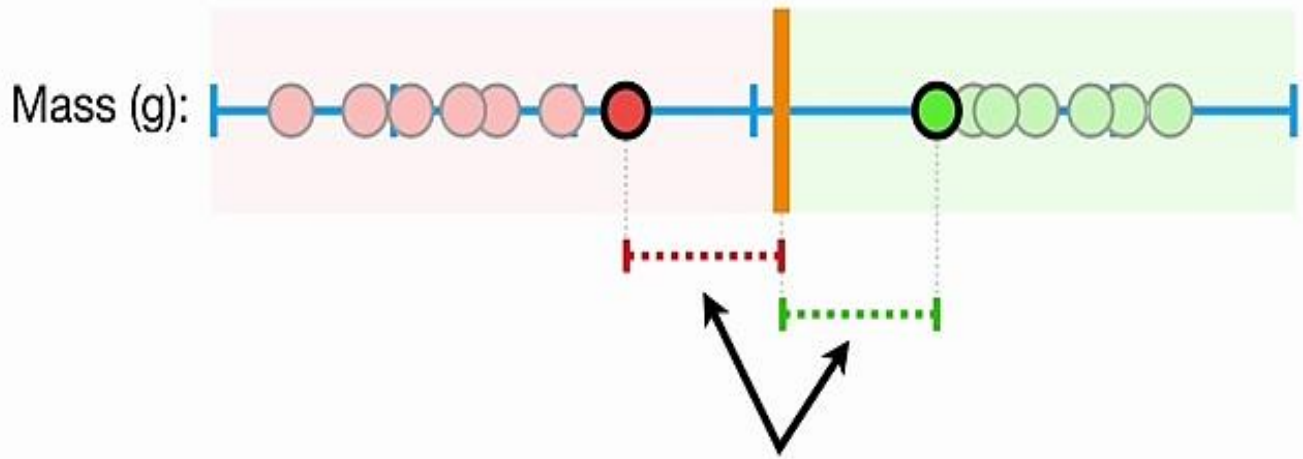


…it will be closer to the
observations that are ***not obese***…

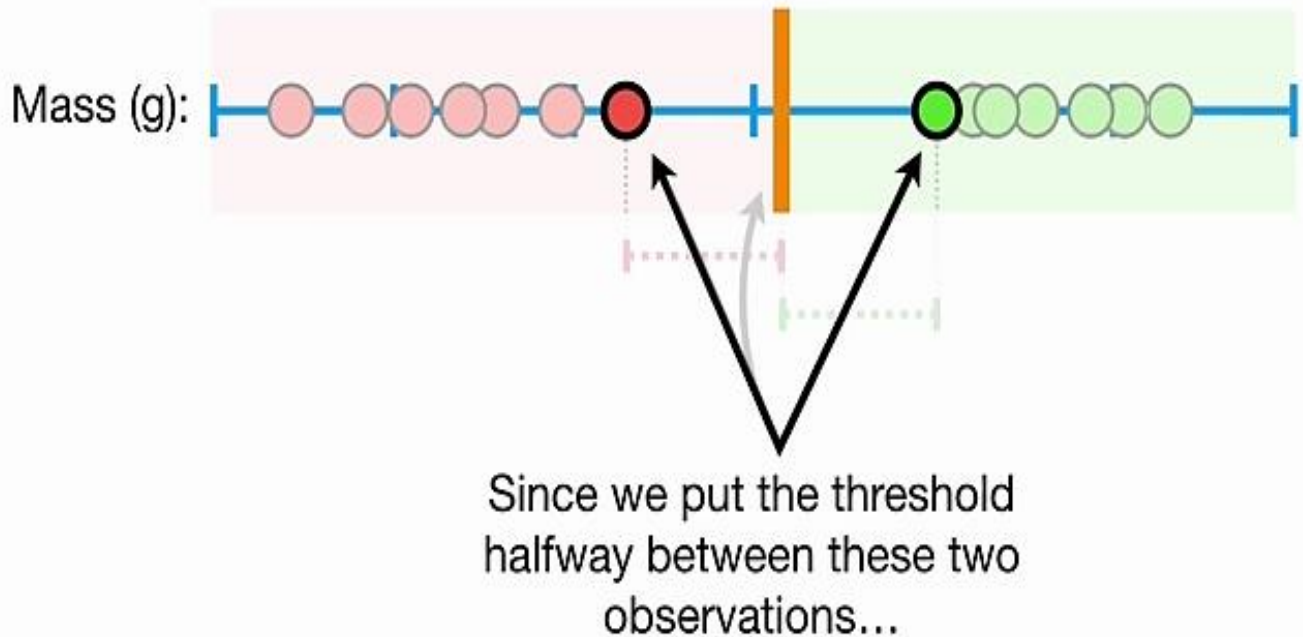


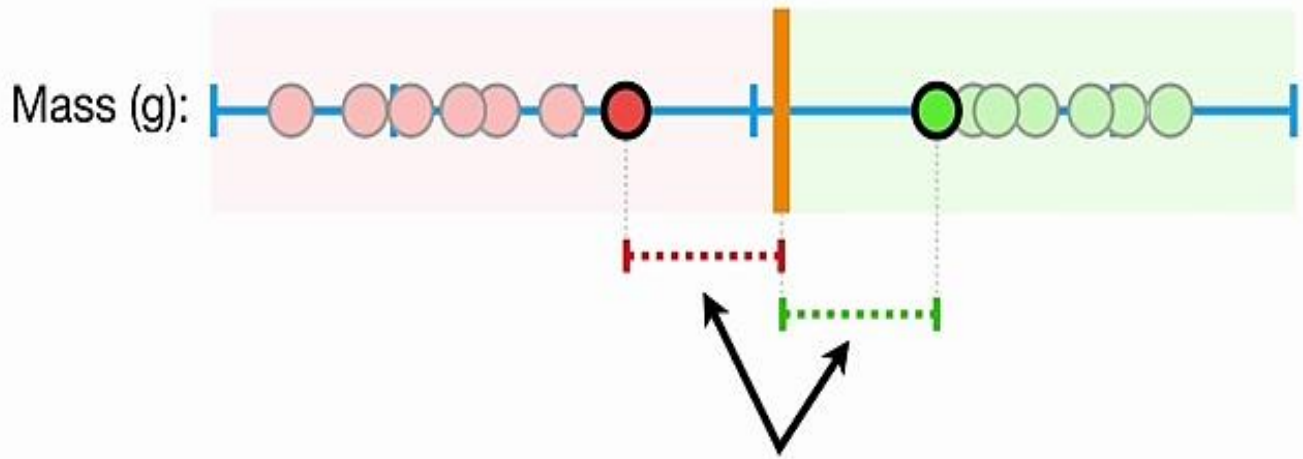
…than it is to the ***obese*** observations.


Mass (g):
So it makes sense to classify this new observation as *not obese*.

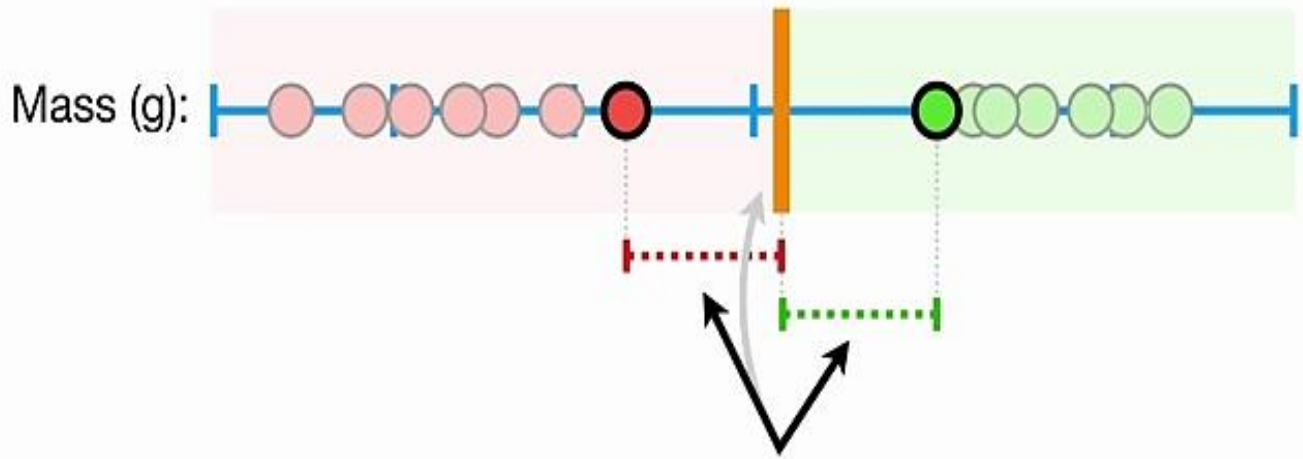


The shortest distance between the observations and the threshold is called the **margin.**

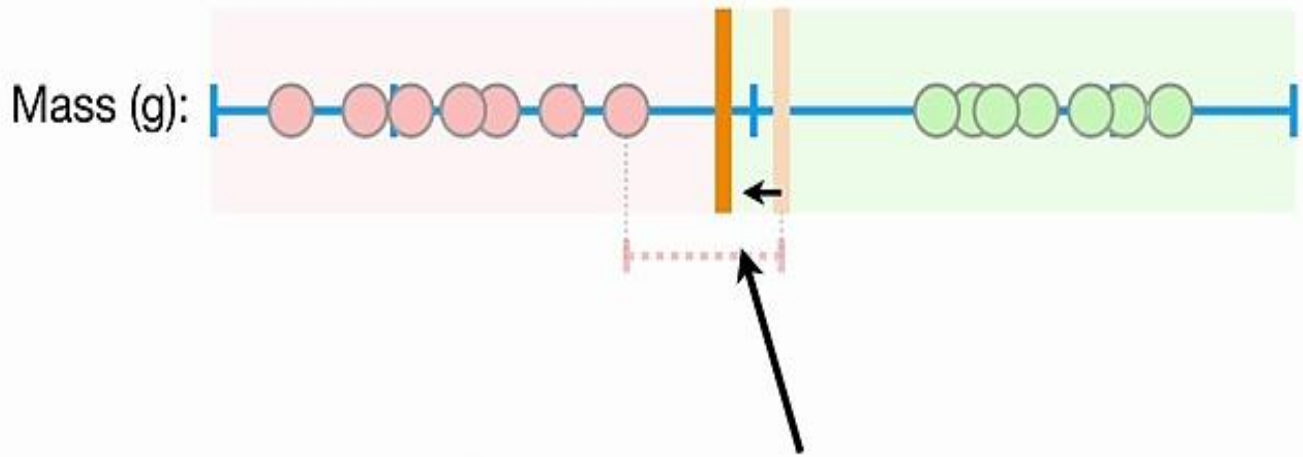

Mass (g):
Since we put the threshold halfway between these two observations…

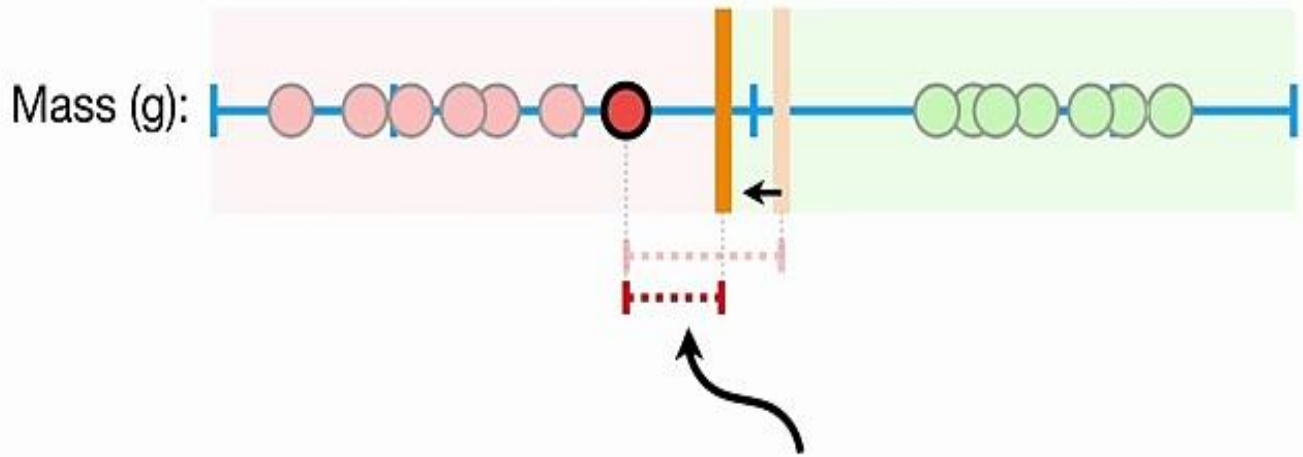


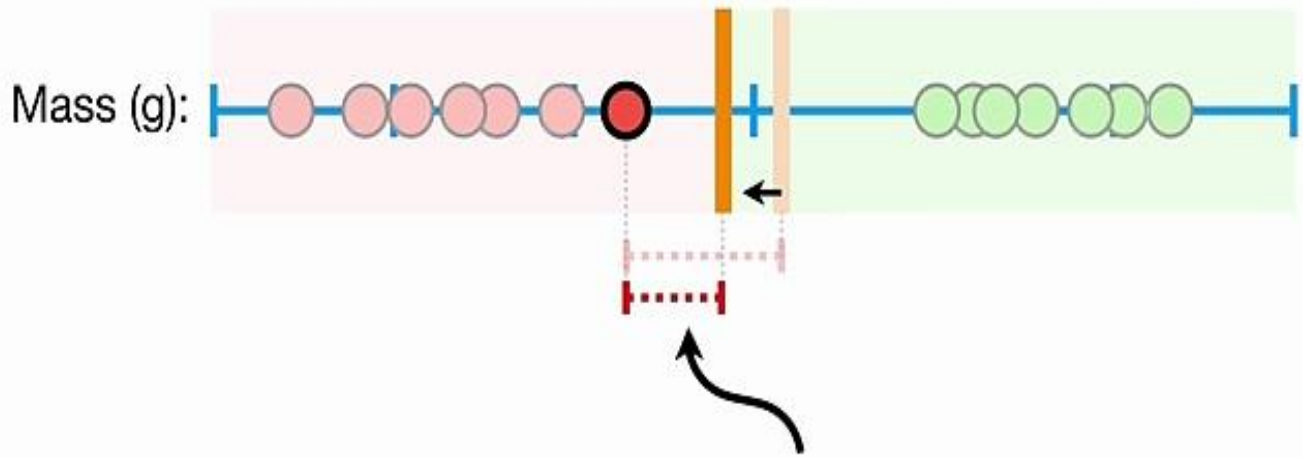
…the distances between the observations and the threshold are the same and both reflect the **margin**.

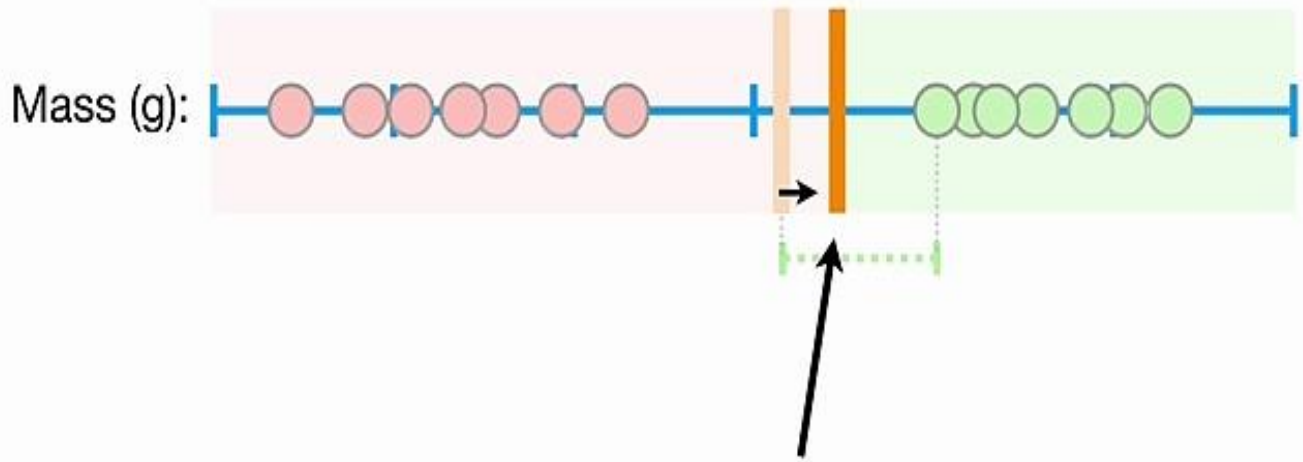


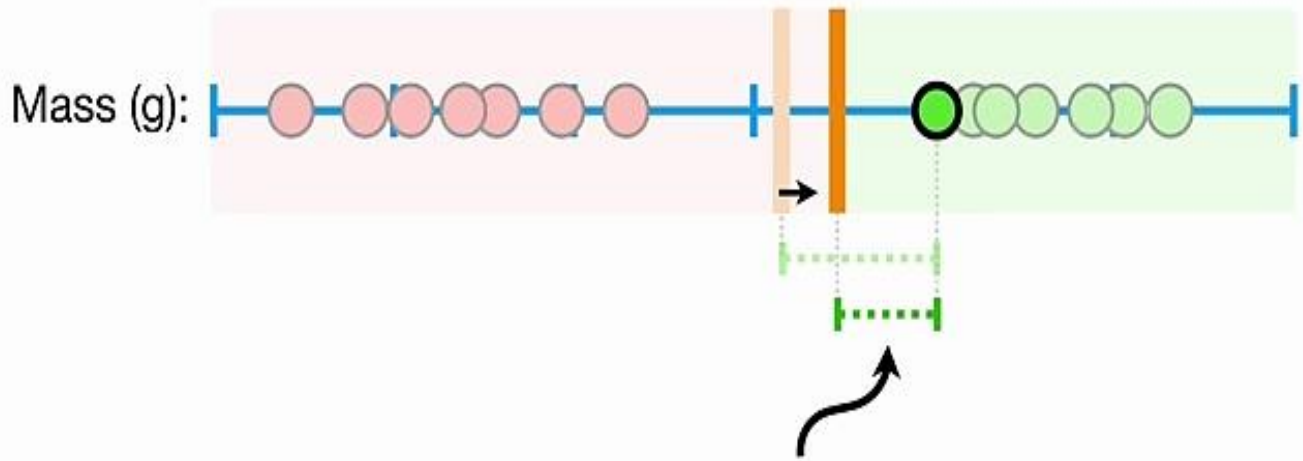
When the threshold is halfway between the two observations, the **margin** is as large as it can be.

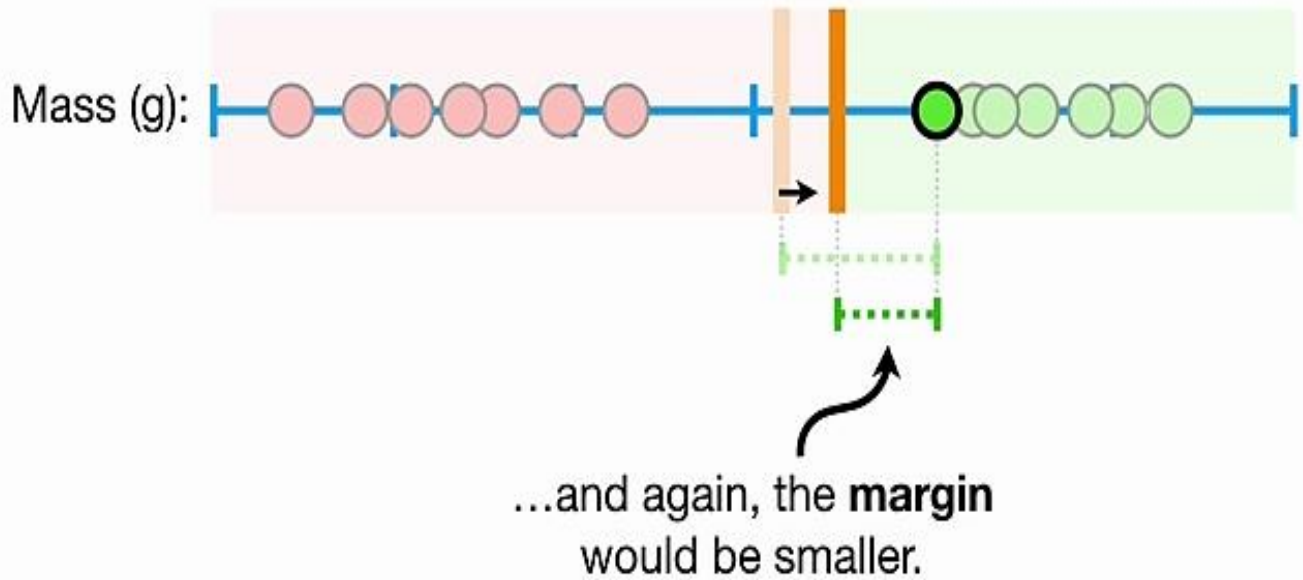

Mass (g):
For example, if we moved the threshold to the left a little bit…

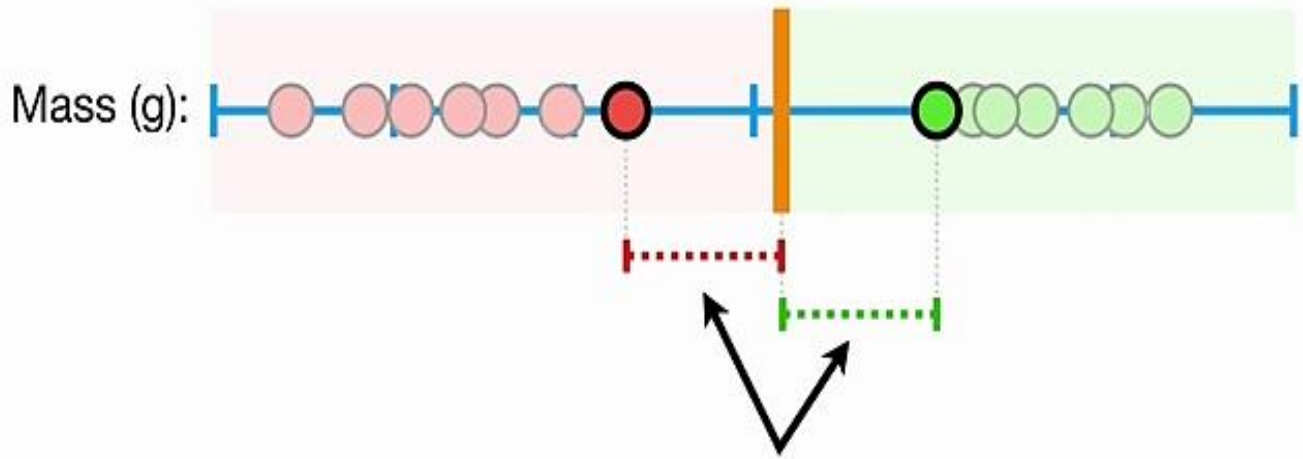

Mass (g):
...then the distance between the threshold and the observation that is *not obese* would be smaller...


Mass (g):
…and thus, the **margin** would be smaller than it was before.

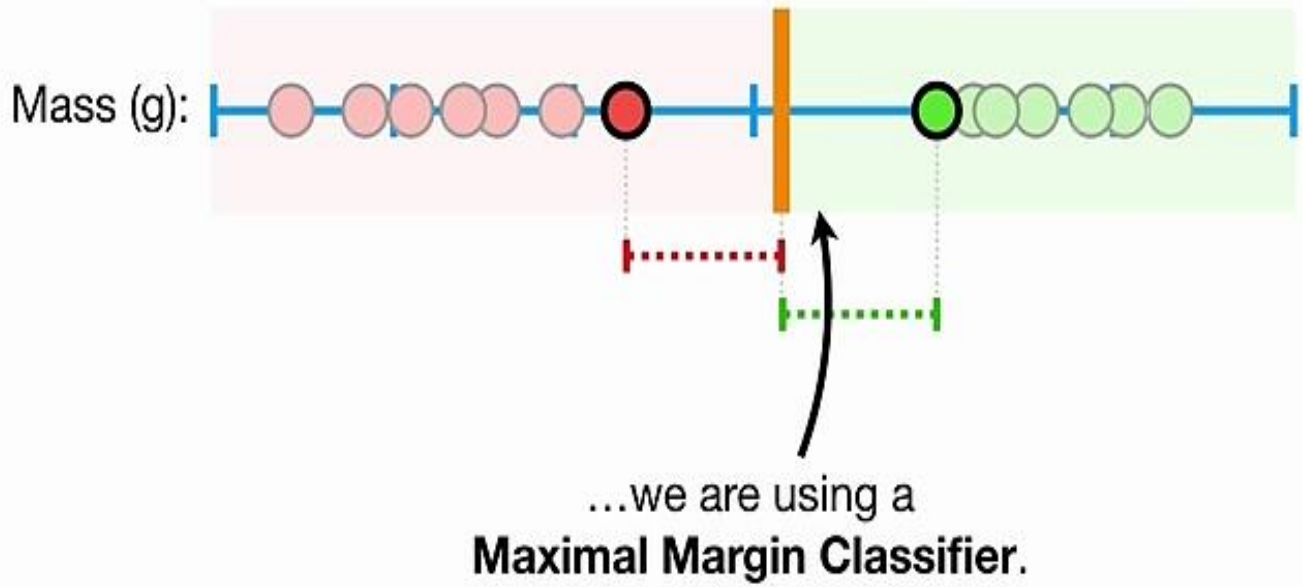

Mass (g):
And if we moved the threshold to
the right a little bit…

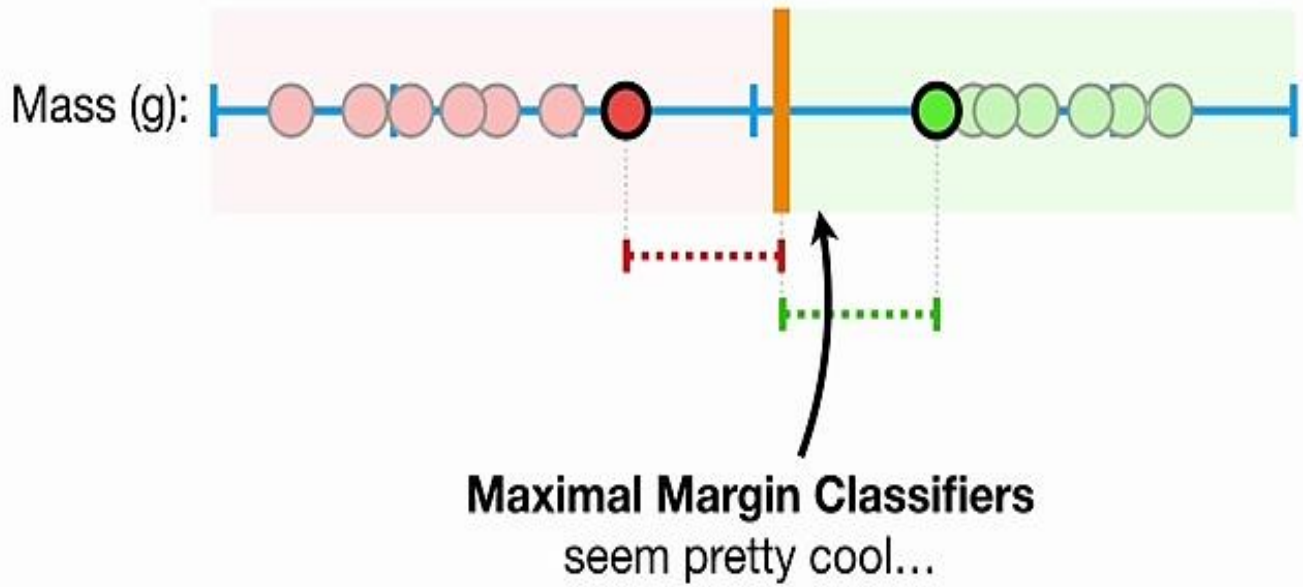

Mass (g):
...then the distance between the
obese observation and the
threshold would get smaller...

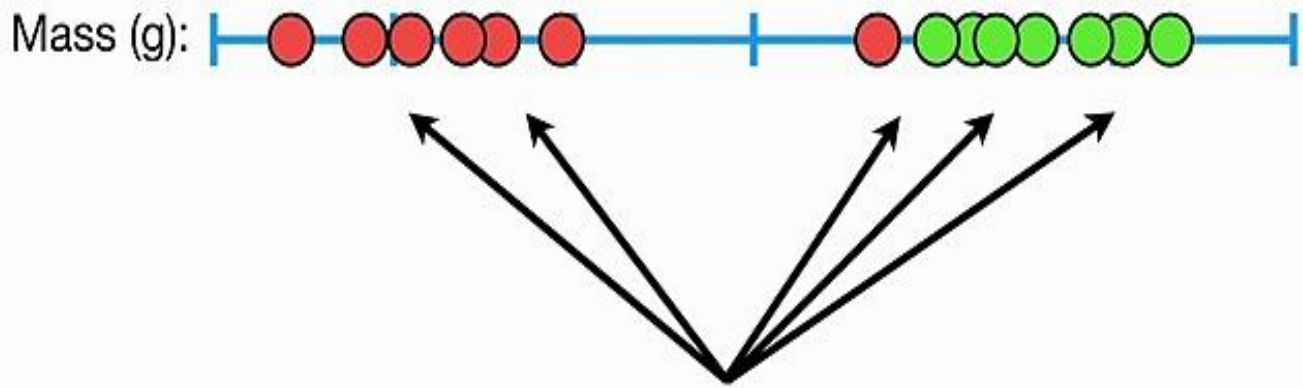

Mass (g):
…and again, the **margin**
would be smaller.



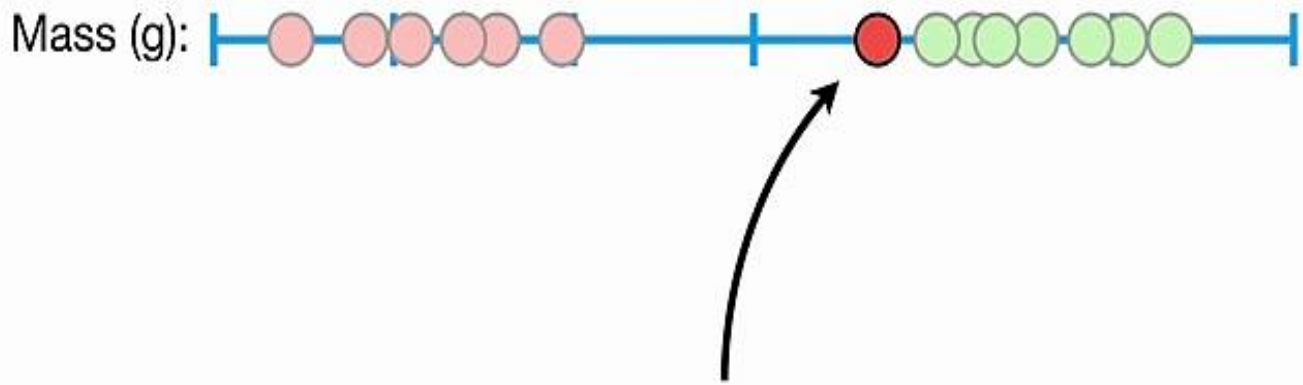
When we use the threshold that gives us the largest **margin** to make classifications…

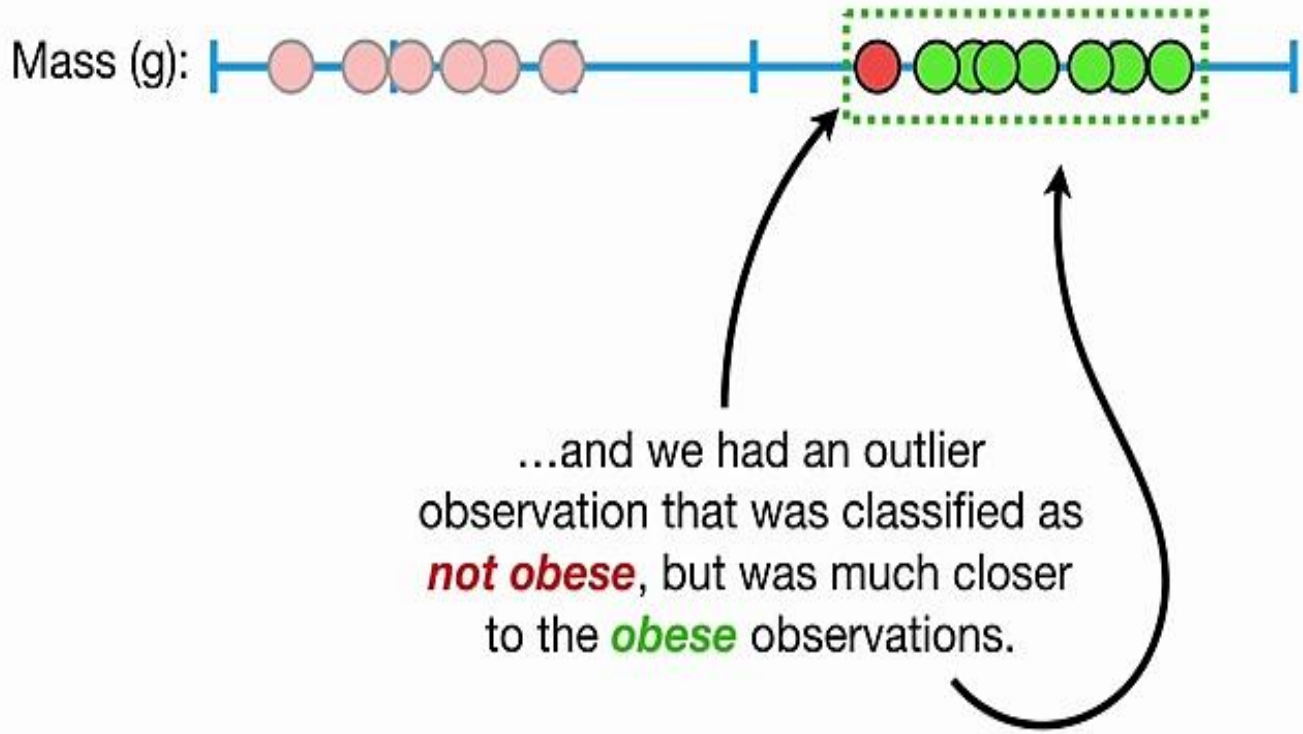

Mass (g):
…we are using a
Maximal Margin Classifier.


Mass (g):
Maximal Margin Classifiers
seem pretty cool…



…but what if our training data looked like this….


Mass (g):
…and we had an outlier observation that was classified as not obese, but was much closer to the obese observations.


Mass (g):
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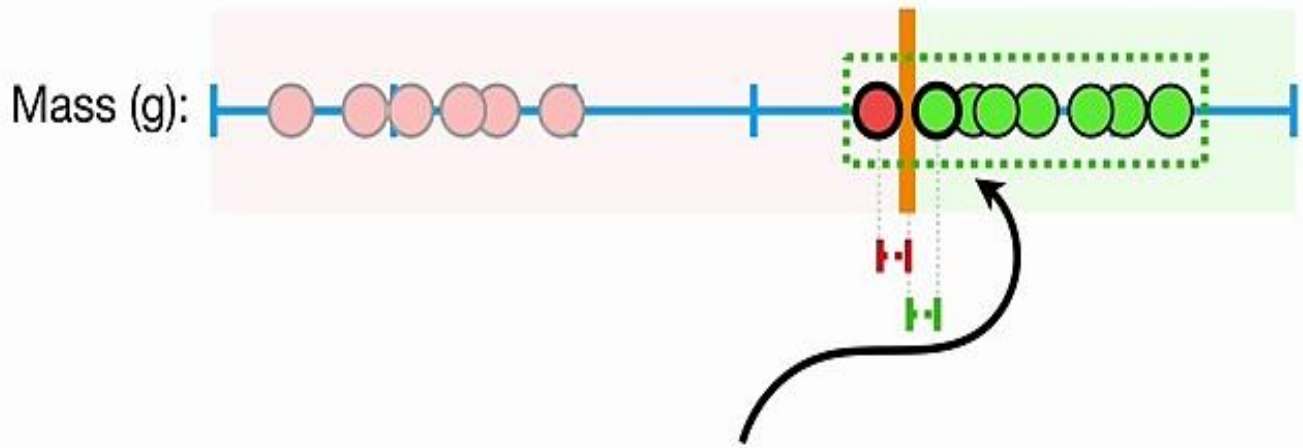
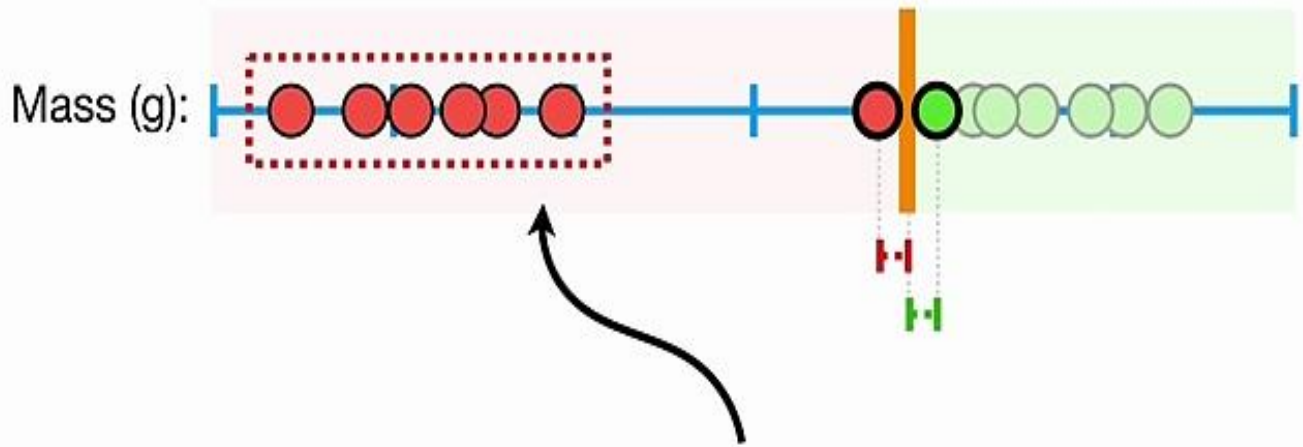
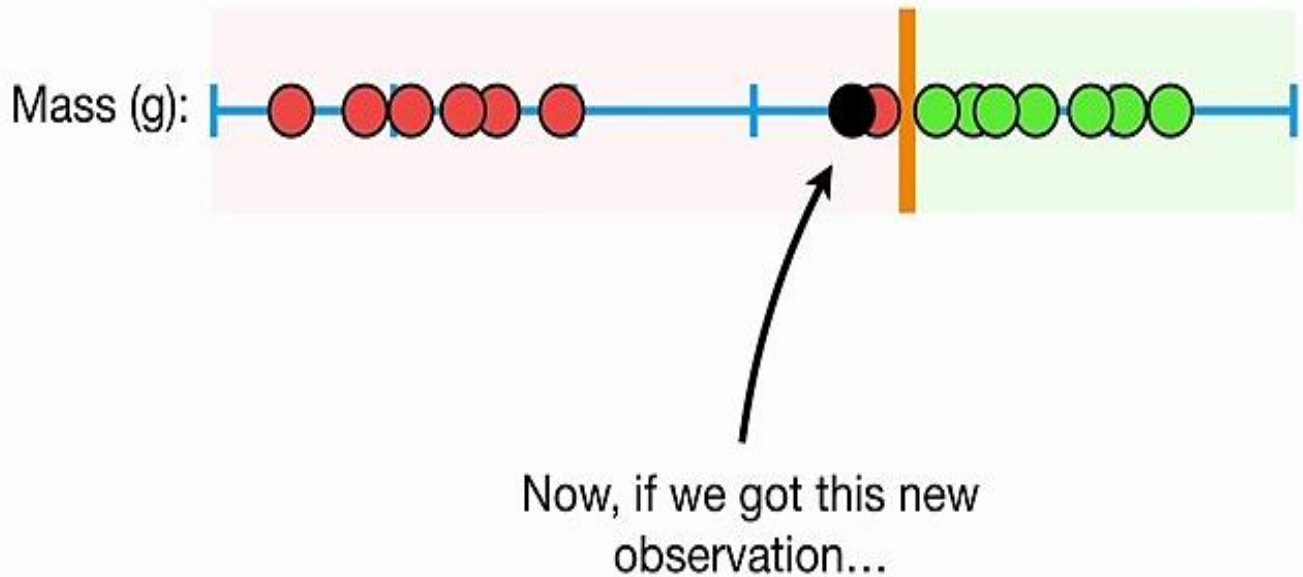
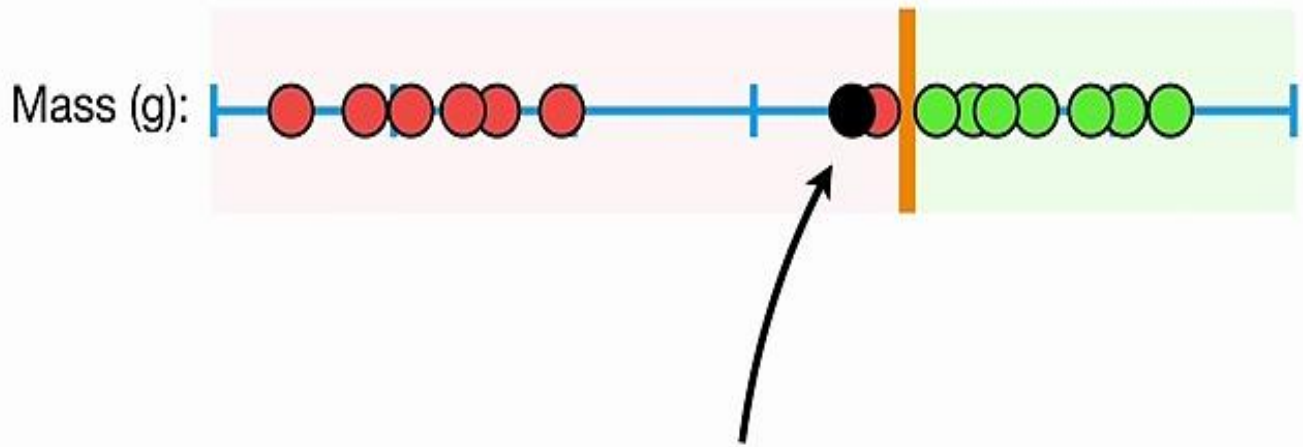


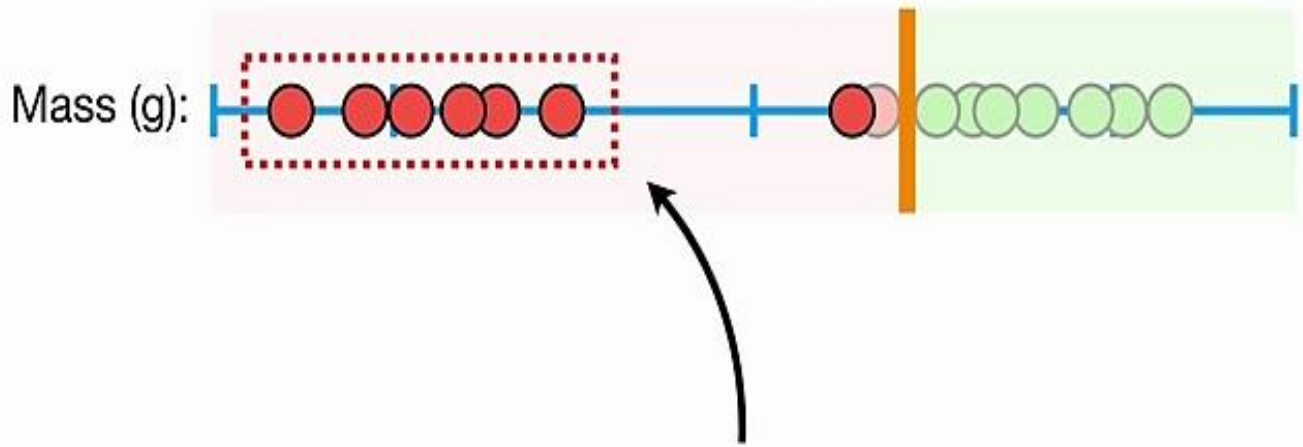
In this case, the **Maximum Margin Classifier** would be super close to the ***obese*** observations...


Mass (g):
…and really far from the majority of the observations that are **not obese**.


Mass (g):
Now, if we got this new observation…



…we would classify it as ***not obese***, even though most of the ***not obese*** observations are much further away than the ***obese*** observations.



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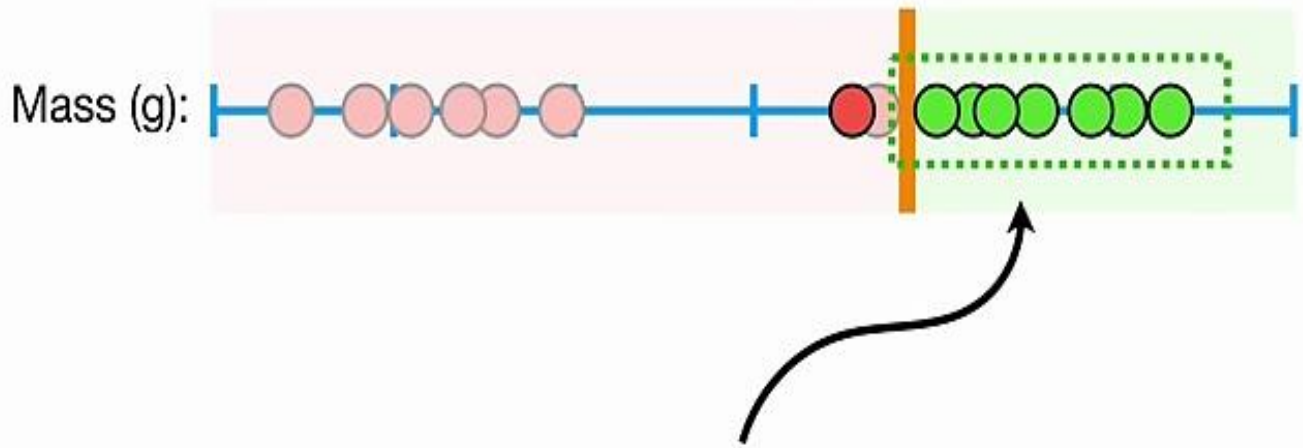
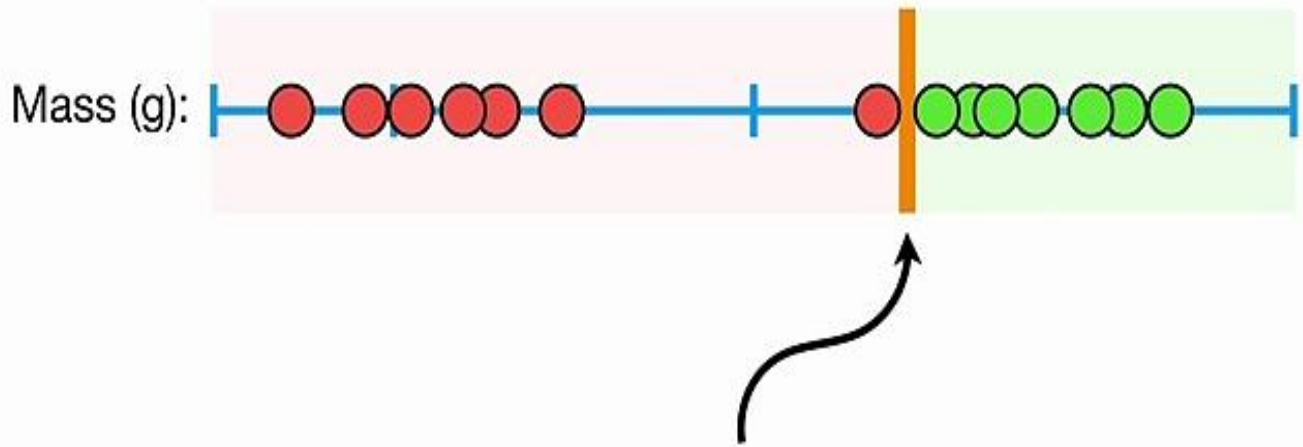
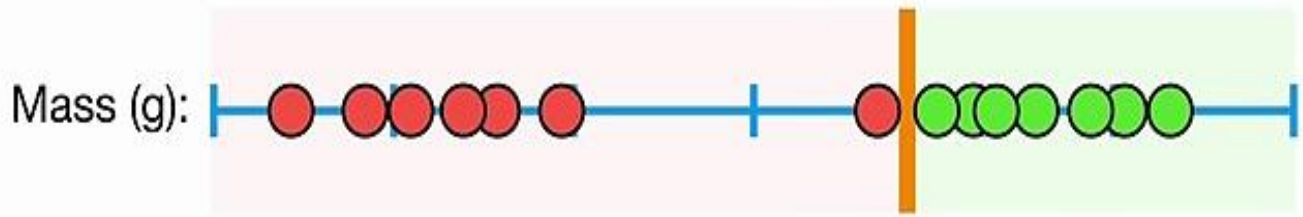


…we would classify it as ***not obese***, even though most of the ***not obese*** observations are much further away than the ***obese*** observations.

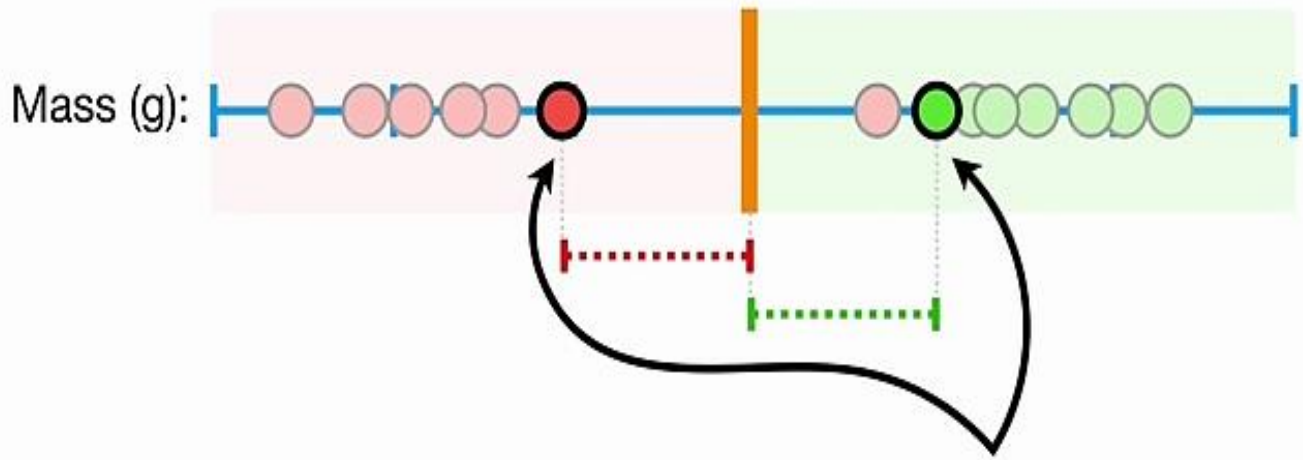


So **Maximal Margin Classifiers** are *super sensitive to outliers* in the training data and that makes them pretty lame.

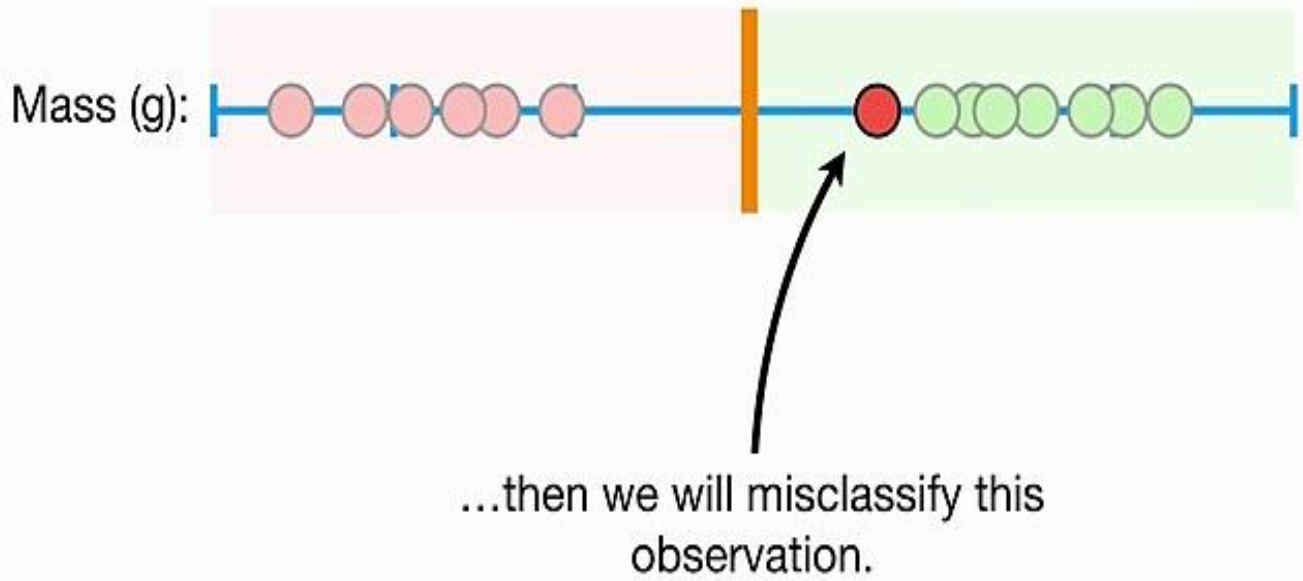


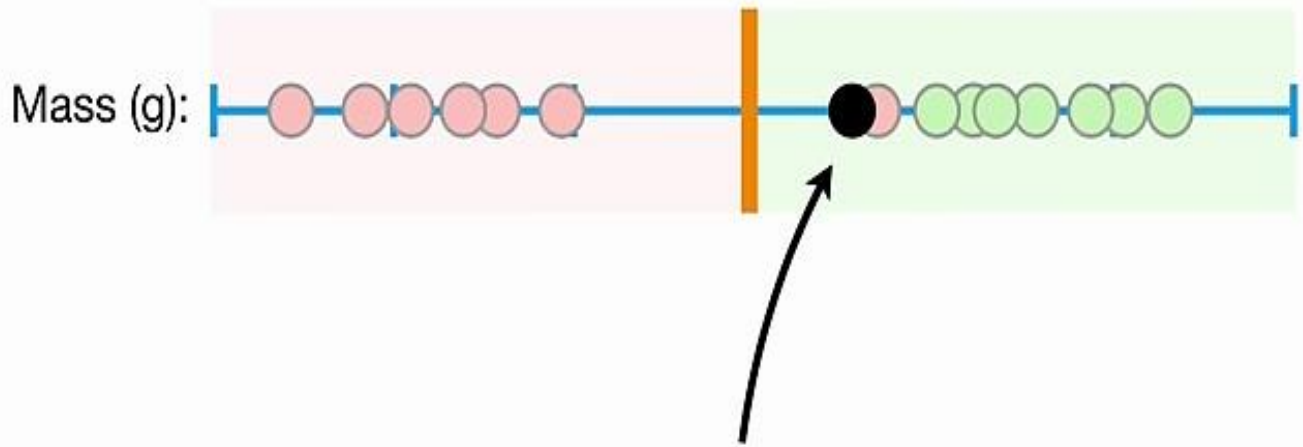
Can we do better?

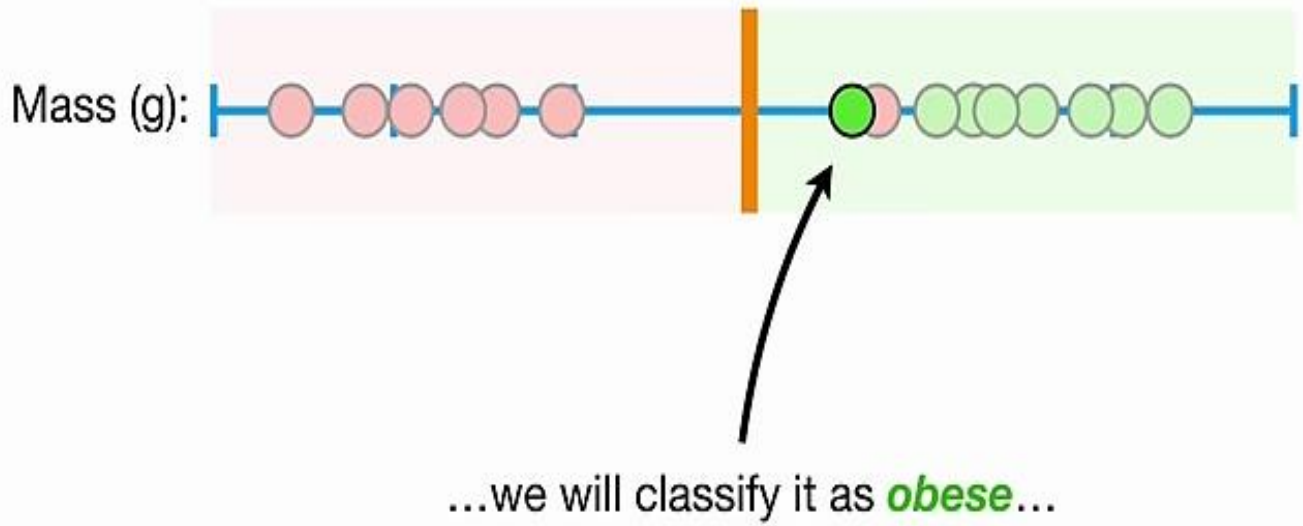
To make a threshold that is not so sensitive to outliers we must **allow misclassifications**.

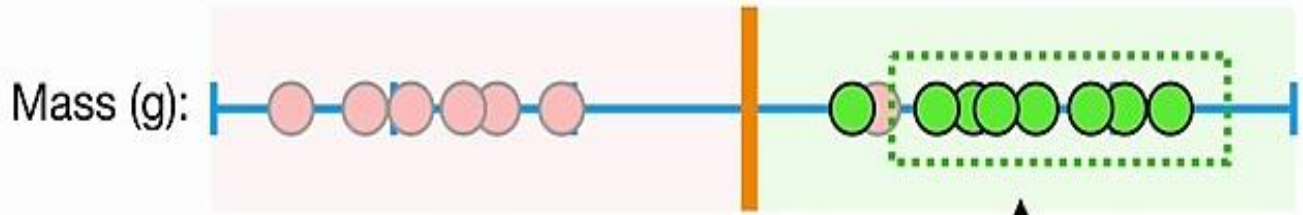


For example, if we put the threshold halfway between these two observations…

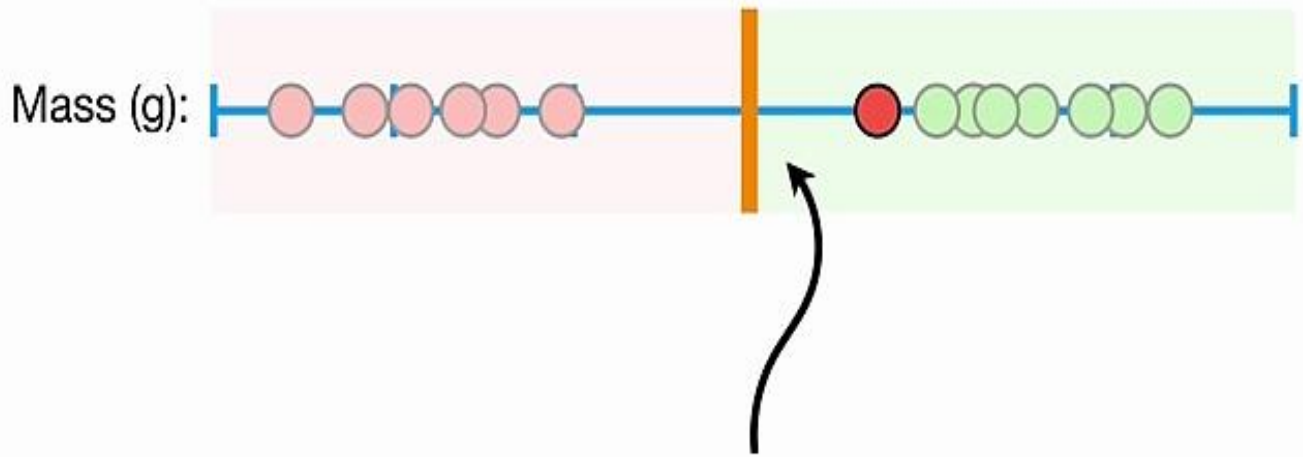

Mass (g):
…then we will misclassify this observation.


Mass (g):
However, now when we get a
new observation here…

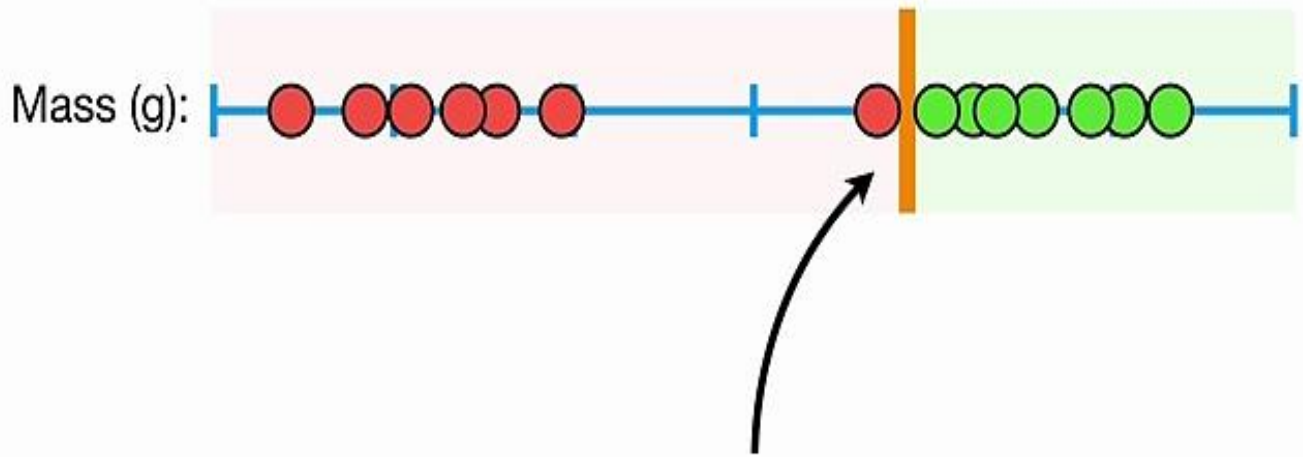

Mass (g):
…we will classify it as *obese*…

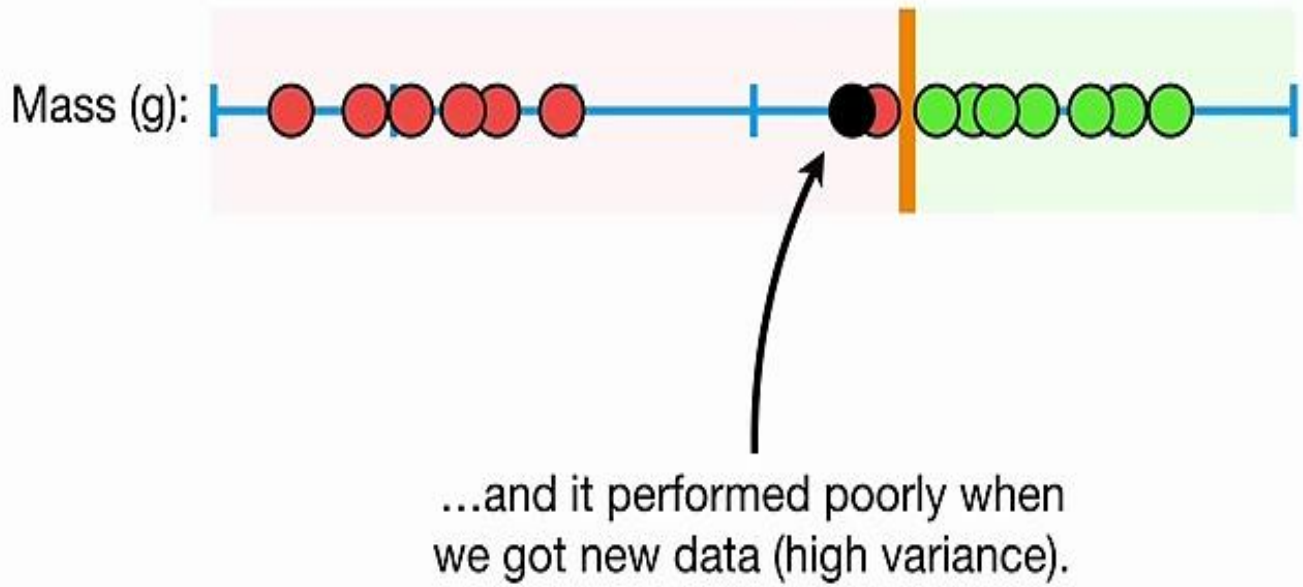


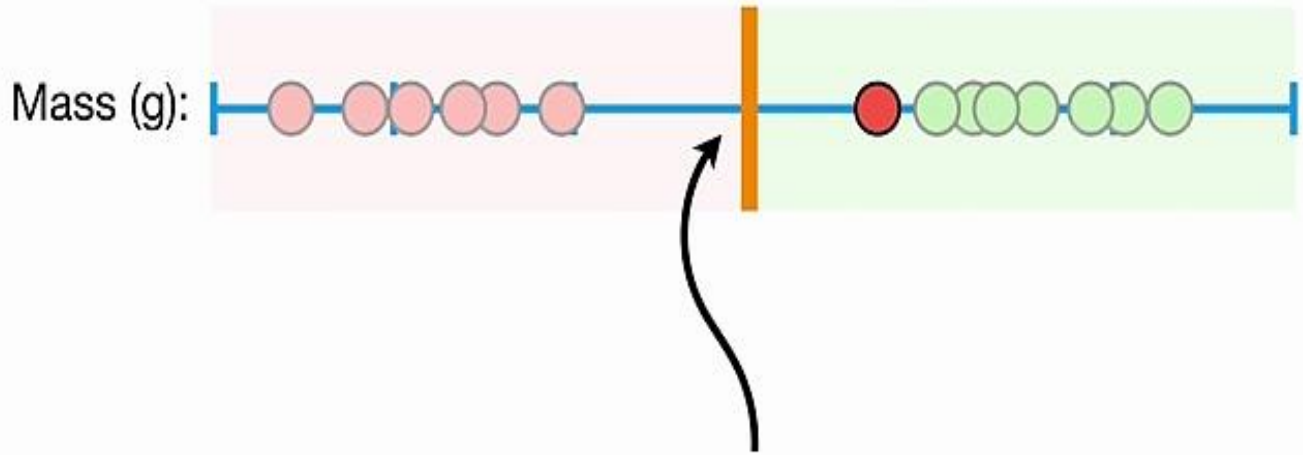
…and that makes sense because it is closer to most of the ***obese*** observations.

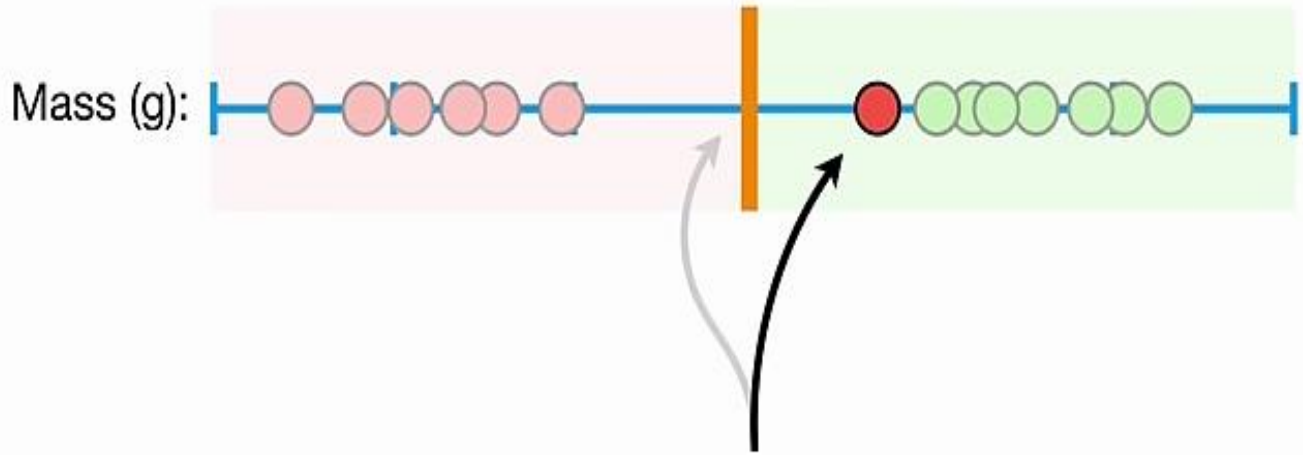


Choosing a threshold that allows misclassifications is an example of the **Bias/Variance Tradeoff** that plagues all of machine learning.


Mass (g):
In other words, before we allowed misclassifications, we picked a threshold that was very sensitive to the training data (low bias)…


Mass (g):
…and it performed poorly when
we got new data (high variance).


Mass (g):
In contrast, when we picked a threshold that was less sensitive to the training data and allowed misclassifications (higher bias)…



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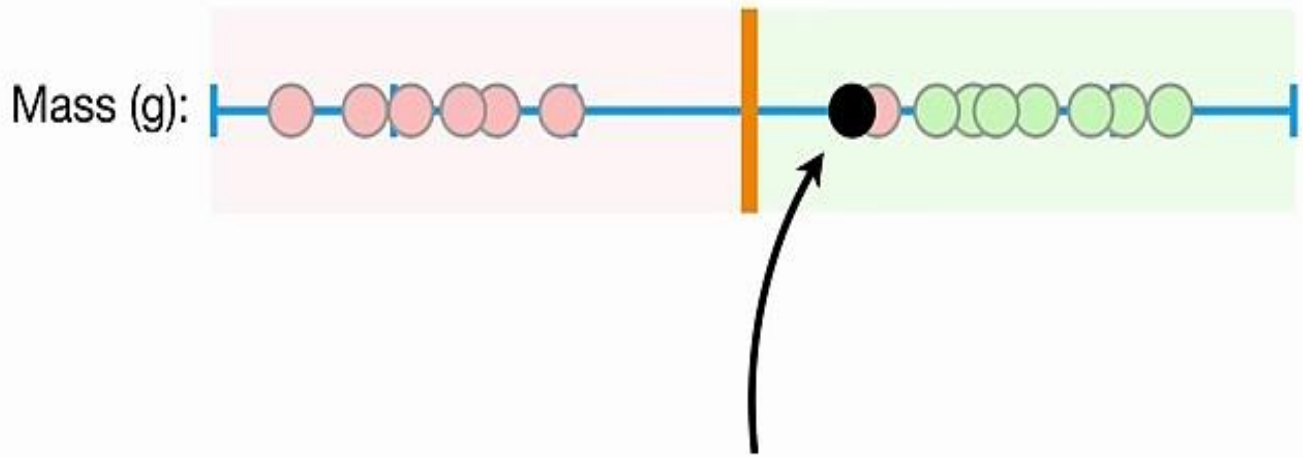
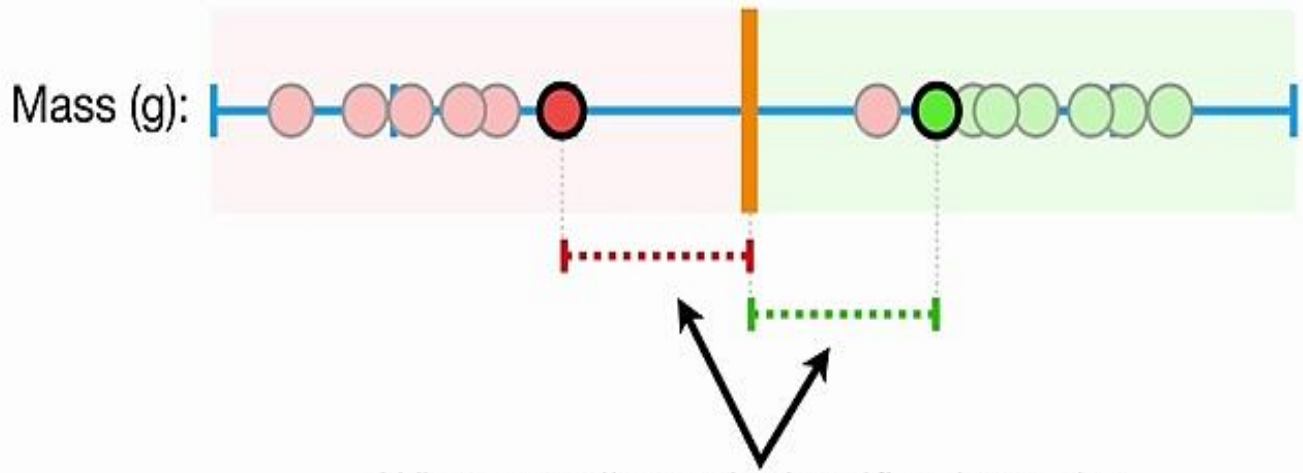
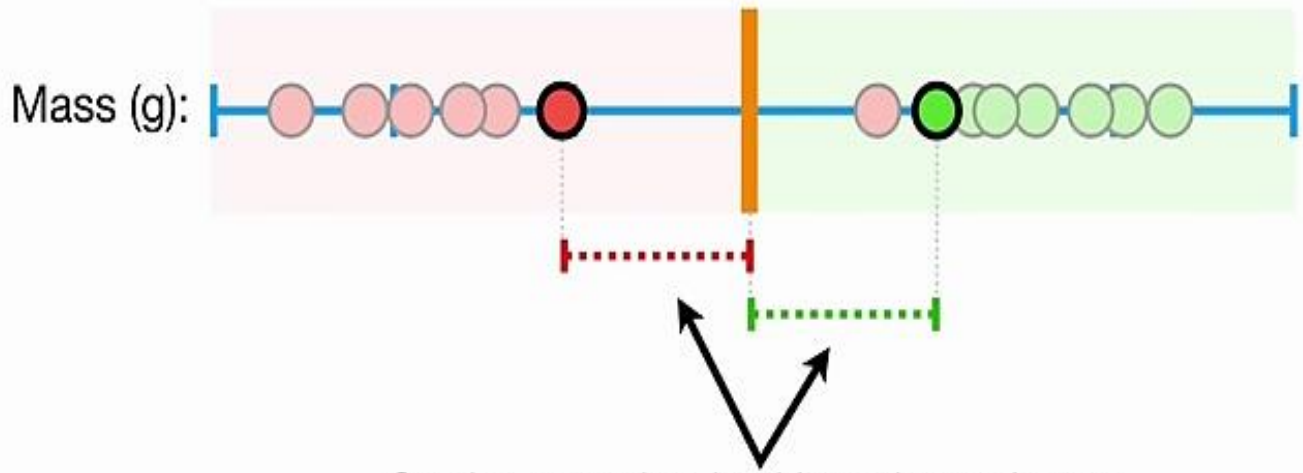
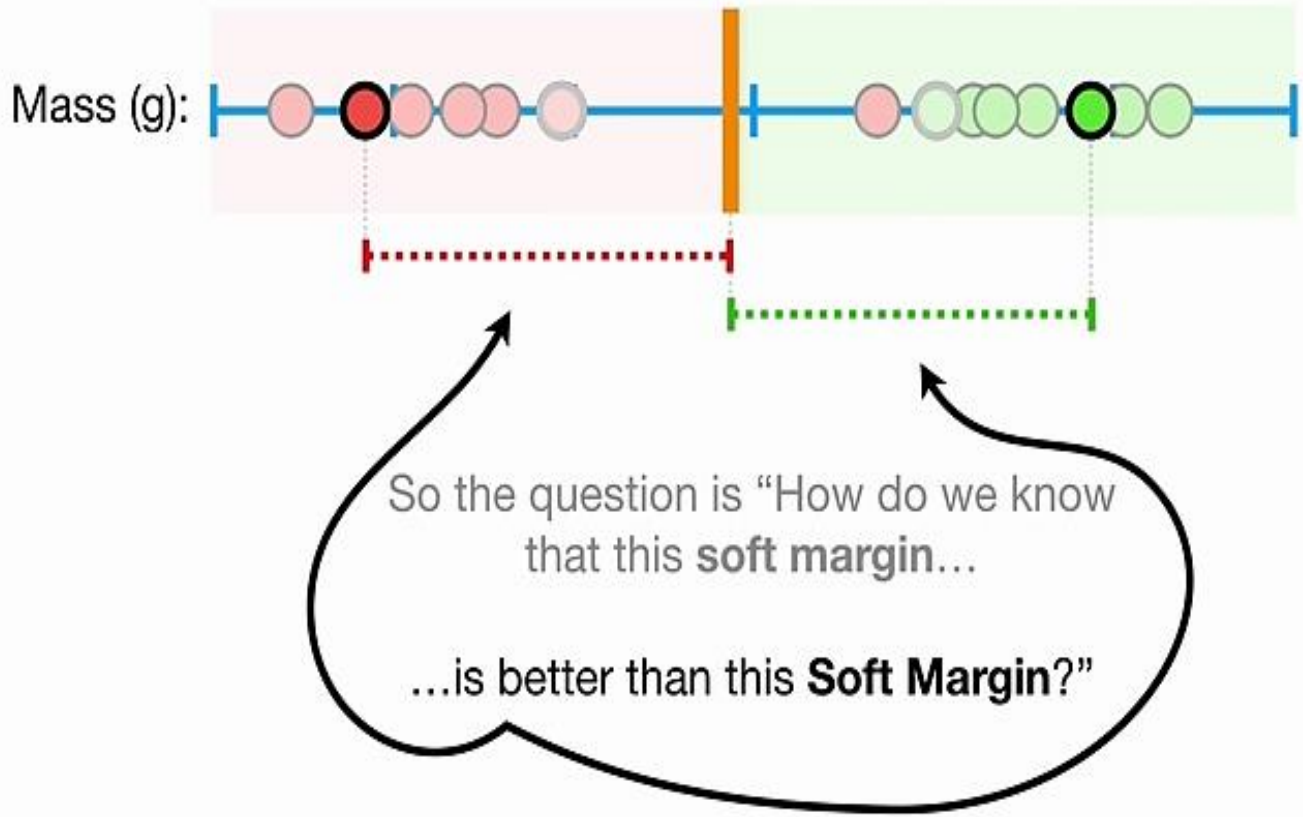

Mass (g):
...it performed better when we got
new data (low variance).

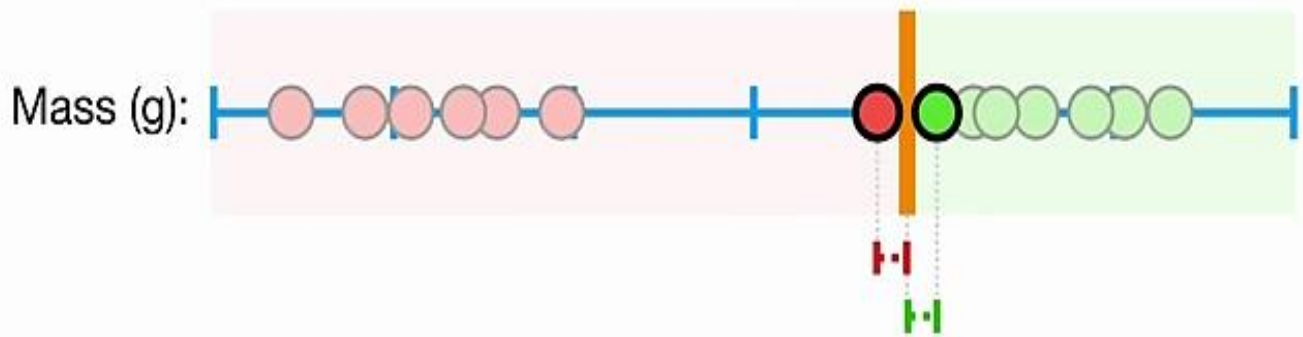


When we allow misclassifications, the distance between the observations and the threshold is called a **Soft Margin**.

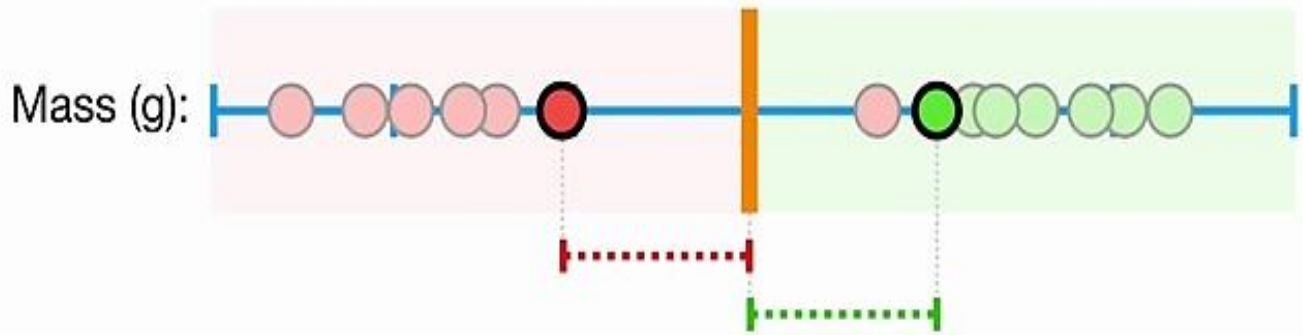


So the question is “How do we know that this **soft margin**…


Mass (g):
So the question is “How do we know that this **soft margin**…
…is better than this **Soft Margin**?”



We can determine how many misclassifications and observations to allow inside of the **Soft Margin** to get the best classification.



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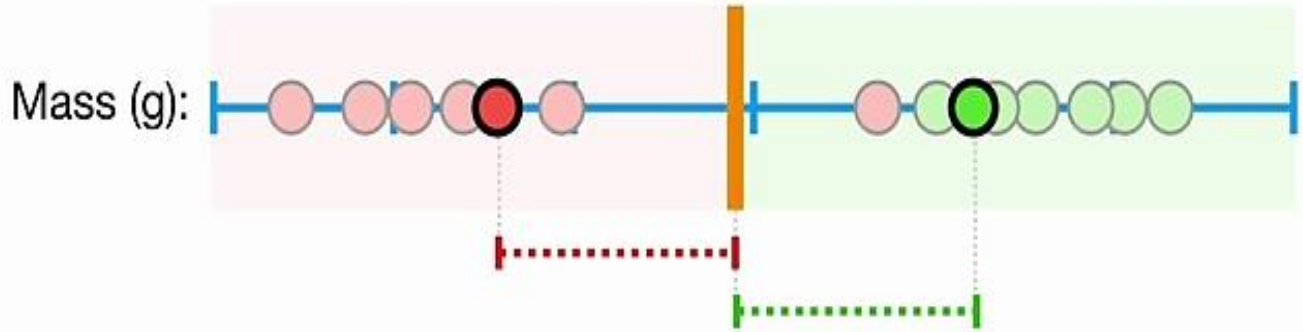

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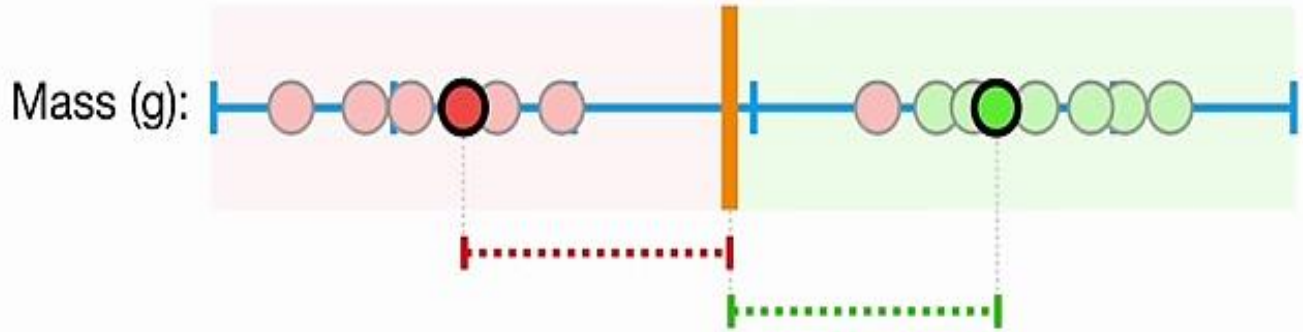

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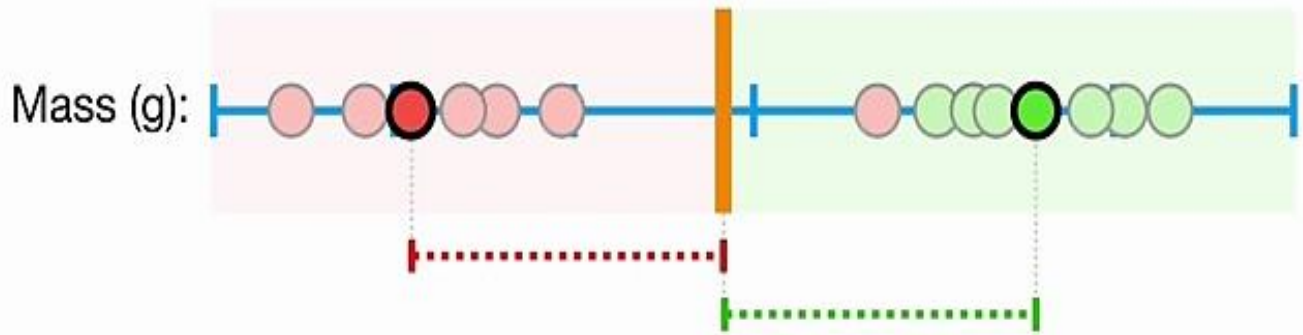

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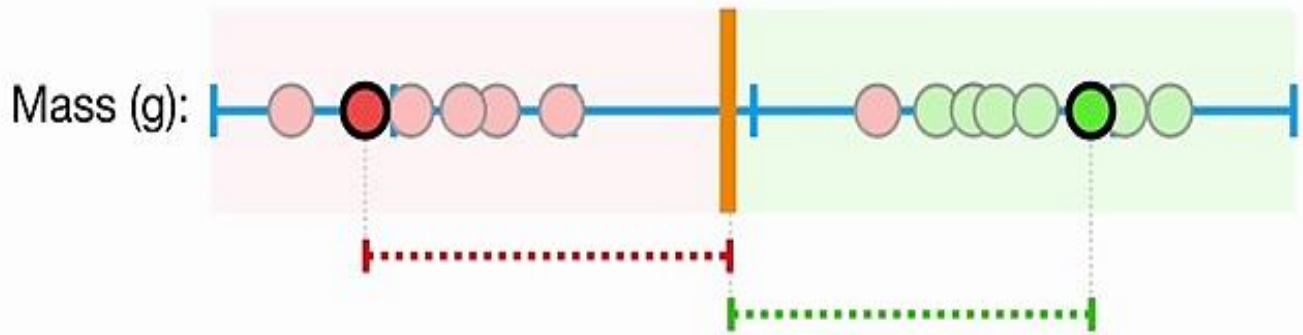

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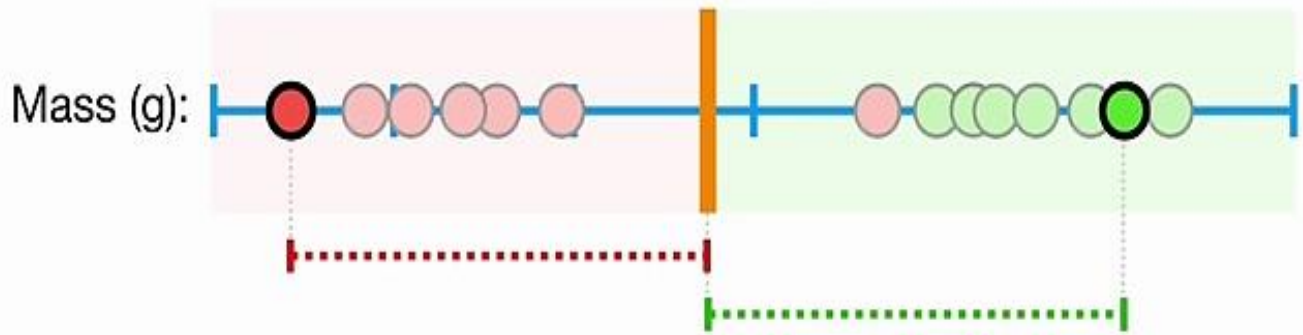

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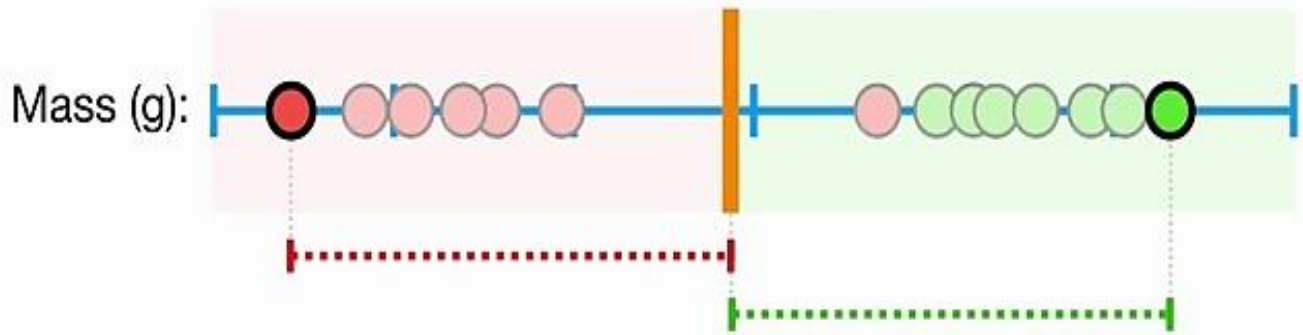

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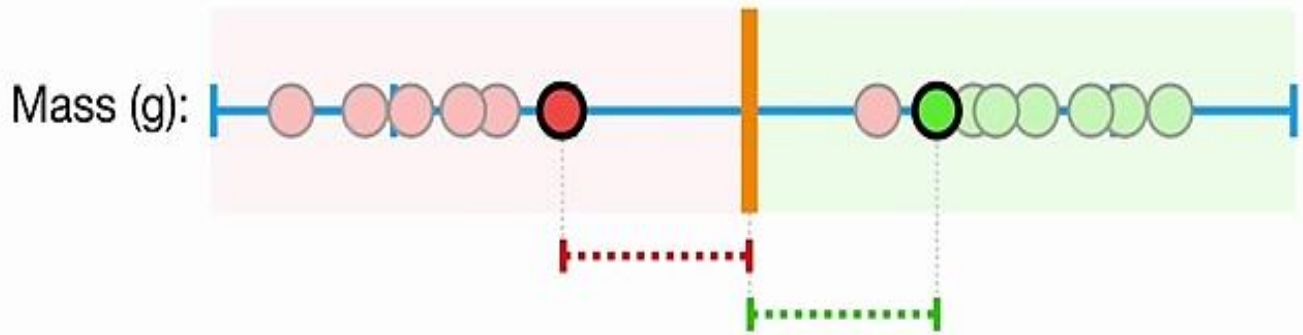
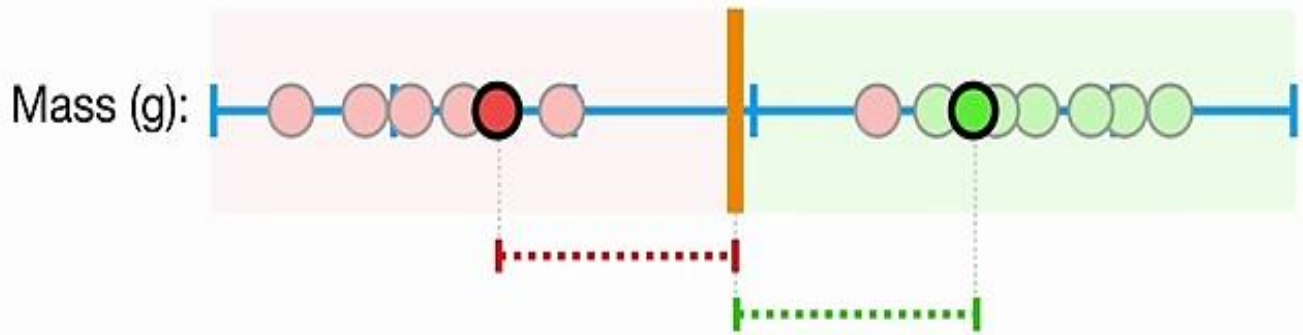
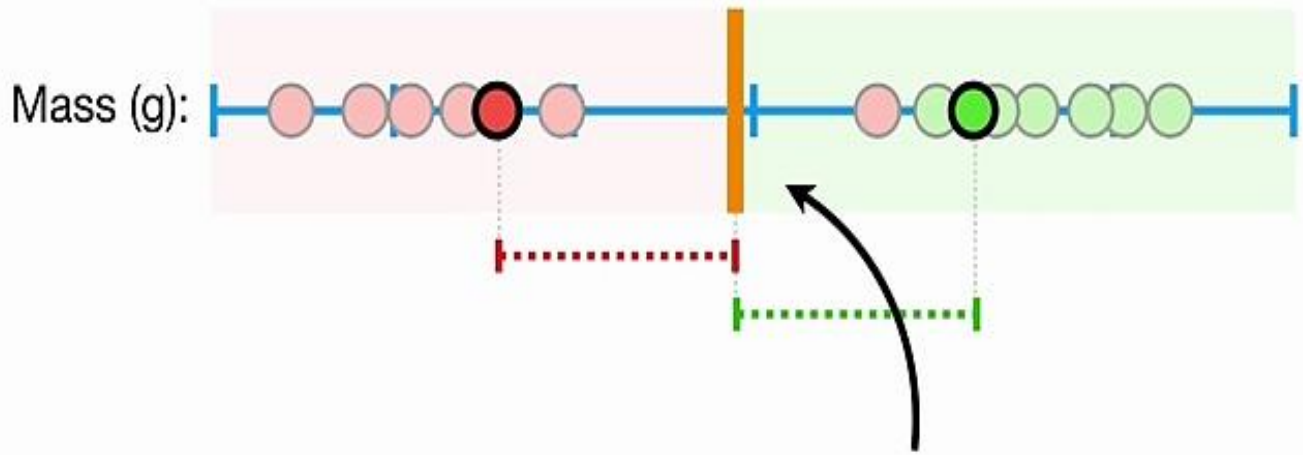


We can determine how many misclassifications and observations to allow inside of the **Soft Margin** to get the best classification.

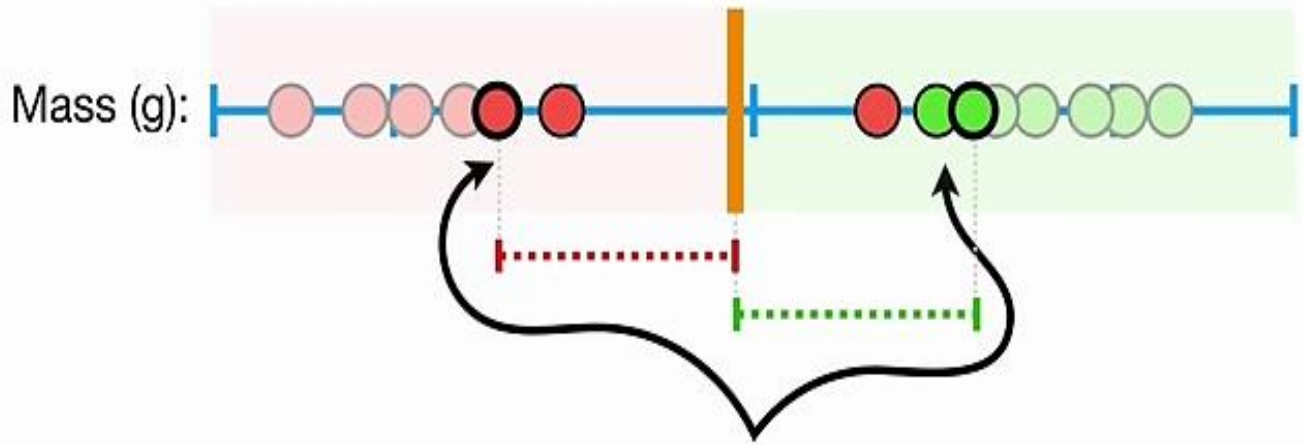
Ideally we should minimize the number of misclassification and the number of observation within the margin to avoid overfitting



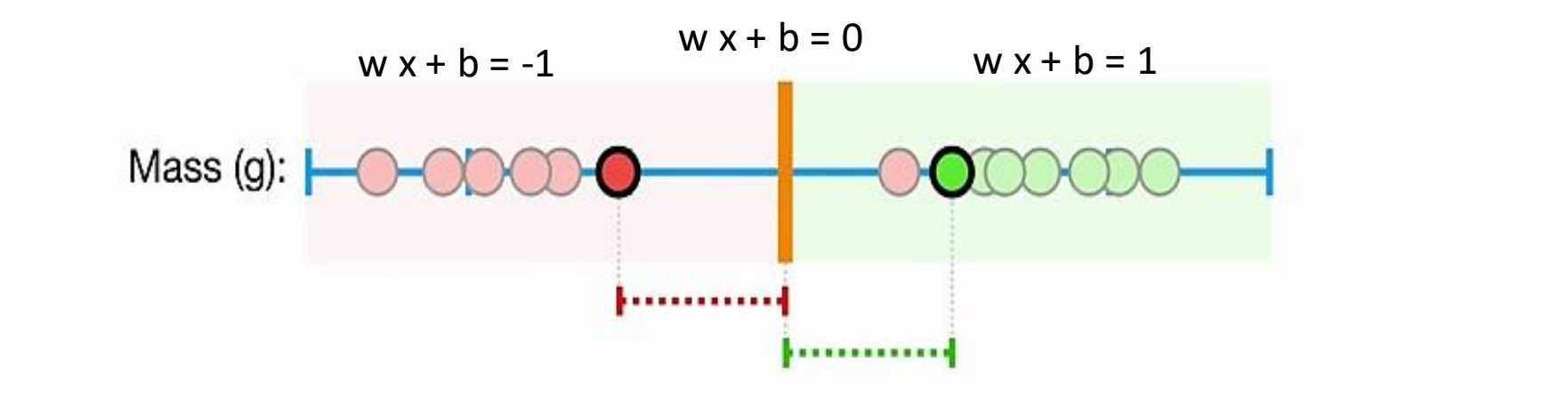
When we use a **Soft Margin** to determine the location of a threshold…



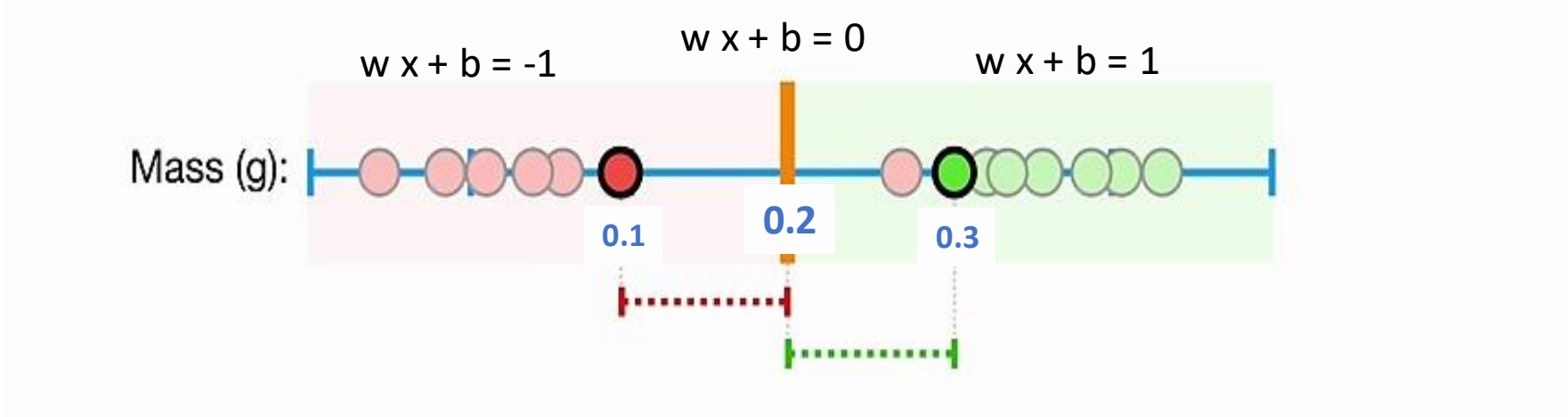
...then we are using a **Soft Margin Classifier** aka a **Support Vector Classifier** to classify observations.



The name **Support Vector Classifier** comes from the fact that the observations on the edge *and within* the **Soft Margin** are called **Support Vectors.**



GREEN if w x + b >= 1
RED if w x + b <= -1

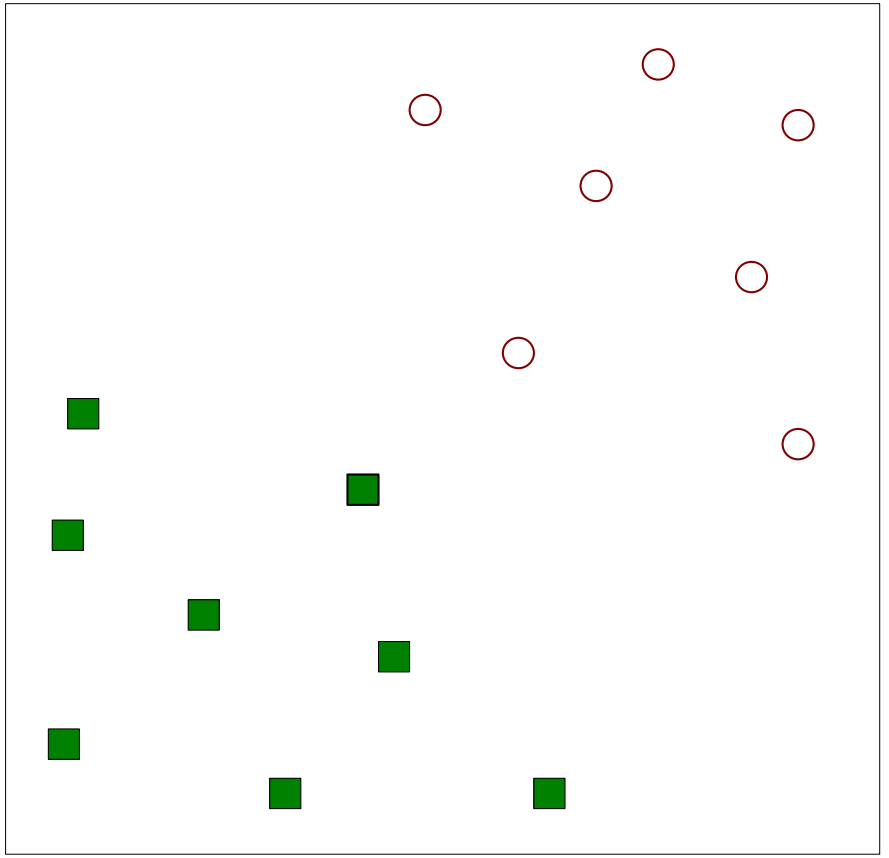


GREEN if 10 x + -2 >= 1
RED if 10 x + -2 <= -1

From One to Two Dimensions

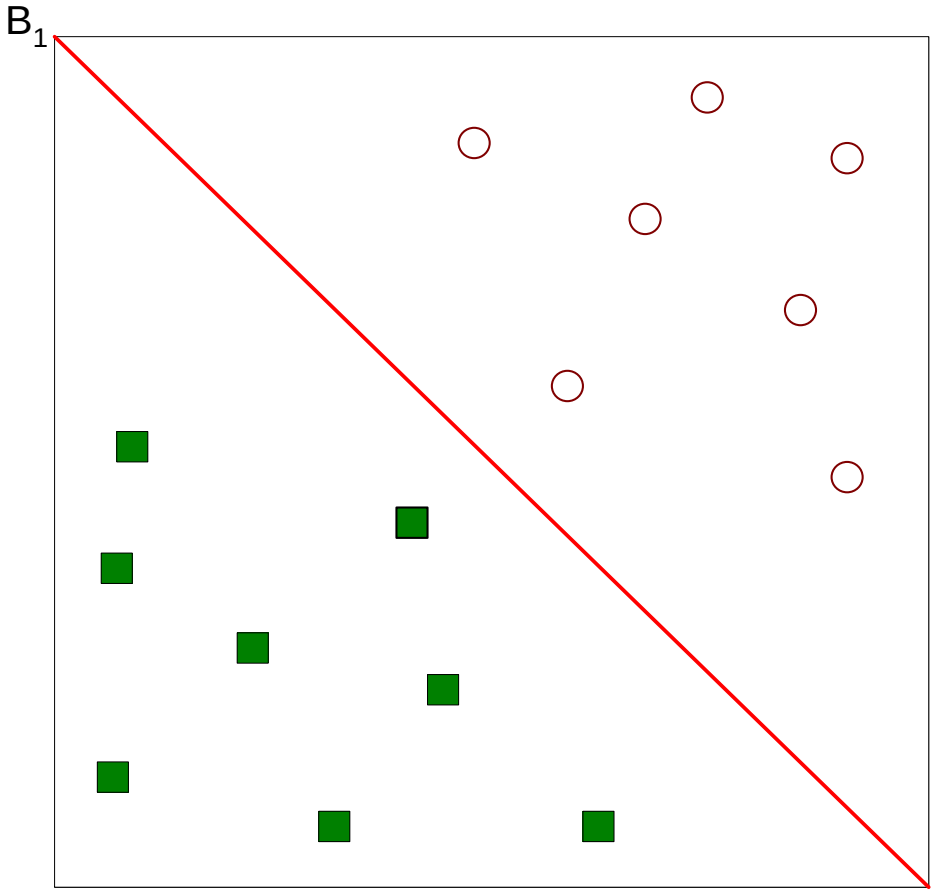
Maximum Margin Hyperplanes

- Find a linear hyperplane (decision boundary) that separates the data.



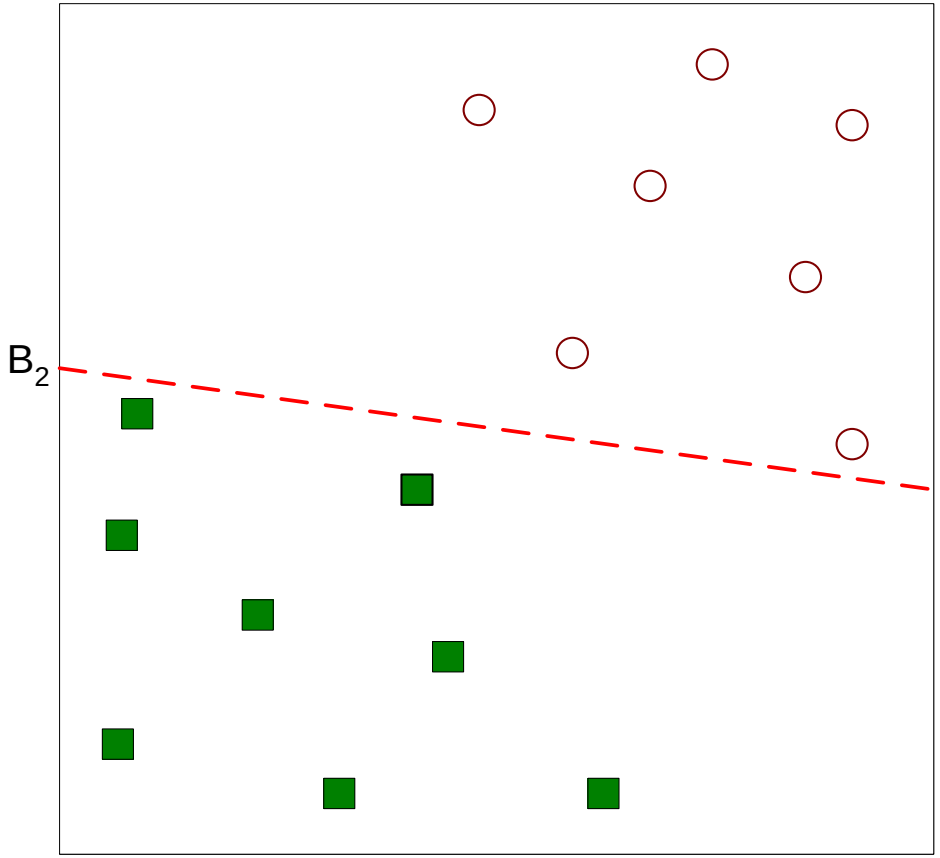
Maximum Margin Hyperplanes

- One possible solution.



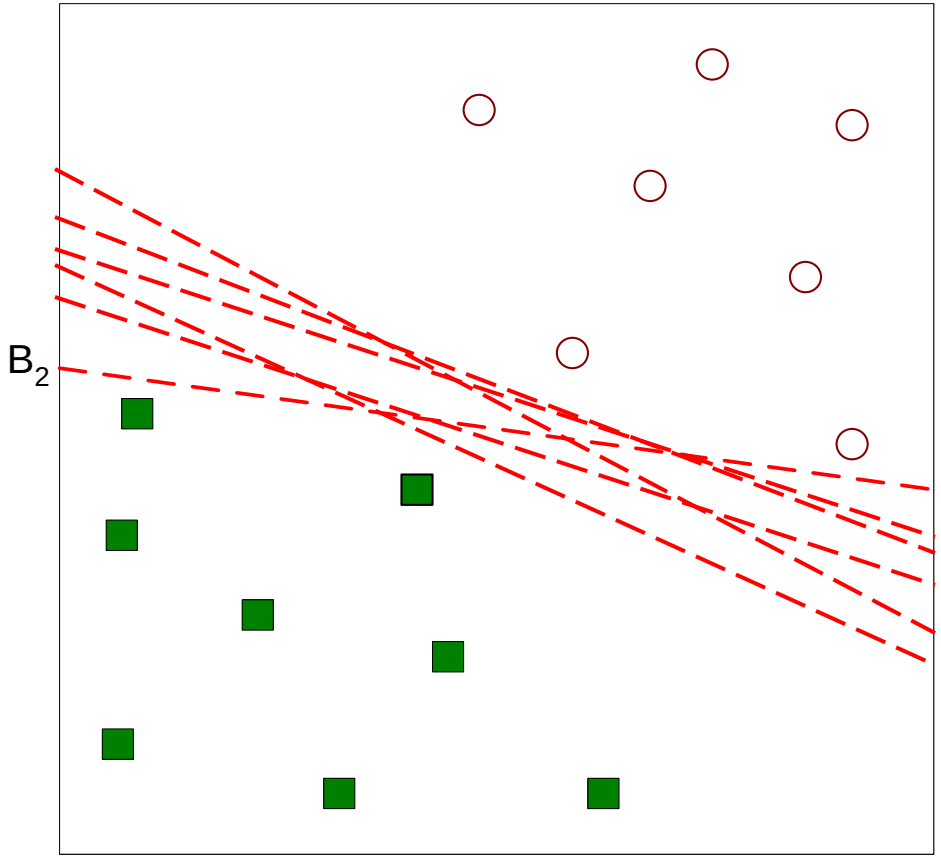
Maximum Margin Hyperplanes

- Another possible solution.



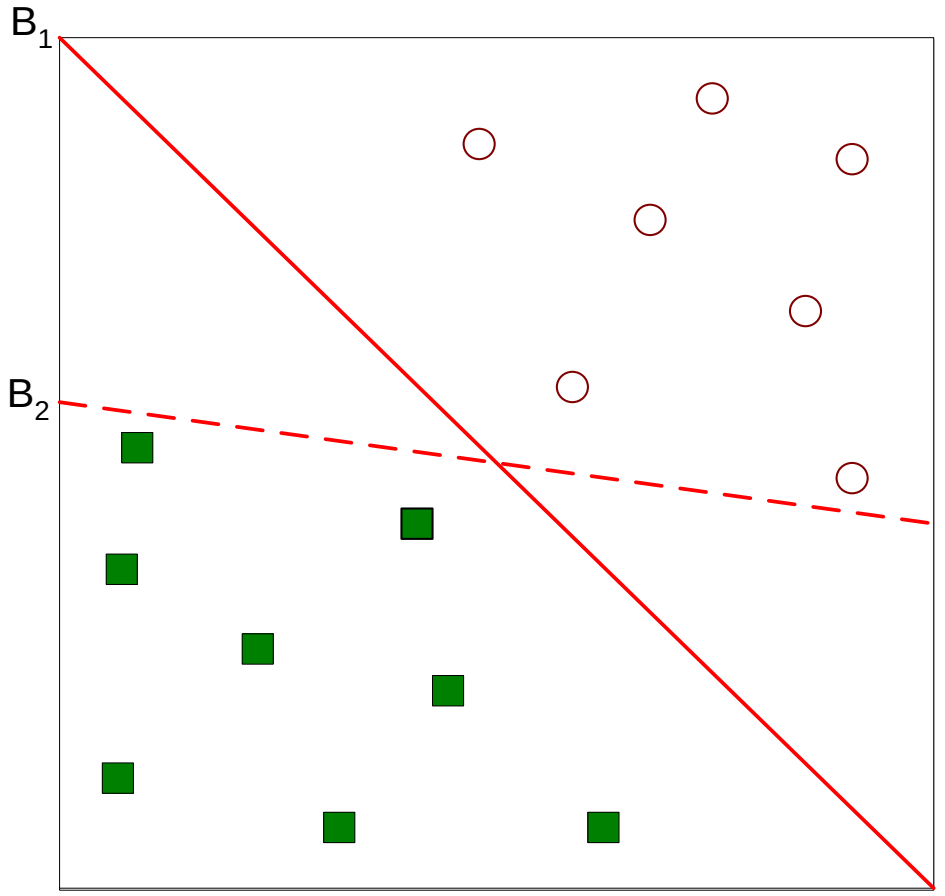
Maximum Margin Hyperplanes

- Other possible solutions.



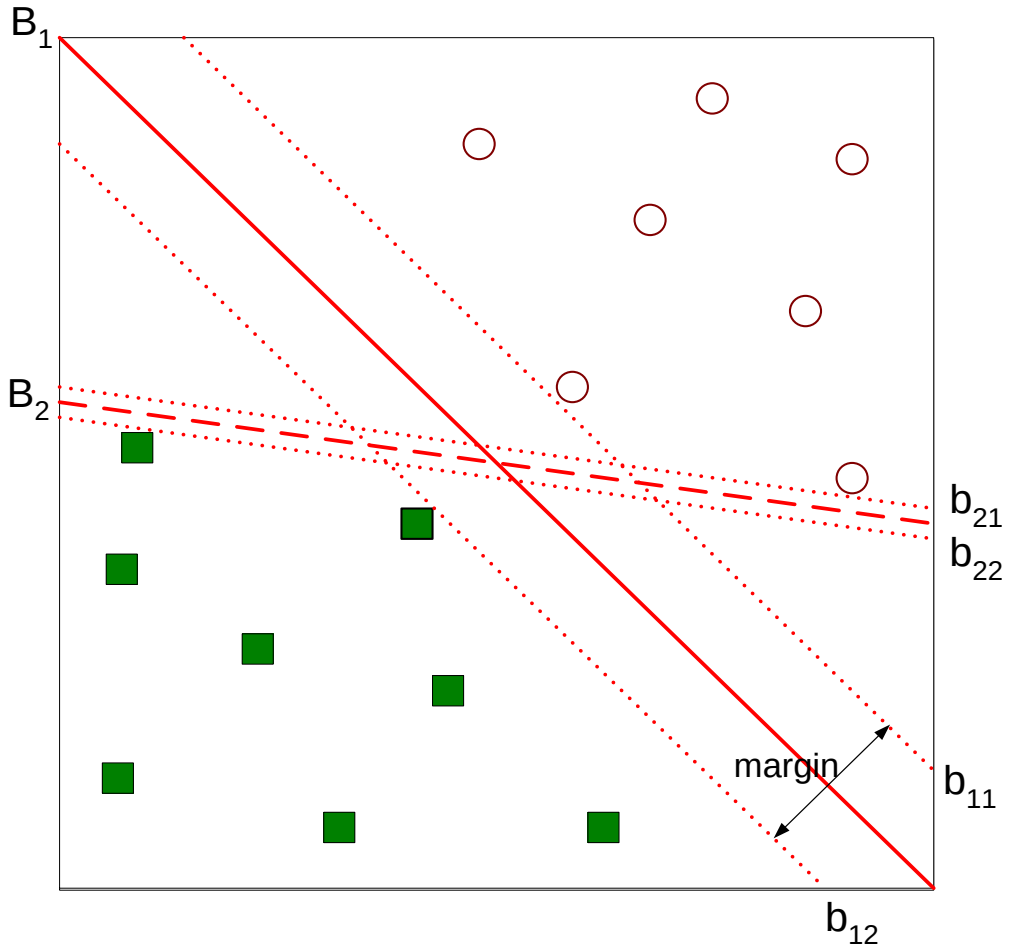
Maximum Margin Hyperplanes

- Let's focus on B_1 and B_2.
- Which one is better?
- How do you define better?



Maximum Margin Hyperplanes

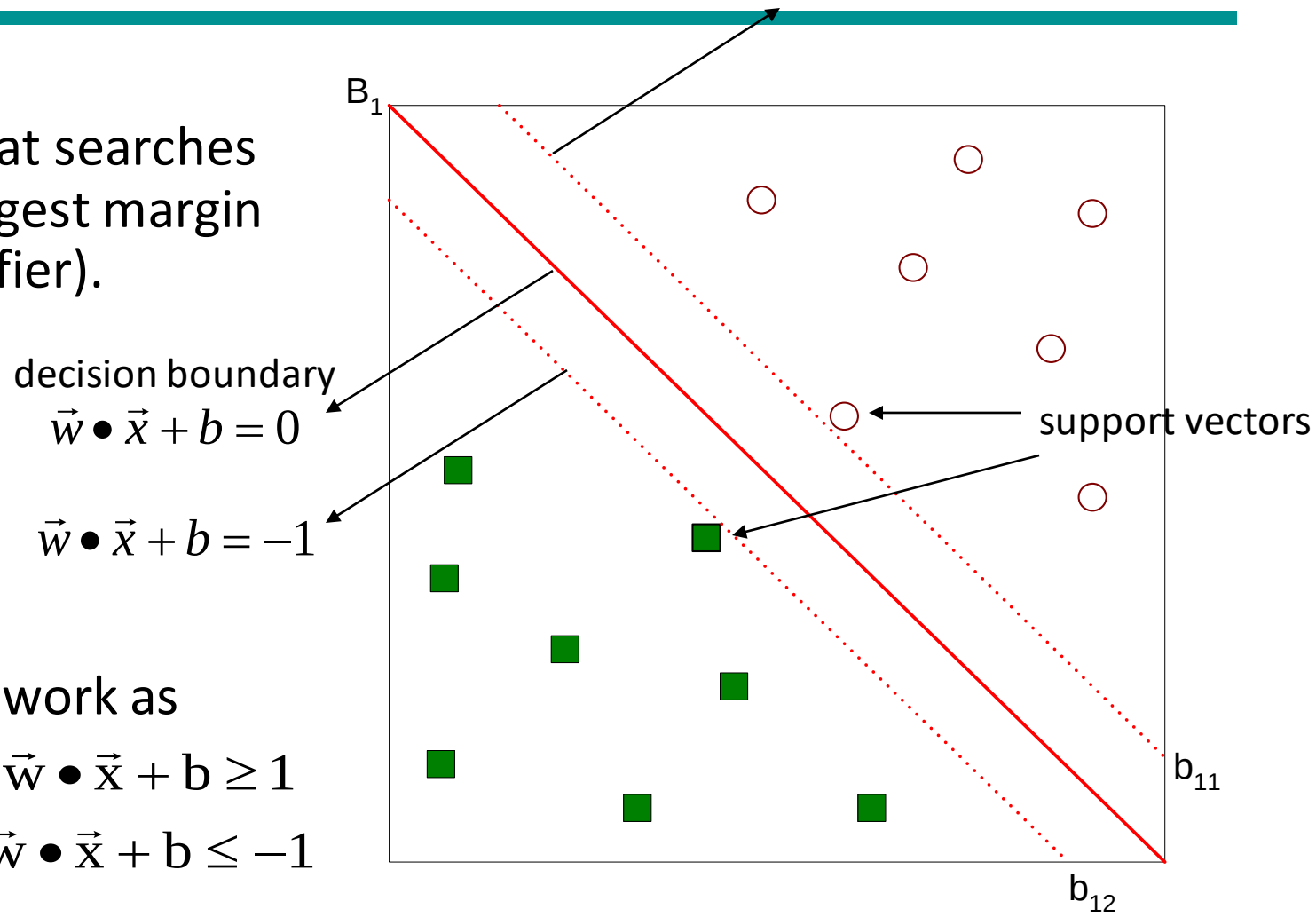
- The best solution is the hyperplane that **maximizes** the **margin**.
- Thus, B_1 is better than B_2.



Linear SVM: Separable Case

- A linear SVM is a classifier that searches for a hyperplane with the largest margin (a.k.a. maximal margin classifier).
- *w* and *b* have to be learned.
- Given *w* and *b* the classifiers work as

$$f(\vec{x}) = \begin{cases} 1 & \text{if } \vec{w} \bullet \vec{x} + b \geq 1 \\ -1 & \text{if } \vec{w} \bullet \vec{x} + b \leq -1 \end{cases}$$



Example calculus dot product

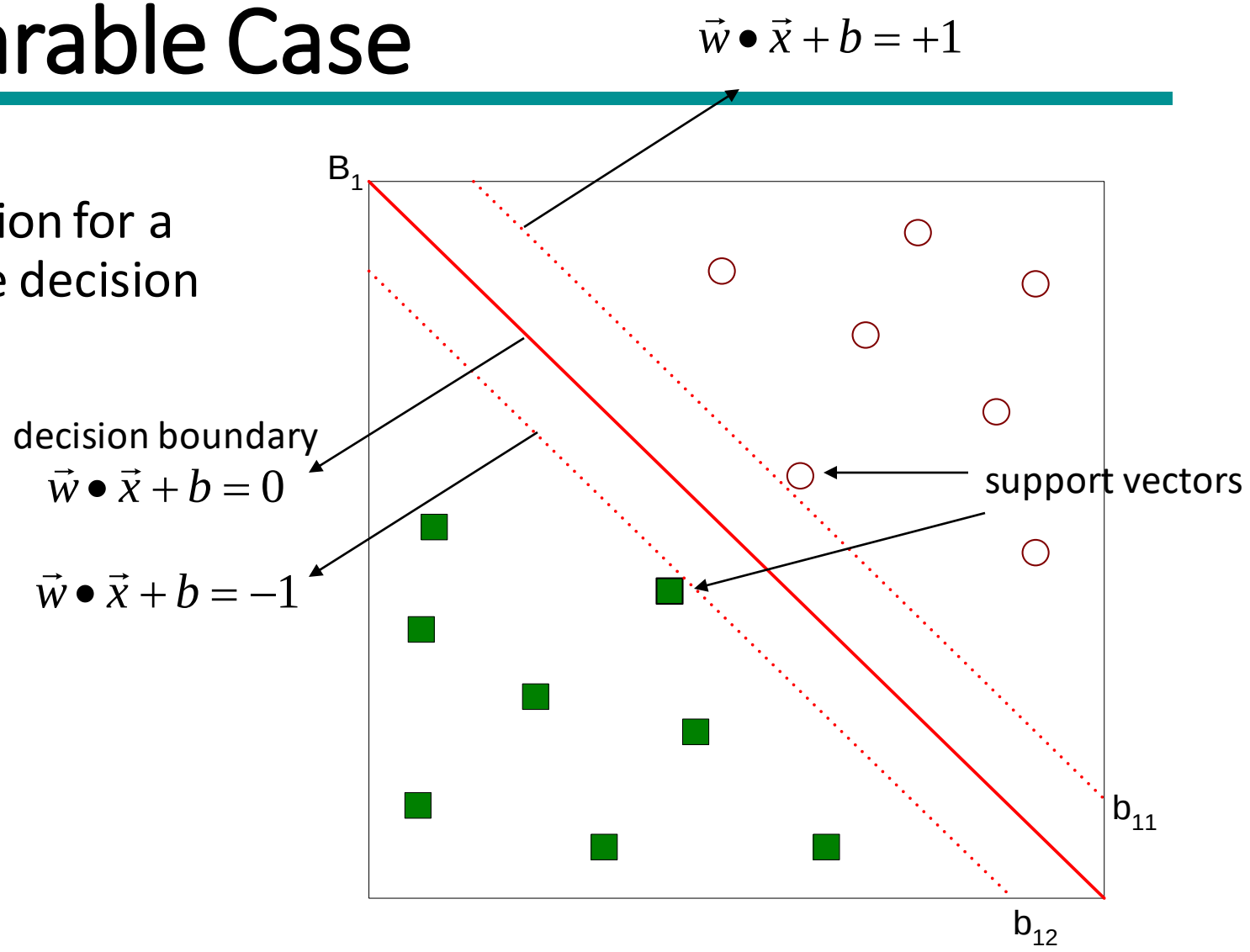
w = [.3 .2] x = [1 2] b = -2

w · x + b = .3*1 + .2*2 +(-2) = -1.3

Linear SVM: Separable Case

- What is the distance expression for a point *x* to a line *wx+b= 0* (the decision boundary)?

$$d(\mathbf{x}) = \frac{|\mathbf{x}\cdot\mathbf{w}+b|}{\sqrt{\|\mathbf{w}\|_2^2}} = \frac{|\mathbf{x}\cdot\mathbf{w}+b|}{\sqrt{\sum_{i=1}^{d} w_i^2}}$$

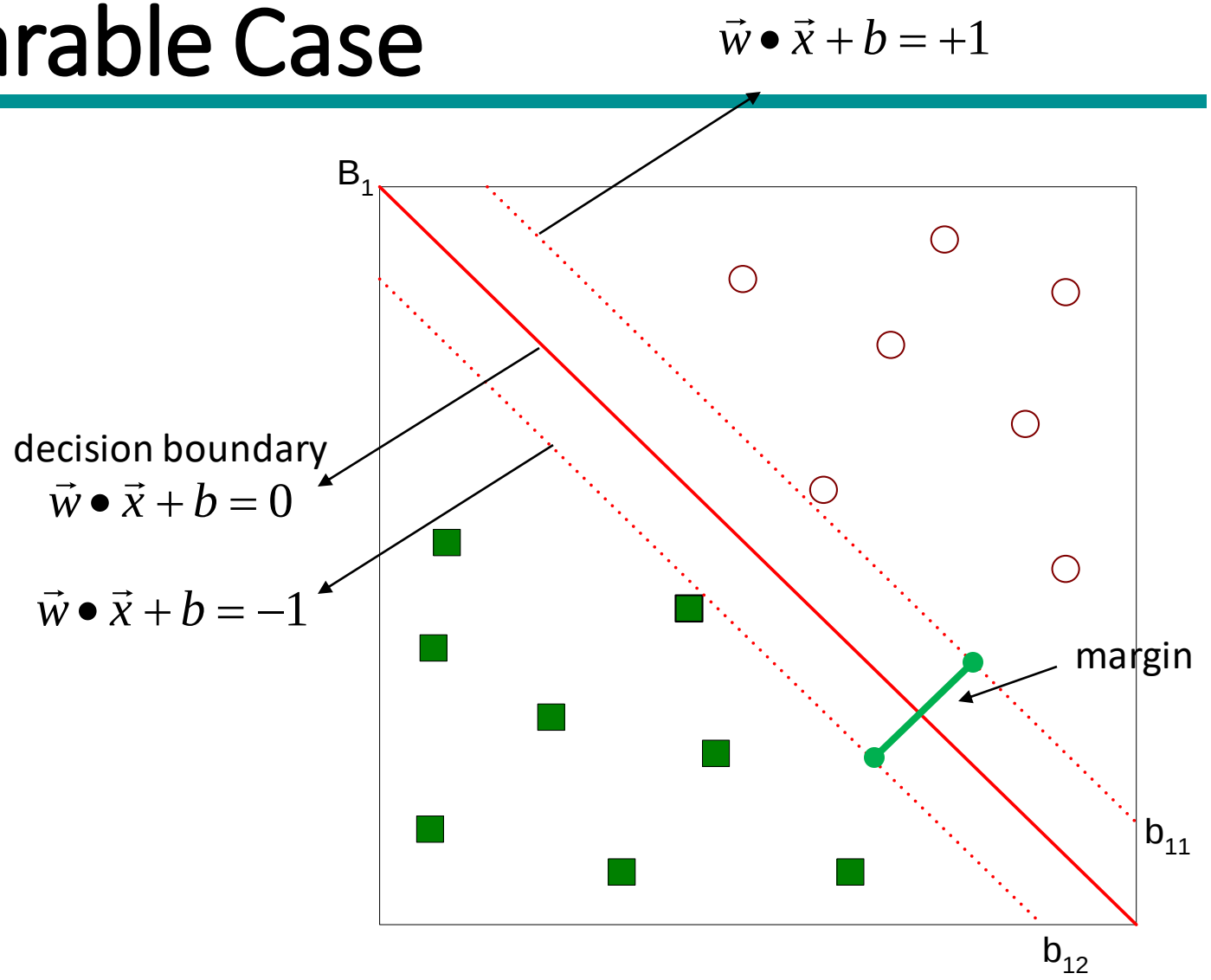


Linear SVM: Separable Case

- The distance between B_1 and b_{11} is $1/\|w\|$
- The distance between b_{11} and b_{12}, i.e., the margin is

$$\text{Margin} = \frac{2}{\|\vec{w}\|}$$

- In order to ***maximize the margin*** we need to minimize $\|w\|$



Learning a Linear SVM

- Learning the SVM model is equivalent to determining *w* and *b.*
- How to find *w* and *b?*
- Objective is to ***maximize the margin***.
- Which is equivalent to minimize
- Subject to to the following constraints
- This is a constrained optimization problem that can be solved using the *Lagrange* multiplier method.
- Introduce Lagrange multiplier λ (or α)

$$\text{Margin} = \frac{2}{\|\vec{w}\|}$$

$$L(\vec{w}) = \frac{\|\vec{w}\|^2}{2}$$

$$y_i = \begin{cases} 1 & \text{if } \vec{\mathrm{w}} \bullet \vec{\mathrm{x}}_\mathrm{i} + \mathrm{b} \geq 1 \\ -1 & \text{if } \vec{\mathrm{w}} \bullet \vec{\mathrm{x}}_\mathrm{i} + \mathrm{b} \leq -1 \end{cases}$$

$$=$$

$$y_i(\mathbf{w} \bullet \mathbf{x}_i + b) \geq 1, \quad i = 1,2,\ldots,N$$

Constrained Optimization Problem

Minimize $\| \mathbf{w} \| = \langle \mathbf{w} \cdot \mathbf{w} \rangle$ subject to $y_i(\langle \mathbf{x}_i \cdot \mathbf{w} \rangle + b) \geq 1$ for all i

Lagrangian method : maximize $\inf_{\mathbf{w}} L(\mathbf{w}, b, \alpha)$, where

$$L(\mathbf{w}, b, \alpha) = \frac{1}{2} \| \mathbf{w} \|^2 - \sum_i \alpha_i \left[\left(y_i (\mathbf{x}_i \cdot \mathbf{w}) + b \right) - 1 \right]$$

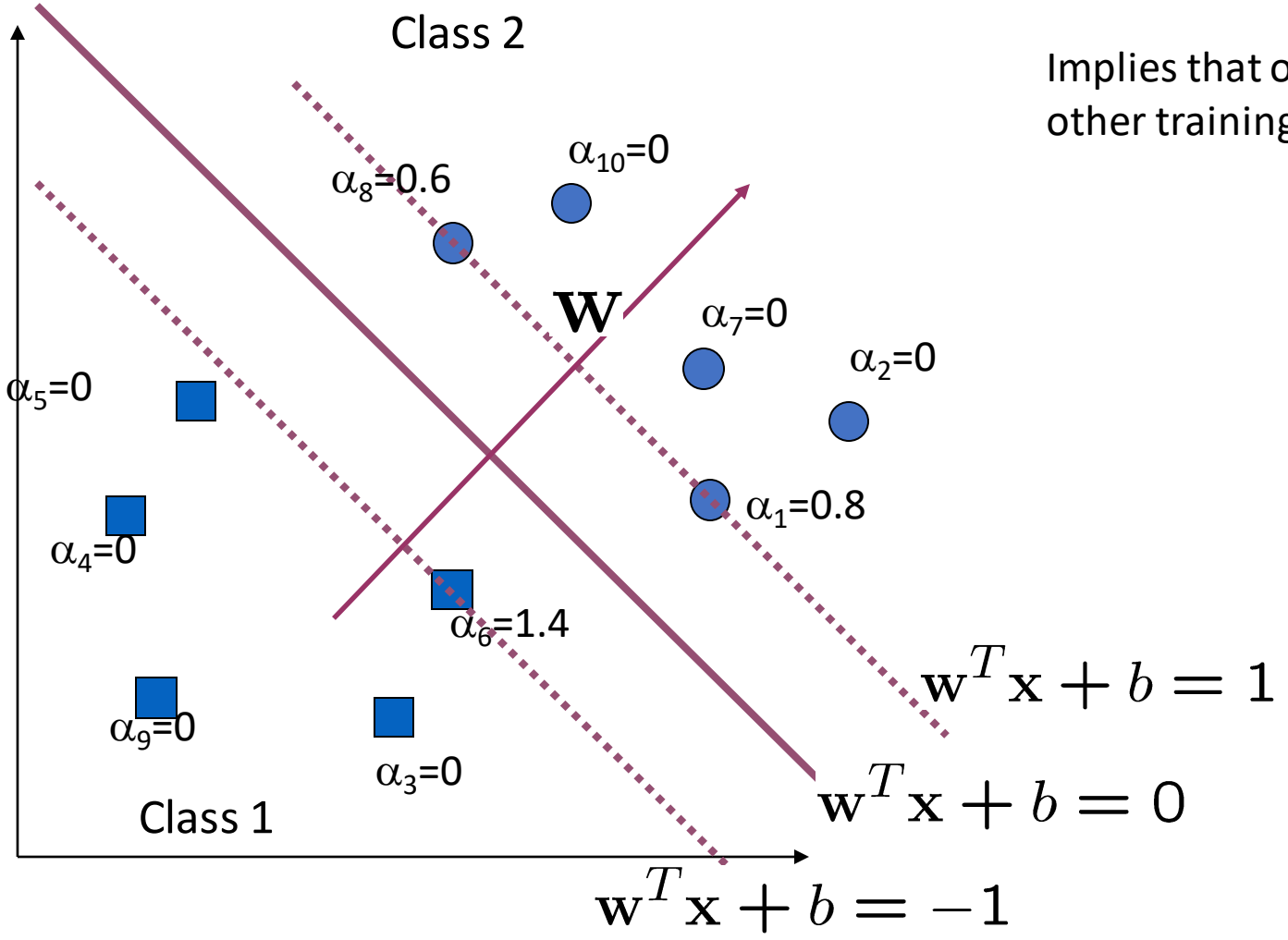
At the extremum, the partial derivative of L with respect both $\mathbf{w}$ and b must be 0. Taking the derivatives, setting them to 0, substituting back into L, and simplifying yields :

$$\text{Maximize } \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} y_i y_j \alpha_i \alpha_j \langle \mathbf{x}_i \cdot \mathbf{x}_j \rangle$$

$$\text{subject to } \sum_i y_i \alpha_i = 0 \text{ and } \alpha_i \geq 0$$

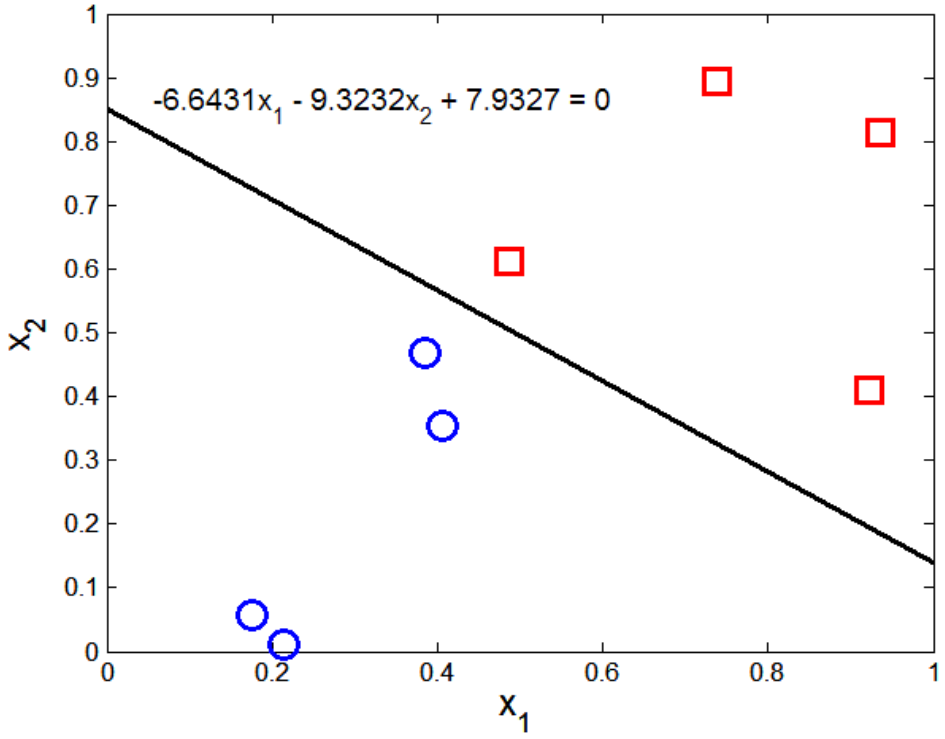
Lagrange multiplier method is a technique for finding a maximum or minimum of a function F subject to a constraint.

A Geometrical Interpretation



Implies that only support vectors matter; other training examples are ignorable.

Example of Linear SVM



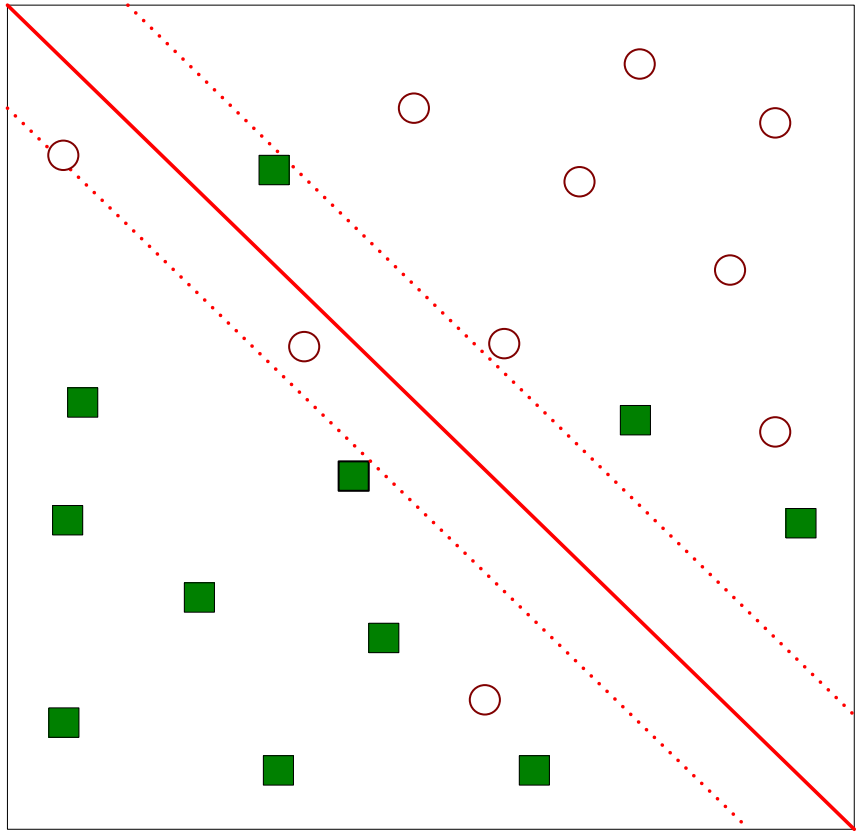
Support vectors

x1	x2	y	λ
0.3858	0.4687	1	65.5261
0.4871	0.611	-1	65.5261
0.9218	0.4103	-1	0
0.7382	0.8936	-1	0
0.1763	0.0579	1	0
0.4057	0.3529	1	0
0.9355	0.8132	-1	0
0.2146	0.0099	1	0

$\lambda = \alpha$

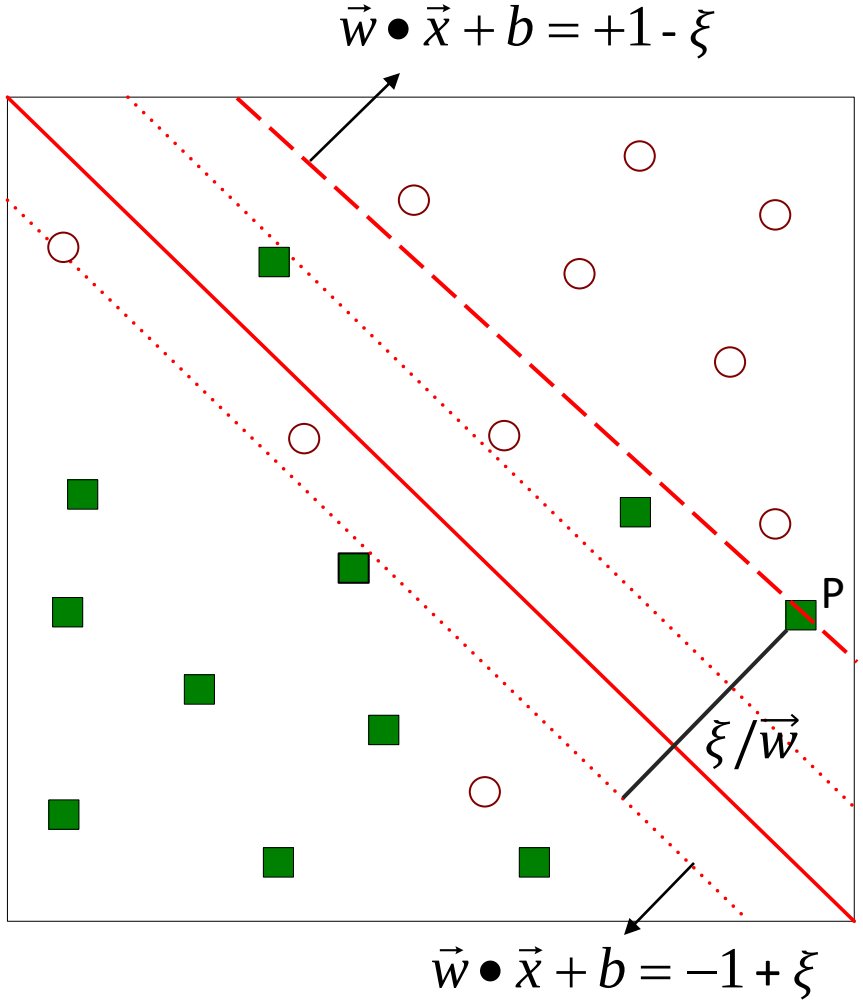
Linear SVM: Non-separable Case

- What if the problem is not linearly separable?
- We must allow for errors in our solution.



Slack Variables

- The inequality constraints must be relaxed to accommodate the nonlinearly separable data.
- This is done introducing slack variables ξ (xi) into the constrains of the optimization problem.
- ξ provides an estimate of the error of the decision boundary on the misclassified training examples.



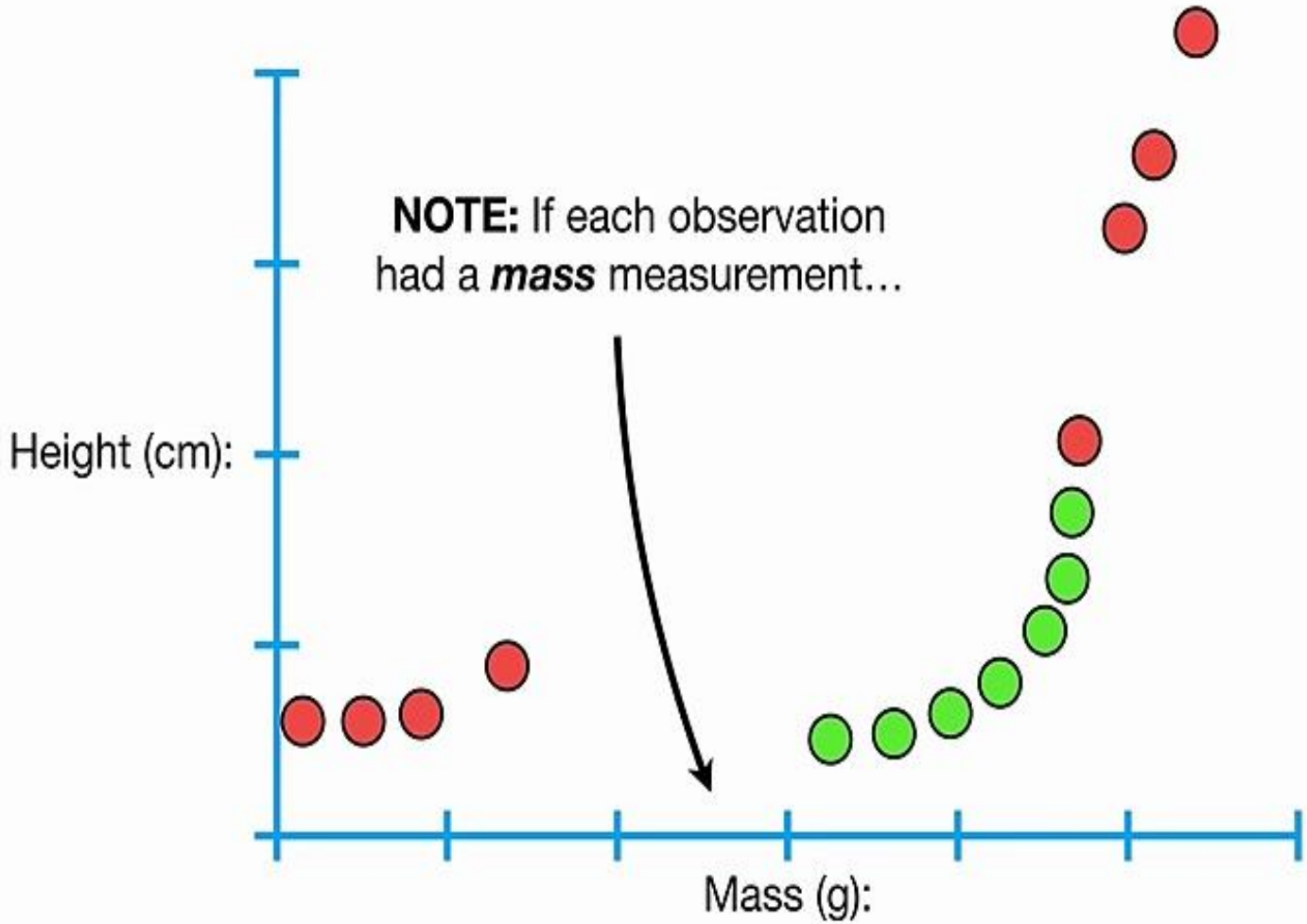
Learning a Non-separable Linear SVM

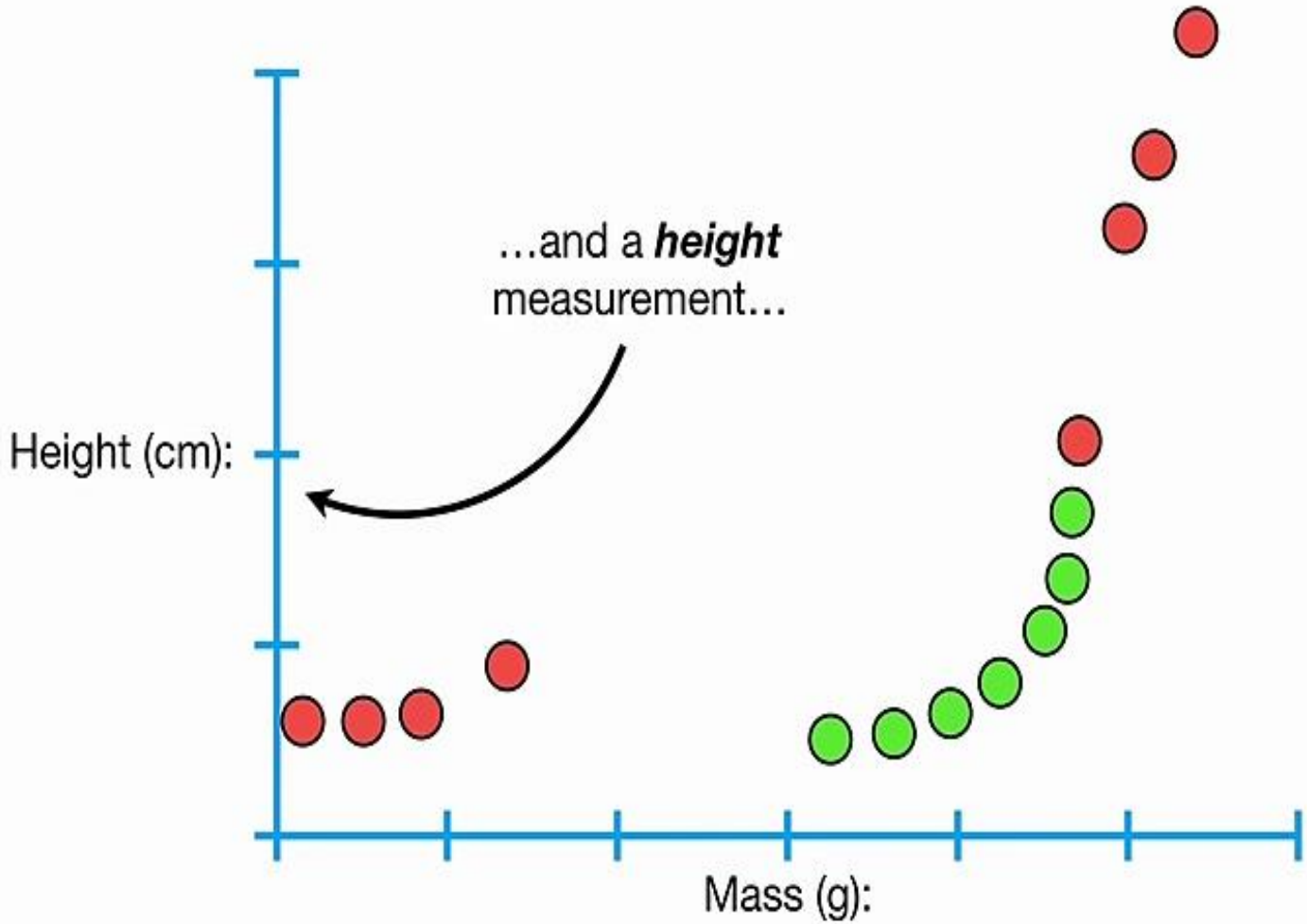
- Objective is to minimize
- Subject to to the constraints
- where *C* and *k* are user-specified parameters representing the penalty of misclassifying the training instances
- Lagrangian multipliers are constrained to $0 \leq \lambda \leq C$.

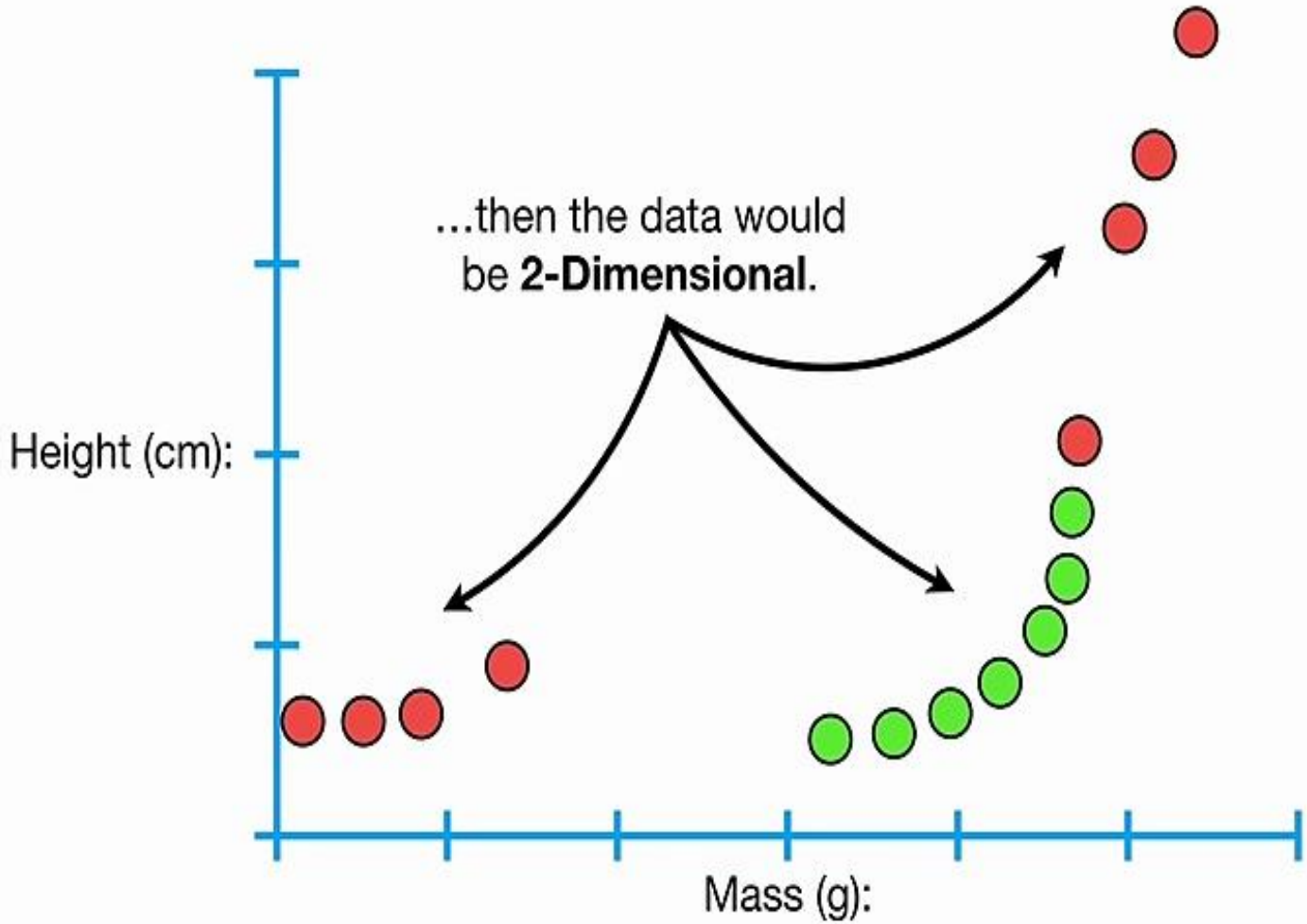
$$L(w) = \frac{\| \vec{w} \|^2}{2} + C\left(\sum_{i=1}^{N} \xi_i^k \right)$$

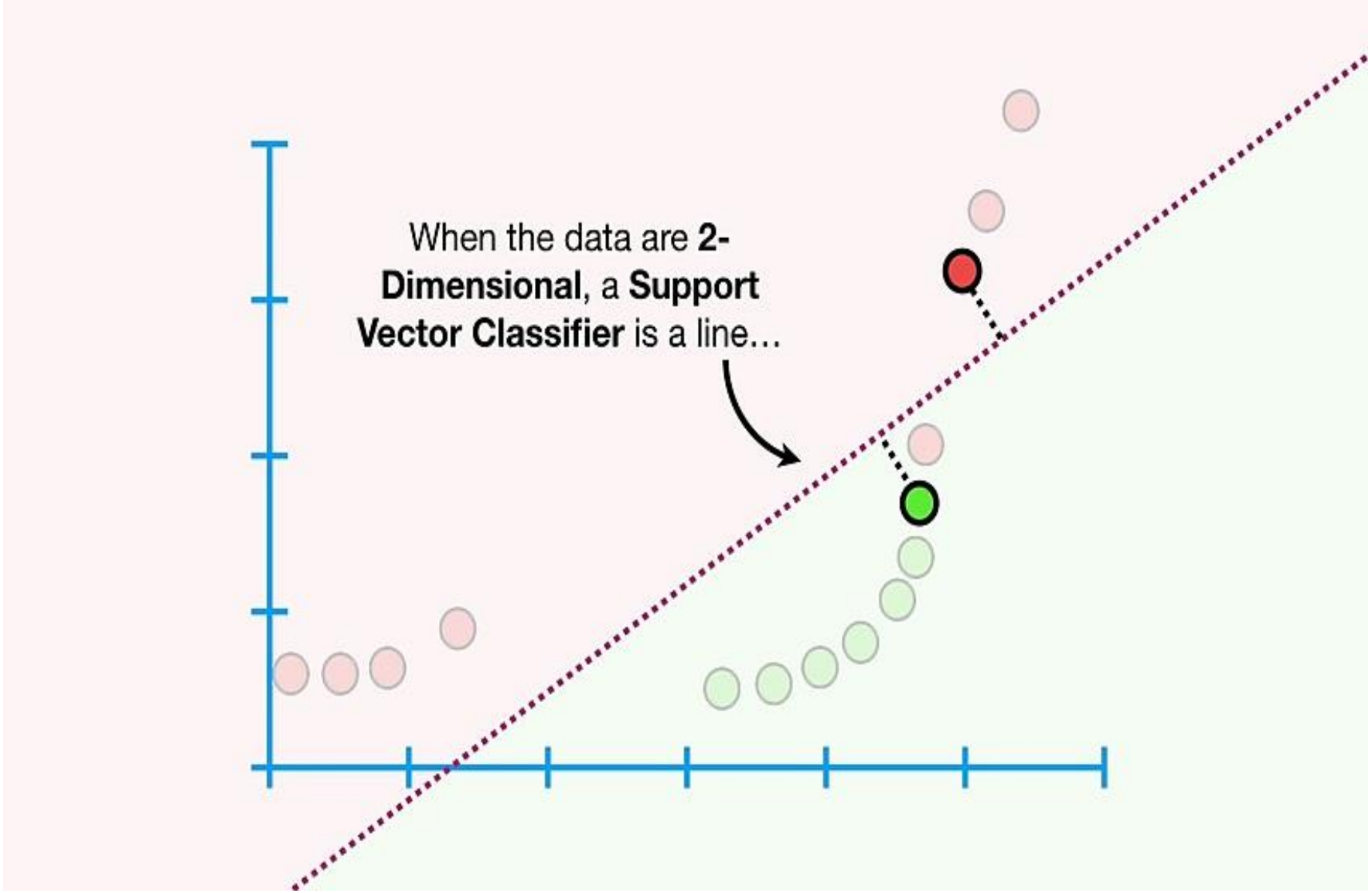
$$y_i = \begin{cases} 1 & \text{if } \vec{w} \bullet \vec{x}_i + b \geq 1 - \xi_i \\ -1 & \text{if } \vec{w} \bullet \vec{x}_i + b \leq -1 + \xi_i \end{cases}$$

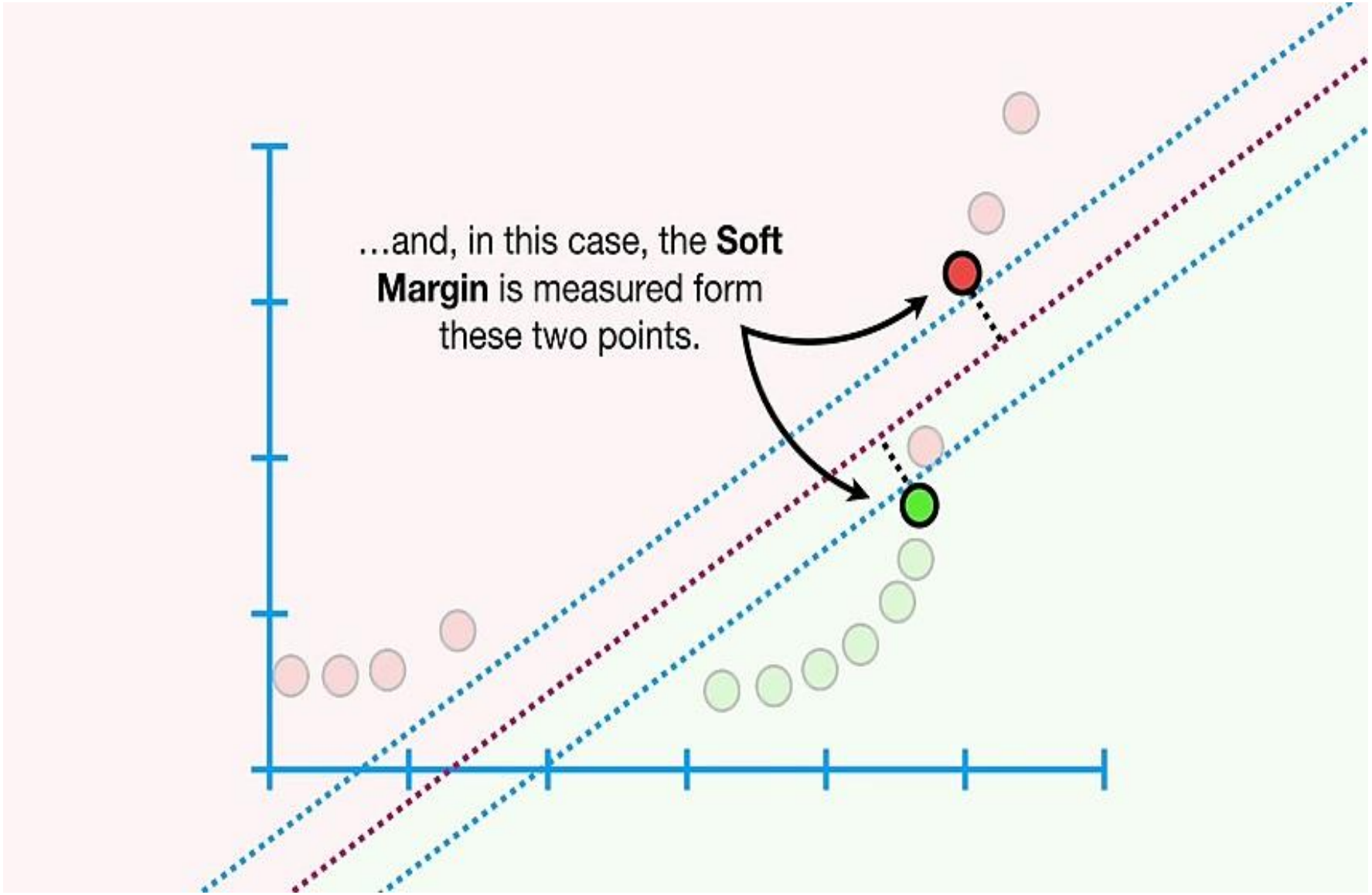
https://scikit-learn.org/stable/auto_examples/svm/plot_linearsvc_support_vectors.html#sphx-glr-auto-examples-svm-plot-linearsvc-support-vectors-py

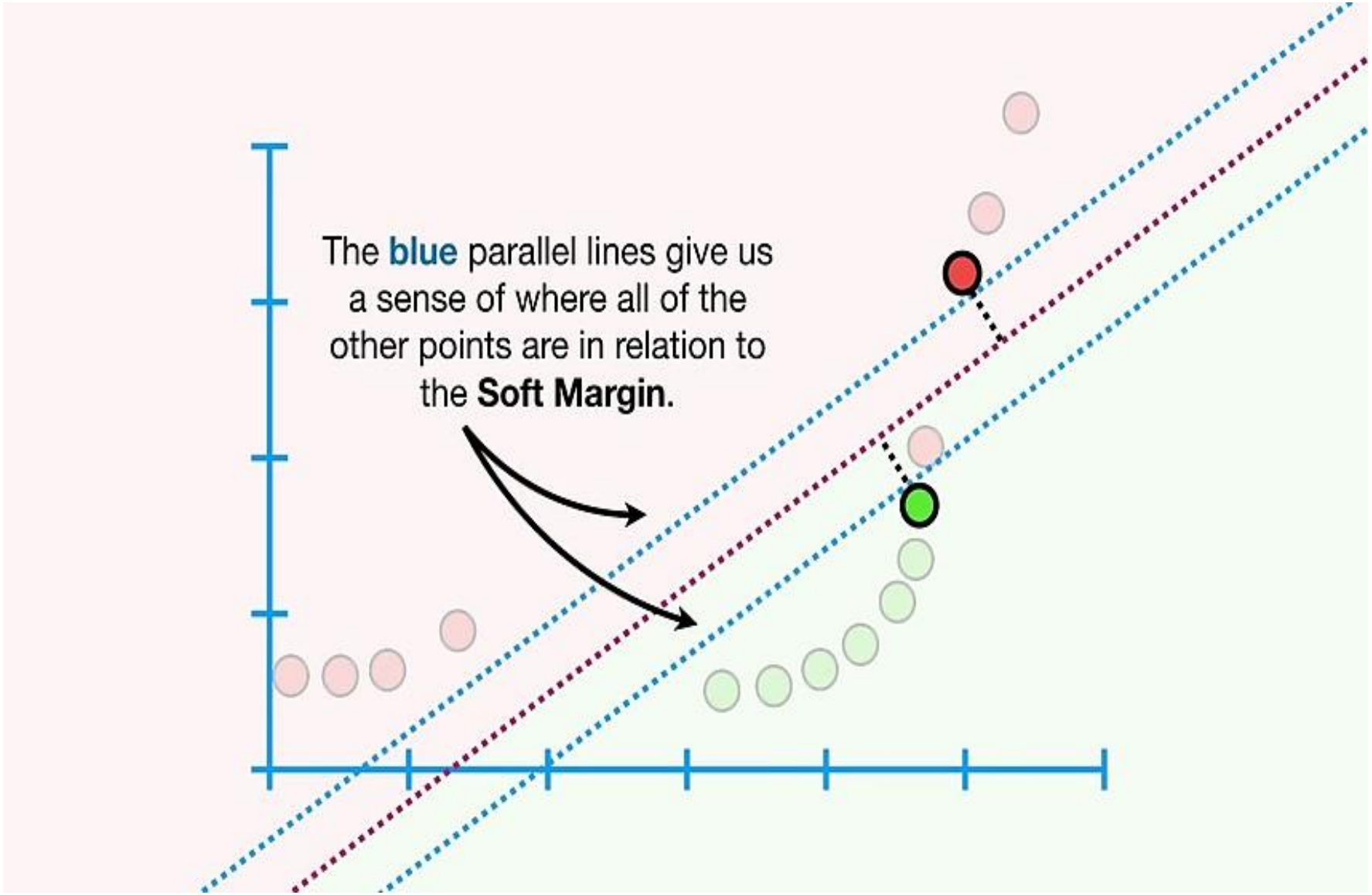

NOTE: If each observation had a *mass* measurement…
Height (cm):
Mass (g):

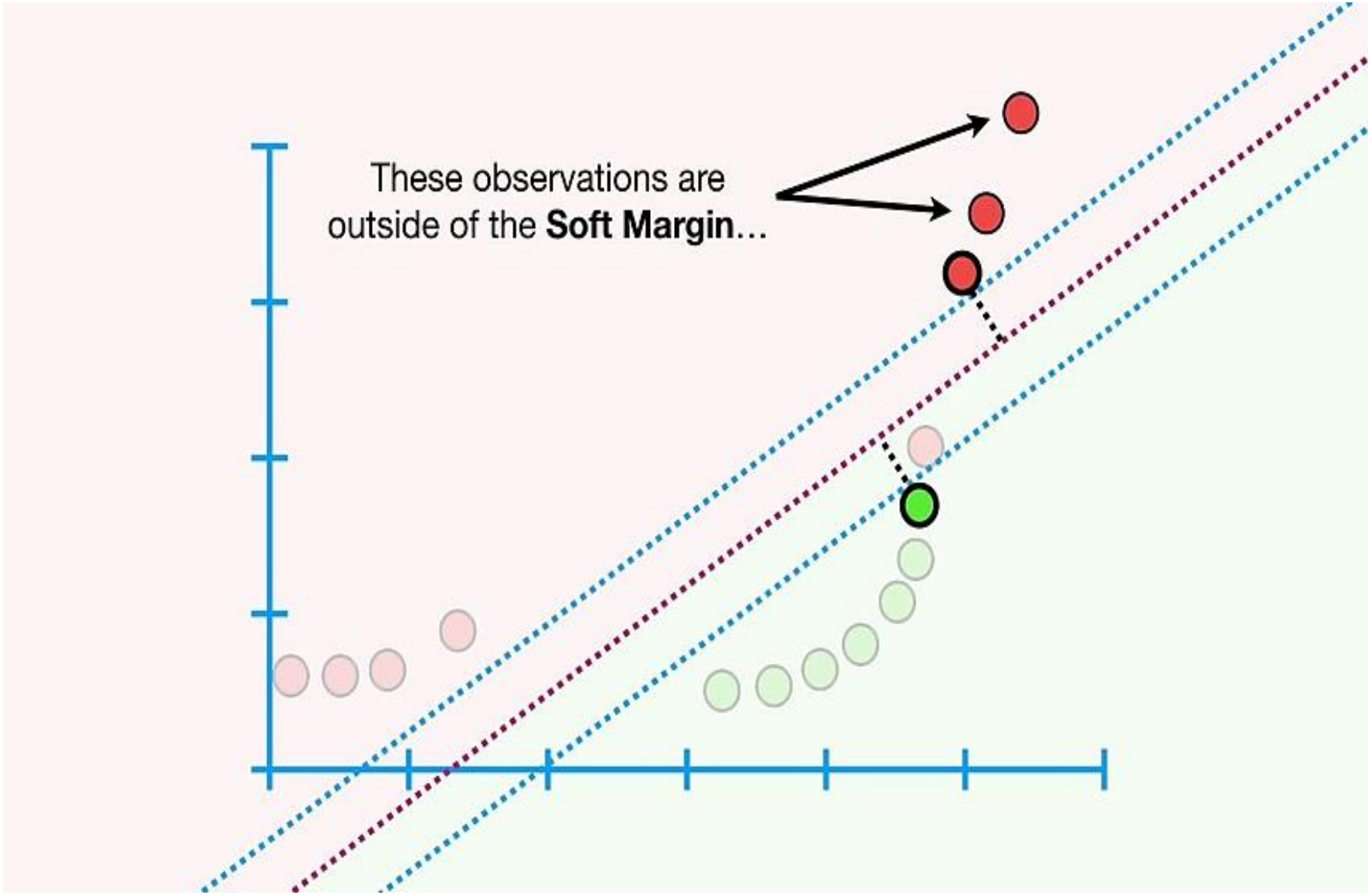

…and a *height* measurement…
Height (cm):
Mass (g):

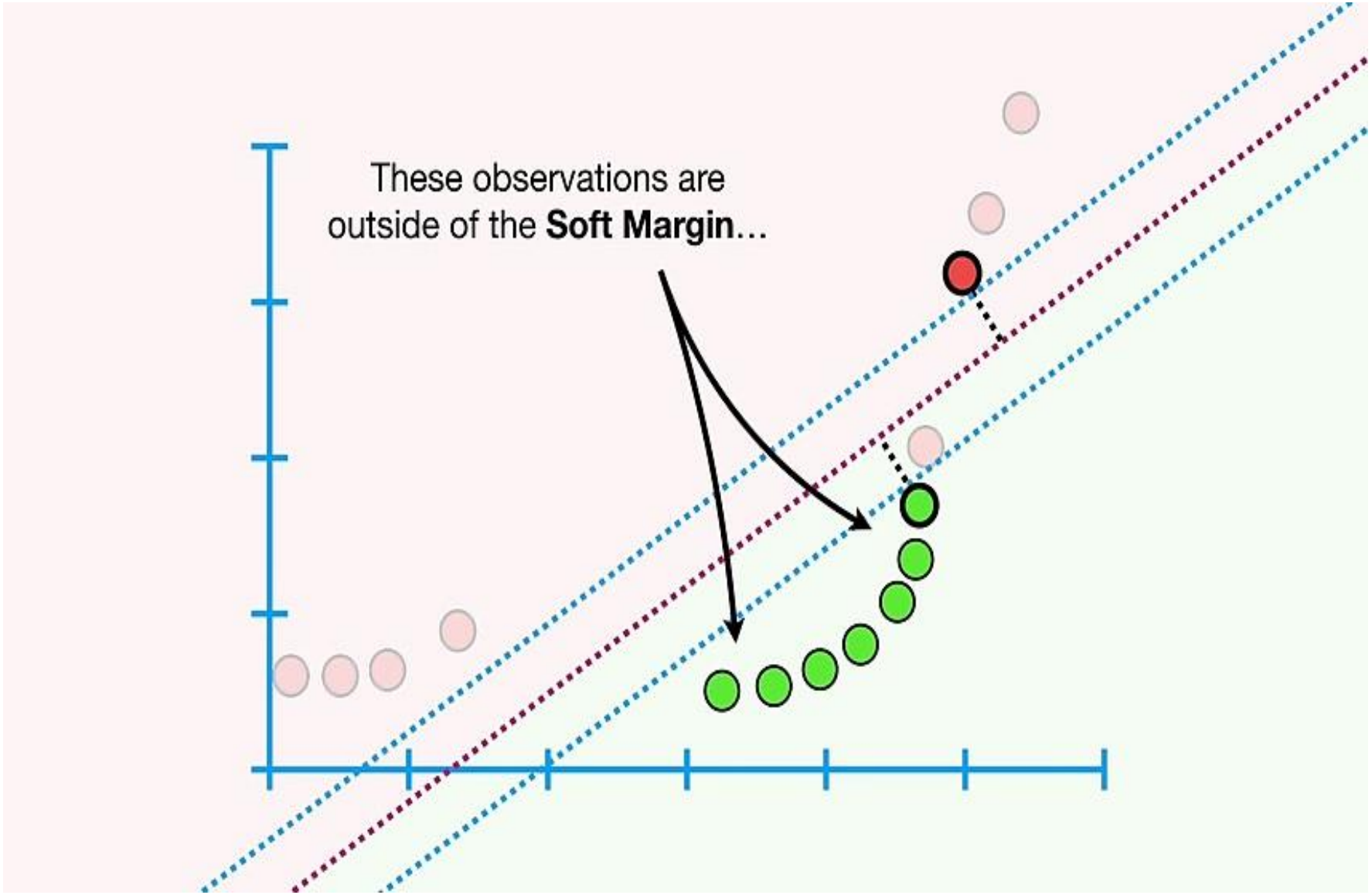

...then the data would
be **2-Dimensional**.
Height (cm):
Mass (g):

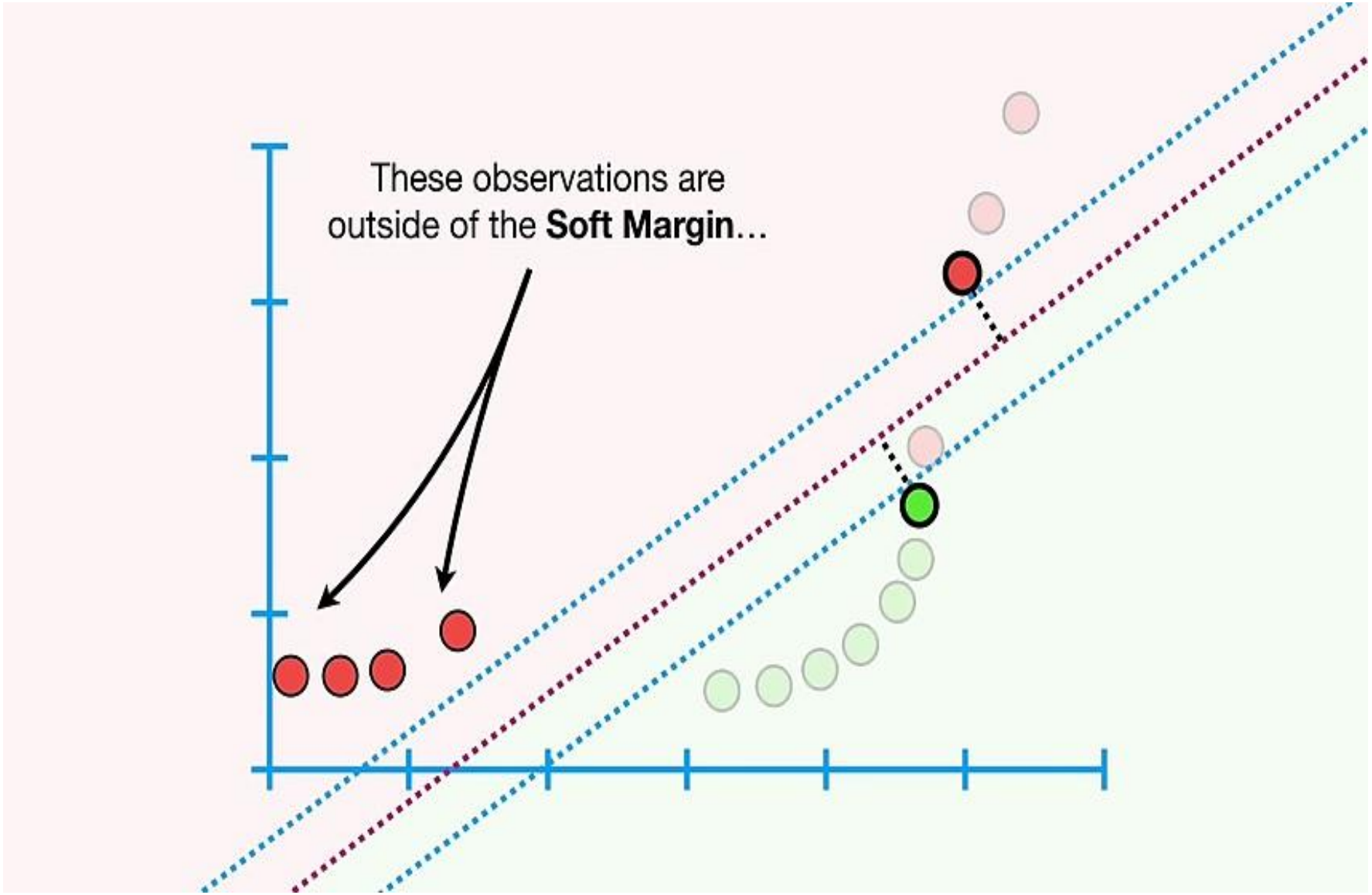

When the data are **2-Dimensional**, a **Support Vector Classifier** is a line...

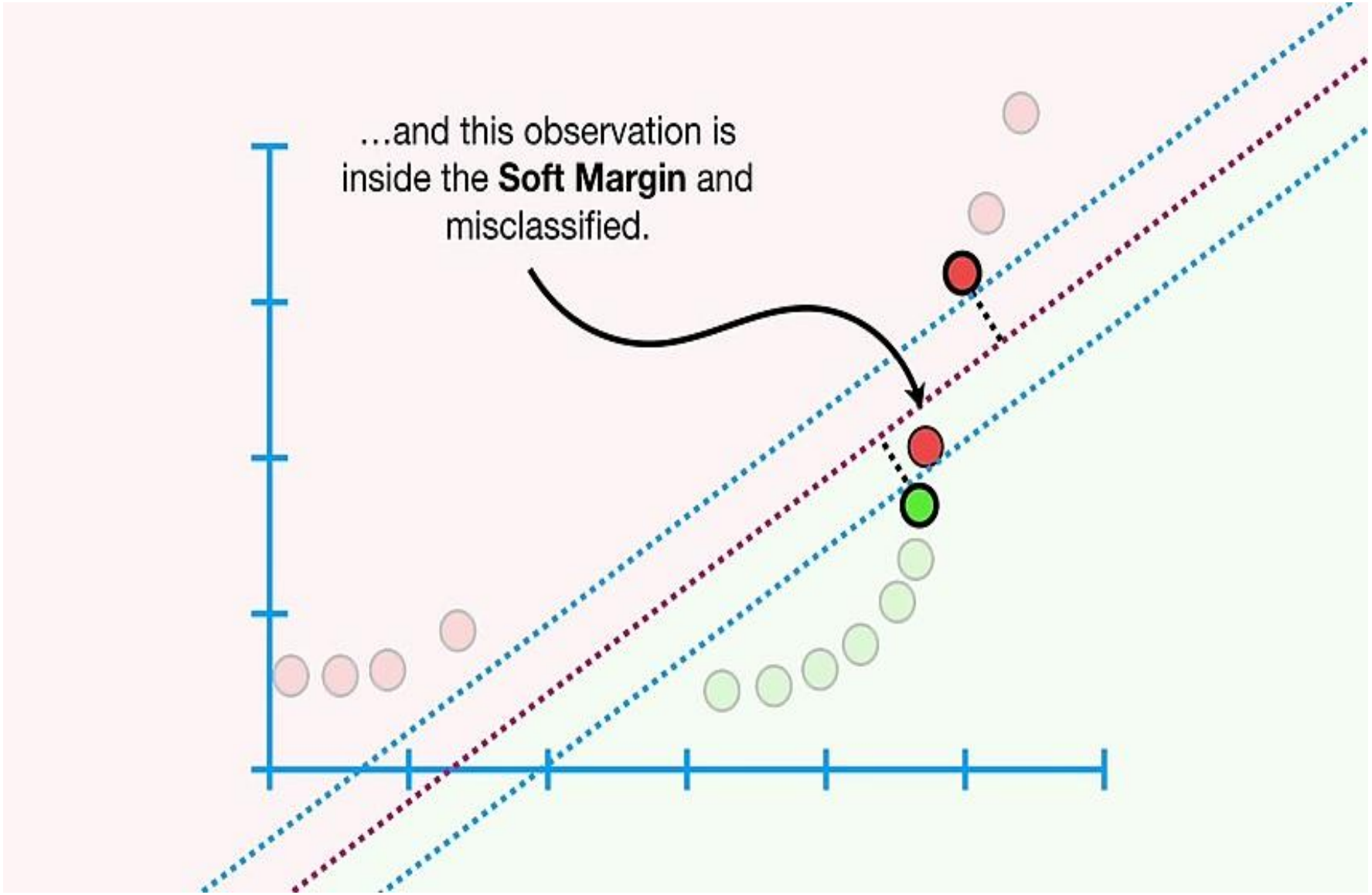

...and, in this case, the **Soft Margin** is measured form these two points.

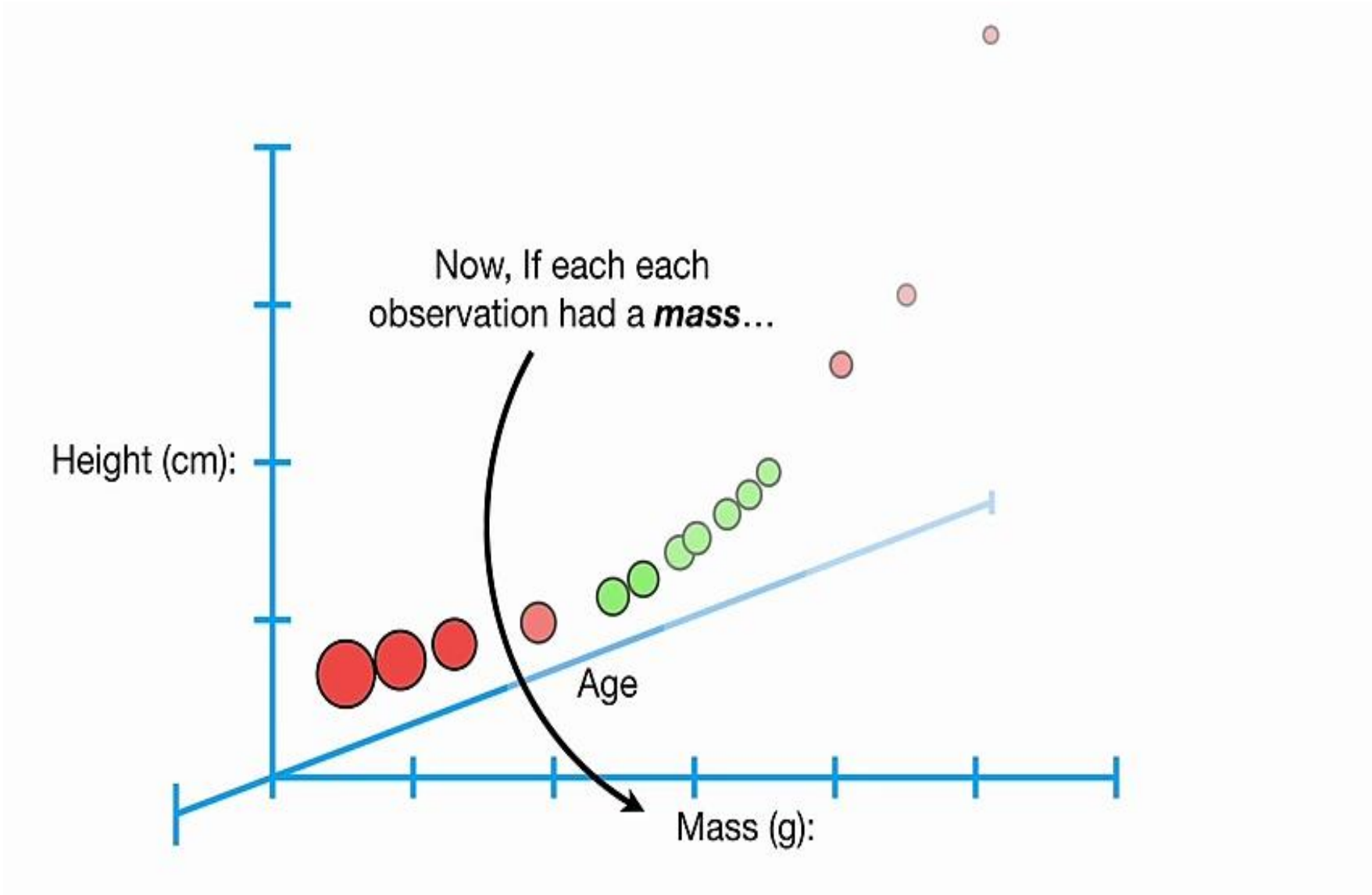

The blue parallel lines give us a sense of where all of the other points are in relation to the Soft Margin.

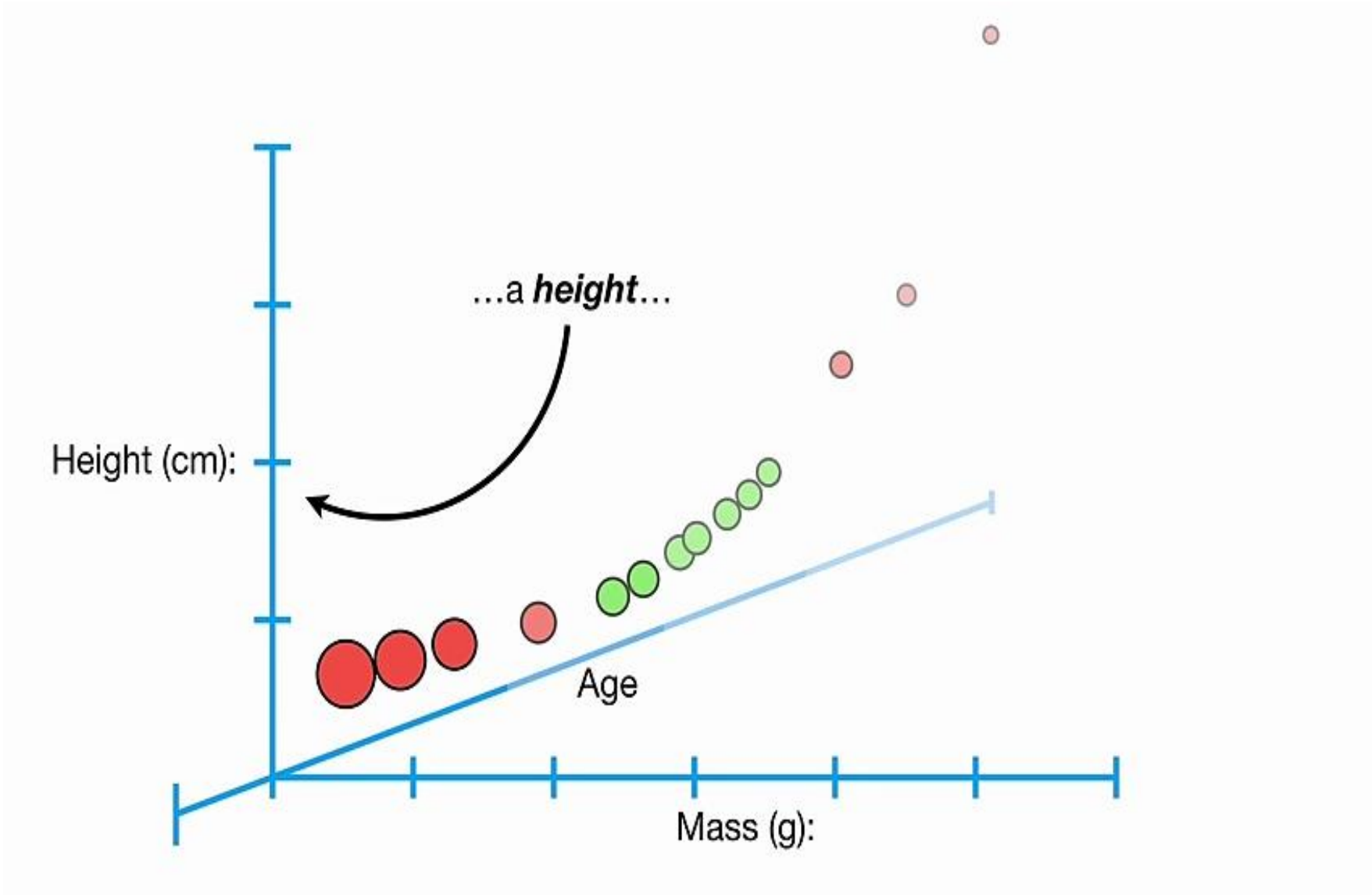

These observations are
outside of the **Soft Margin**...

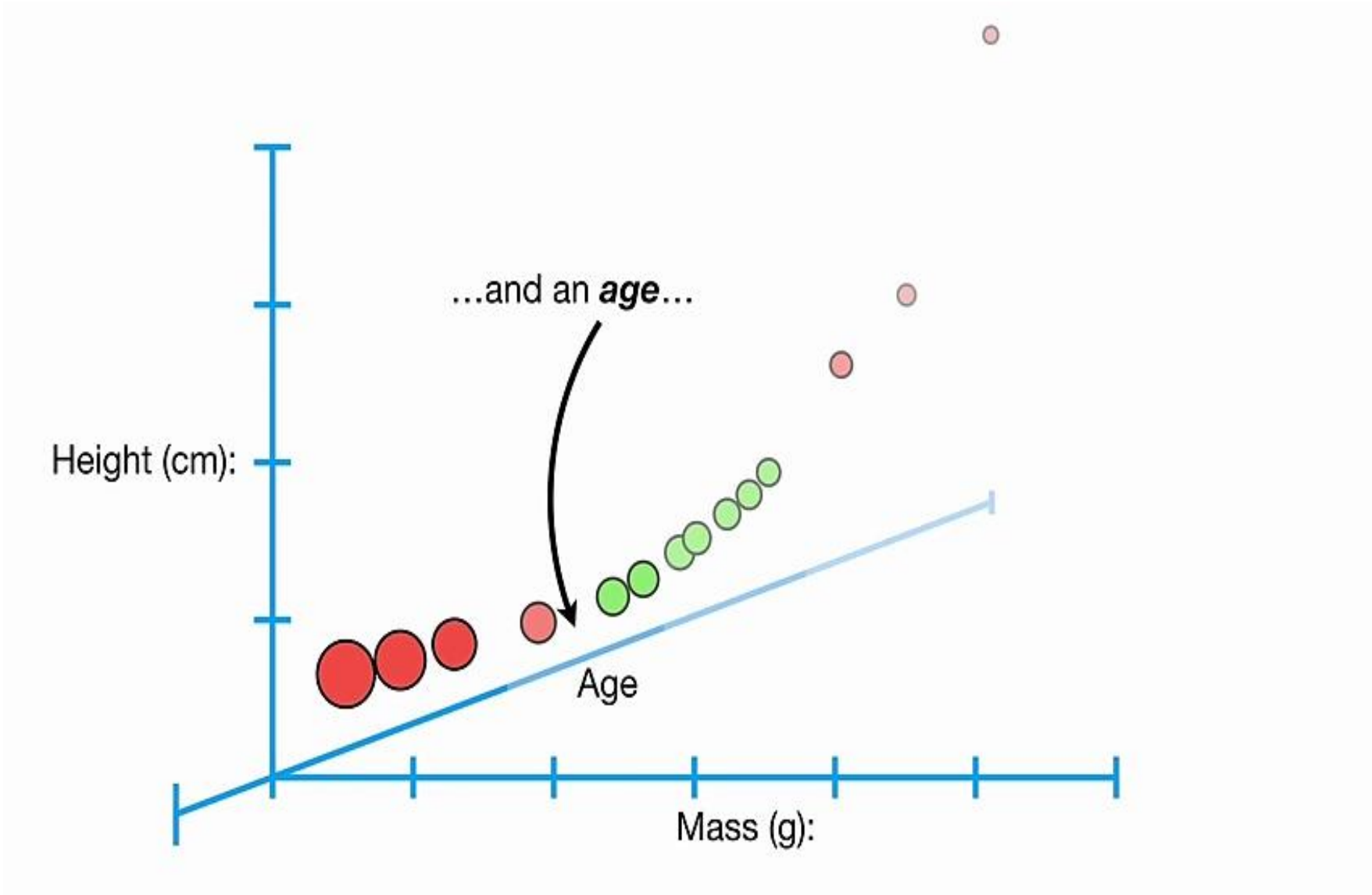

These observations are
outside of the **Soft Margin**...

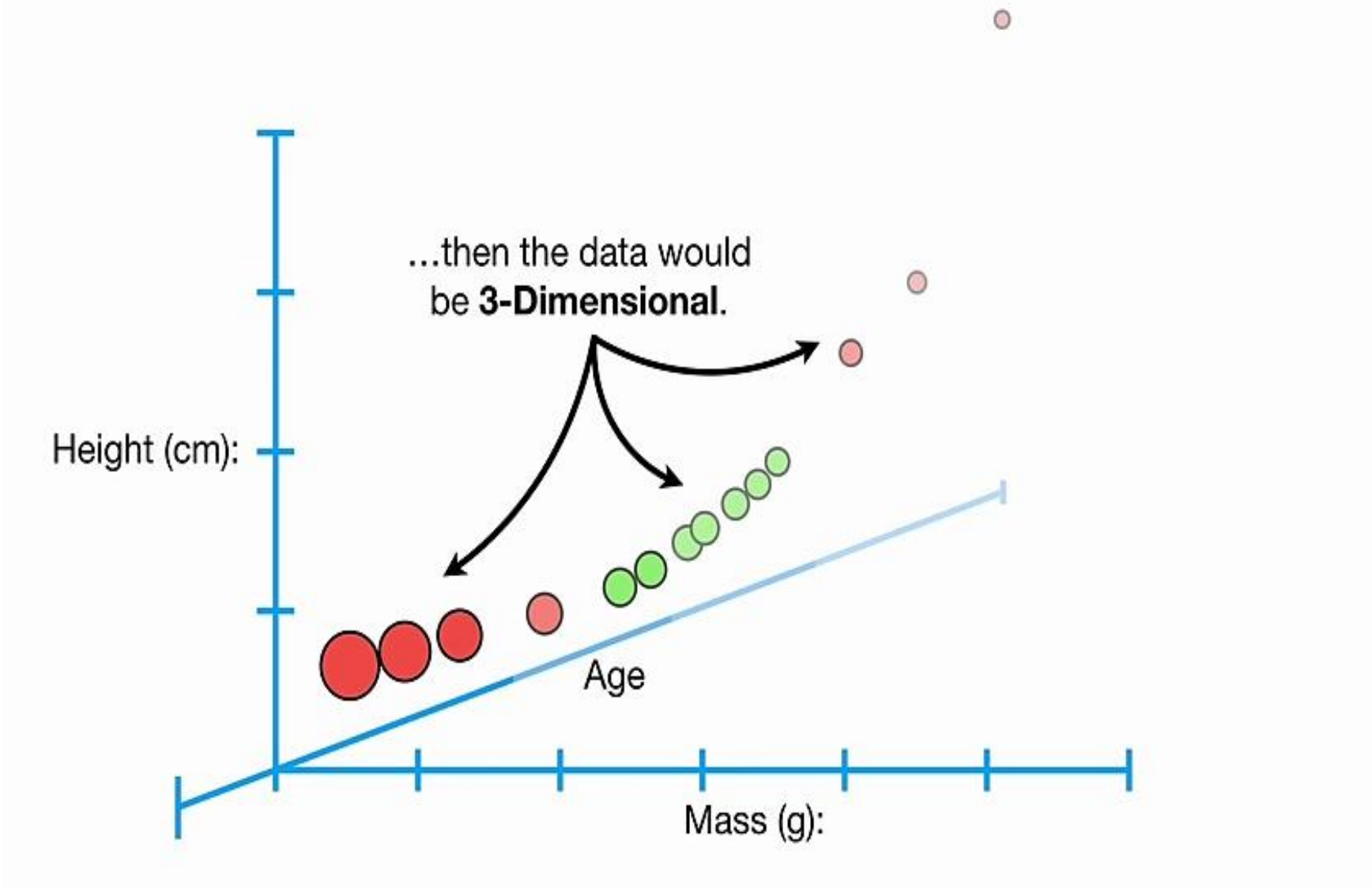

These observations are
outside of the **Soft Margin**...

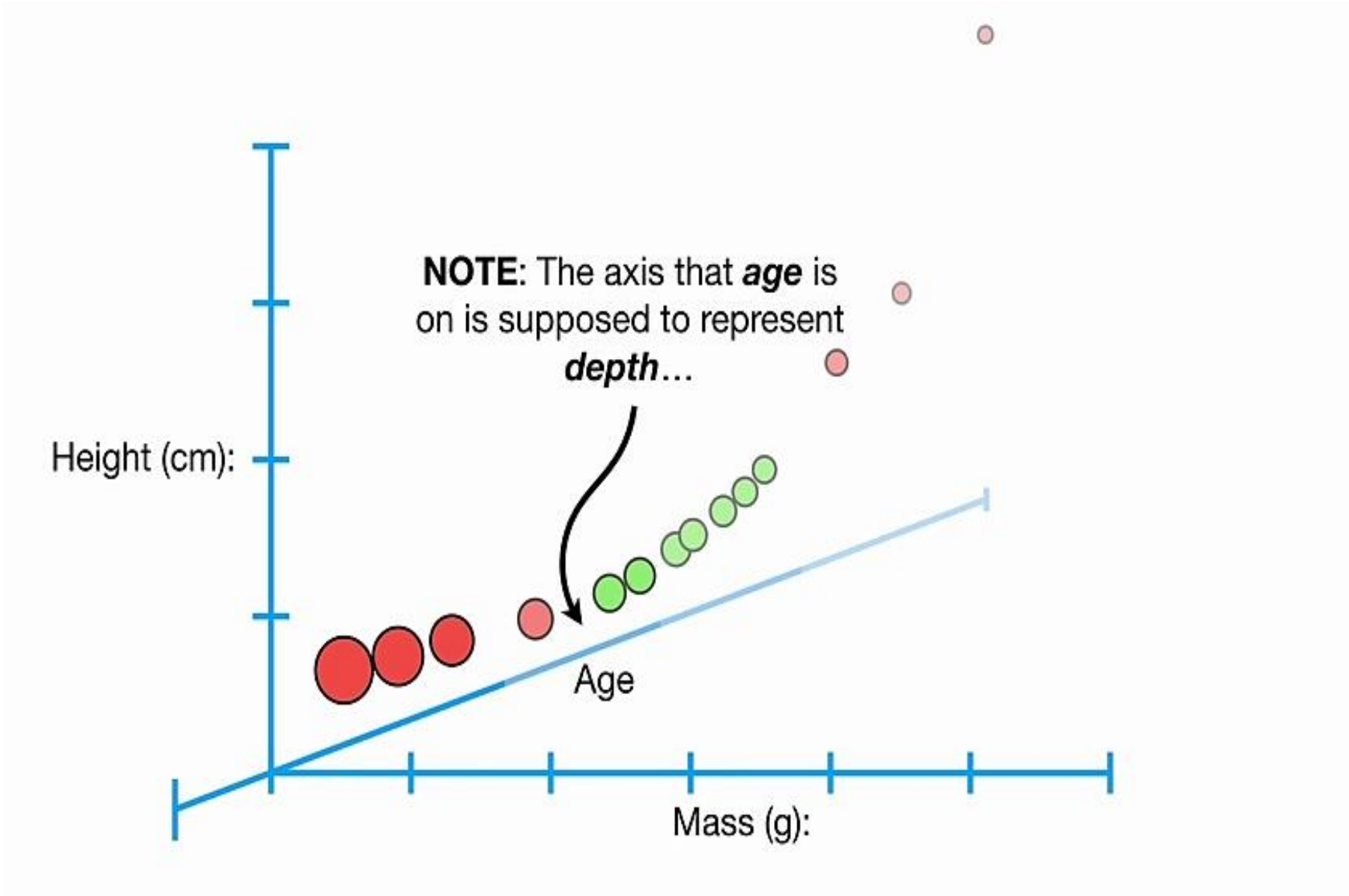

…and this observation is
inside the **Soft Margin** and
misclassified.

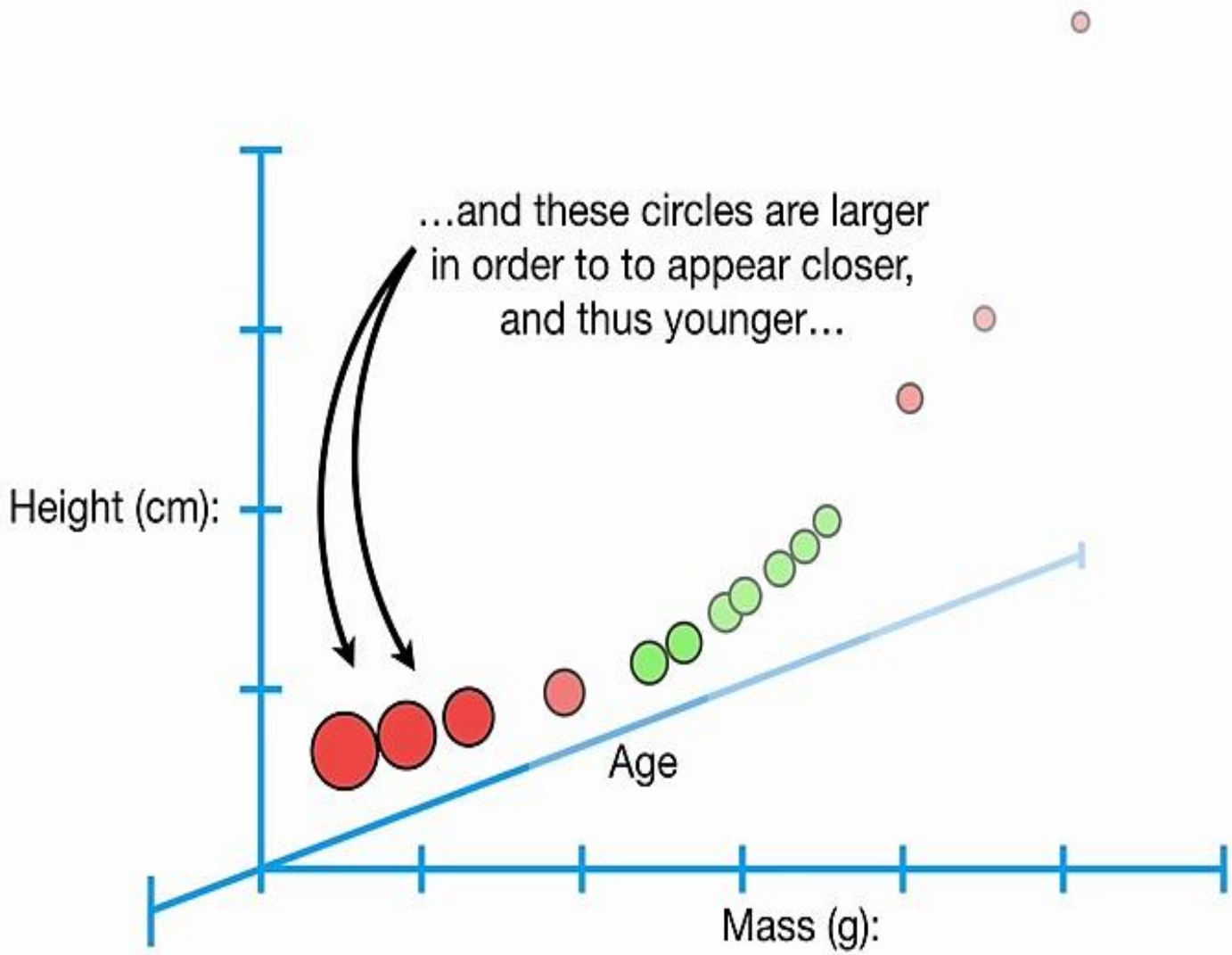

Now, If each each
observation had a *mass*...
Height (cm):
Age
Mass (g):

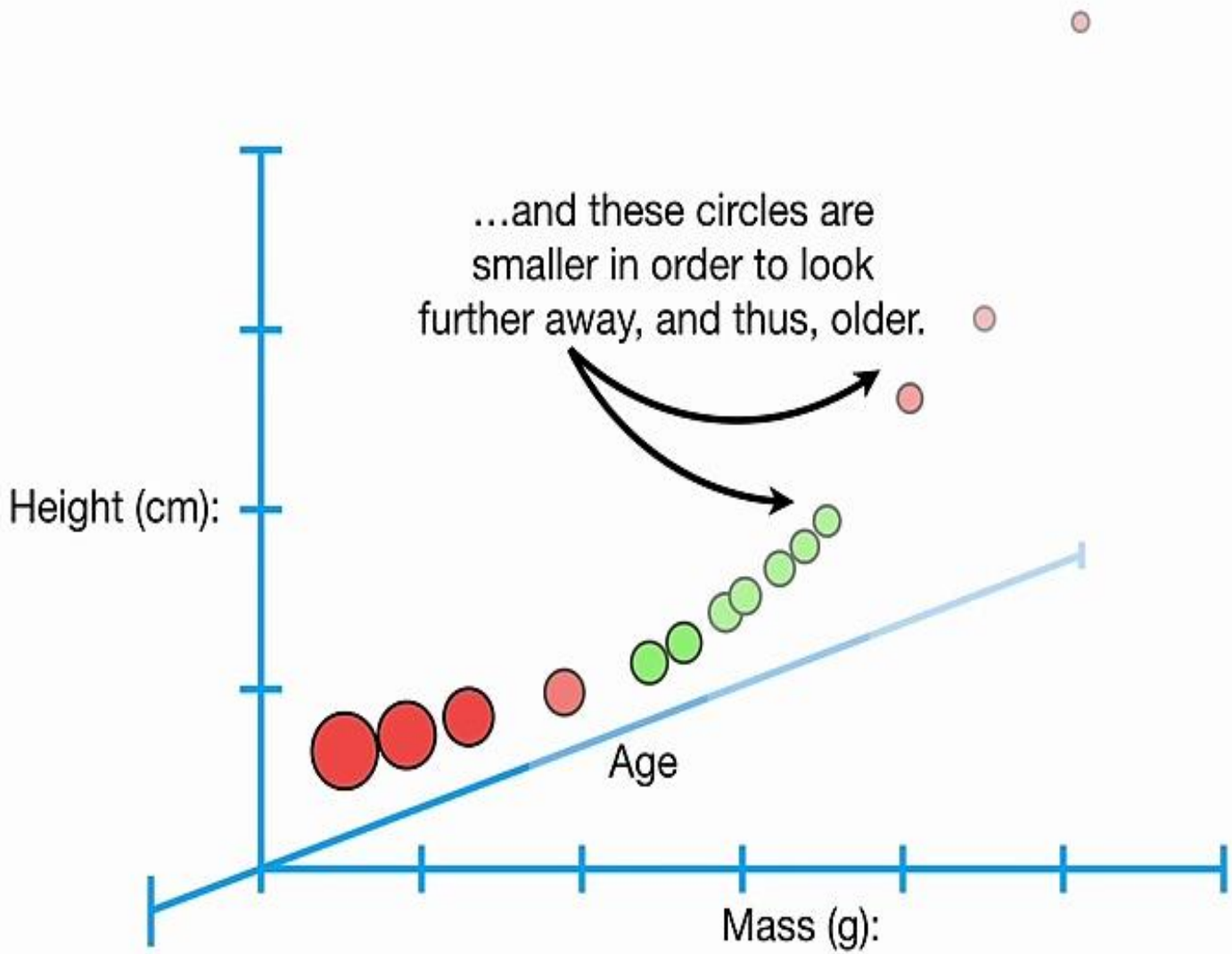

…a height…
Height (cm):
Age
Mass (g):

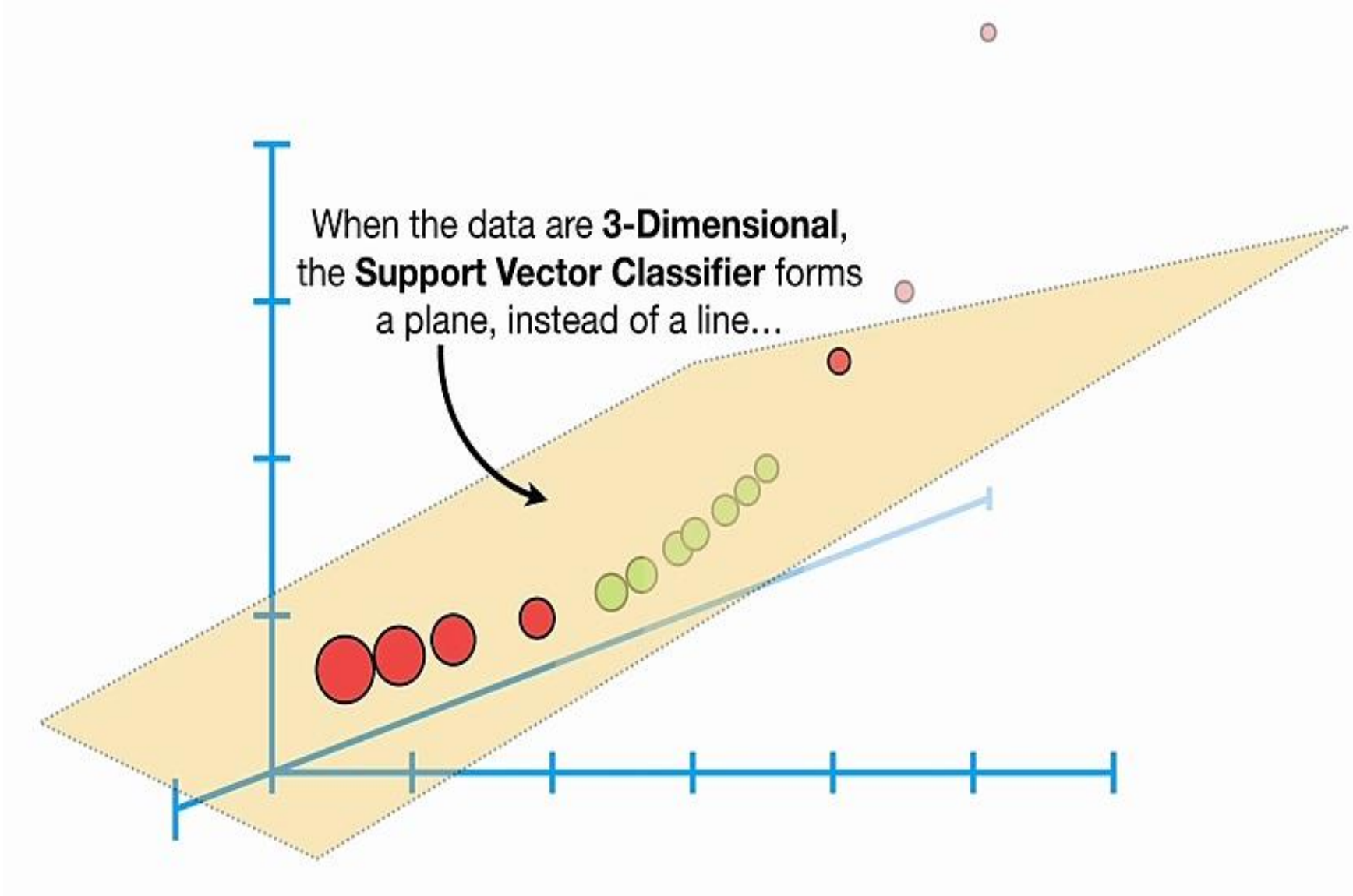

…and an *age*…
Height (cm):
Age
Mass (g):

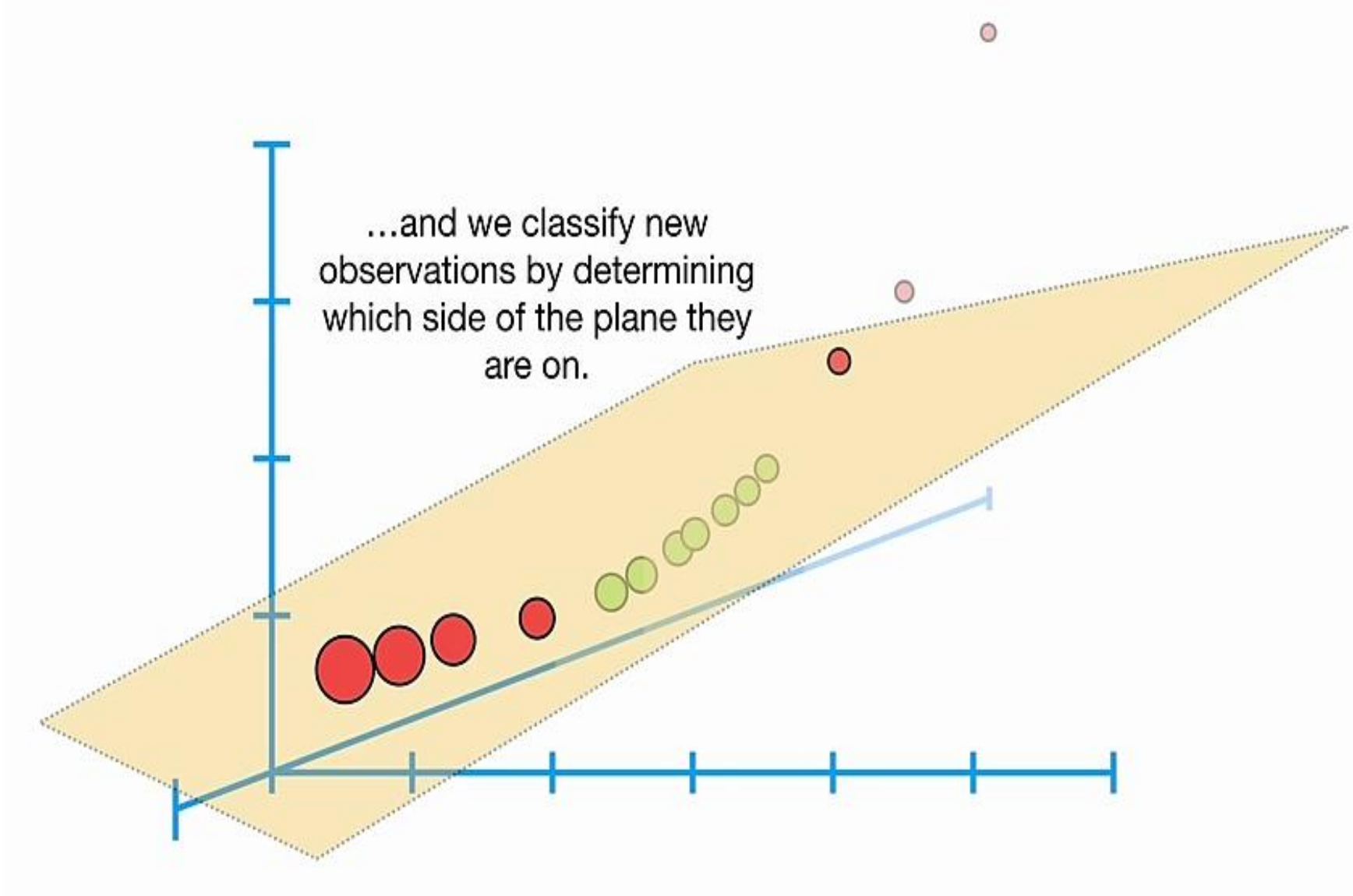

...then the data would be 3-Dimensional.
Height (cm):
Age
Mass (g):

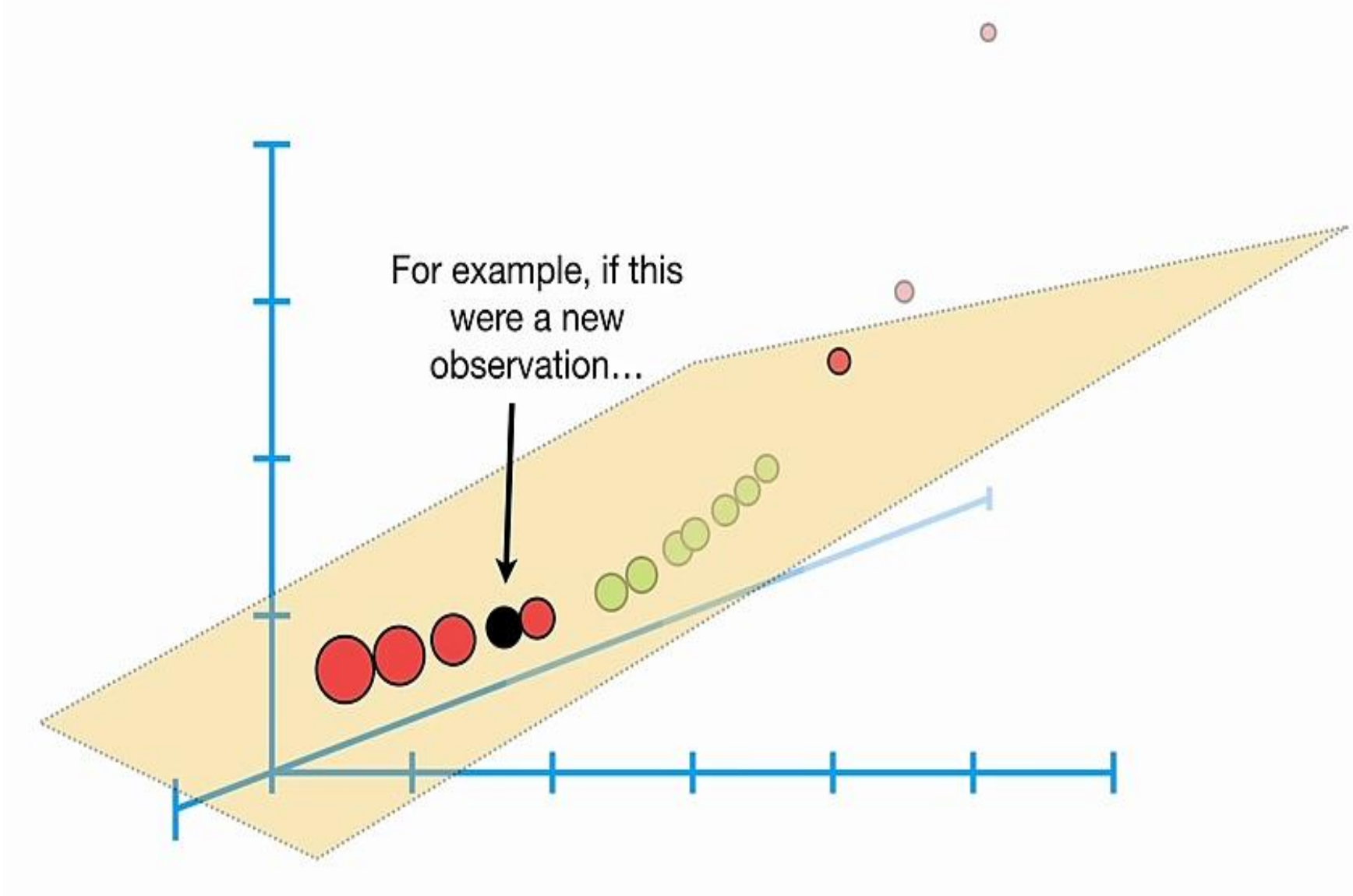

NOTE: The axis that age is on is supposed to represent depth...
Height (cm):
Age
Mass (g):

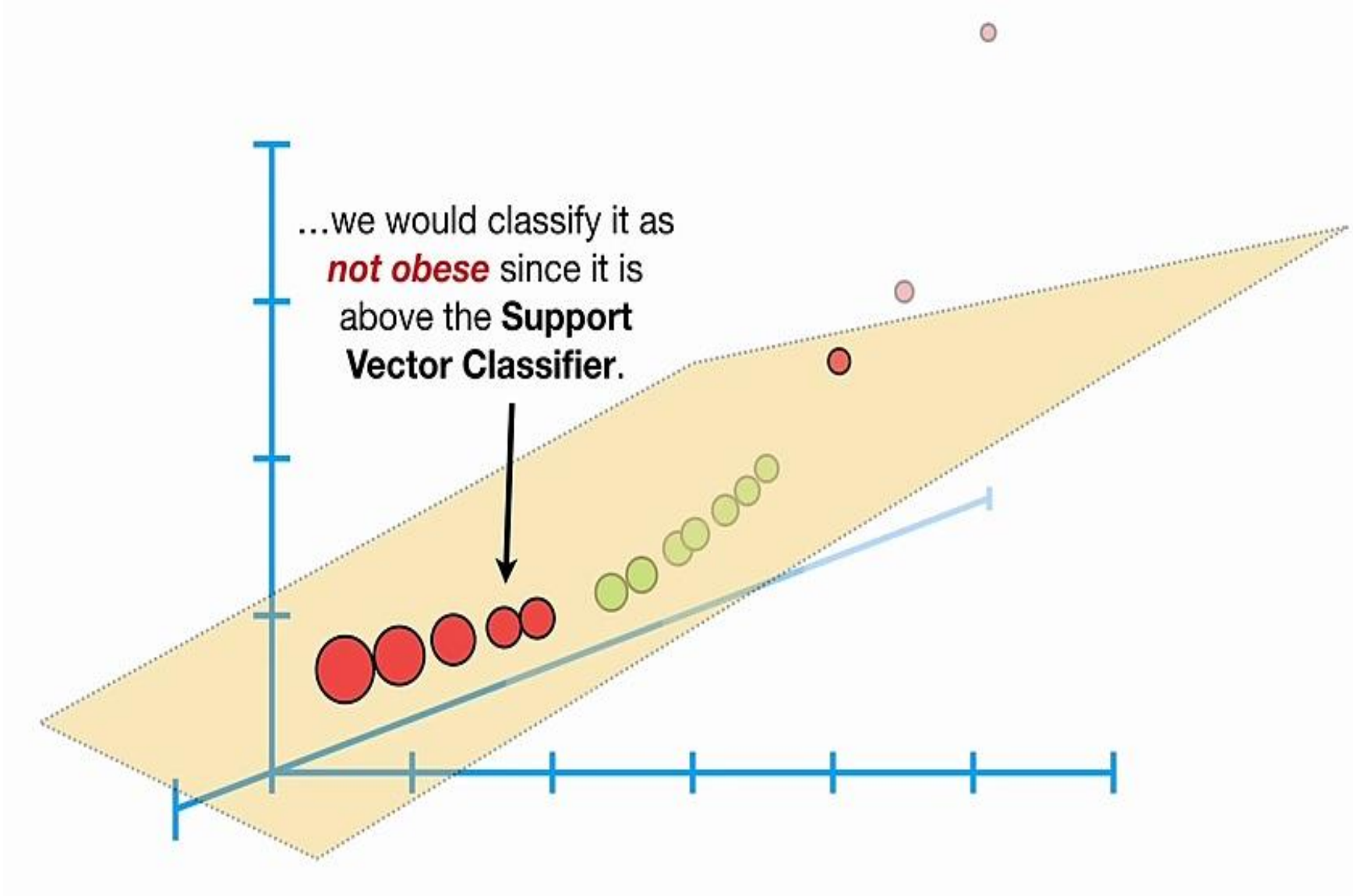

…and these circles are larger
in order to to appear closer,
and thus younger…
Height (cm):
Age
Mass (g):


...and these circles are
smaller in order to look
further away, and thus, older.
Height (cm):
Age
Mass (g):

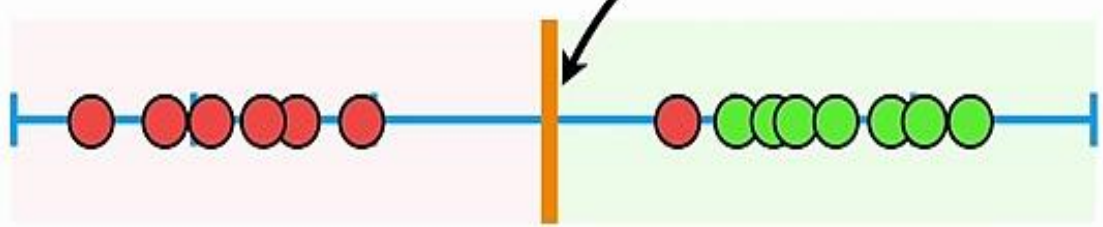

When the data are **3-Dimensional**,
the **Support Vector Classifier** forms
a plane, instead of a line...

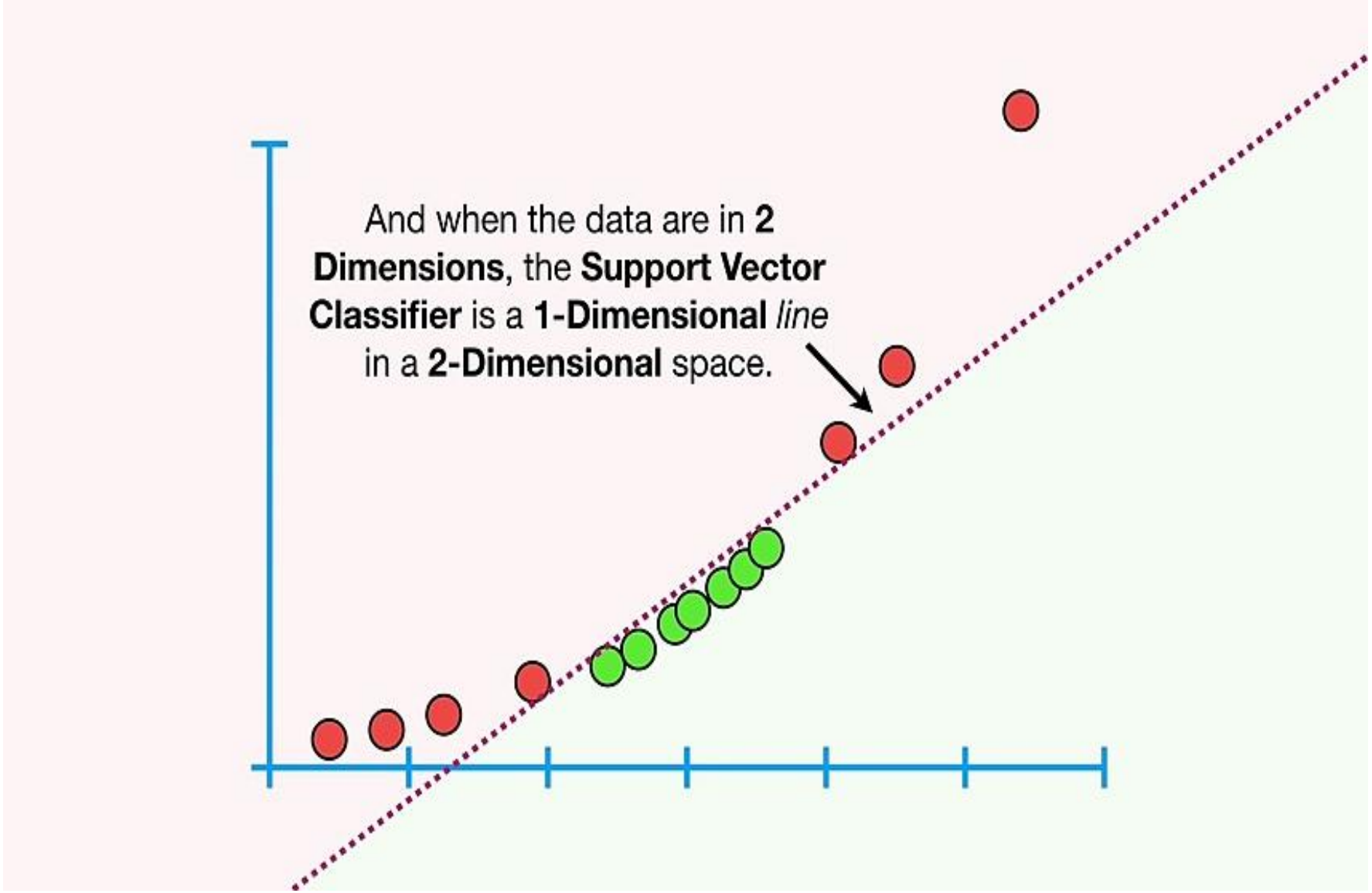

…and we classify new observations by determining which side of the plane they are on.

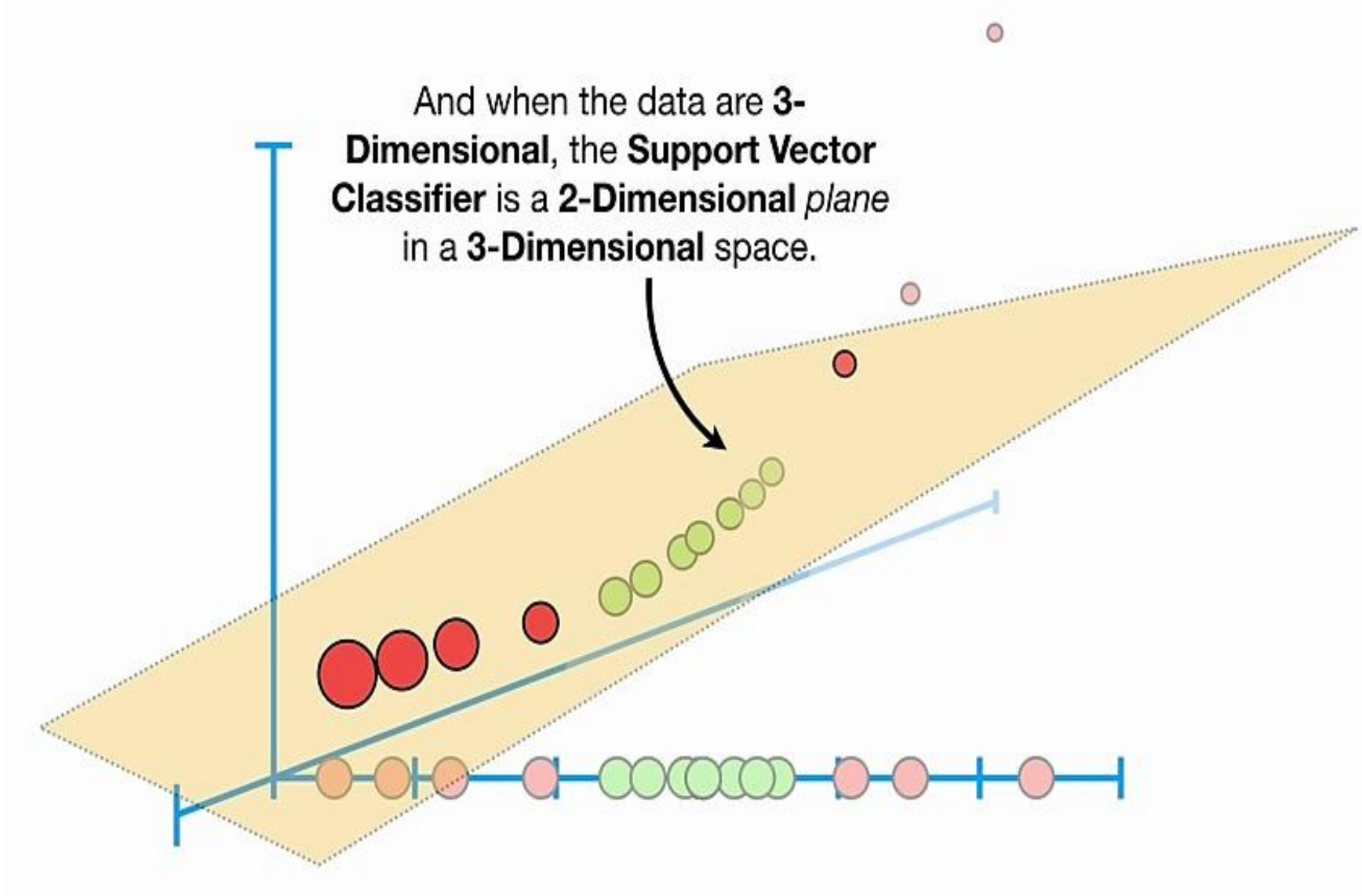

For example, if this were a new observation…


…we would classify it as
not obese since it is
above the Support
Vector Classifier.

But we know that when the data are **1-Dimensional**, the **Support Vector Classifier** is a single *point* on a **1-Dimensional** number line.



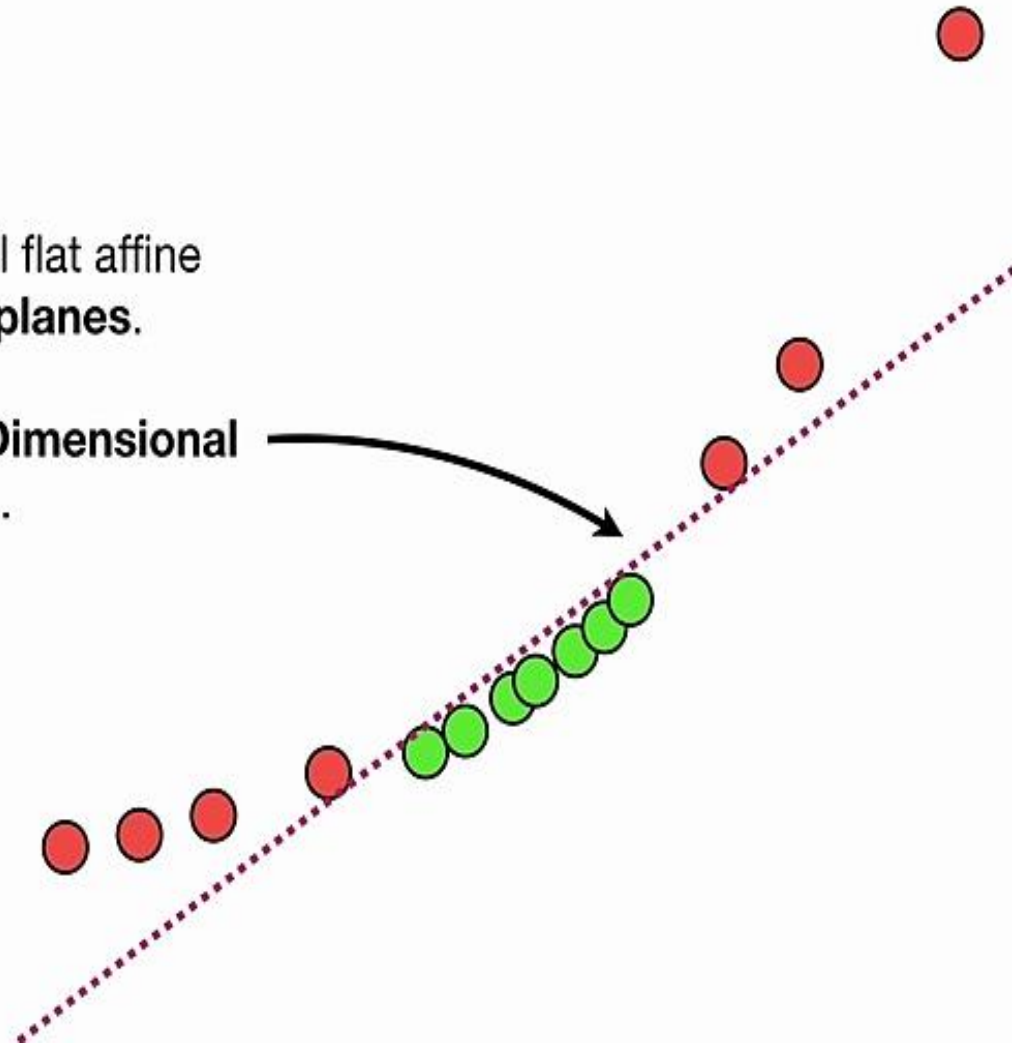

And when the data are in **2 Dimensions**, the **Support Vector Classifier** is a **1-Dimensional** *line* in a **2-Dimensional** space.


And when the data are **3-Dimensional**, the **Support Vector Classifier** is a **2-Dimensional** *plane* in a **3-Dimensional** space.

And when the data are in **4 or more Dimensions**, the **Support Vector Classifier** is a *hyperplane*.

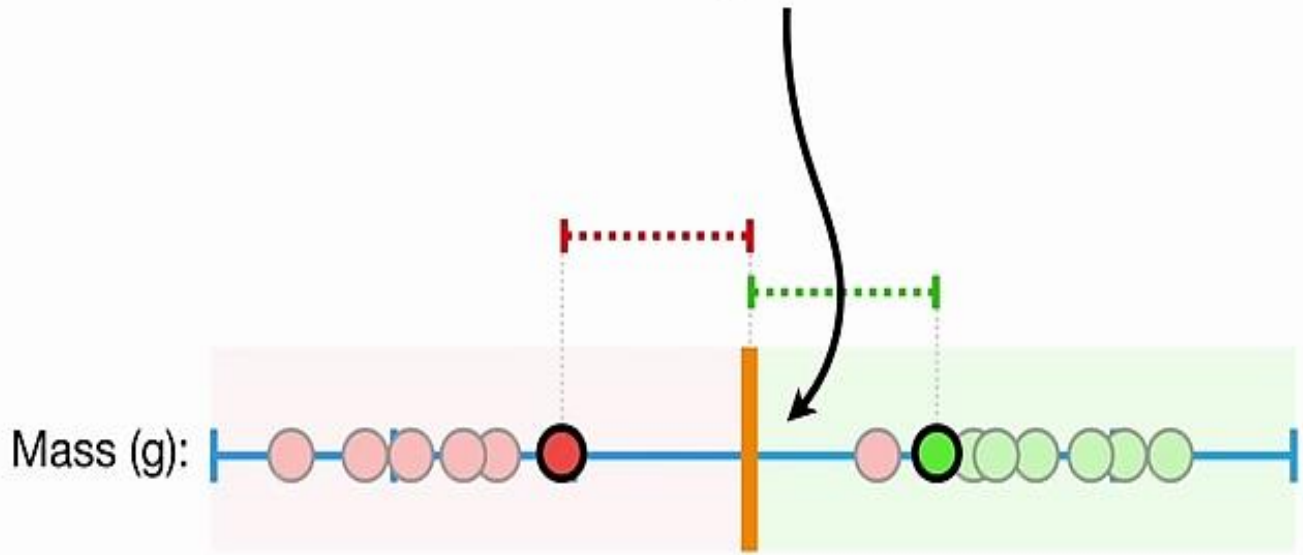
NOTE: Technically speaking, all flat affine subspaces are called **hyperplanes**.

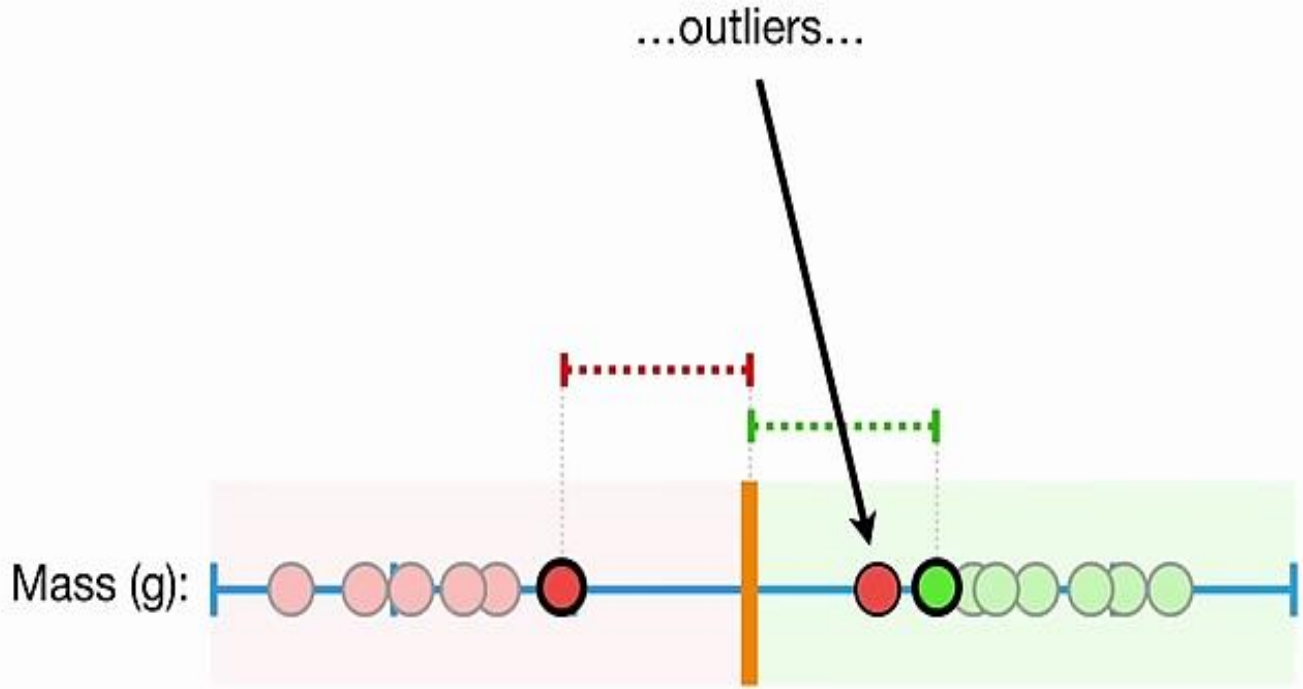
So, technically speaking, this **1-Dimensional** *line* is a **hyperplane**…

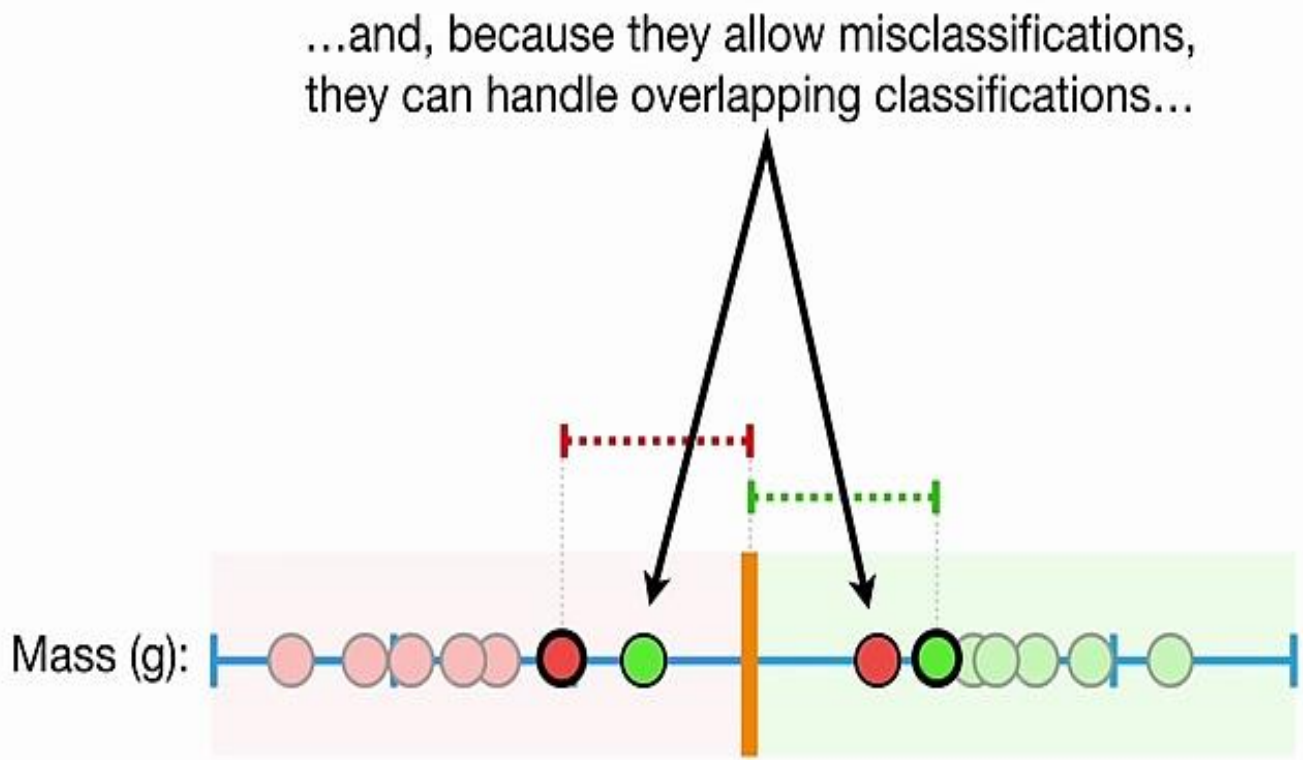


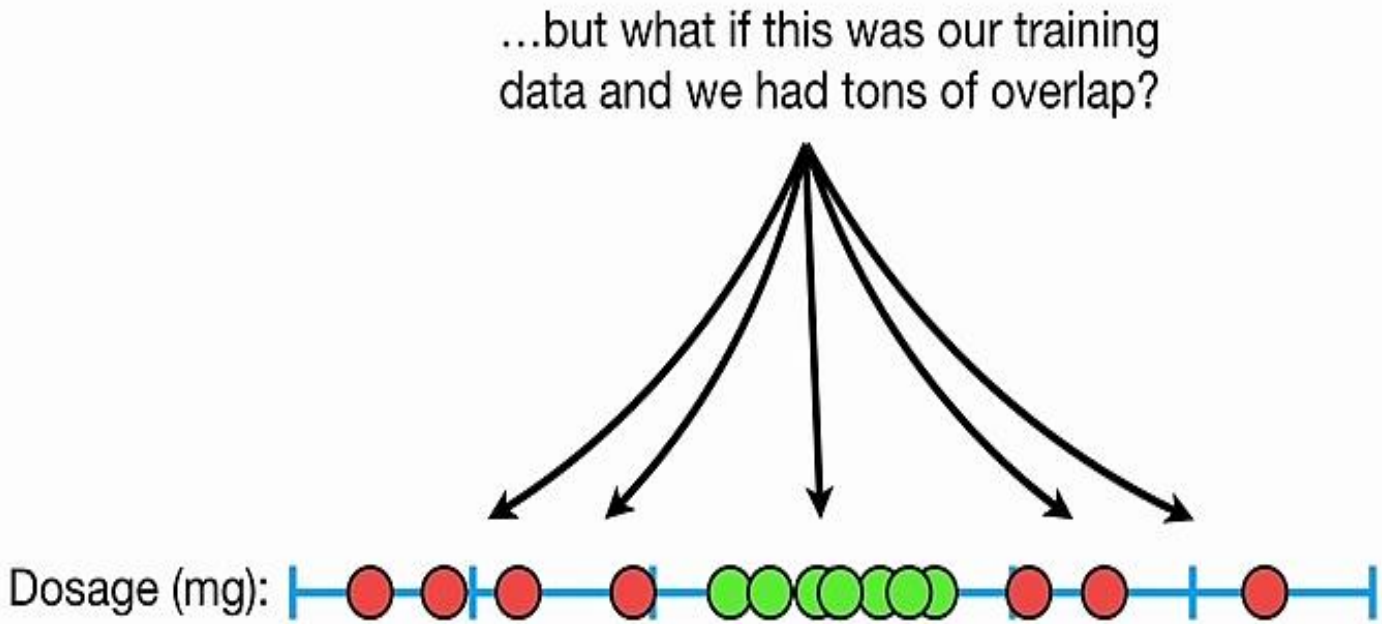
Non-linear SVM

Support Vector Classifiers seem pretty cool because they can handle...

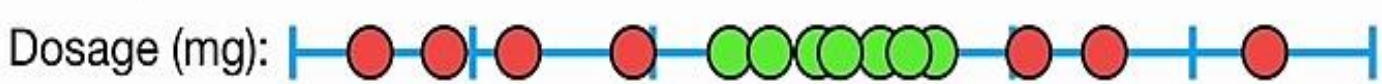


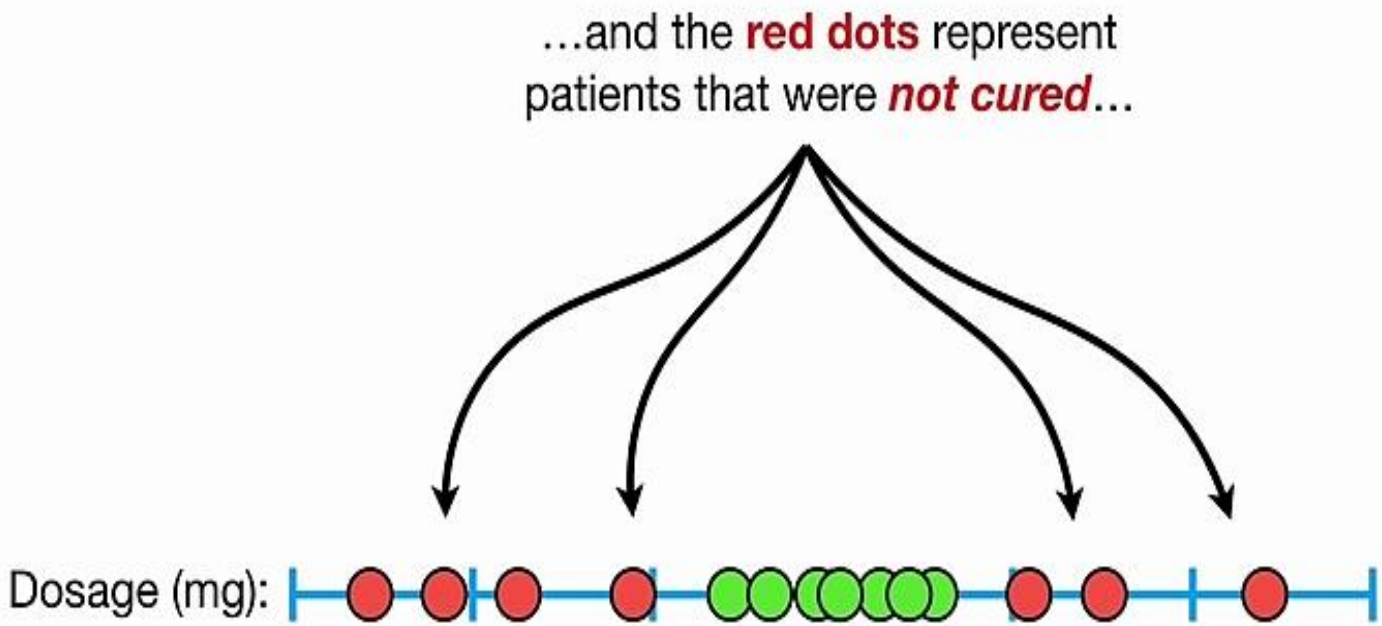

…outliers…
Mass (g):

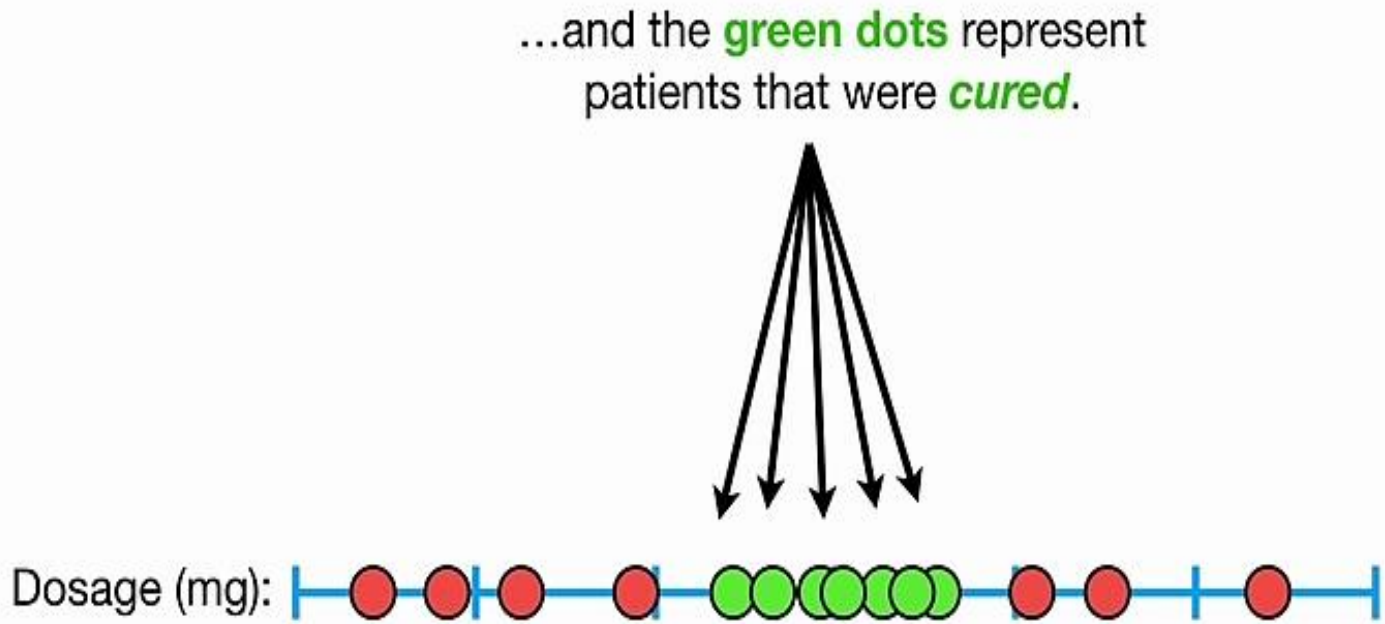

…and, because they allow misclassifications,
they can handle overlapping classifications…
Mass (g):

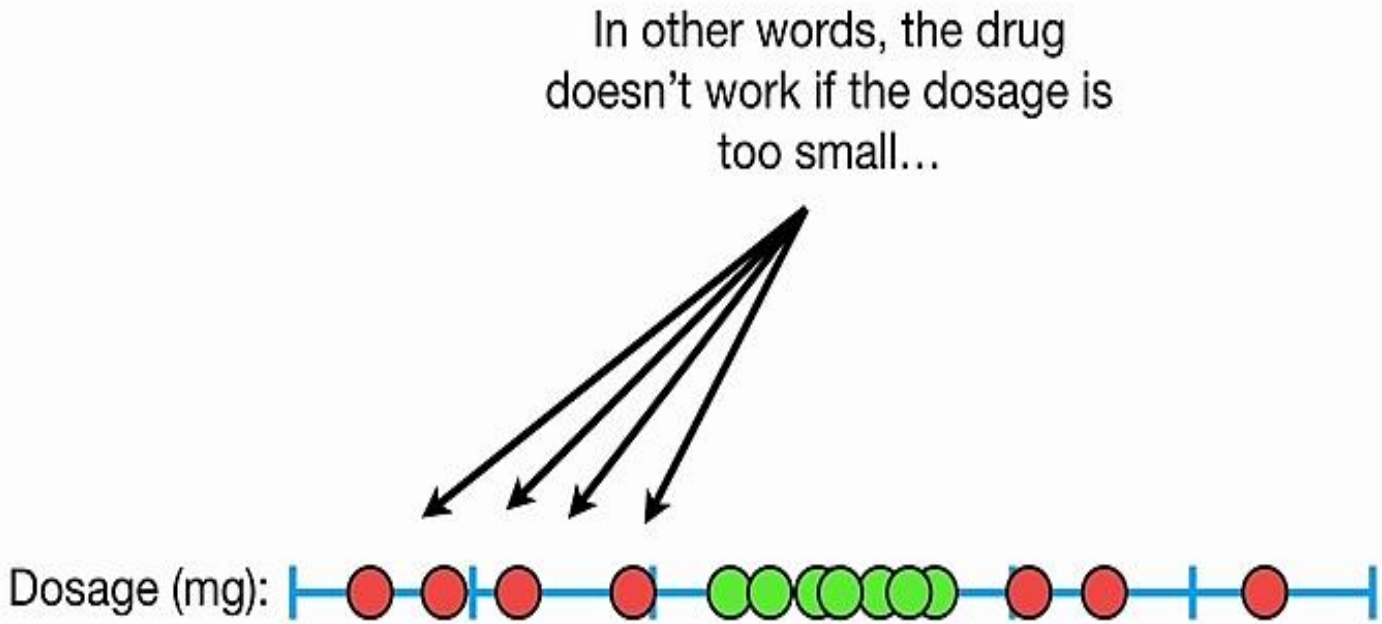

…but what if this was our training data and we had tons of overlap?
Dosage (mg):

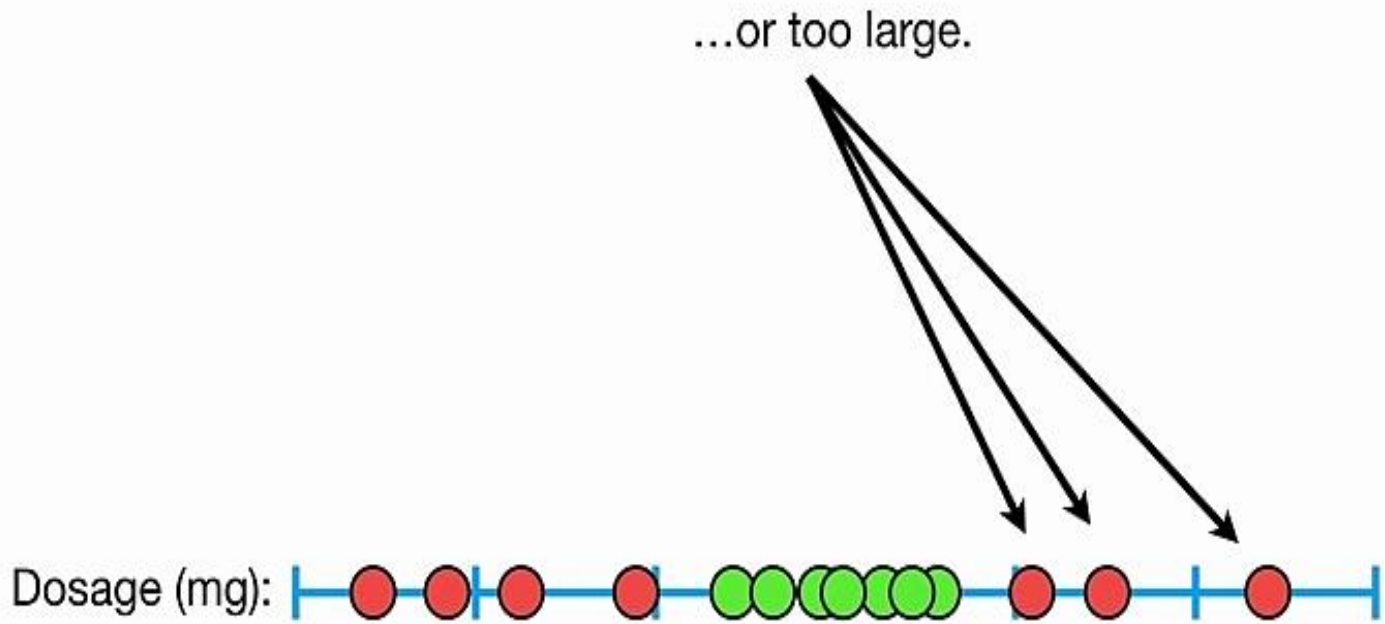
In this new example, with tons of overlap, we are now looking at **Drug Dosages**…

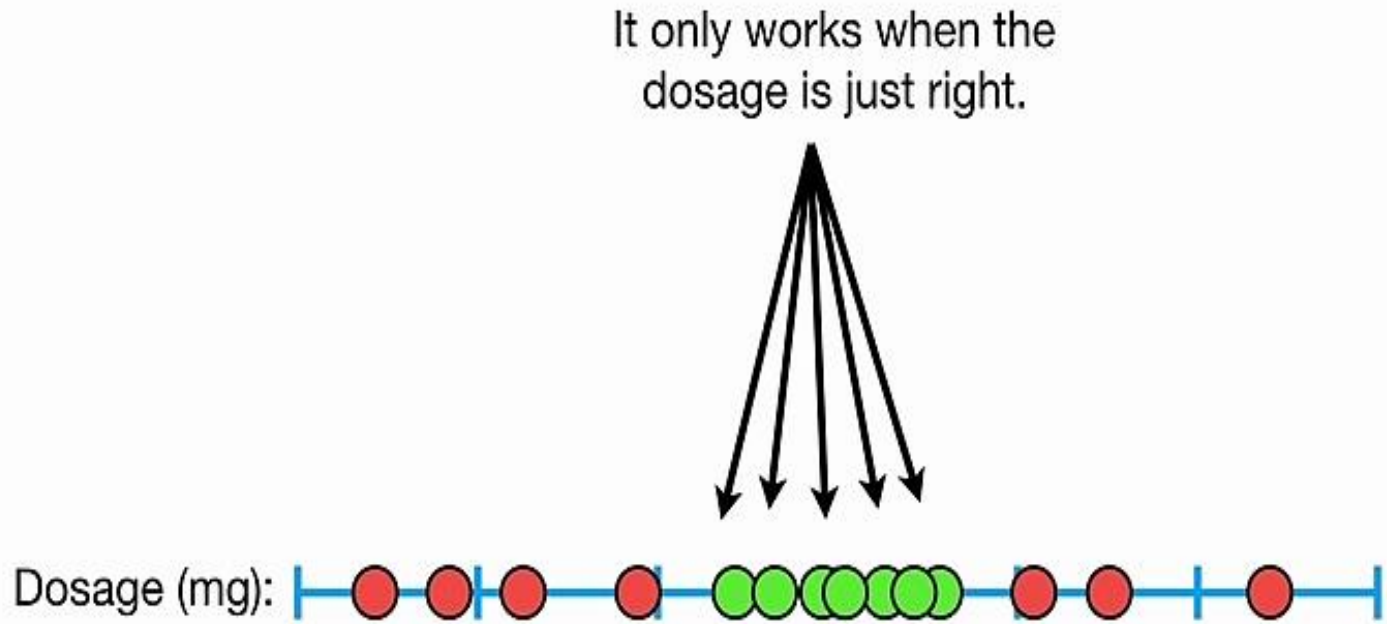


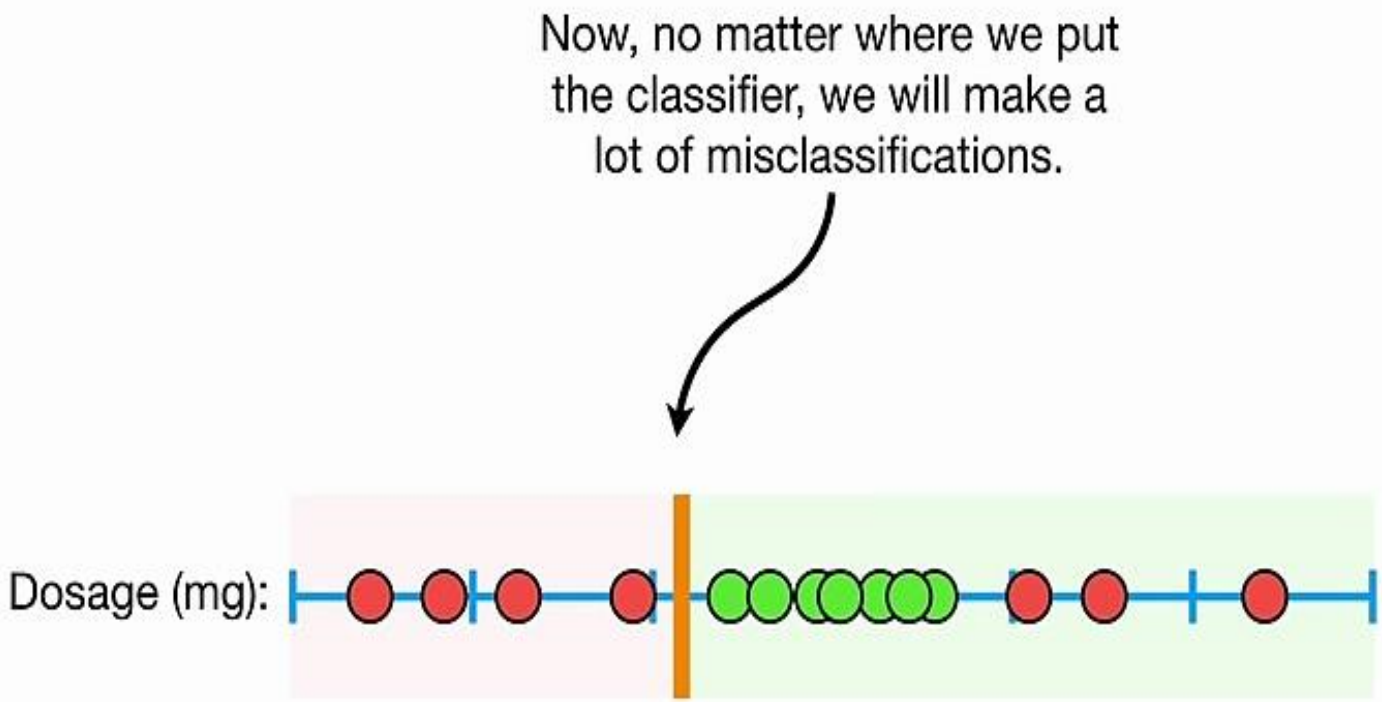

…and the red dots represent
patients that were not cured…
Dosage (mg):

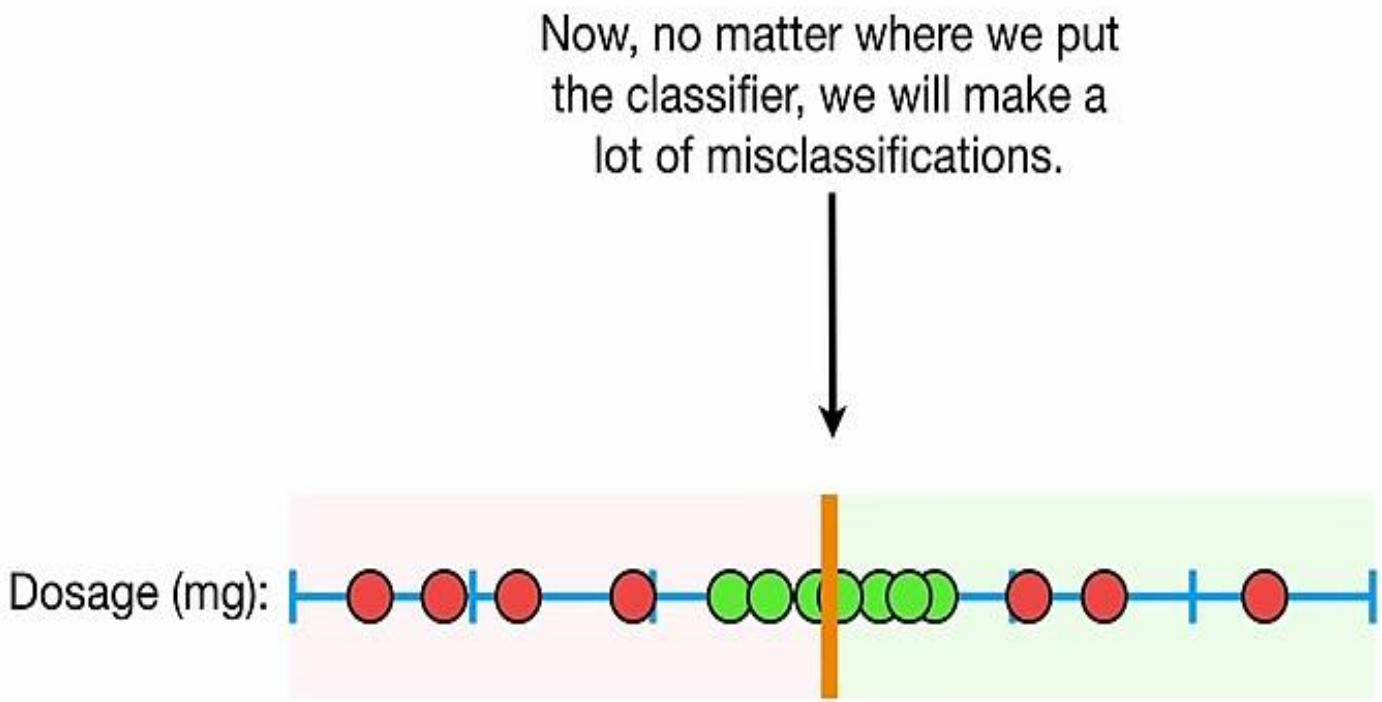

...and the green dots represent
patients that were cured.
Dosage (mg):

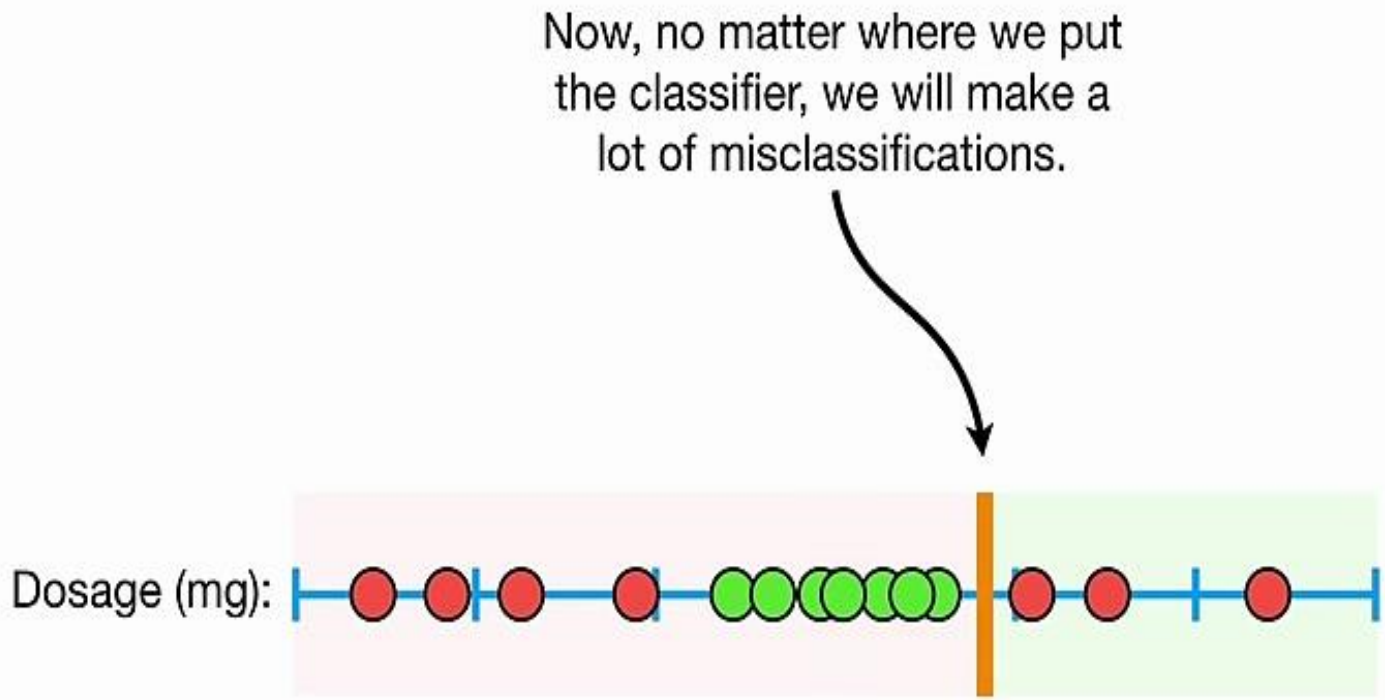

In other words, the drug
doesn't work if the dosage is
too small…
Dosage (mg):


...or too large.
Dosage (mg):

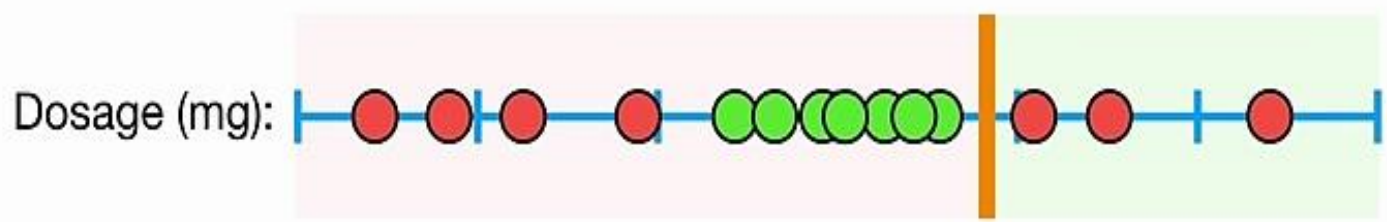

It only works when the
dosage is just right.
Dosage (mg):


Now, no matter where we put the classifier, we will make a lot of misclassifications.
Dosage (mg):

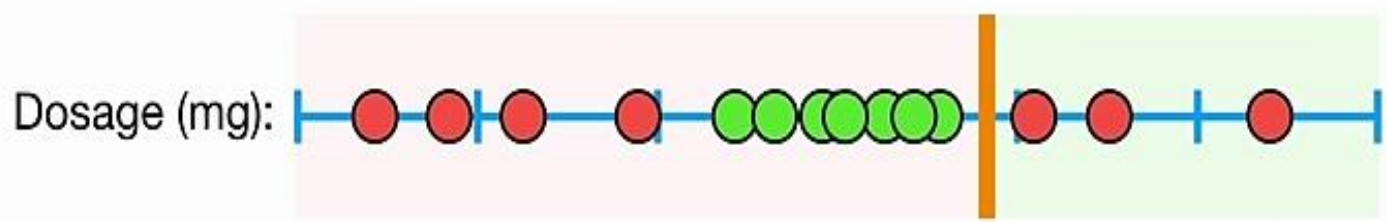

Now, no matter where we put
the classifier, we will make a
lot of misclassifications.
Dosage (mg):

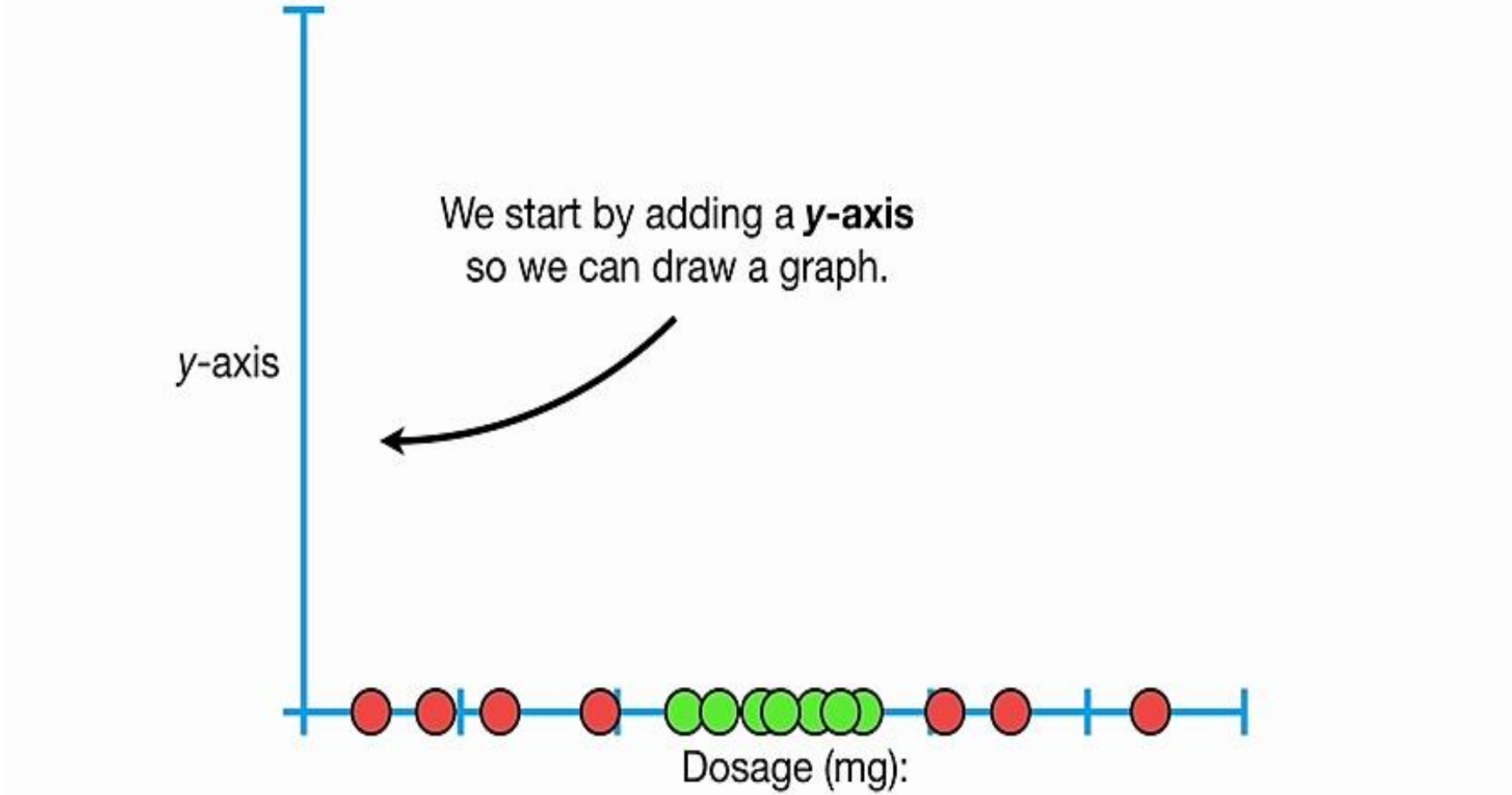

Now, no matter where we put the classifier, we will make a lot of misclassifications.
Dosage (mg):

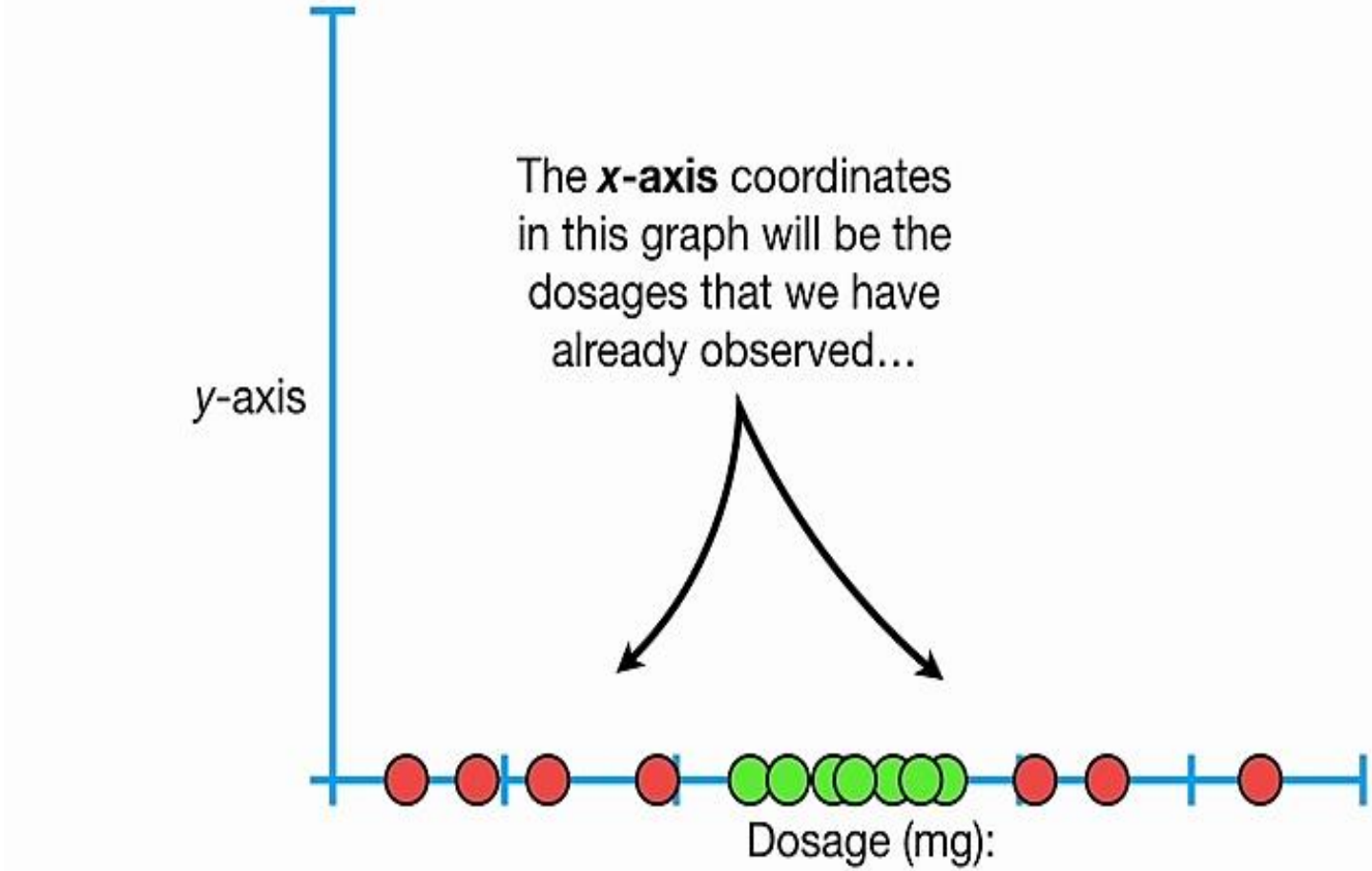
So **Support Vector Classifiers** are are only semi-cool, since they don't perform well with this type of data.

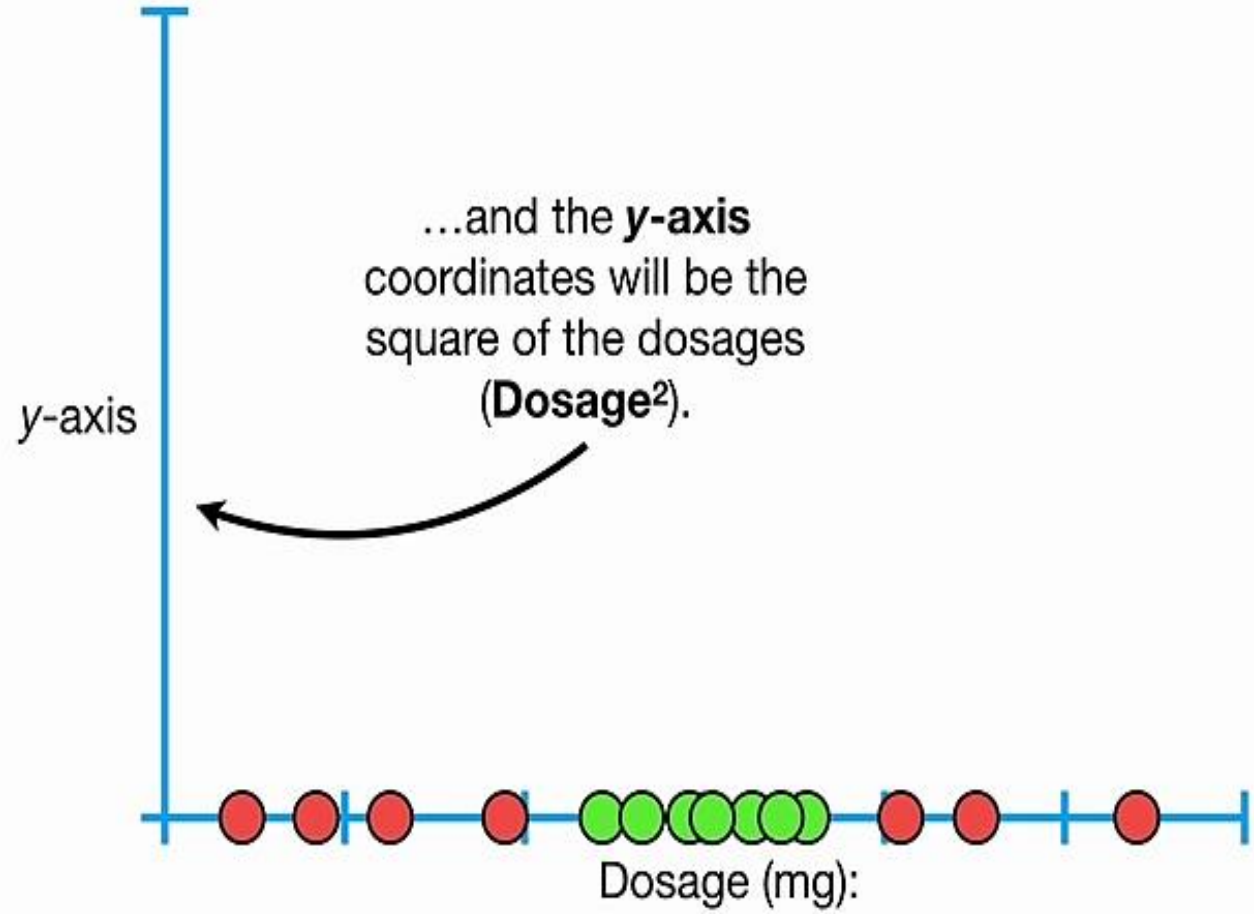


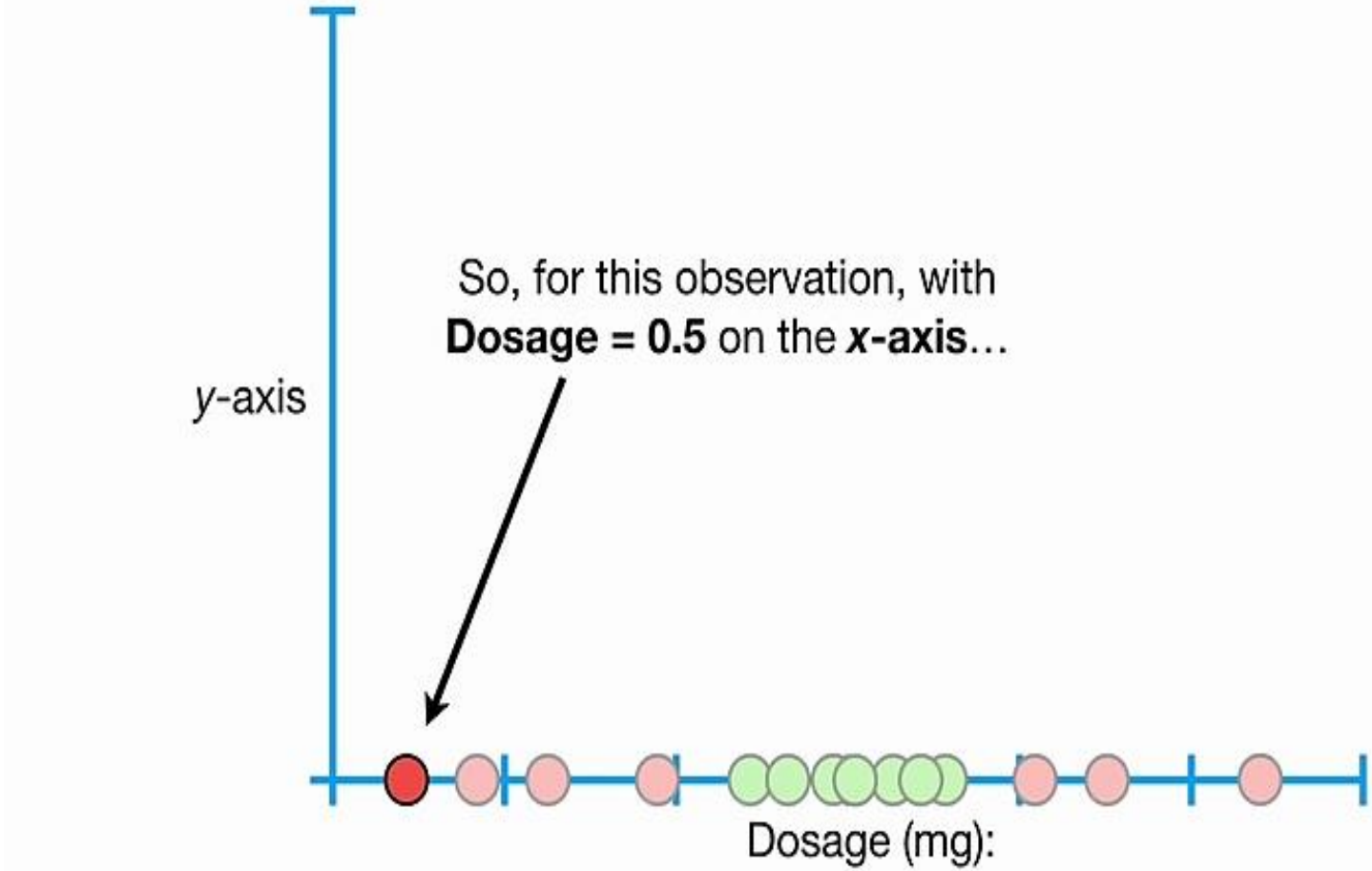
Can we do better than **Maximal Margin Classifiers** and **Support Vector Classifiers**?

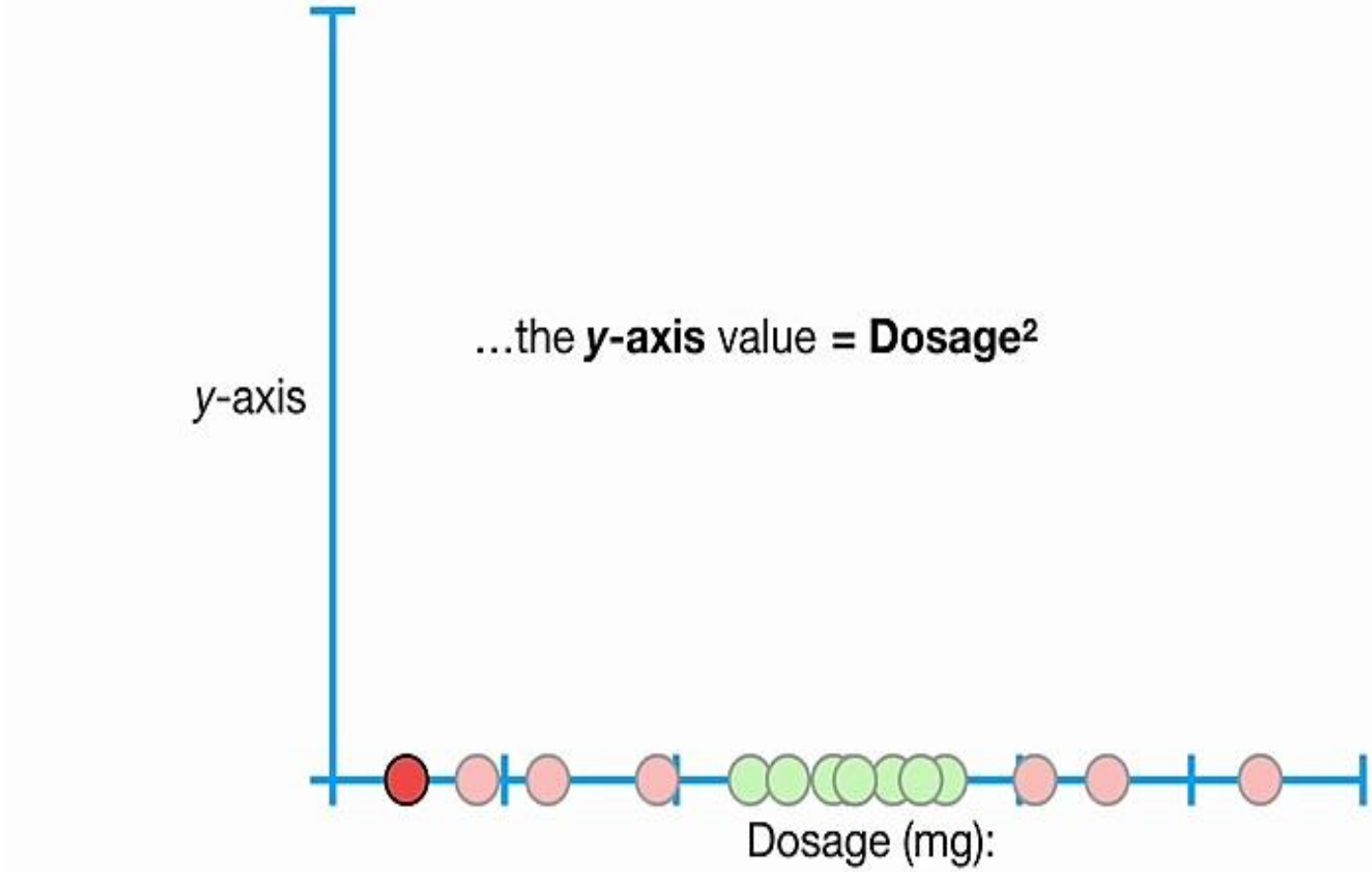


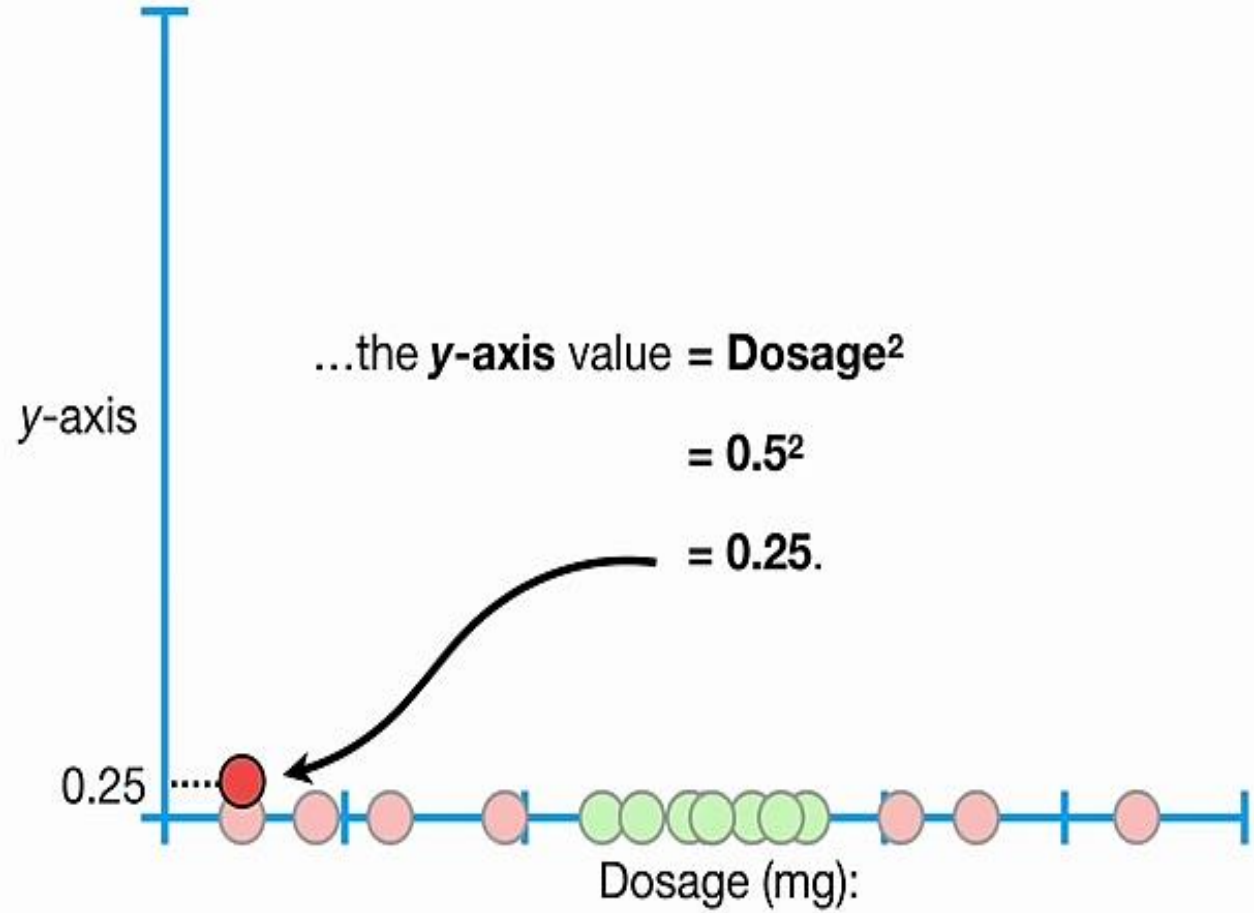

We start by adding a **y-axis**
so we can draw a graph.
y-axis
Dosage (mg):

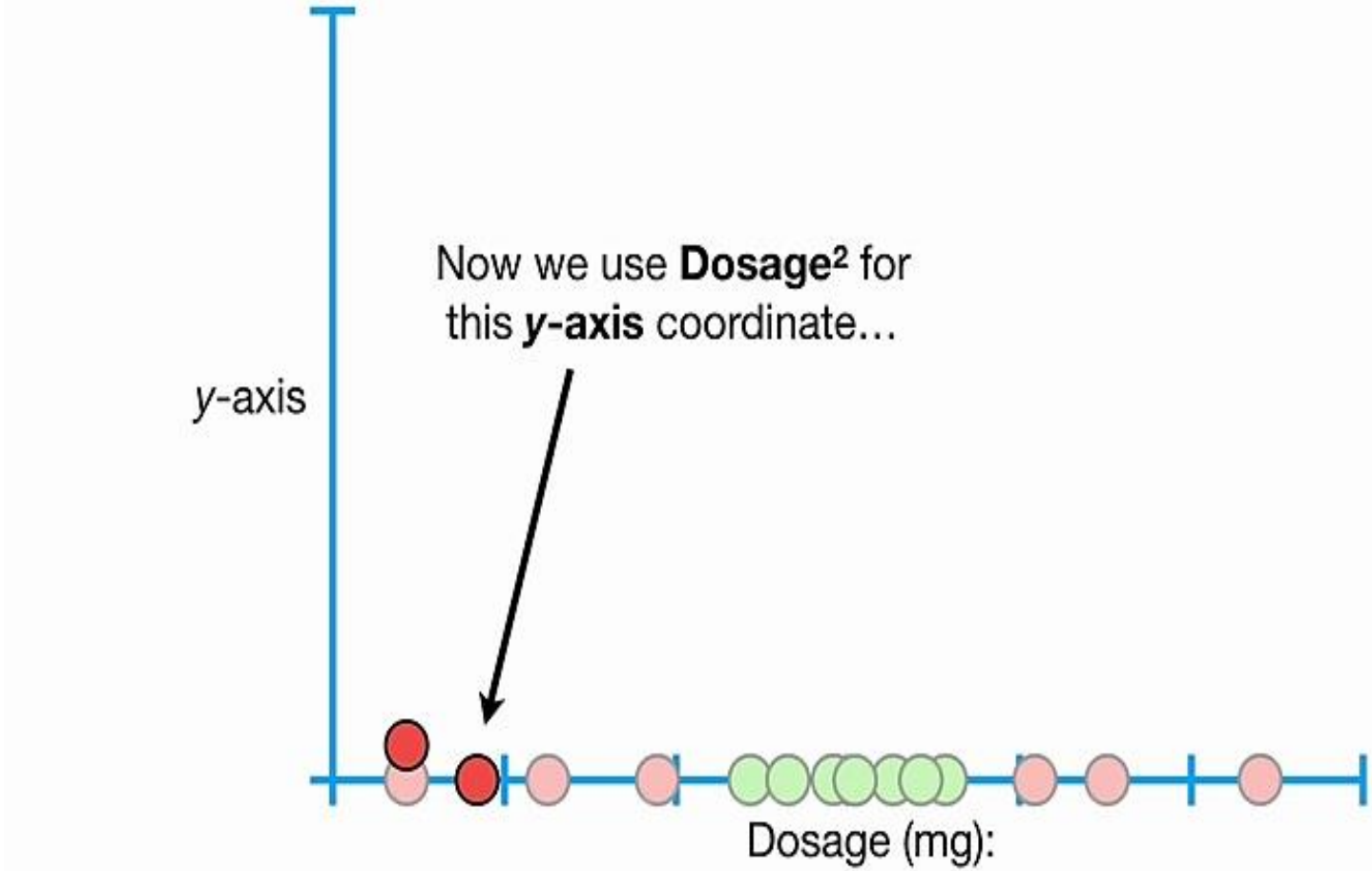

The x-axis coordinates in this graph will be the dosages that we have already observed…
y-axis
Dosage (mg):

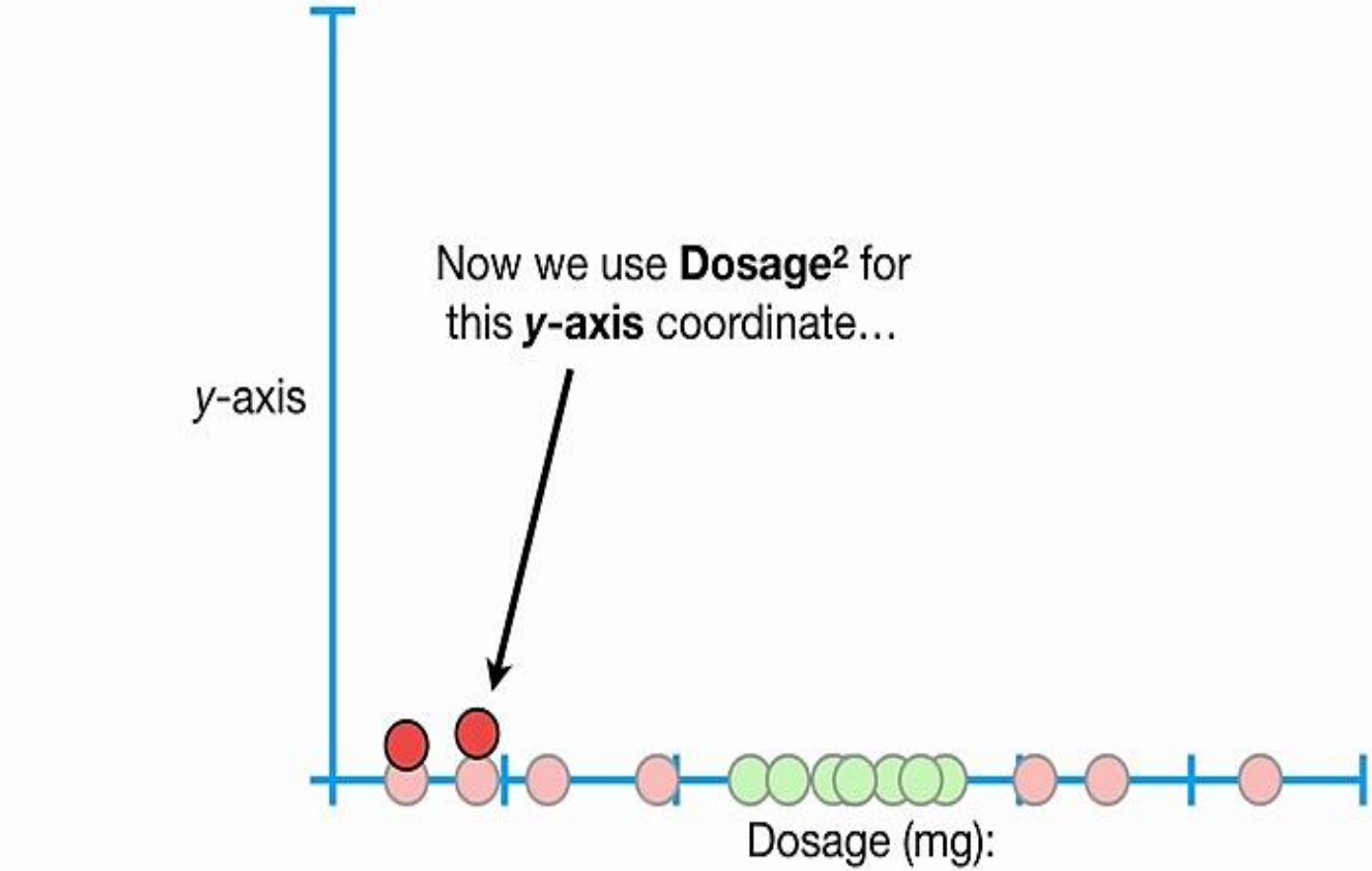

…and the **y-axis** coordinates will be the square of the dosages (**Dosage²**).
y-axis
Dosage (mg):

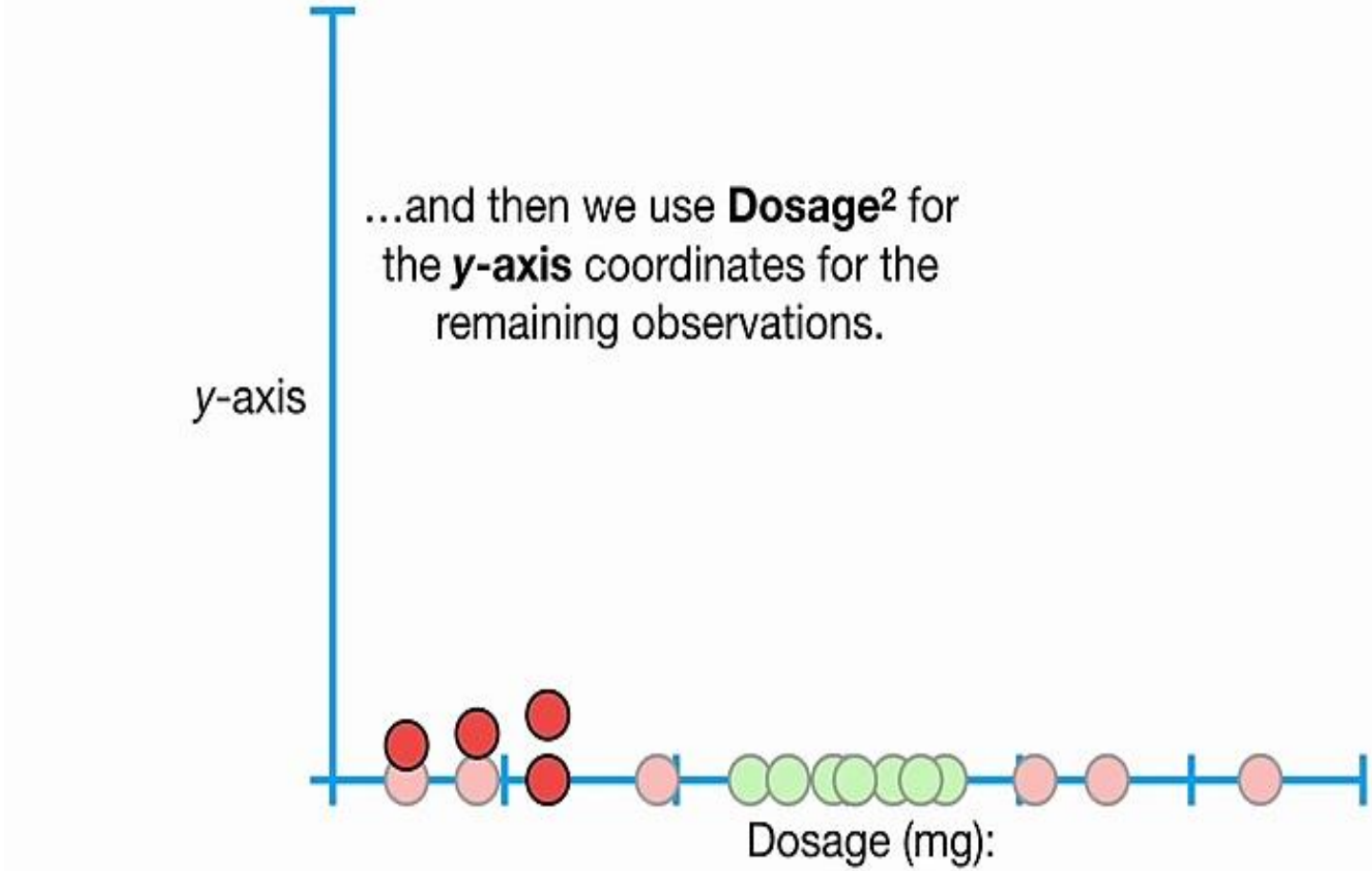

So, for this observation, with
Dosage = 0.5 on the ***x*-axis**…
y-axis
Dosage (mg):

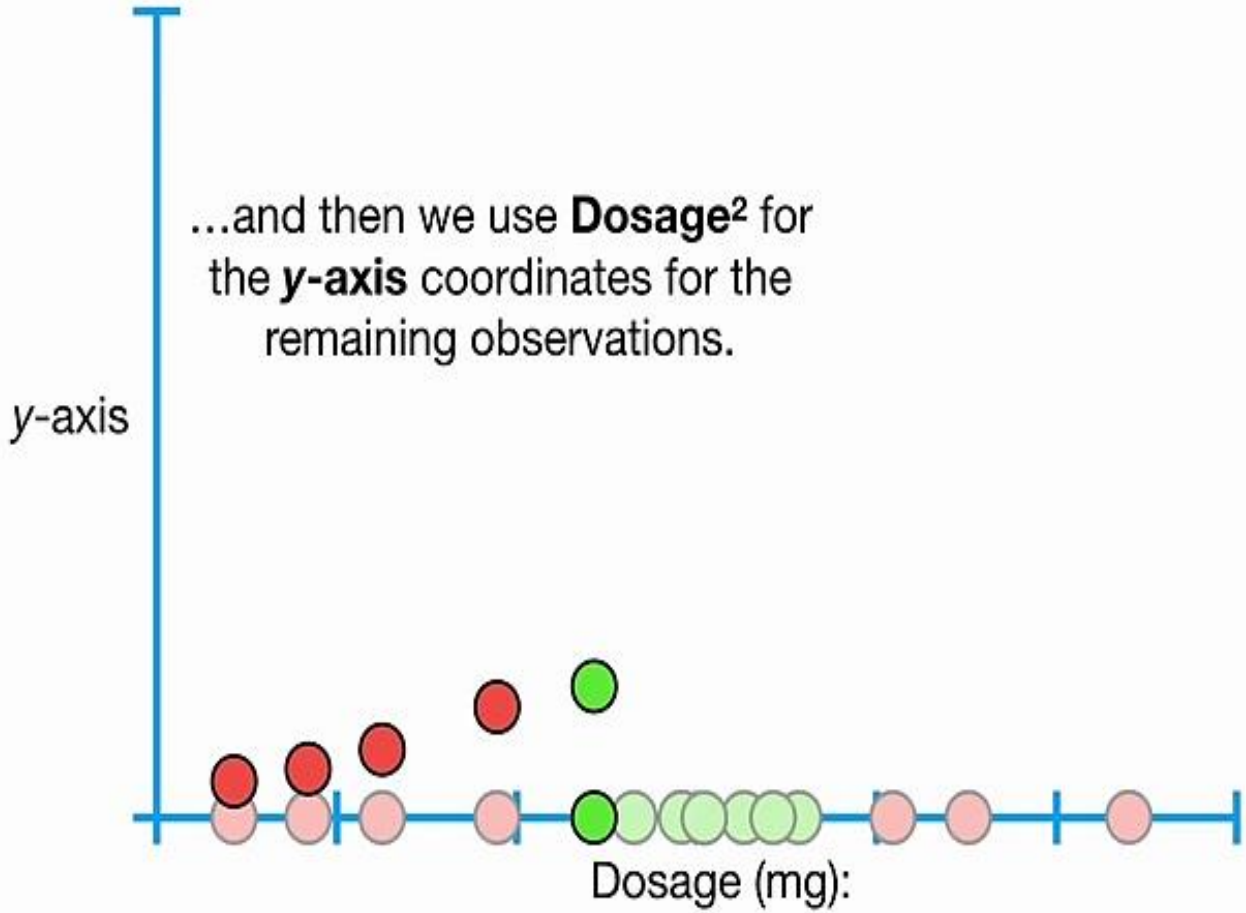

…the **y-axis** value = **Dosage²**
y-axis
Dosage (mg):

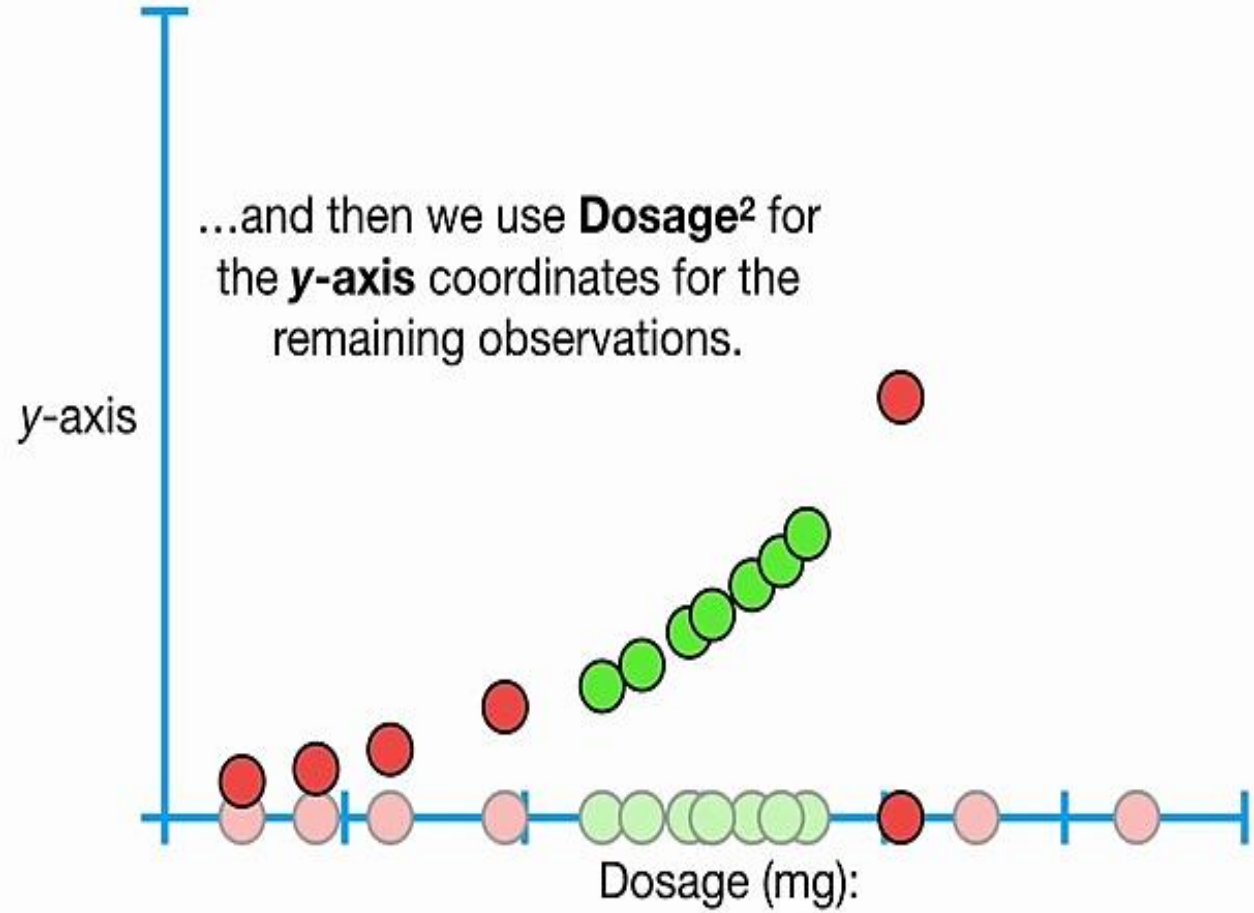

y-axis
…the y-axis value = Dosage²
= 0.5²
= 0.25.
0.25
Dosage (mg):

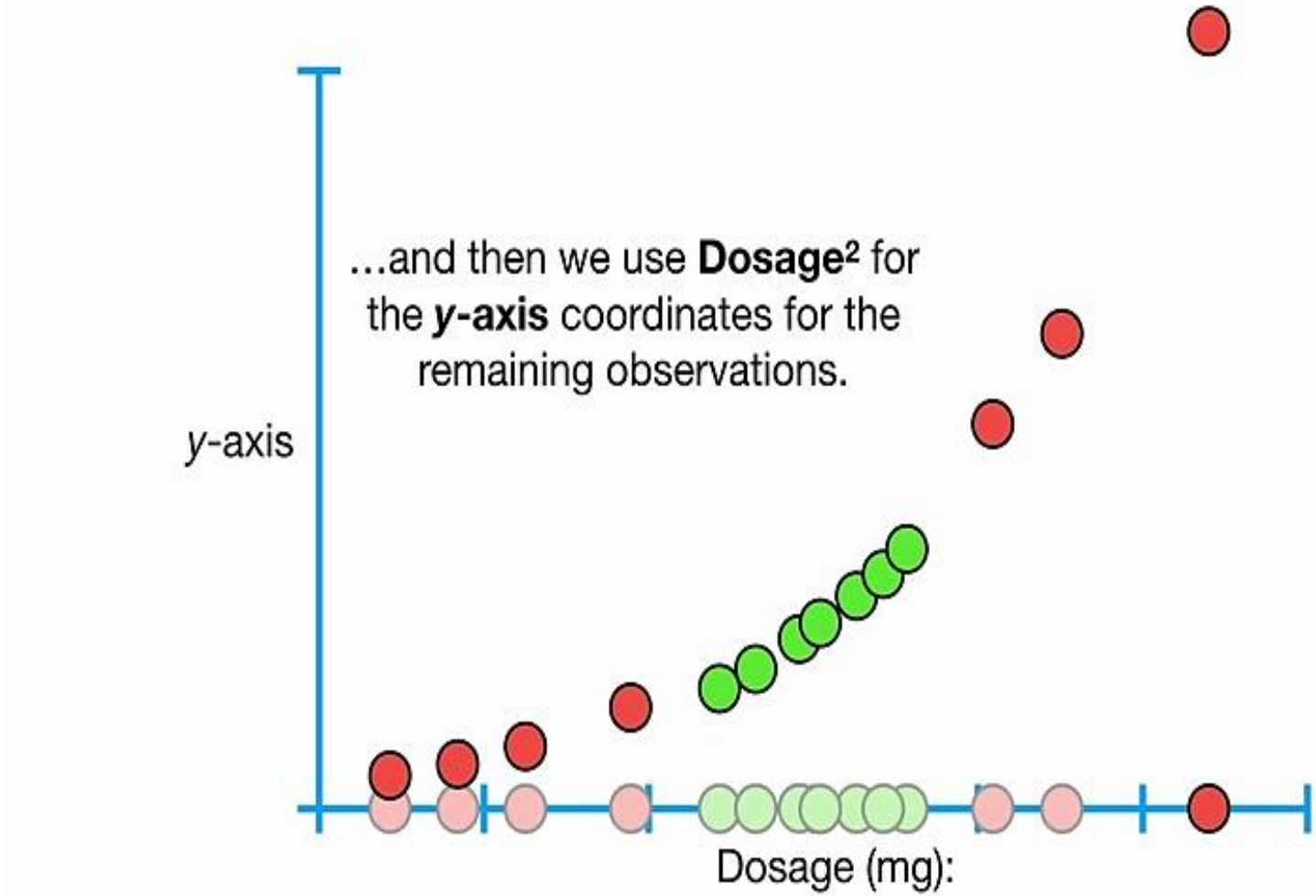

Now we use **Dosage²** for this ***y*-axis** coordinate…
y-axis
Dosage (mg):

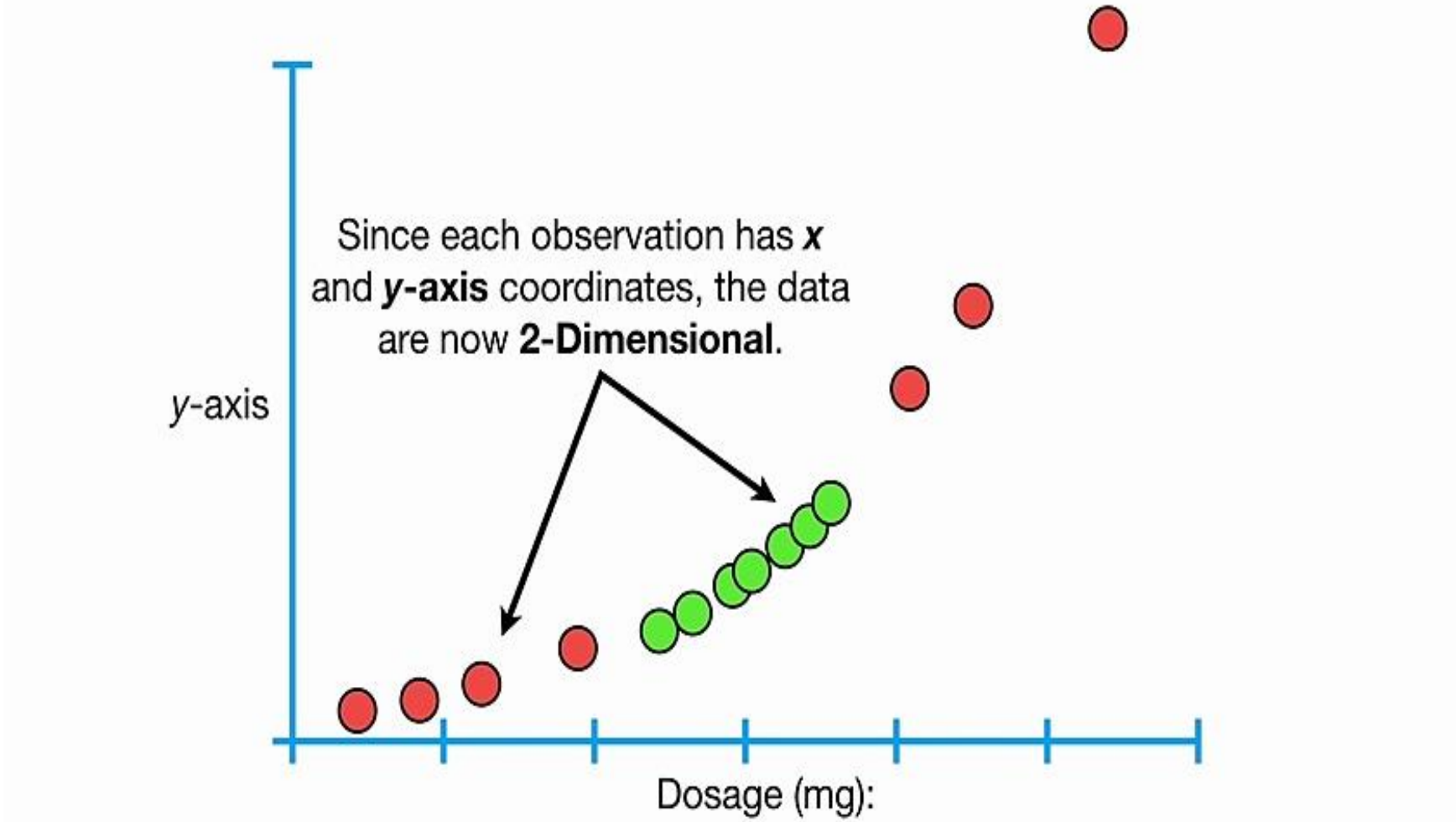

Now we use **Dosage²** for this ***y*-axis** coordinate…
y-axis
Dosage (mg):

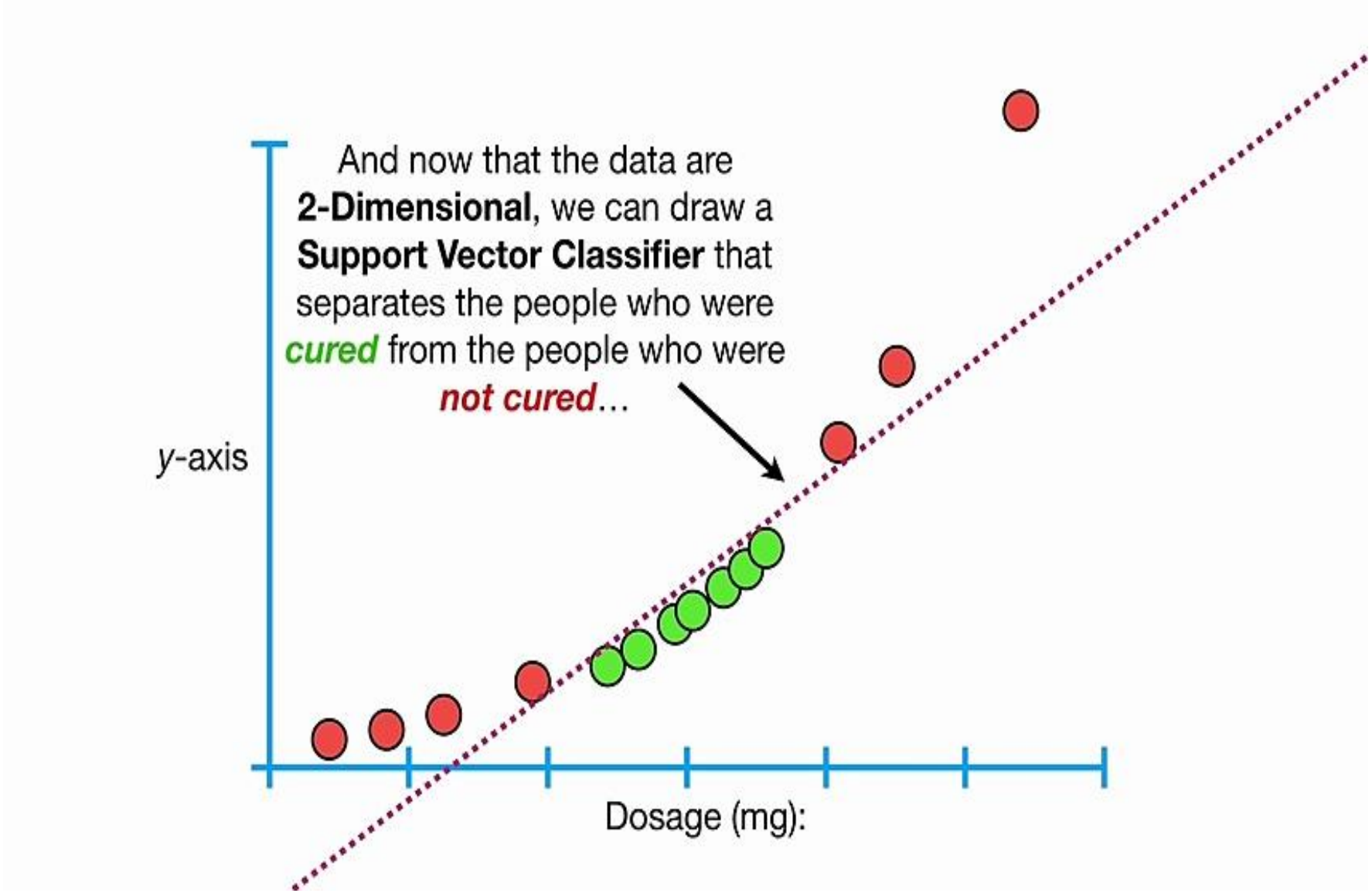

...and then we use **Dosage²** for the ***y*-axis** coordinates for the remaining observations.
y-axis
Dosage (mg):

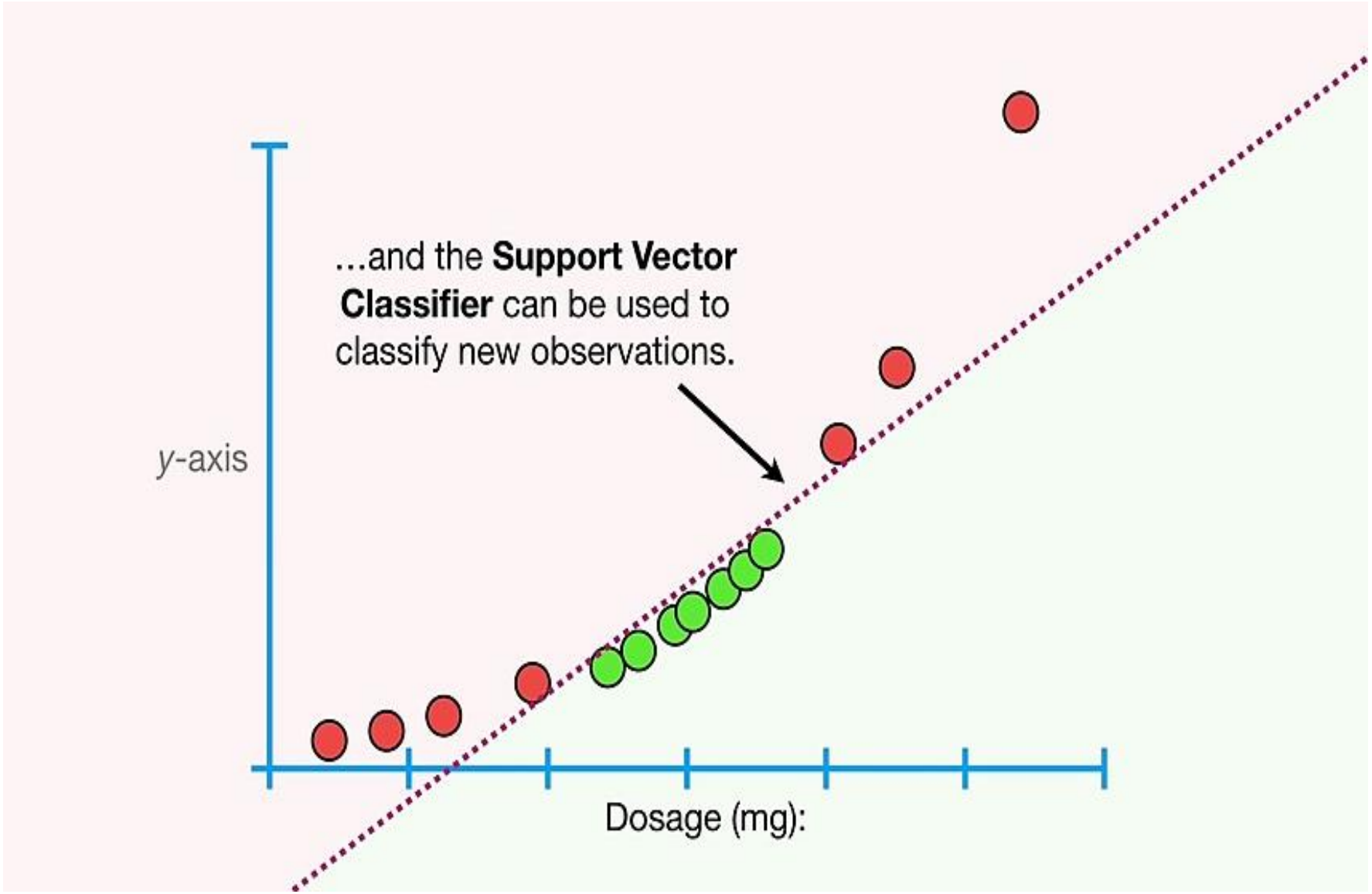

...and then we use **Dosage²** for the ***y*-axis** coordinates for the remaining observations.
y-axis
Dosage (mg):

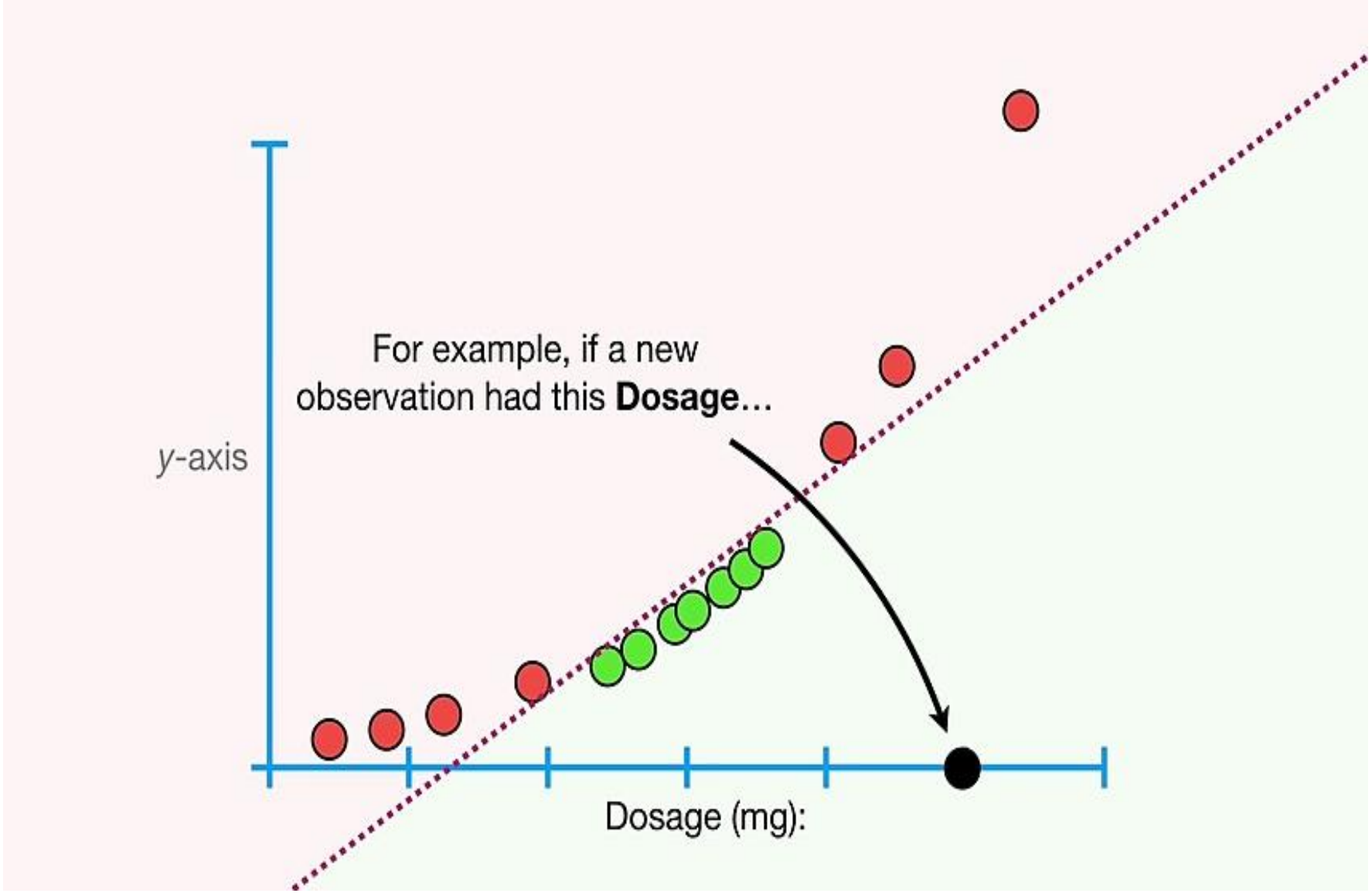

...and then we use **Dosage²** for the ***y*-axis** coordinates for the remaining observations.
y-axis
Dosage (mg):

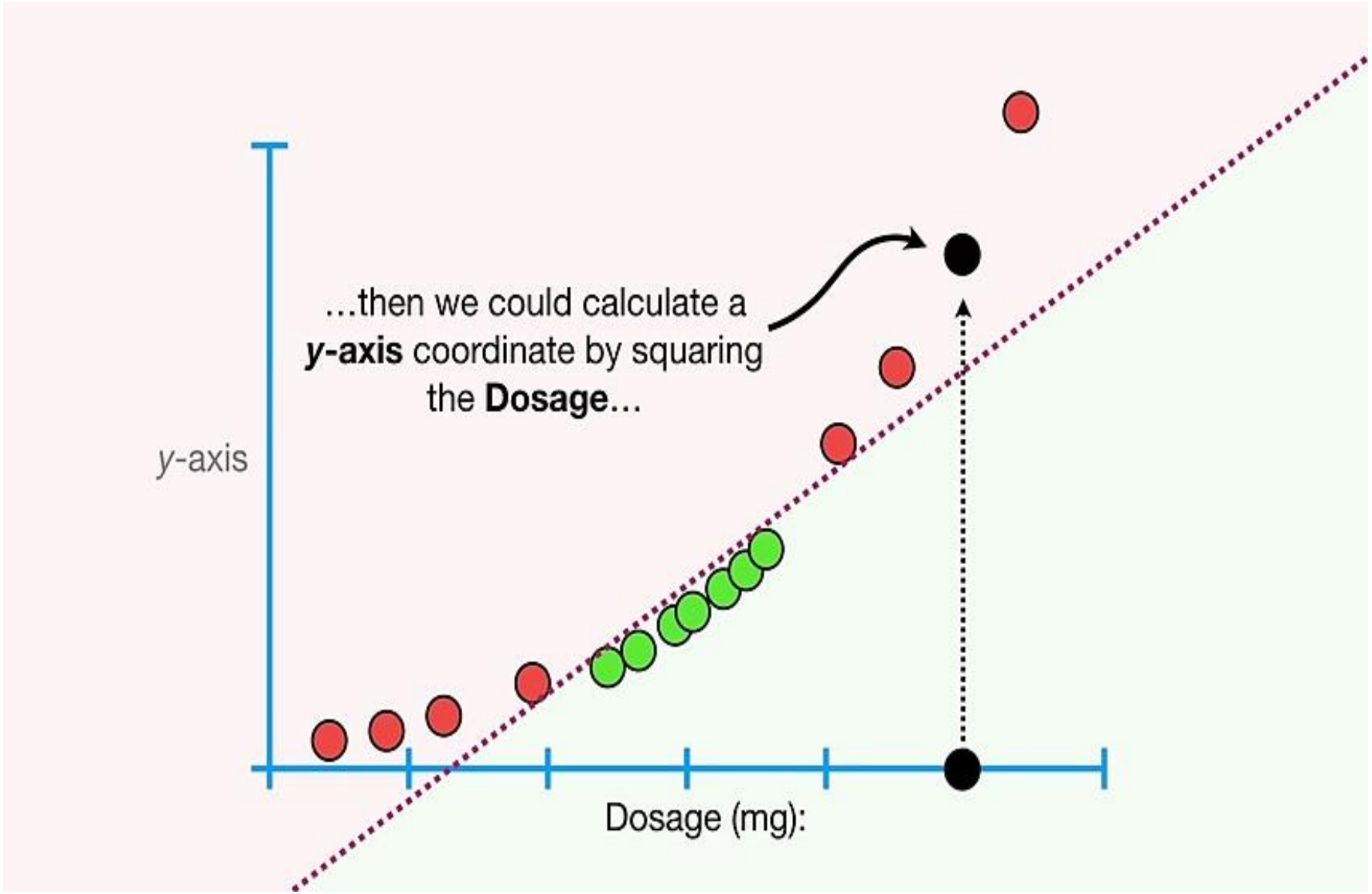

...and then we use **Dosage²** for the ***y*-axis** coordinates for the remaining observations.
y-axis
Dosage (mg):

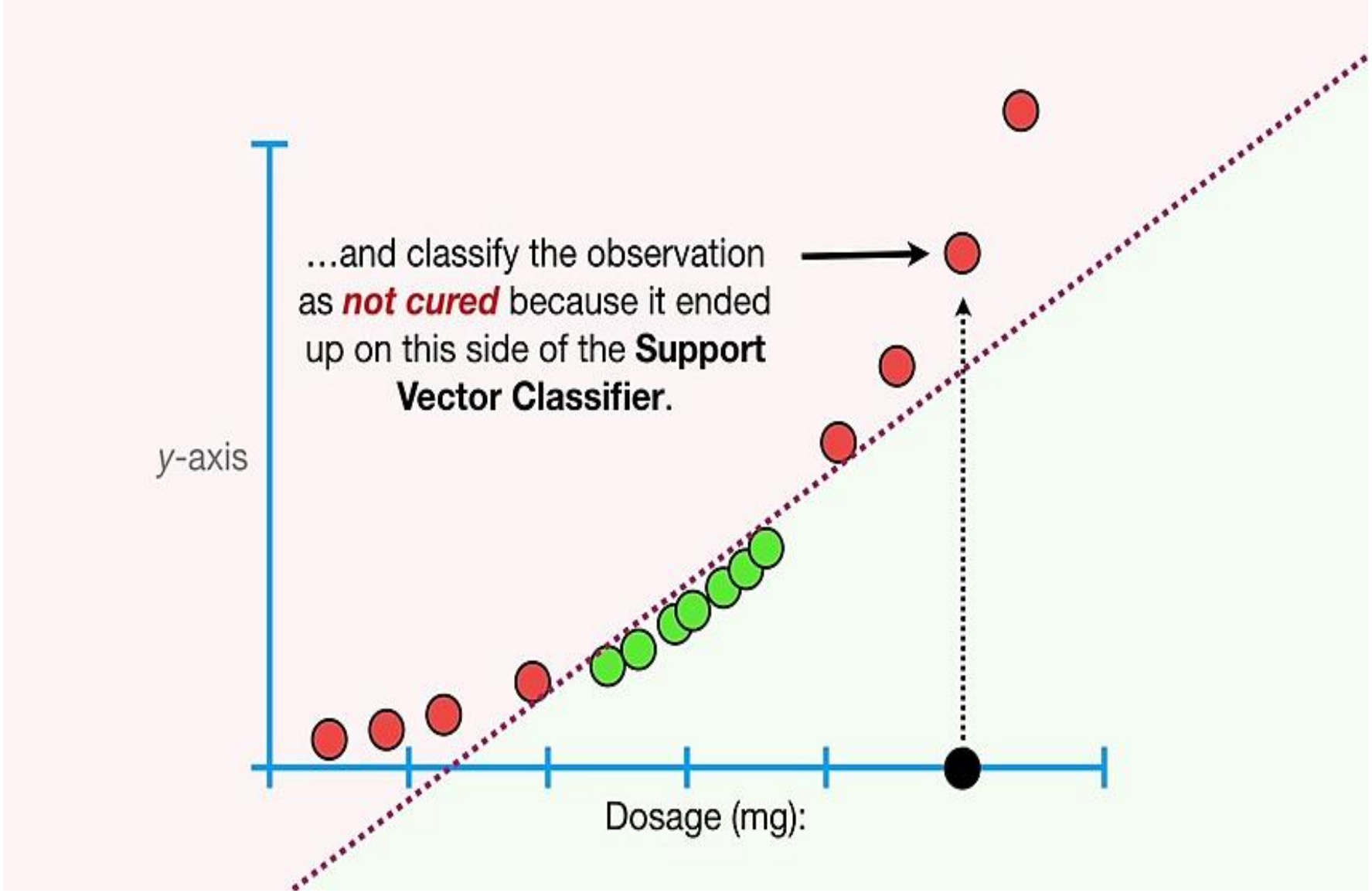

Since each observation has x and y-axis coordinates, the data are now 2-Dimensional.
y-axis
Dosage (mg):

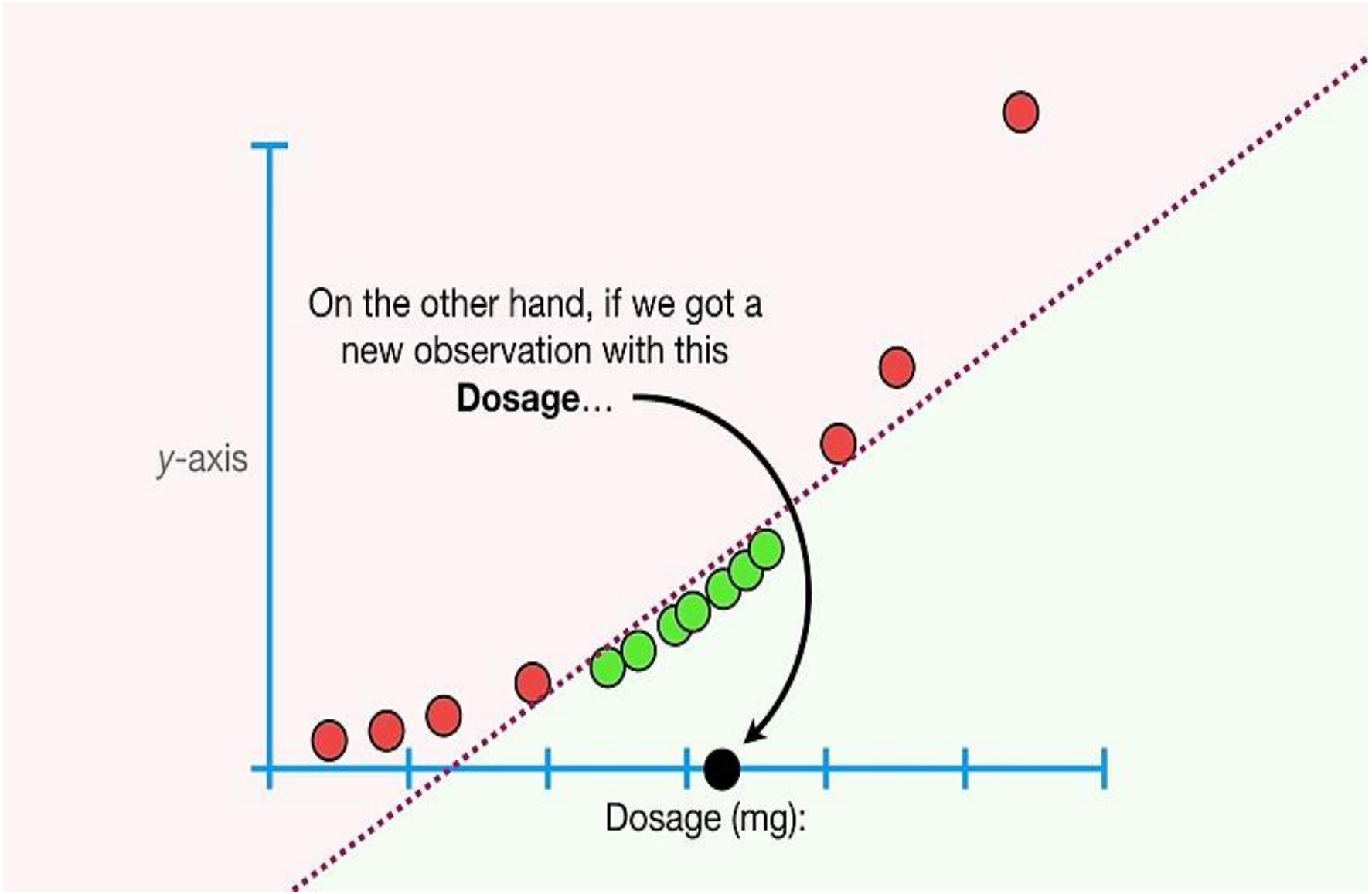

And now that the data are
2-Dimensional, we can draw a
Support Vector Classifier that
separates the people who were
cured from the people who were
not cured…
y-axis
Dosage (mg):

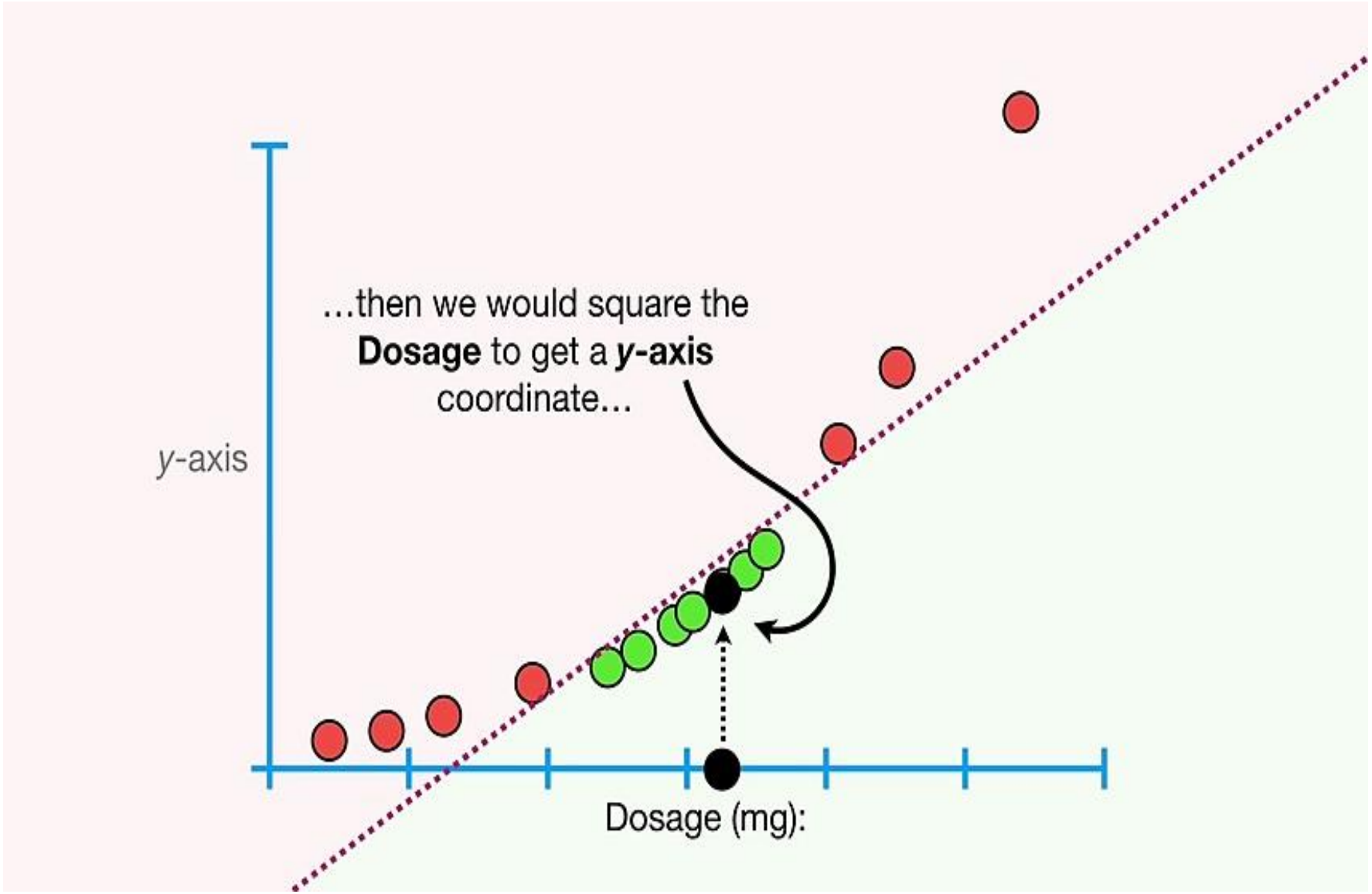

...and the **Support Vector Classifier** can be used to classify new observations.
y-axis
Dosage (mg):

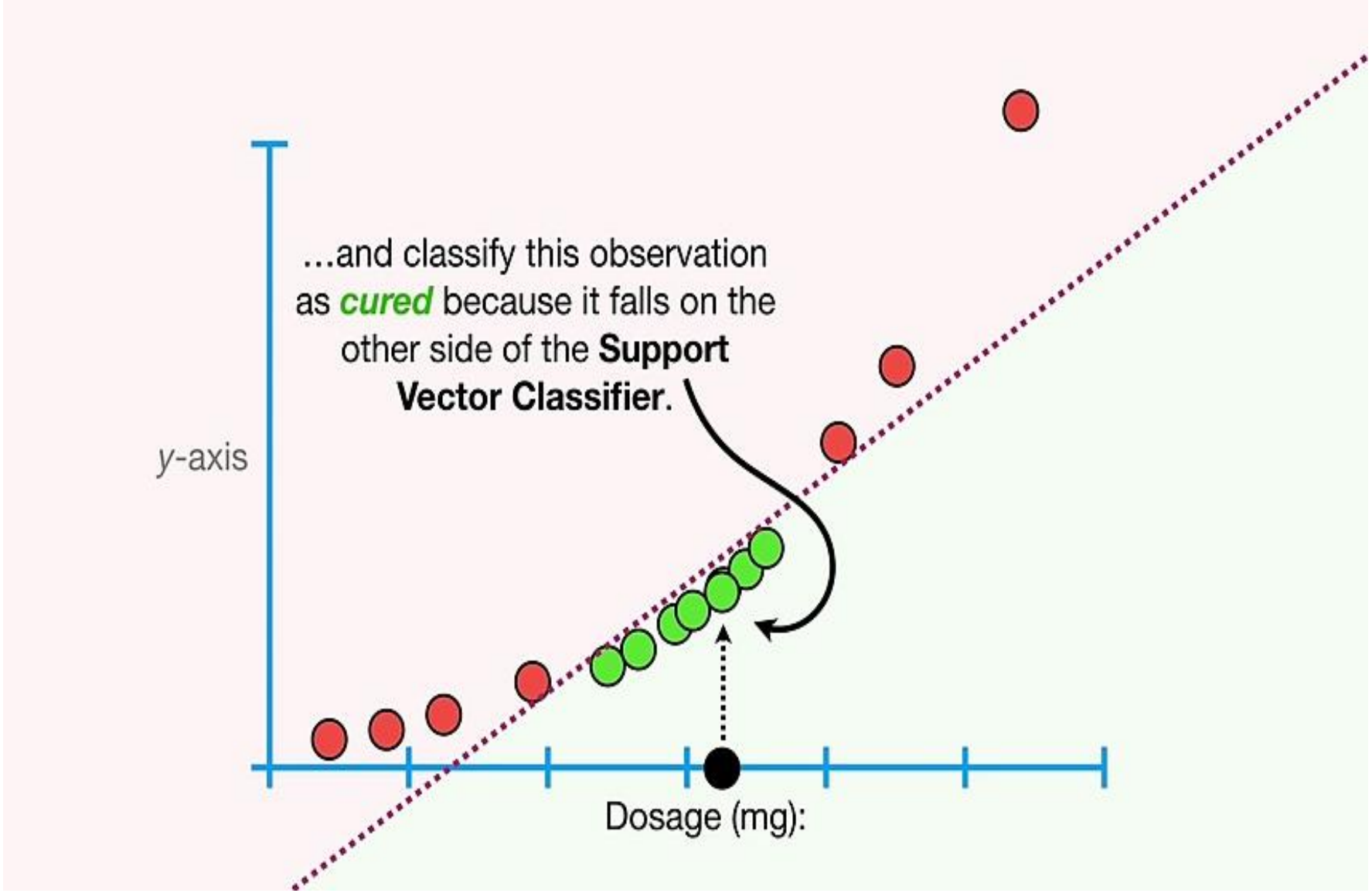

For example, if a new observation had this **Dosage**...
y-axis
Dosage (mg):

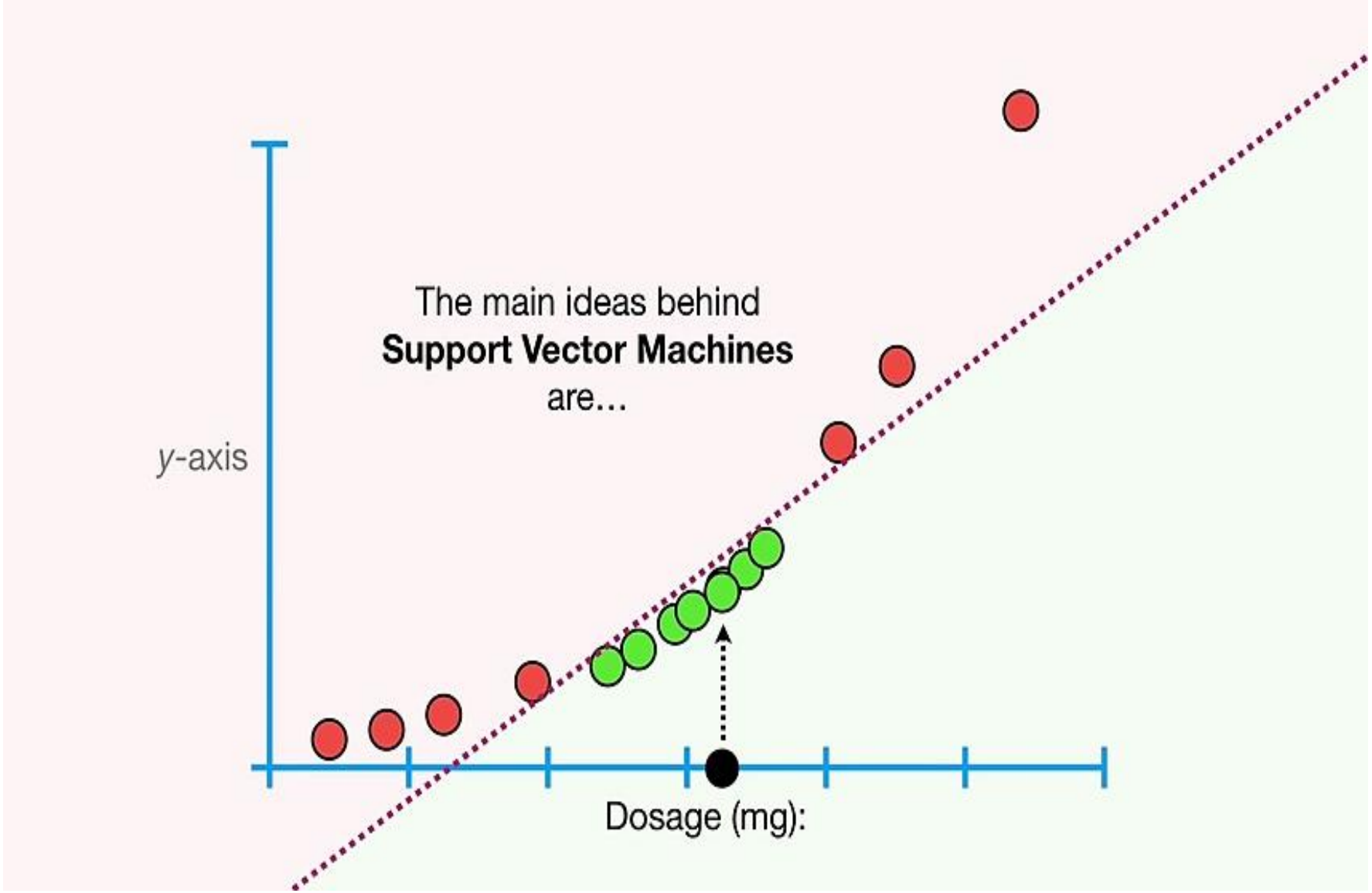

...then we could calculate a
y-axis coordinate by squaring
the Dosage...
y-axis
Dosage (mg):

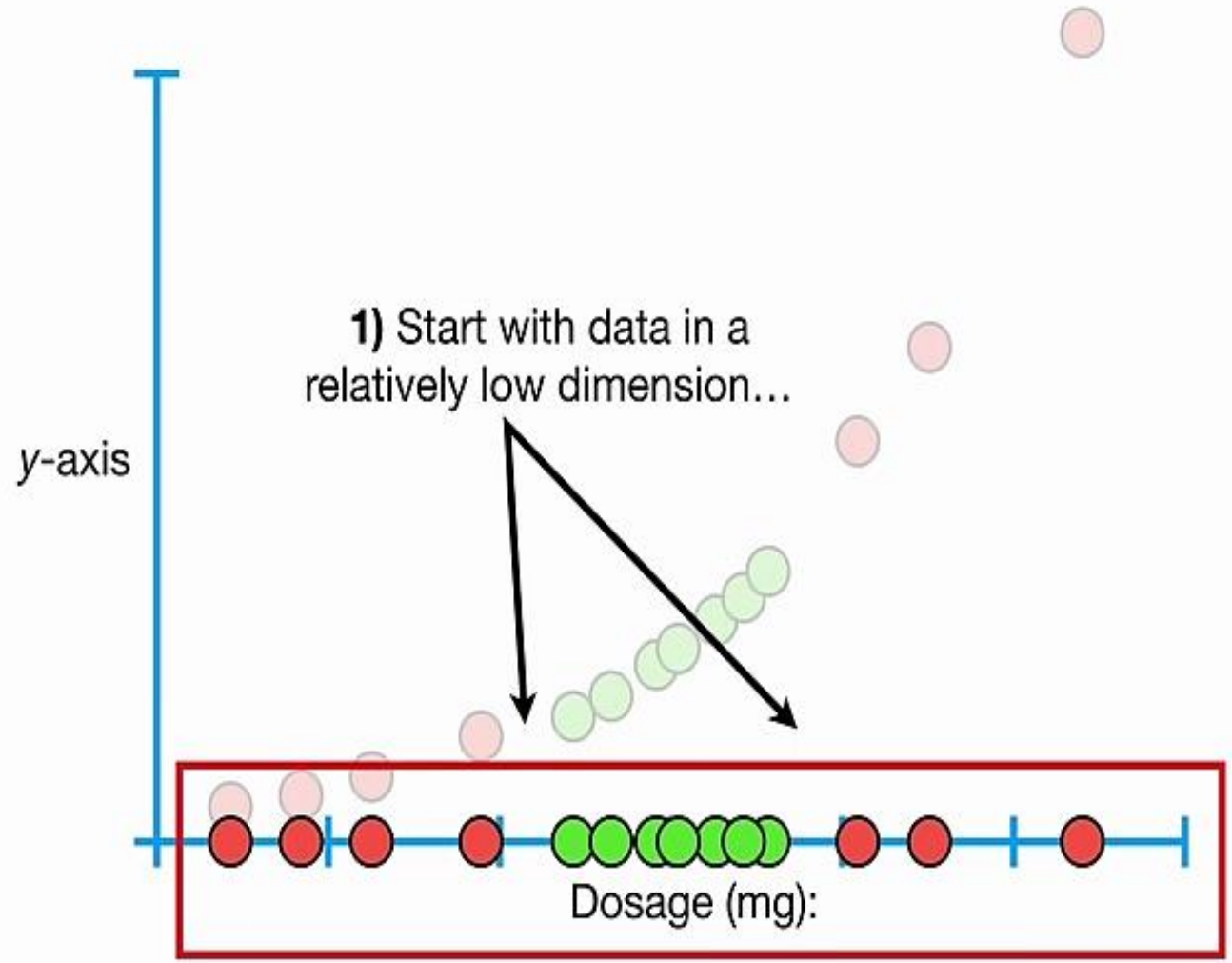

...and classify the observation as not cured because it ended up on this side of the Support Vector Classifier.
y-axis
Dosage (mg):

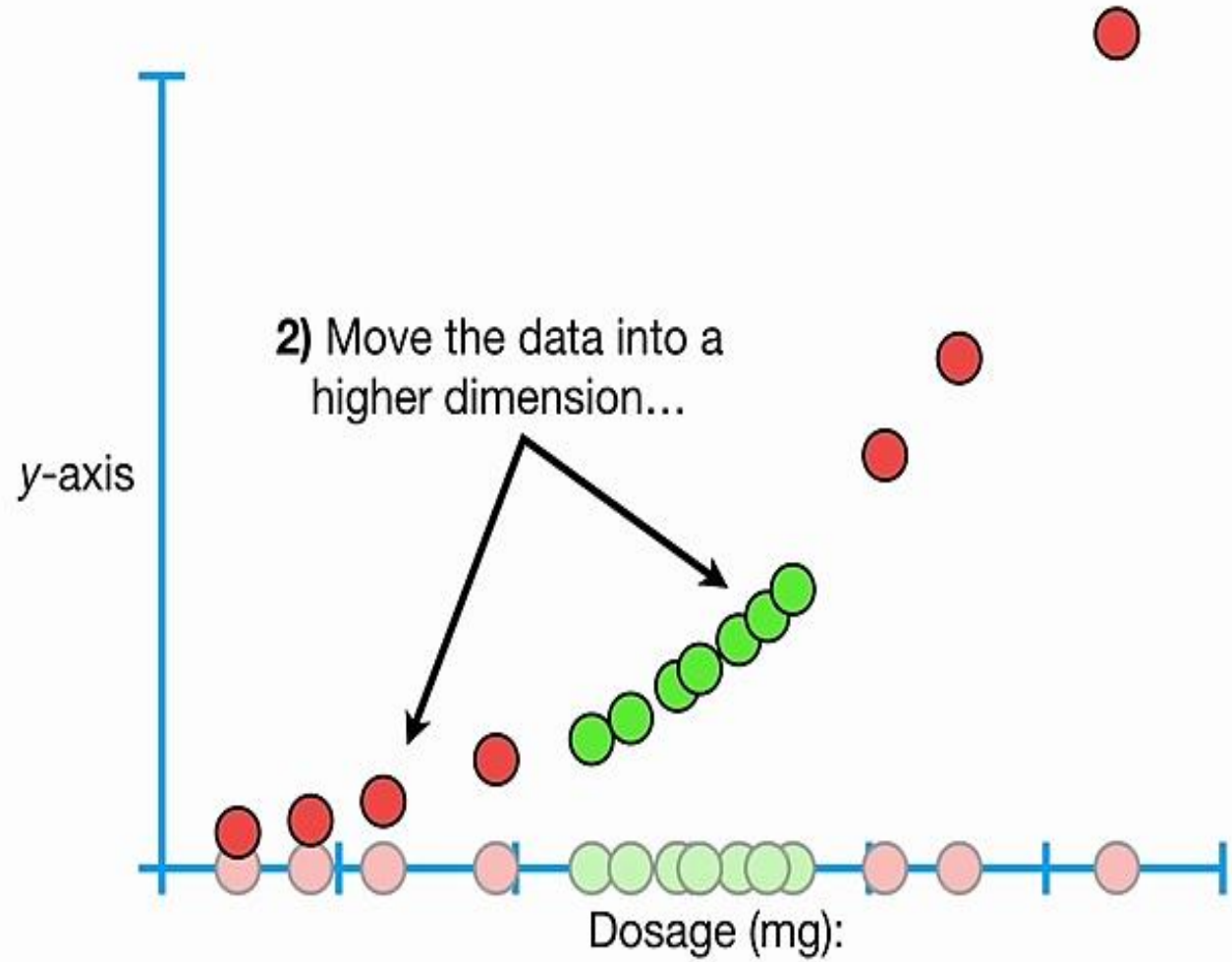

On the other hand, if we got a new observation with this **Dosage**...
y-axis
Dosage (mg):

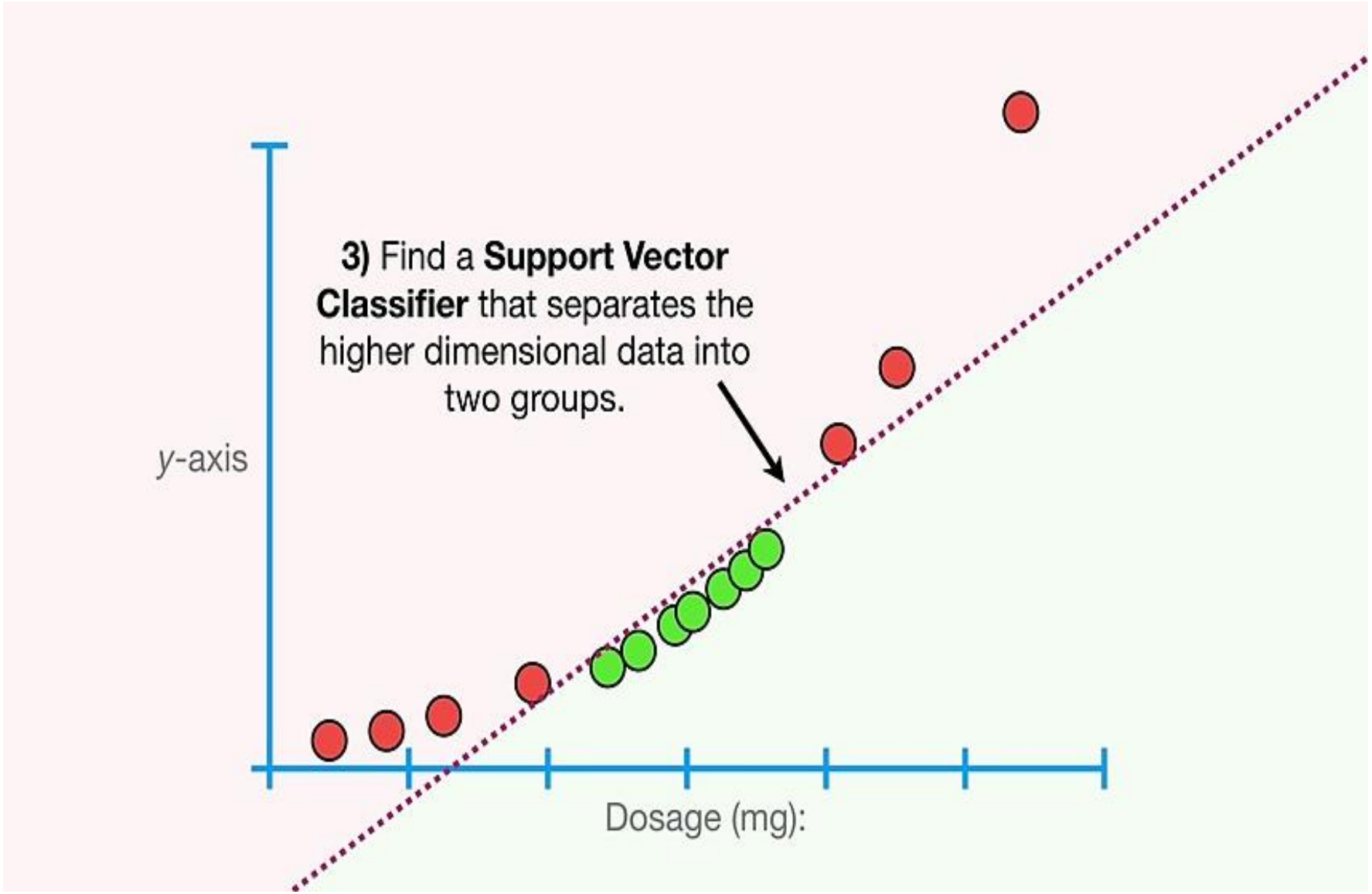

...then we would square the
Dosage to get a ***y*-axis**
coordinate...
y-axis
Dosage (mg):

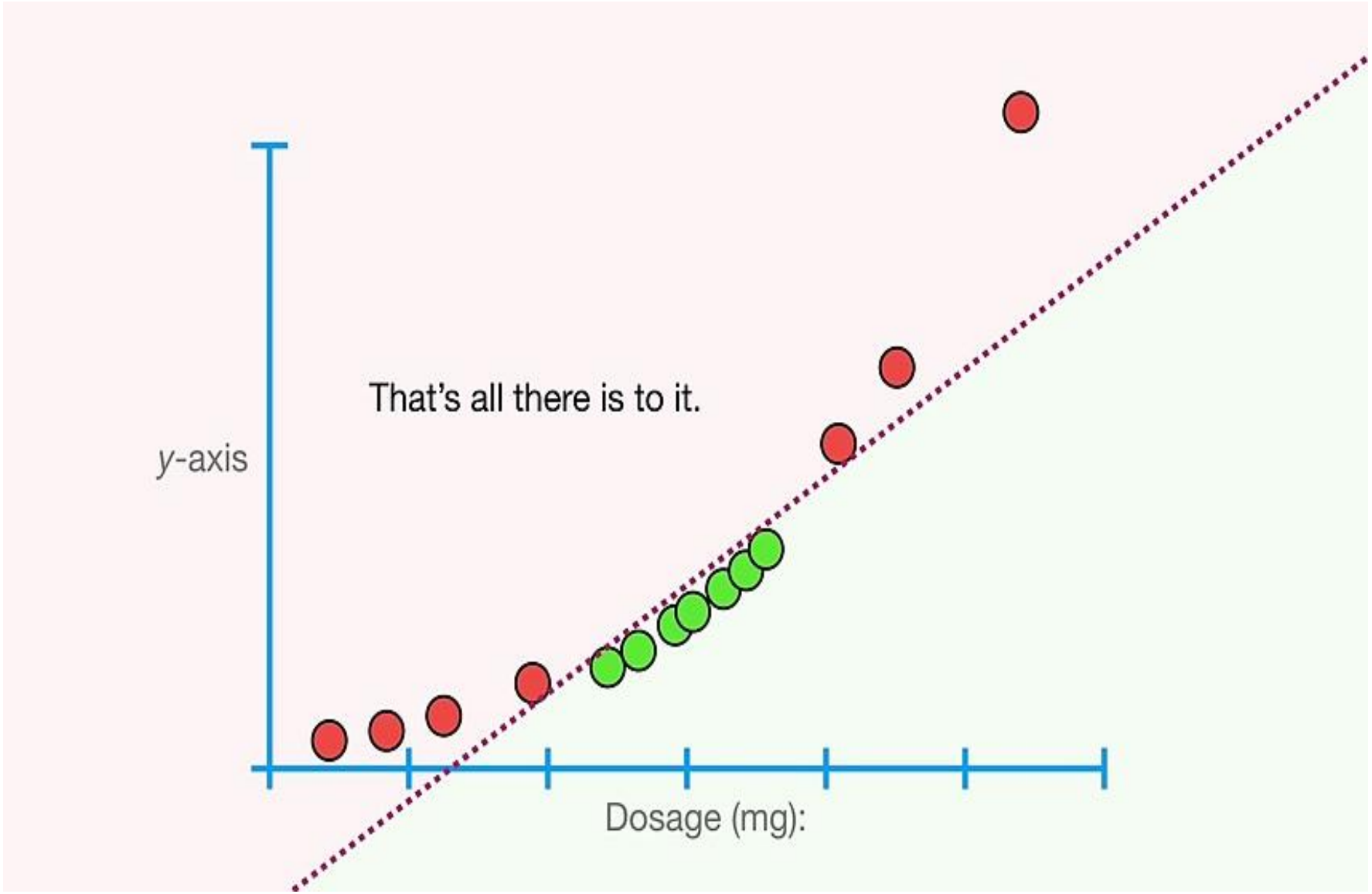

...and classify this observation as cured because it falls on the other side of the Support Vector Classifier.
y-axis
Dosage (mg):


The main ideas behind
Support Vector Machines
are…
y-axis
Dosage (mg):


y-axis
1) Start with data in a relatively low dimension…
Dosage (mg):

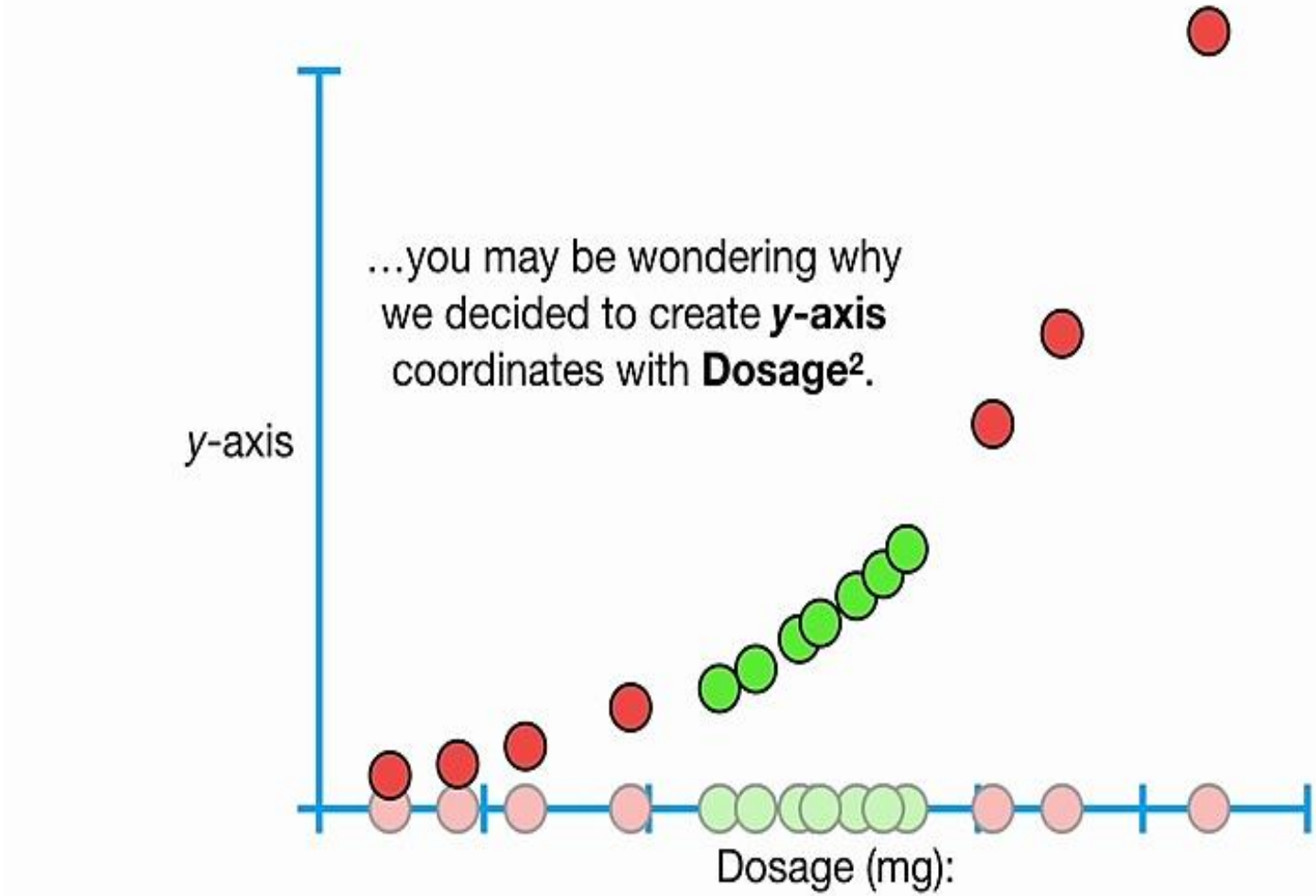

2) Move the data into a higher dimension…
y-axis
Dosage (mg):

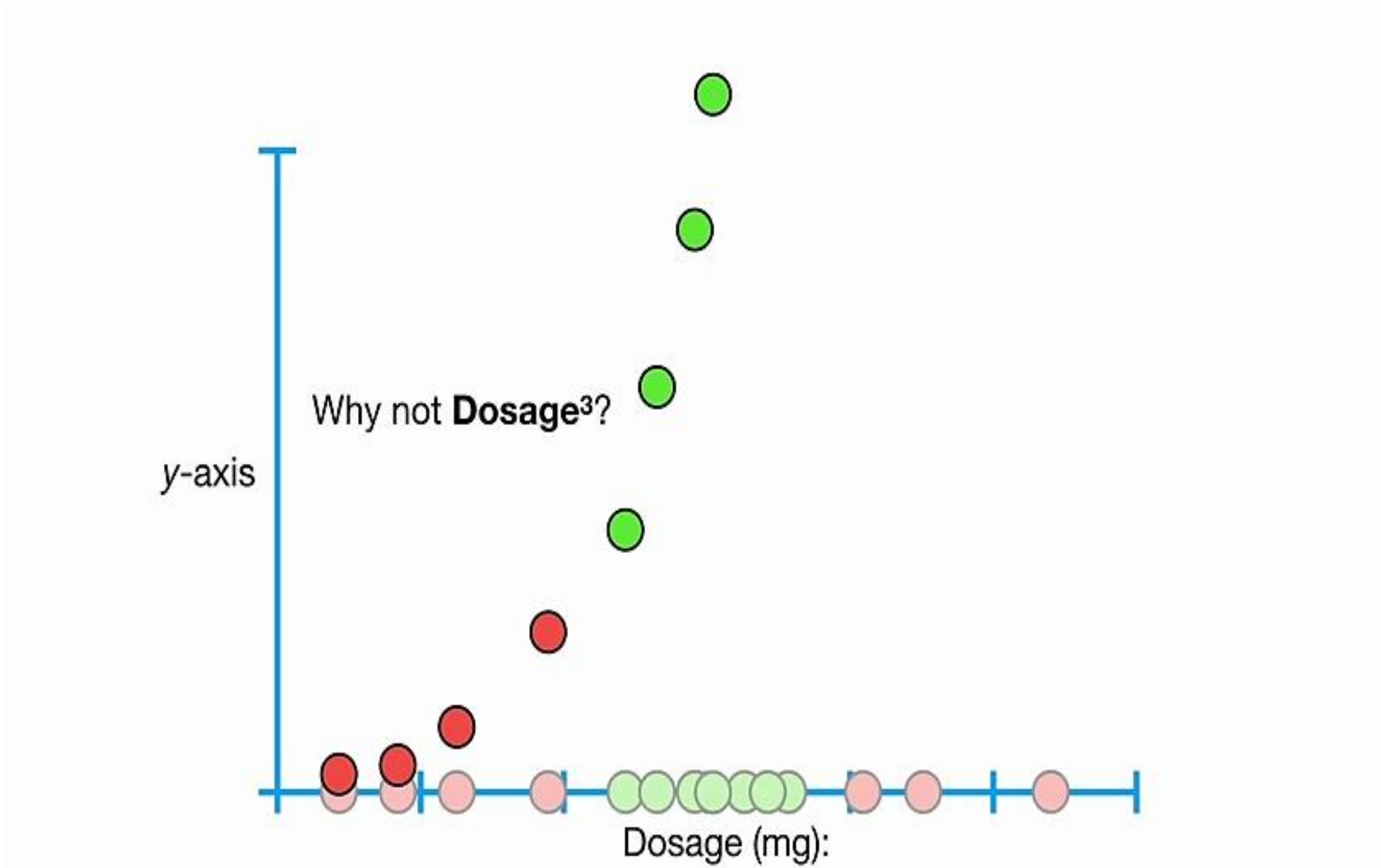

3) Find a **Support Vector Classifier** that separates the higher dimensional data into two groups.
y-axis
Dosage (mg):

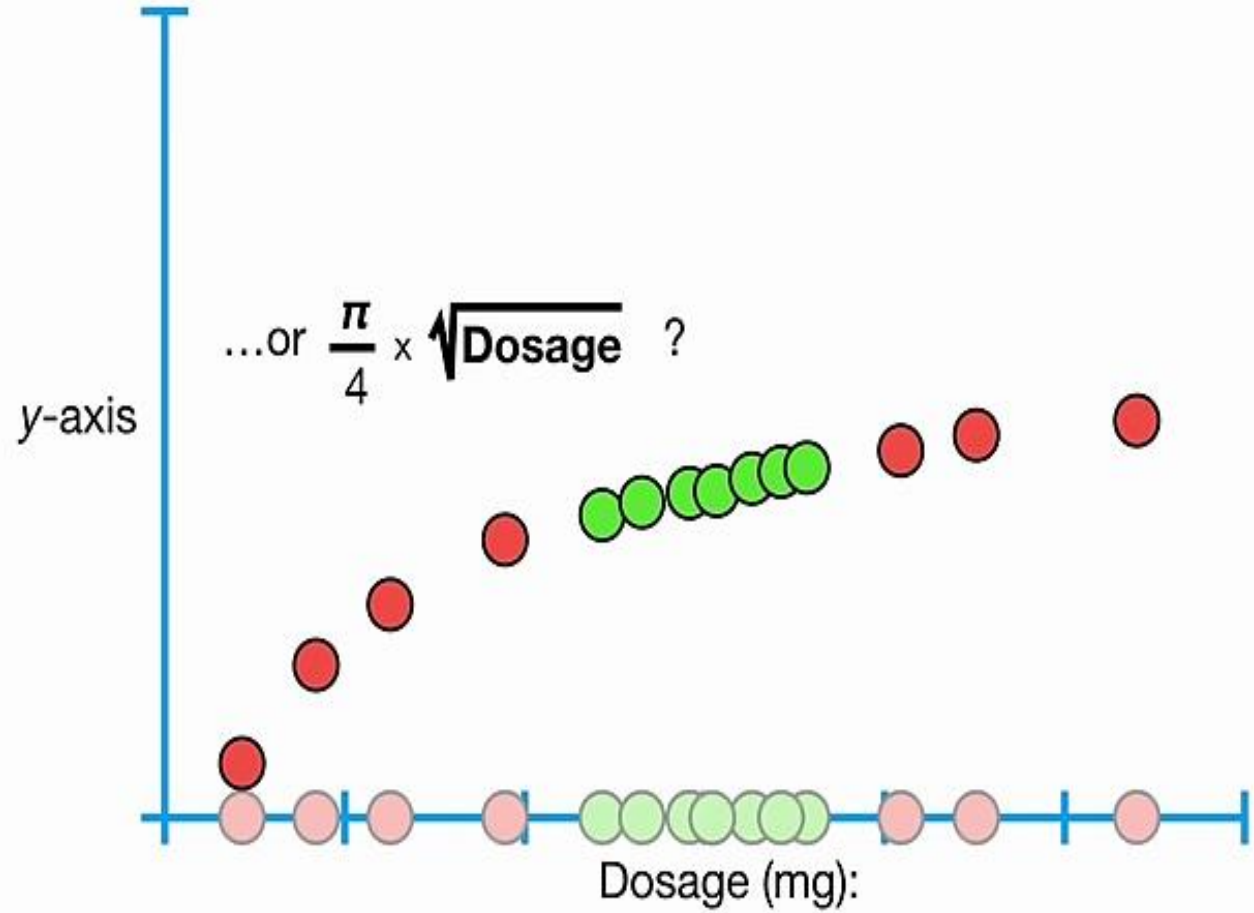

That's all there is to it.
y-axis
Dosage (mg):

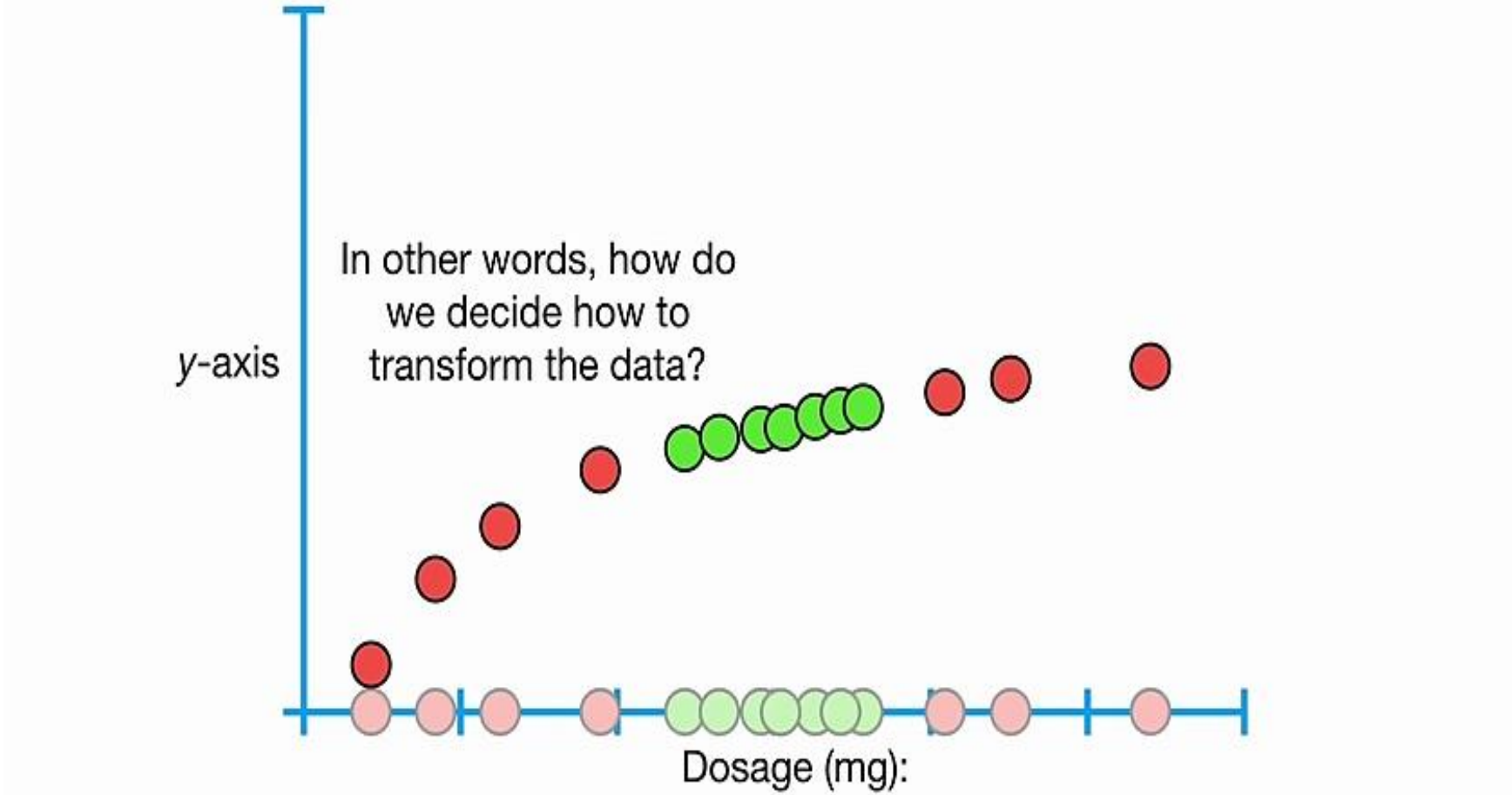
Going back to the original
1-Dimensional data…

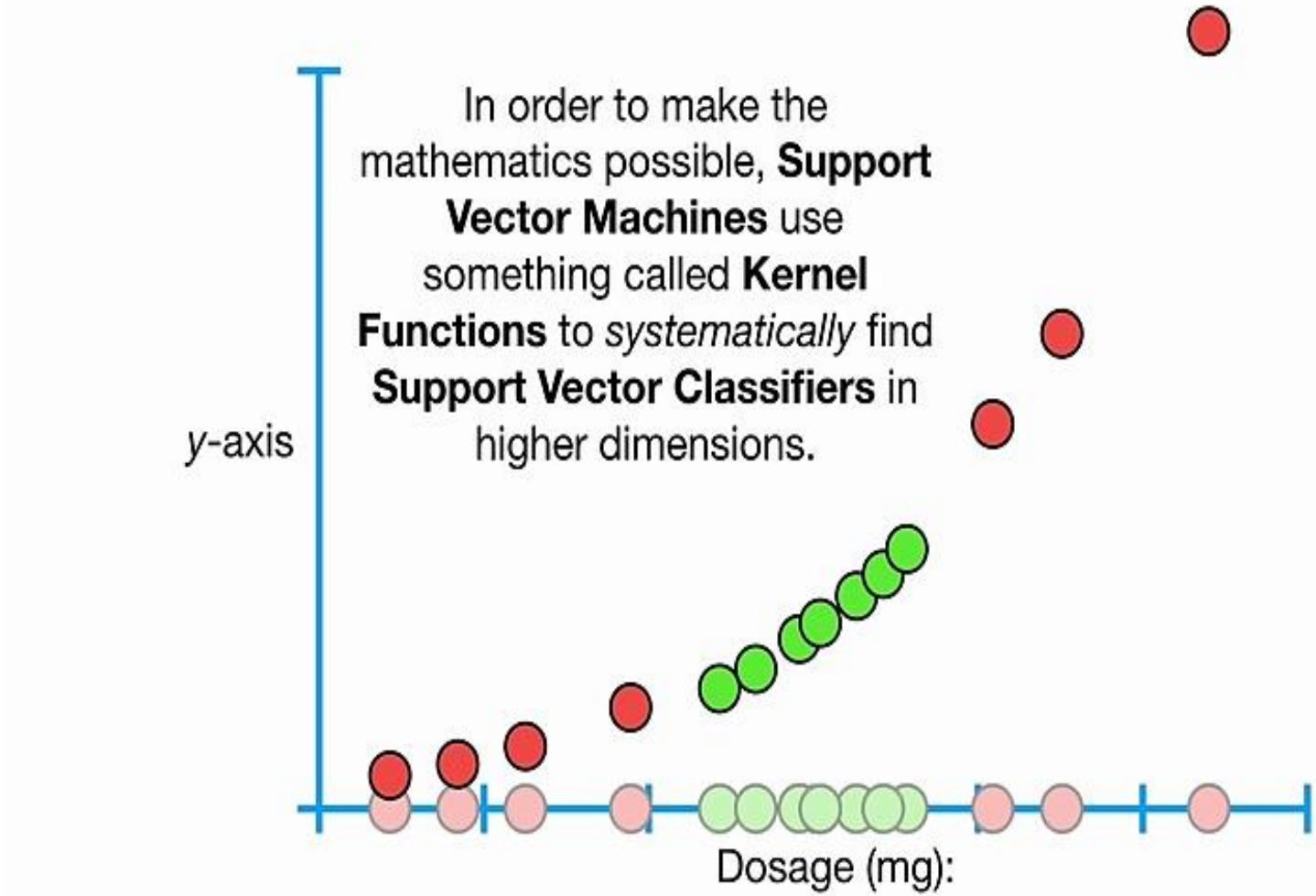
Dosage (mg):

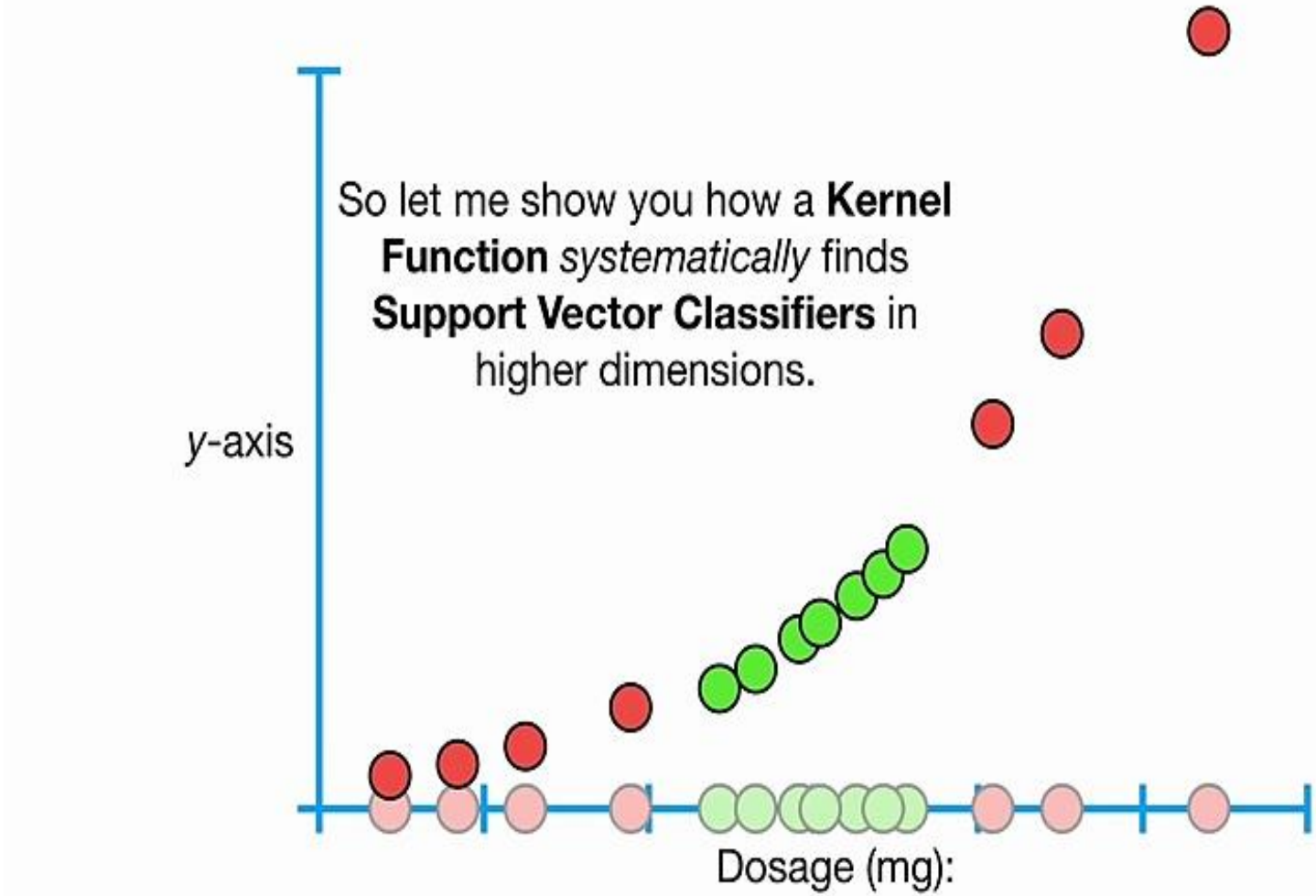

…you may be wondering why we decided to create **y-axis** coordinates with **Dosage²**.
y-axis
Dosage (mg):

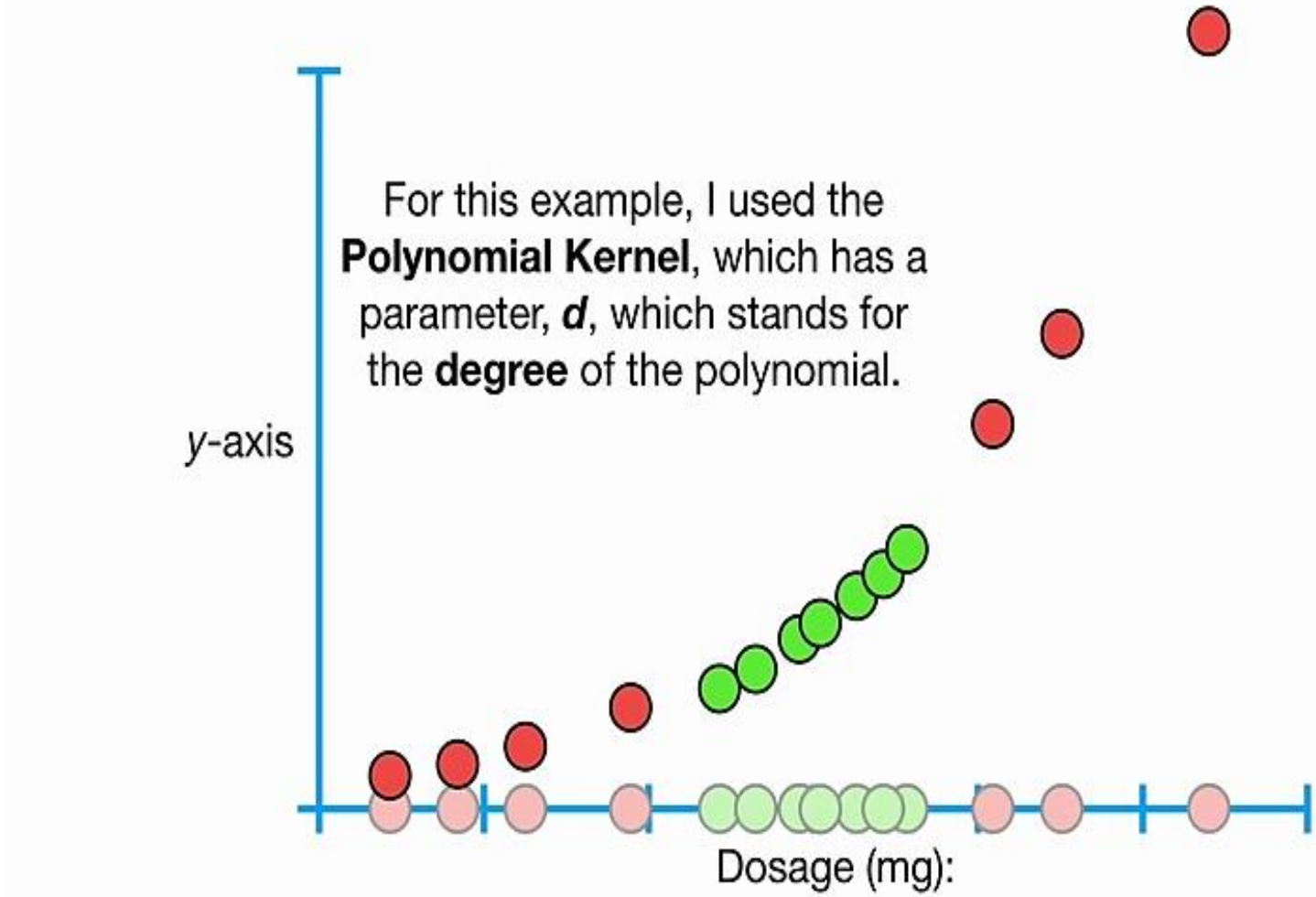

Why not **Dosage**^{3}?
y-axis
Dosage (mg):


y-axis
…or $\frac{\pi}{4} \times \sqrt{\text{Dosage}}$?
Dosage (mg):


y-axis
In other words, how do we decide how to transform the data?
Dosage (mg):

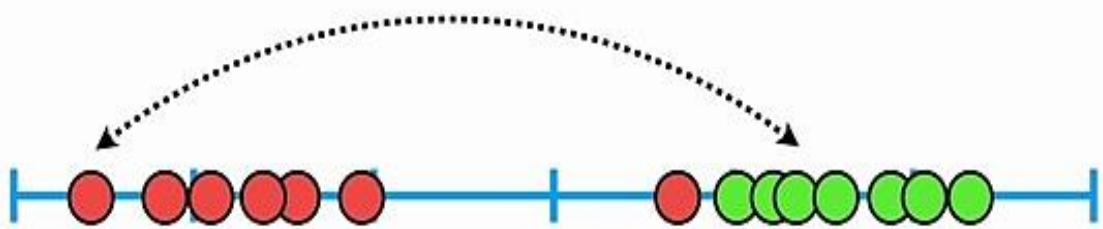

In order to make the mathematics possible, **Support Vector Machines** use something called **Kernel Functions** to *systematically* find **Support Vector Classifiers** in higher dimensions.
y-axis
Dosage (mg):


So let me show you how a **Kernel Function** *systematically* finds **Support Vector Classifiers** in higher dimensions.
y-axis
Dosage (mg):

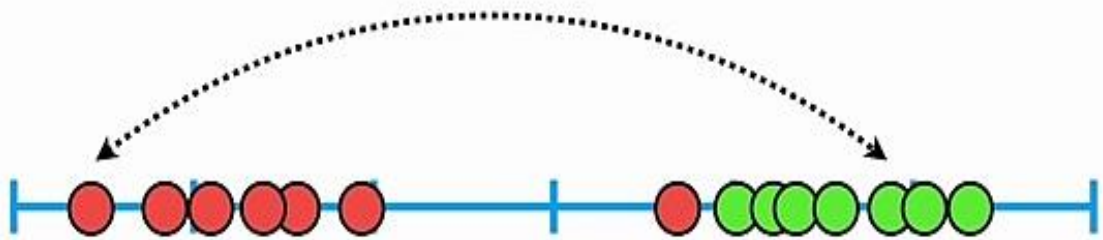

For this example, I used the
Polynomial Kernel, which has a
parameter, ***d***, which stands for
the **degree** of the polynomial.
y-axis
Dosage (mg):

When ***d* = 1**, the **Polynomial Kernel** computes the relationships between each pair of observations in **1-Dimension**…

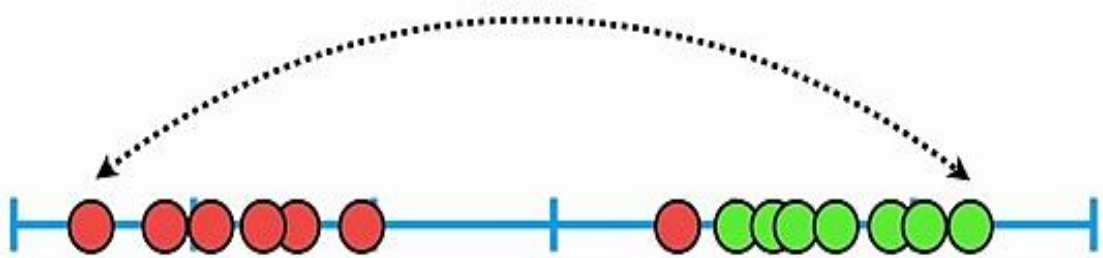
When ***d* = 1**, the **Polynomial Kernel** computes the relationships between each pair of observations in **1-Dimension**…



When ***d* = 1**, the **Polynomial Kernel** computes the relationships between each pair of observations in **1-Dimension**…

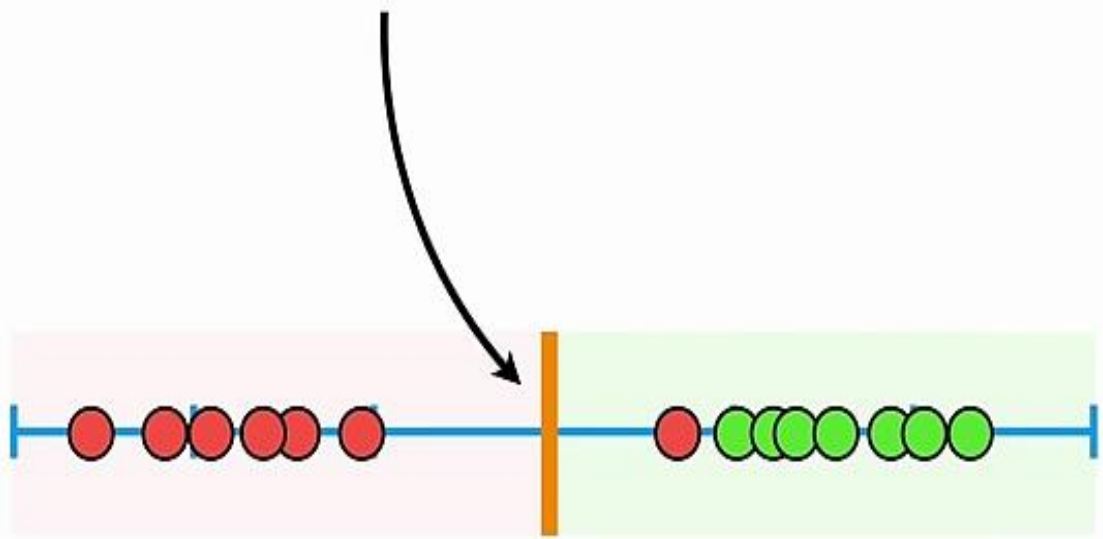


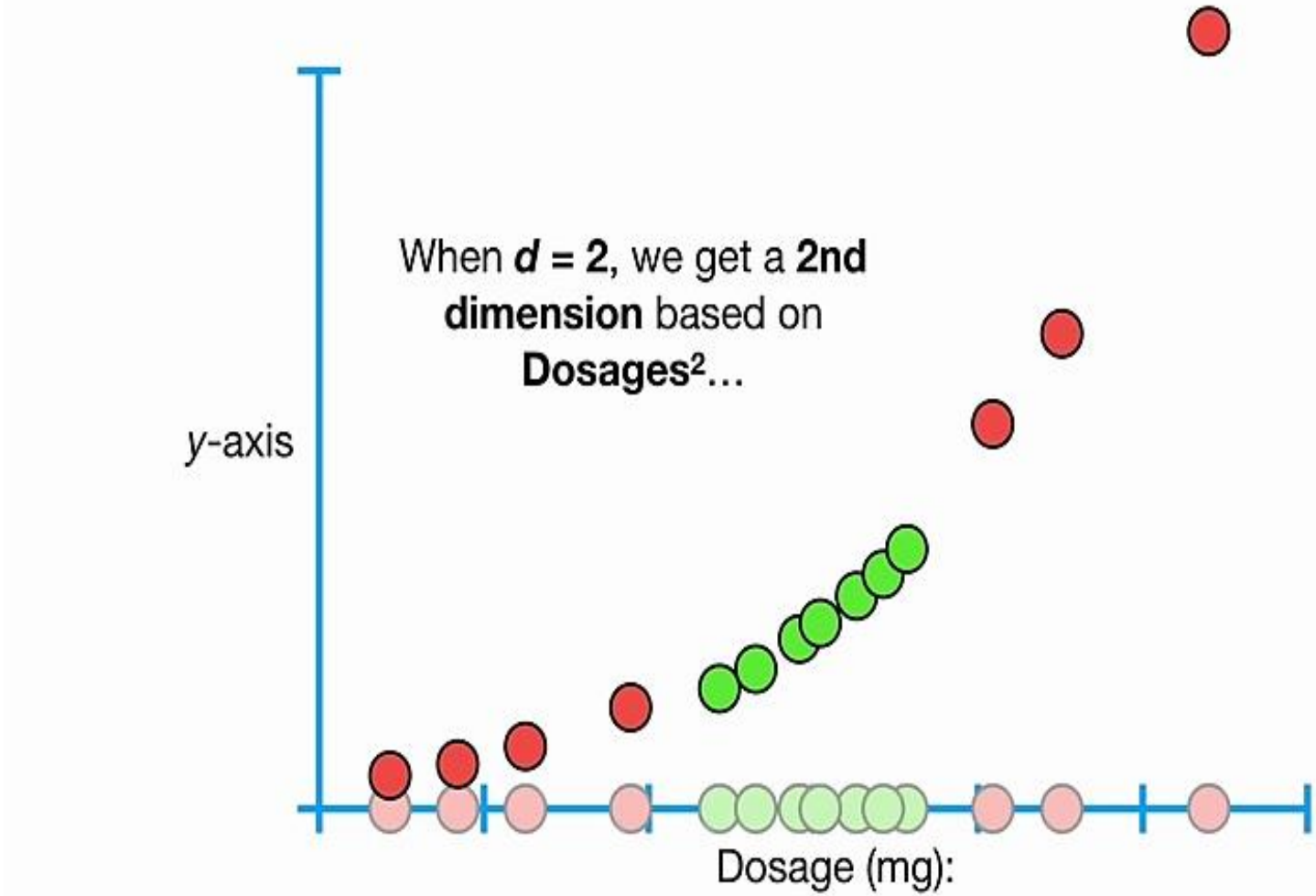
When ***d* = 1**, the **Polynomial Kernel** computes the relationships between each pair of observations in **1-Dimension**…

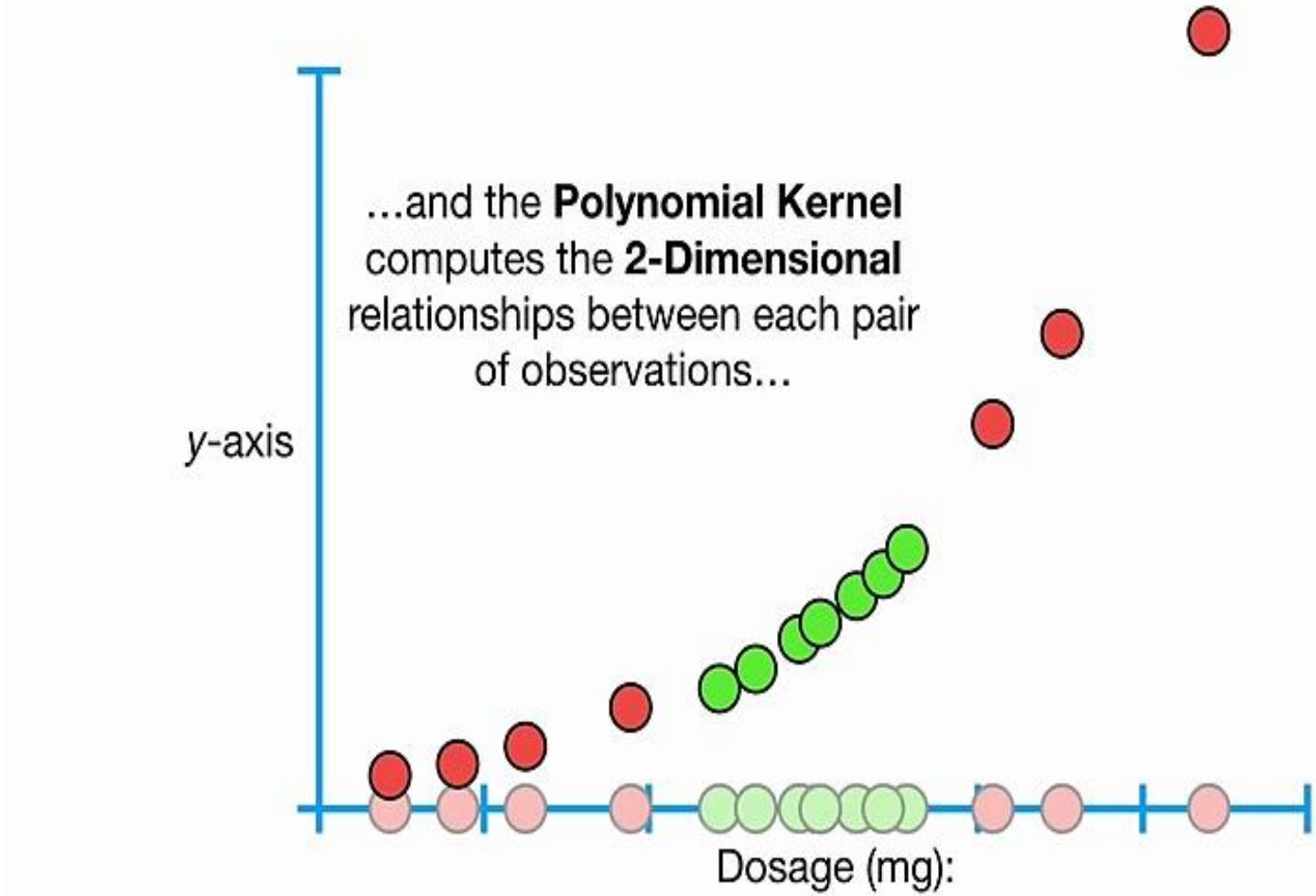


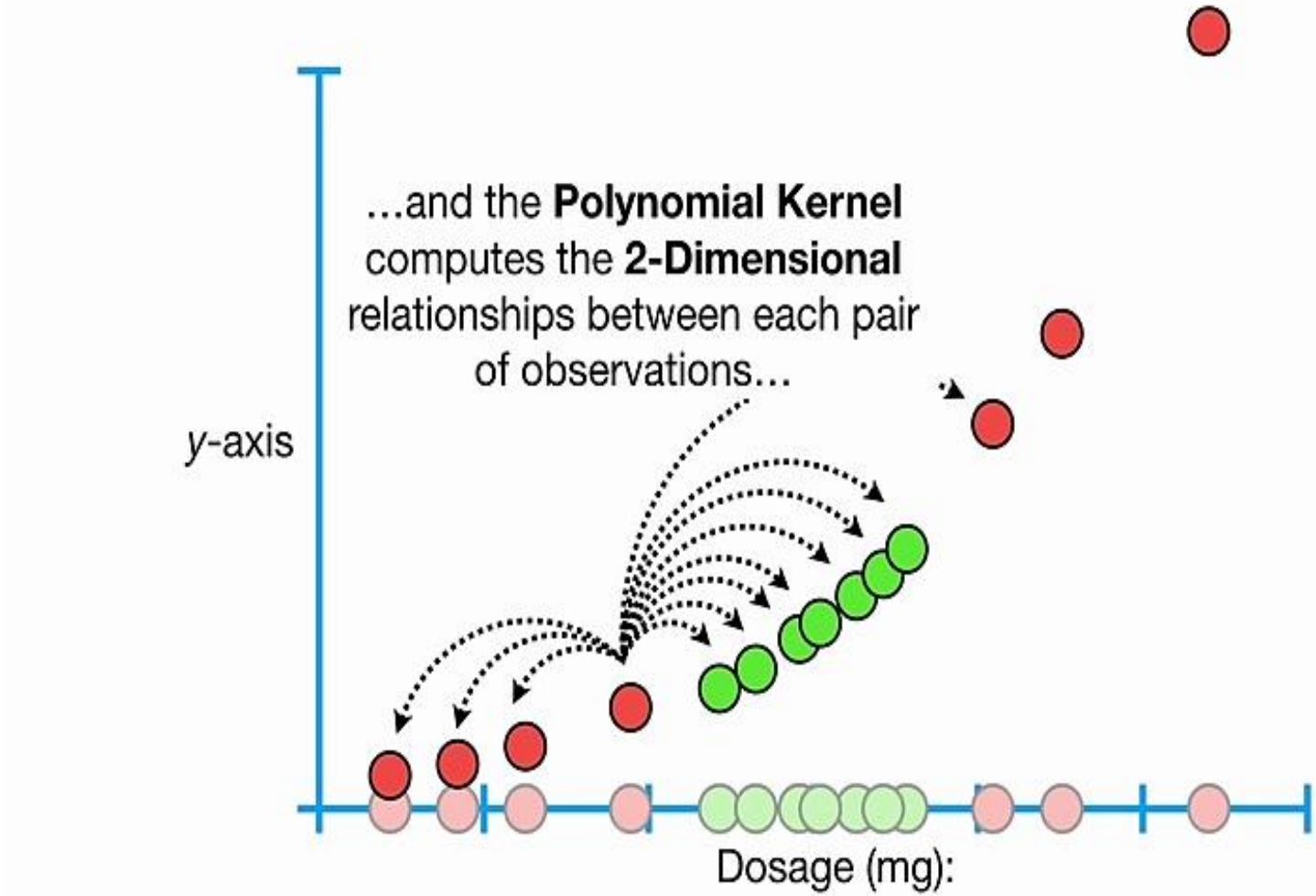
When ***d* = 1**, the **Polynomial Kernel** computes the relationships between each pair of observations in **1-Dimension**…

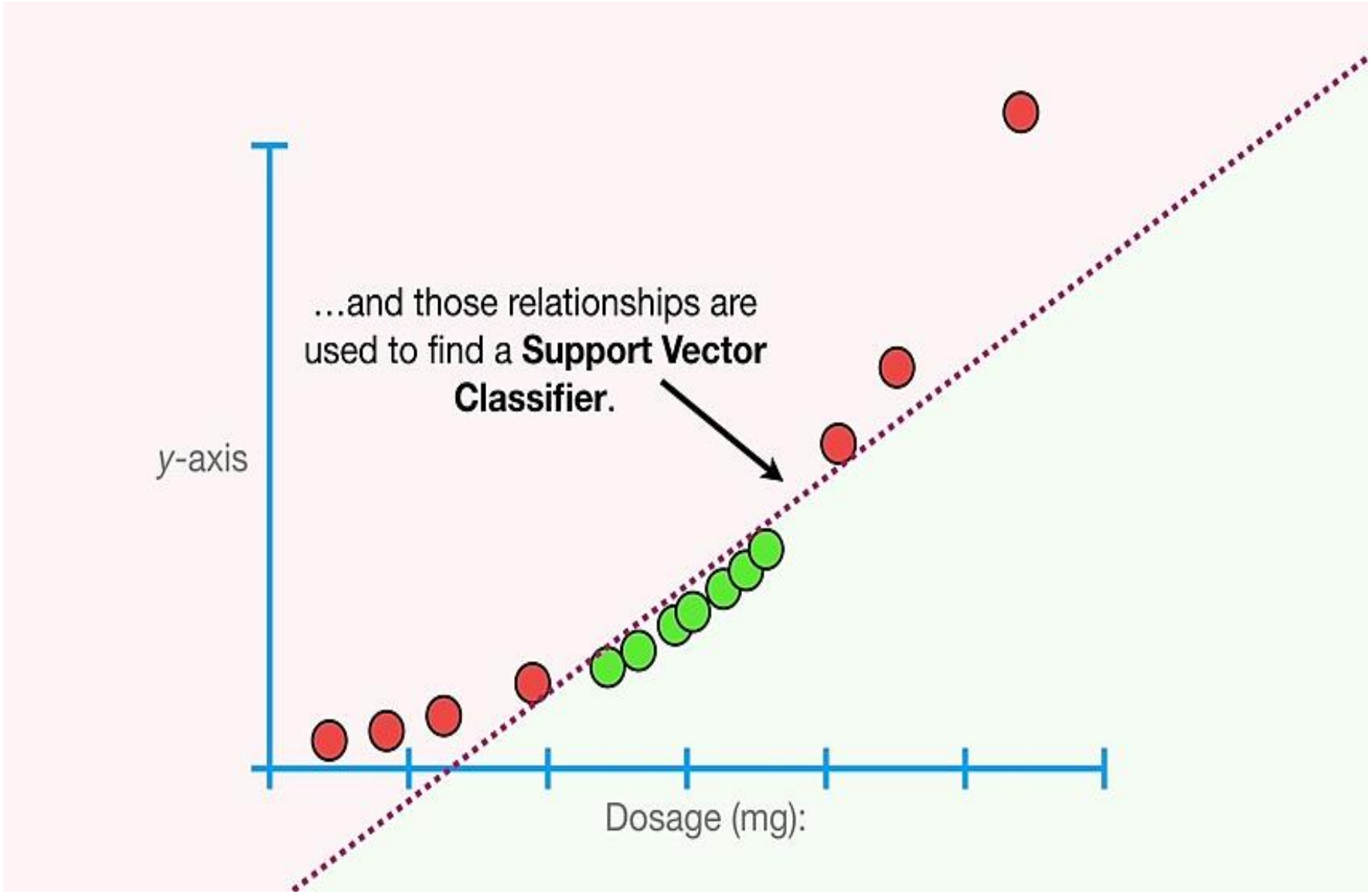
...and these relationships are used to find a **Support Vector Classifier.**

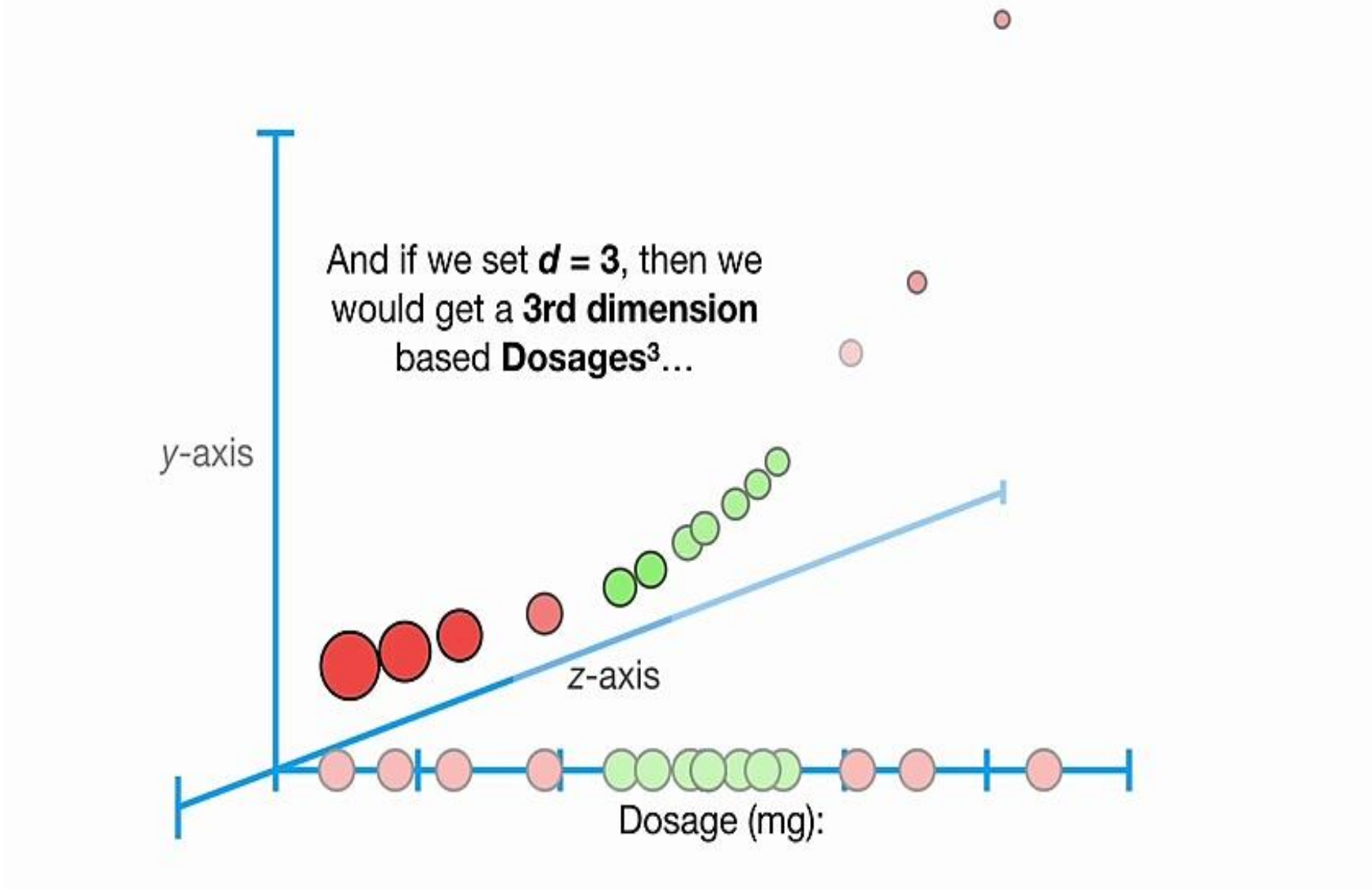


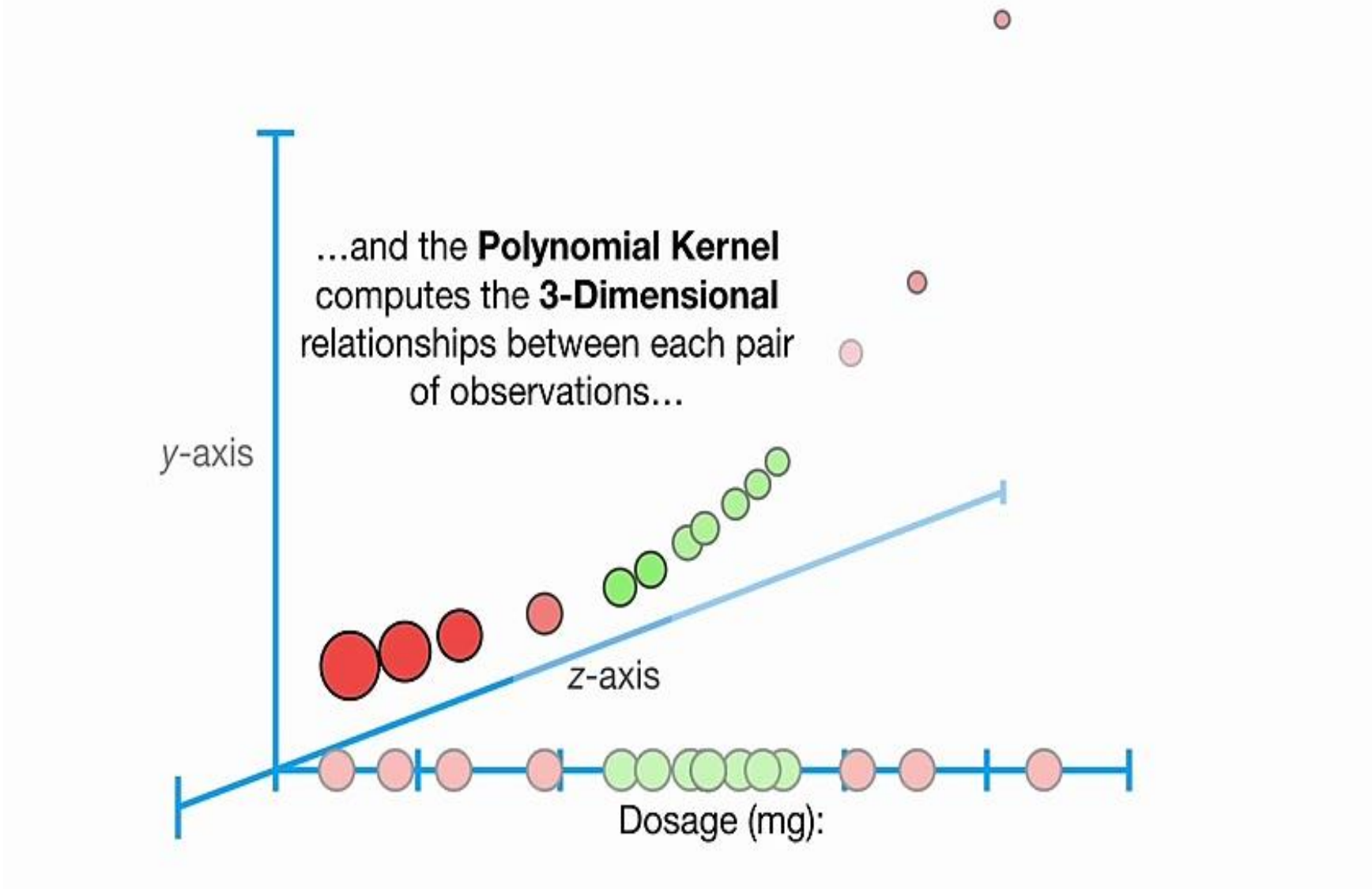

When **d = 2**, we get a **2nd dimension** based on **Dosages²**…
y-axis
Dosage (mg):

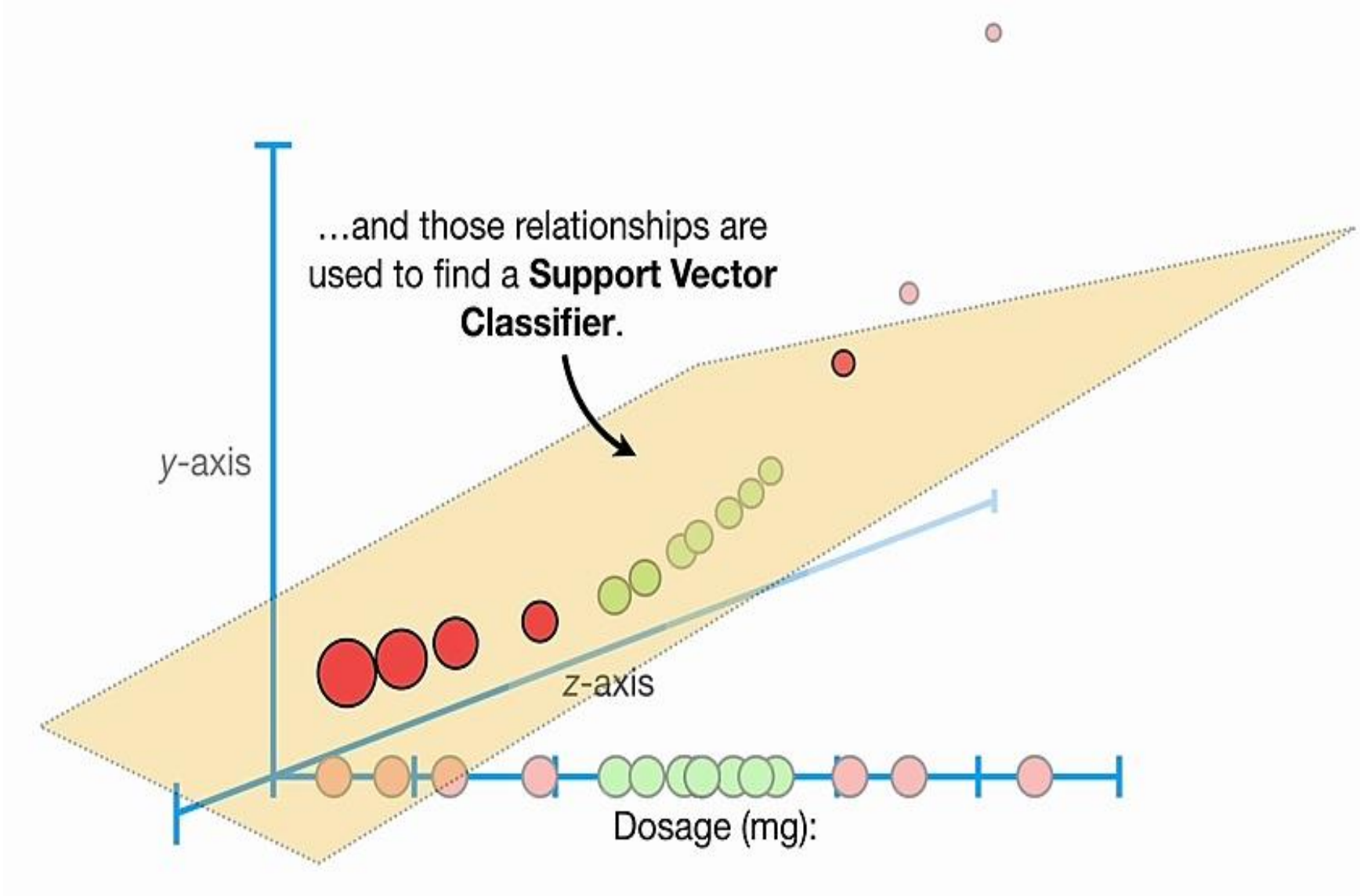

…and the **Polynomial Kernel** computes the **2-Dimensional** relationships between each pair of observations…
y-axis
Dosage (mg):


...and the **Polynomial Kernel** computes the **2-Dimensional** relationships between each pair of observations...
y-axis
Dosage (mg):


…and those relationships are used to find a **Support Vector Classifier.**
y-axis
Dosage (mg):


And if we set **d = 3**, then we would get a **3rd dimension** based **Dosages³**...
y-axis
z-axis
Dosage (mg):


...and the **Polynomial Kernel** computes the **3-Dimensional** relationships between each pair of observations...
y-axis
z-axis
Dosage (mg):

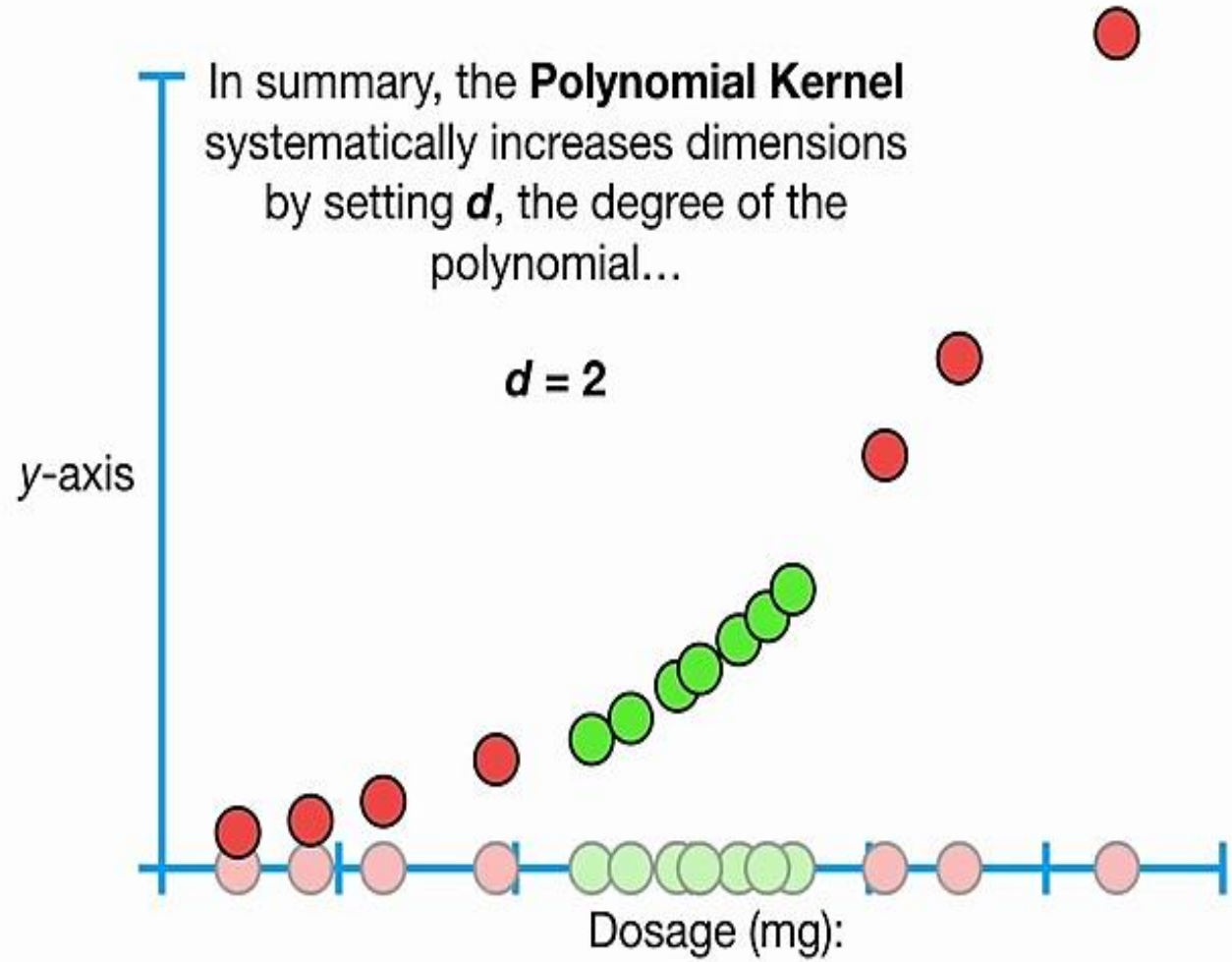

…and those relationships are used to find a **Support Vector Classifier.**
y-axis
z-axis
Dosage (mg):

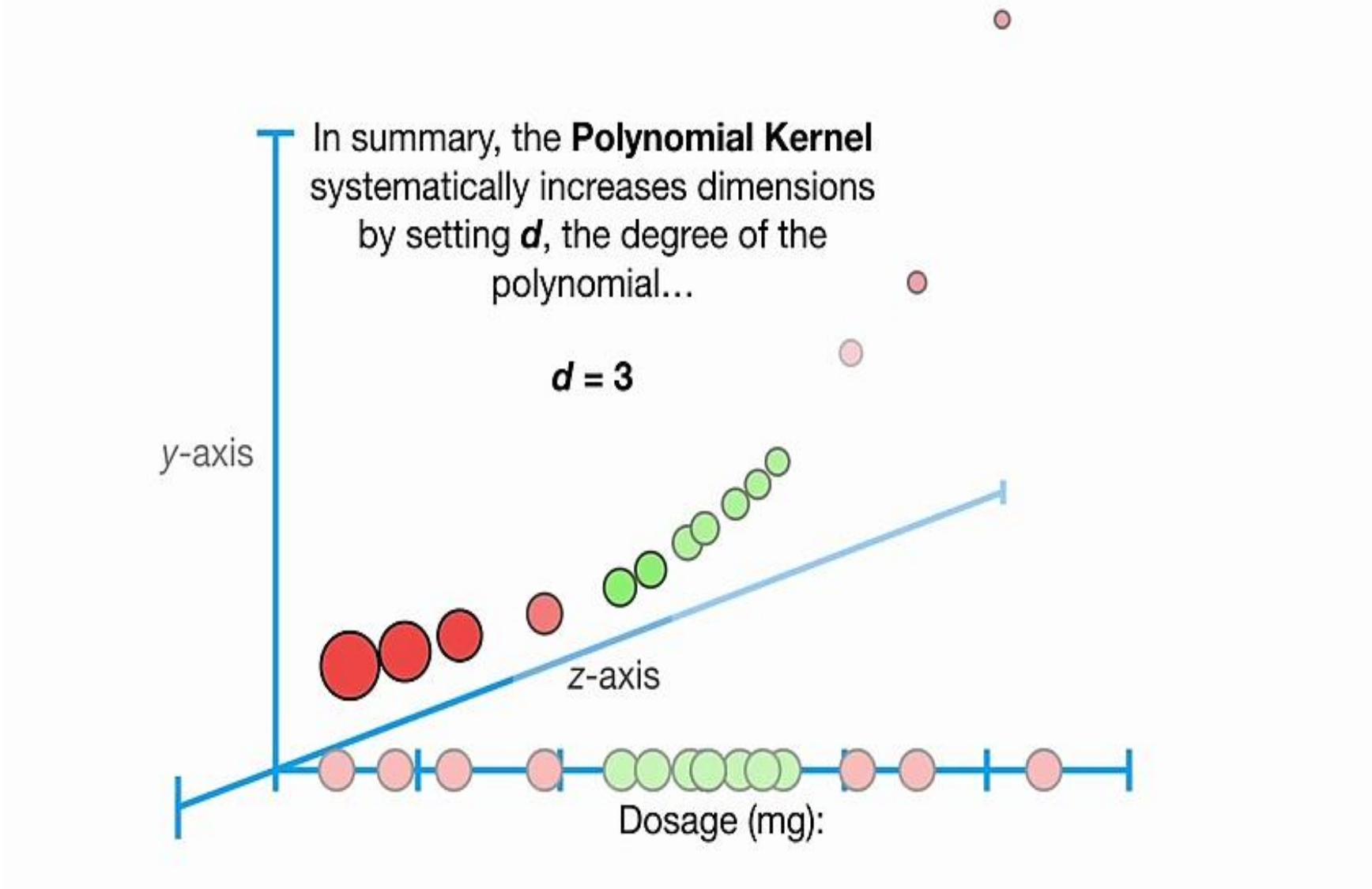
And when ***d* = 4 or more**, then we get even more dimensions to find a **Support Vector Classifier**.

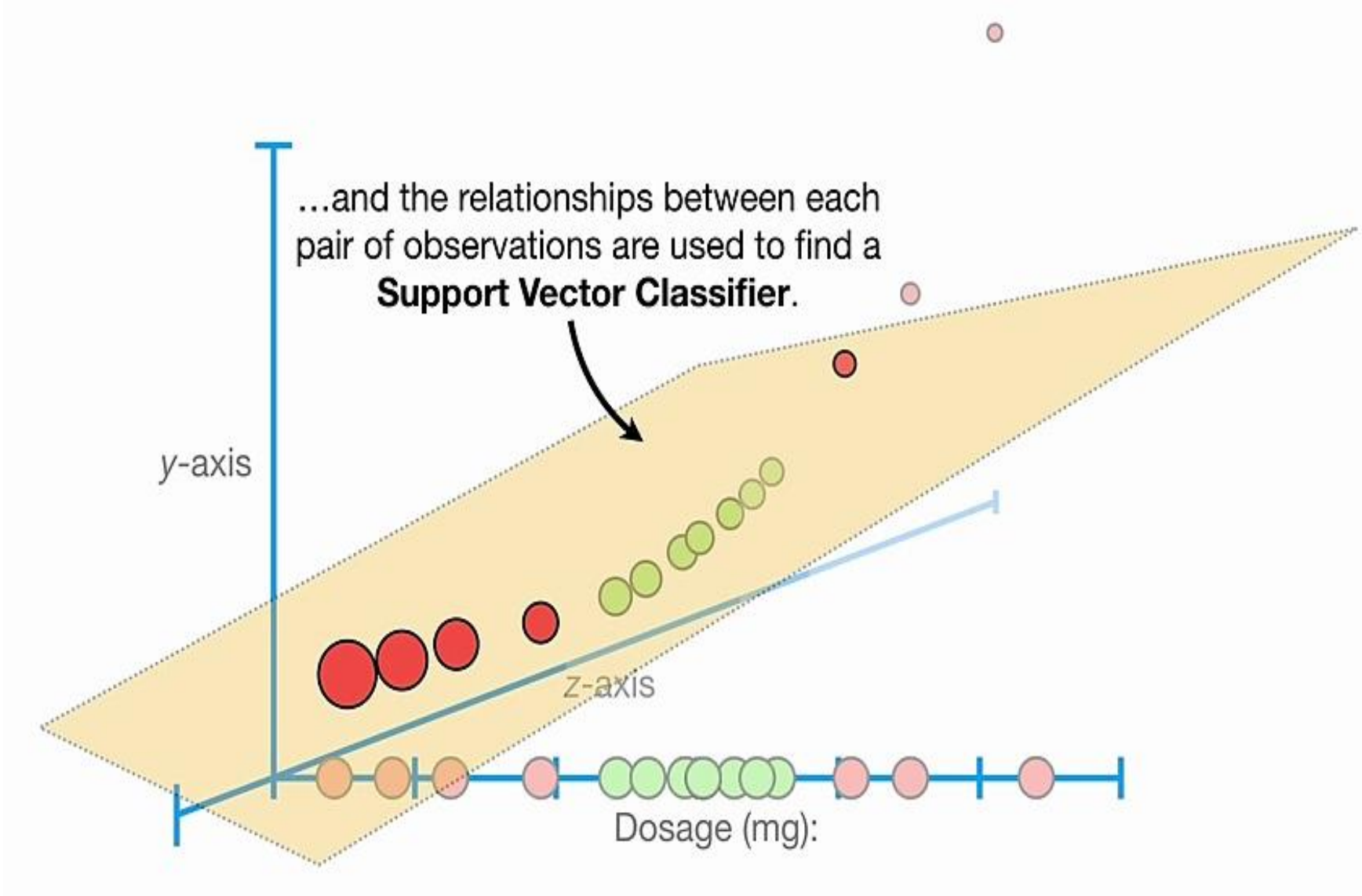
In summary, the **Polynomial Kernel** systematically increases dimensions by setting ***d***, the degree of the polynomial...

***d* = 1**

Dosage (mg):

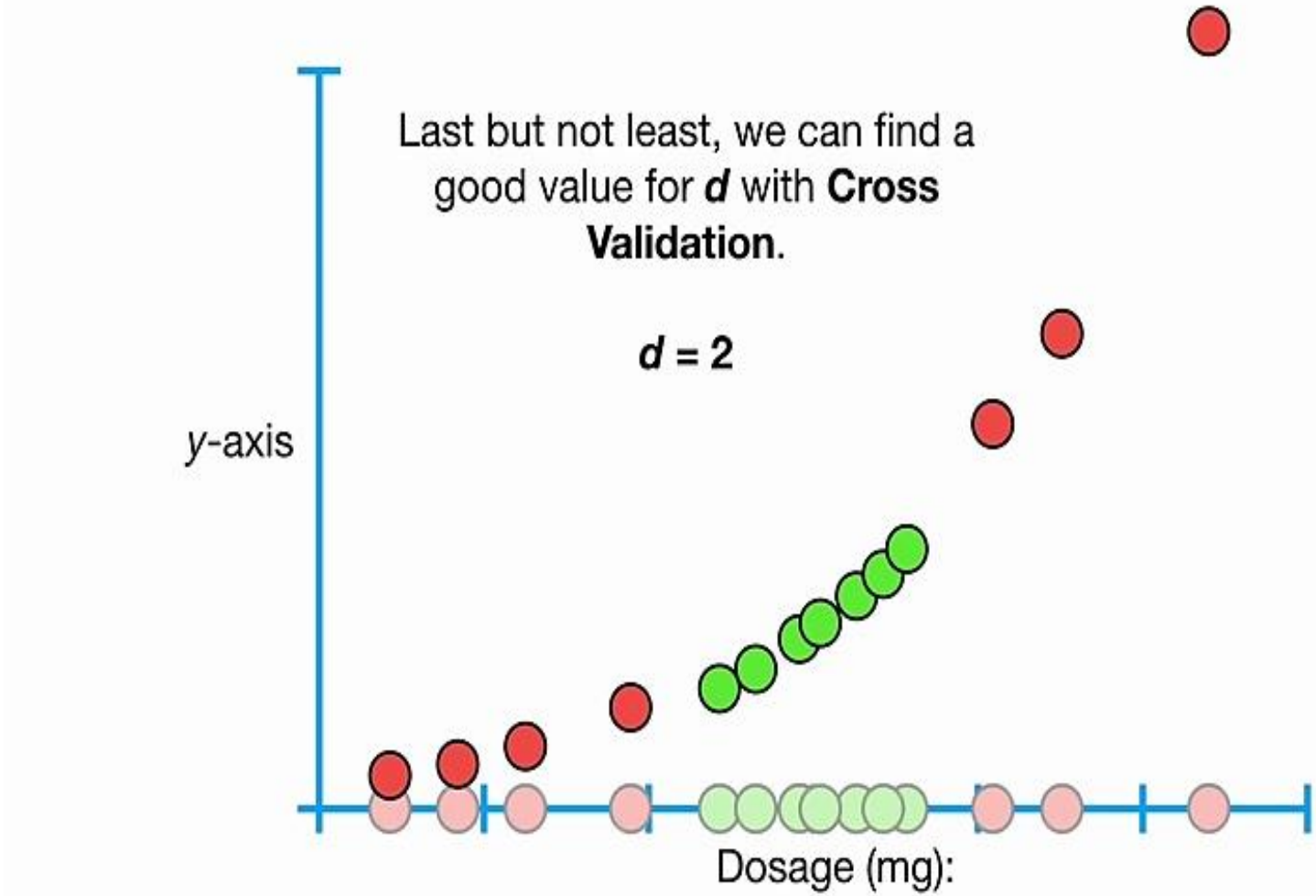

In summary, the **Polynomial Kernel** systematically increases dimensions by setting ***d***, the degree of the polynomial…
***d* = 2**
y-axis
Dosage (mg):

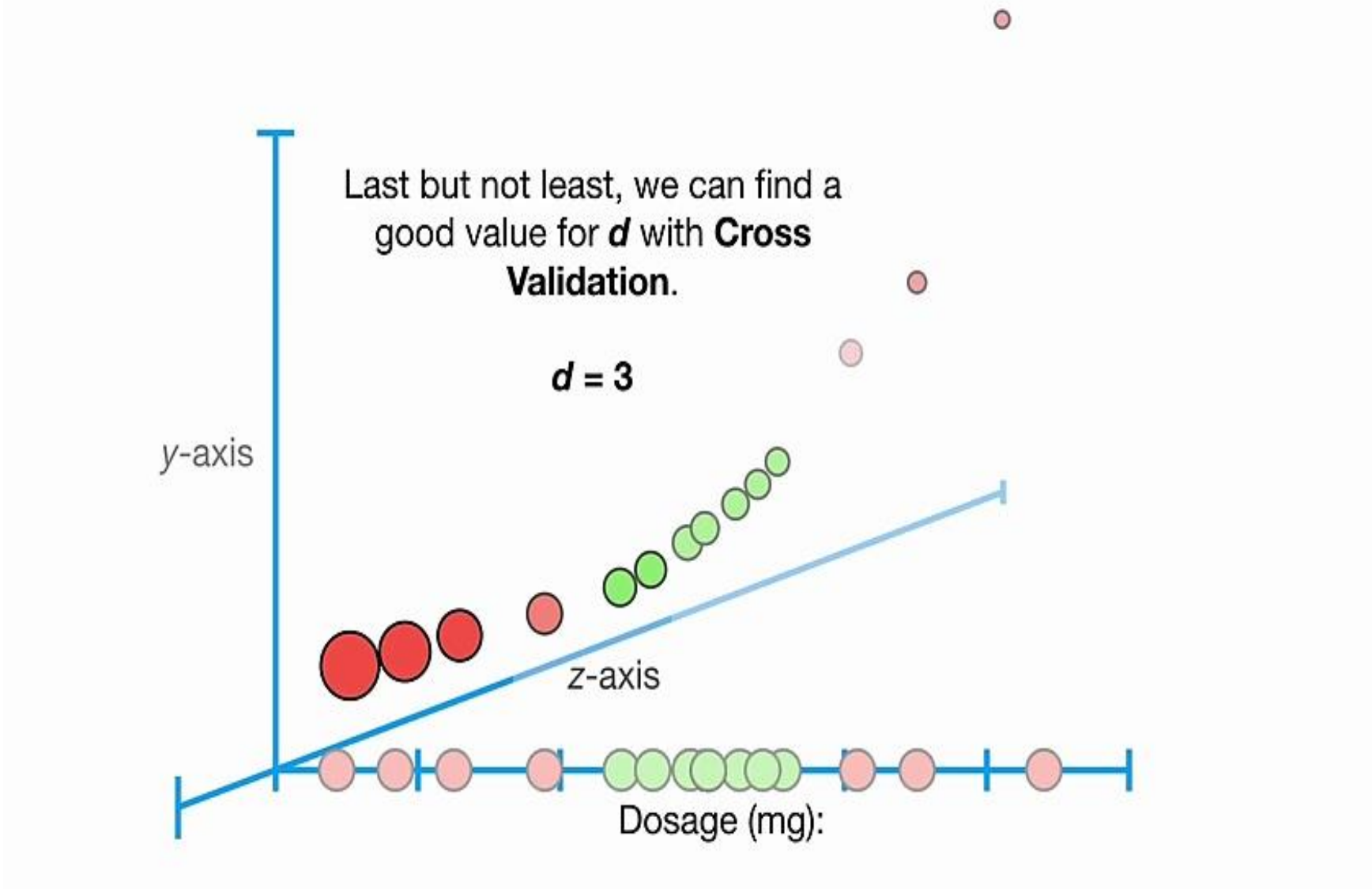

In summary, the **Polynomial Kernel** systematically increases dimensions by setting ***d***, the degree of the polynomial...
***d* = 3**
y-axis
z-axis
Dosage (mg):

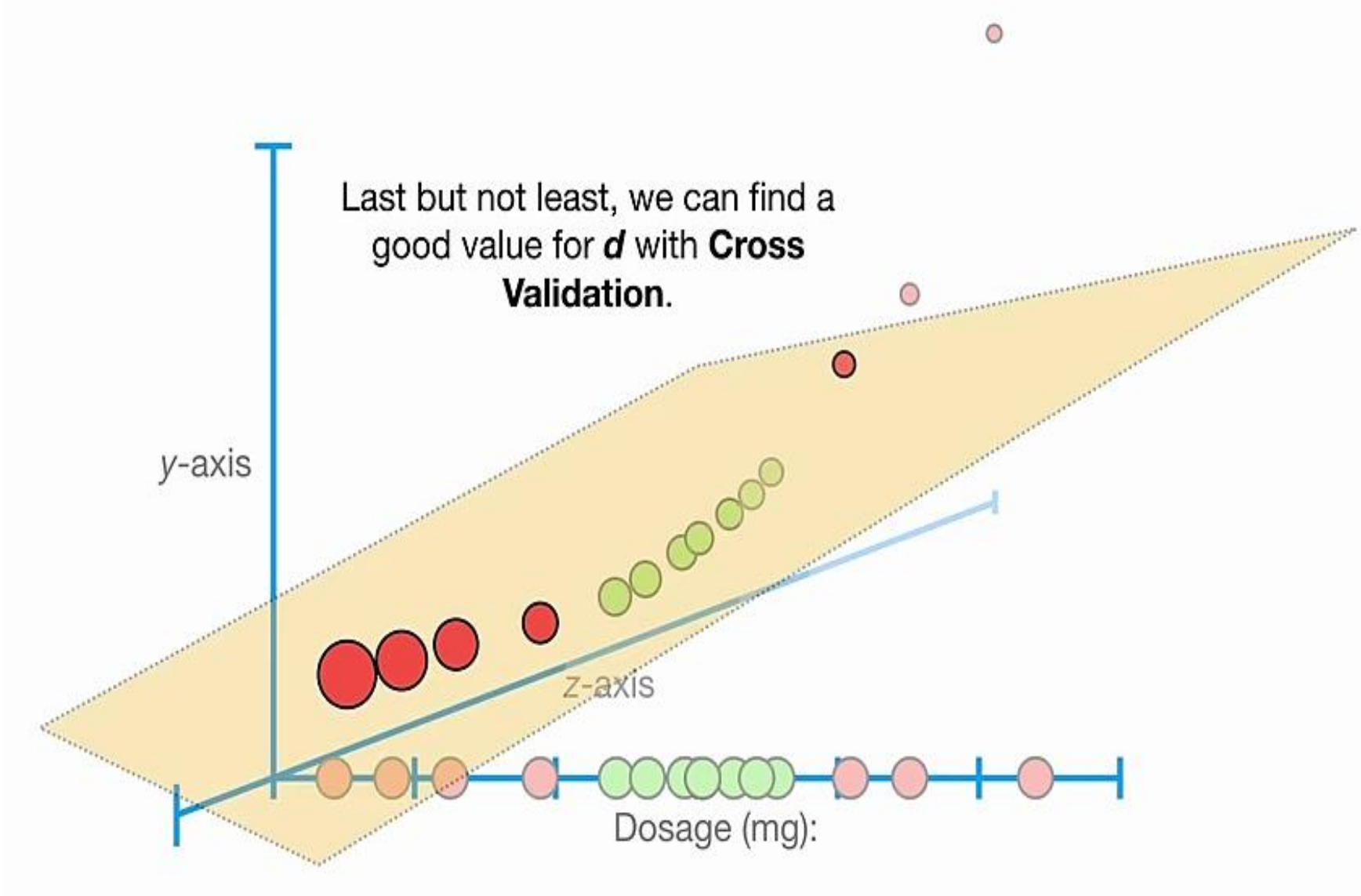

...and the relationships between each pair of observations are used to find a **Support Vector Classifier**.
y-axis
z-axis
Dosage (mg):

Last but not least, we can find a good value for ***d*** with **Cross Validation**.

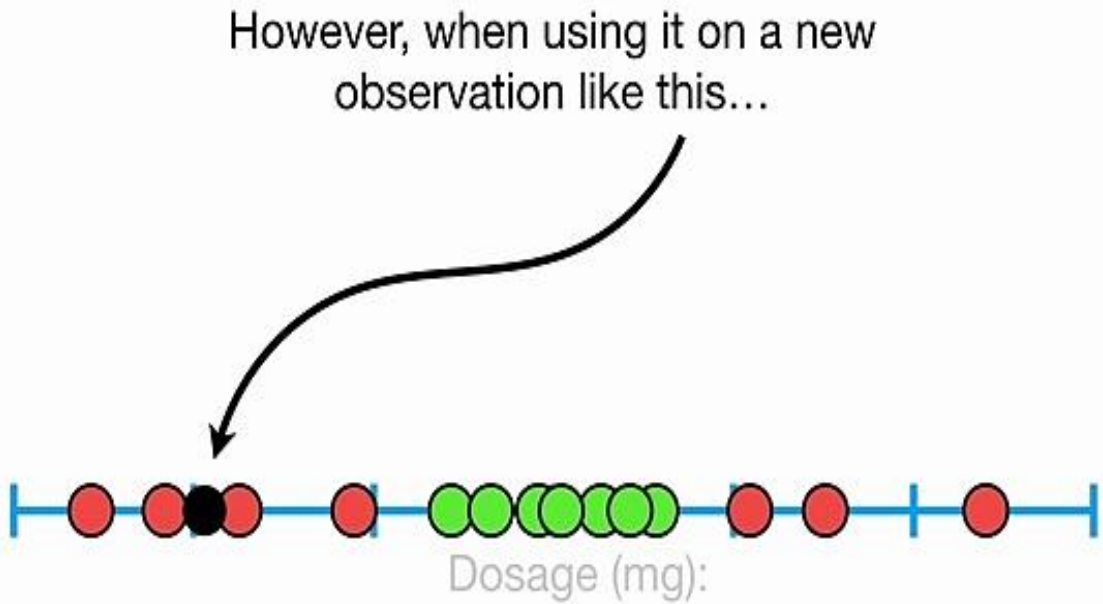
***d* = 1**


Last but not least, we can find a good value for d with Cross Validation.
d = 2
y-axis
Dosage (mg):


Last but not least, we can find a good value for d with Cross Validation.
d = 3
y-axis
z-axis
Dosage (mg):

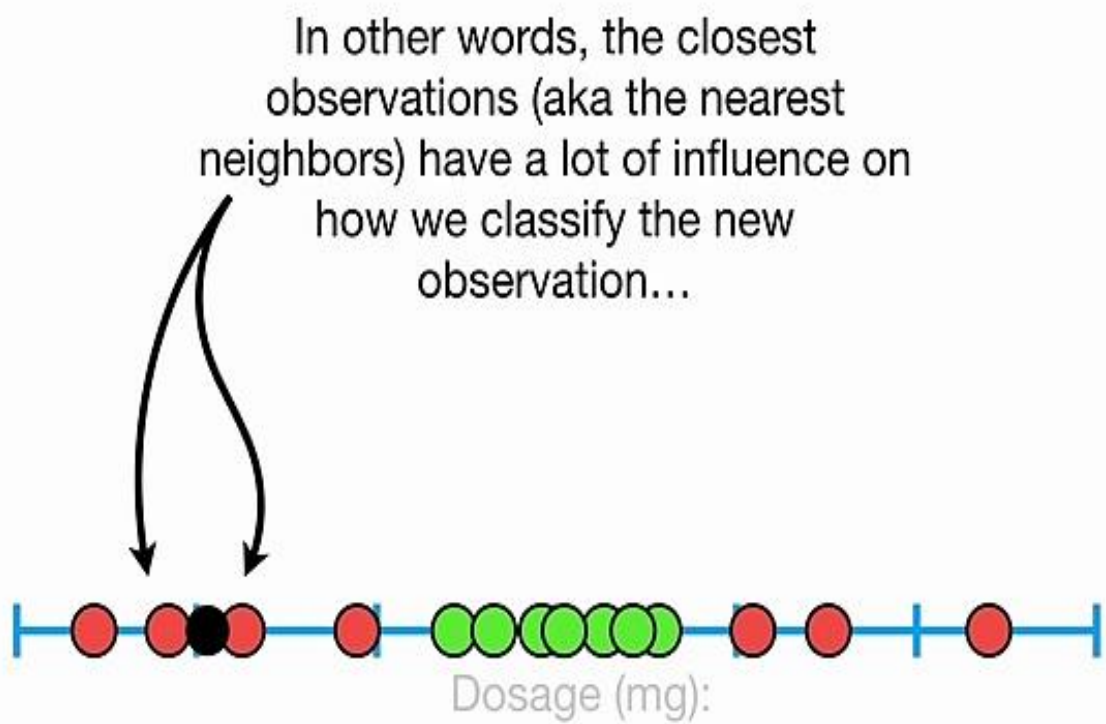

Last but not least, we can find a good value for d with Cross Validation.
y-axis
z-axis
Dosage (mg):

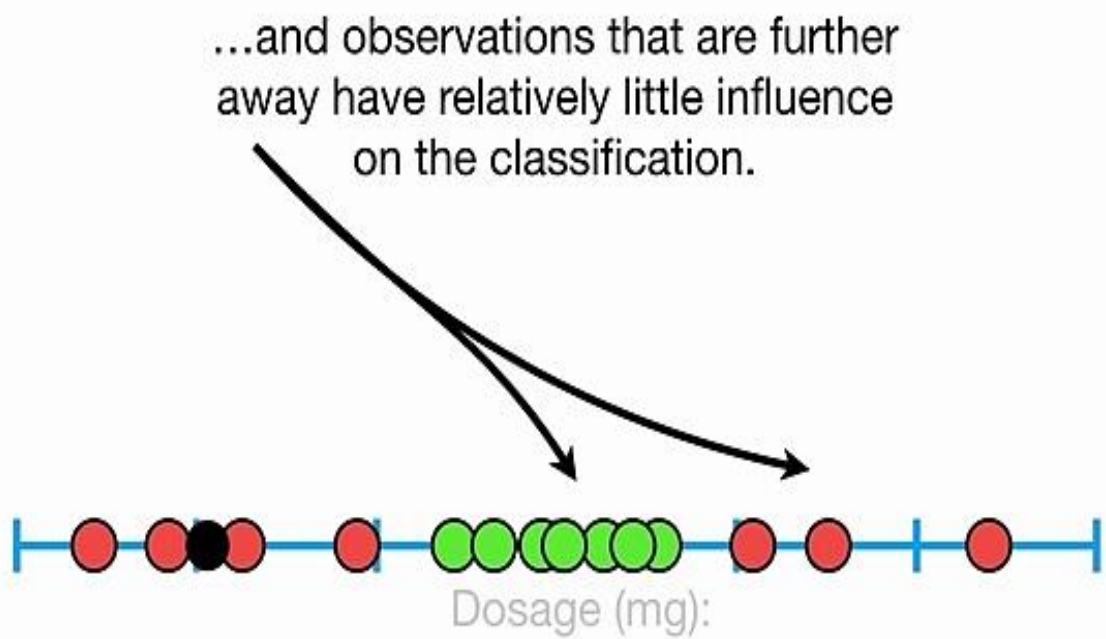
Another very commonly used **Kernel** is the **Radial Kernel**, also known as the **Radial Basis Function (RBF) Kernel**.

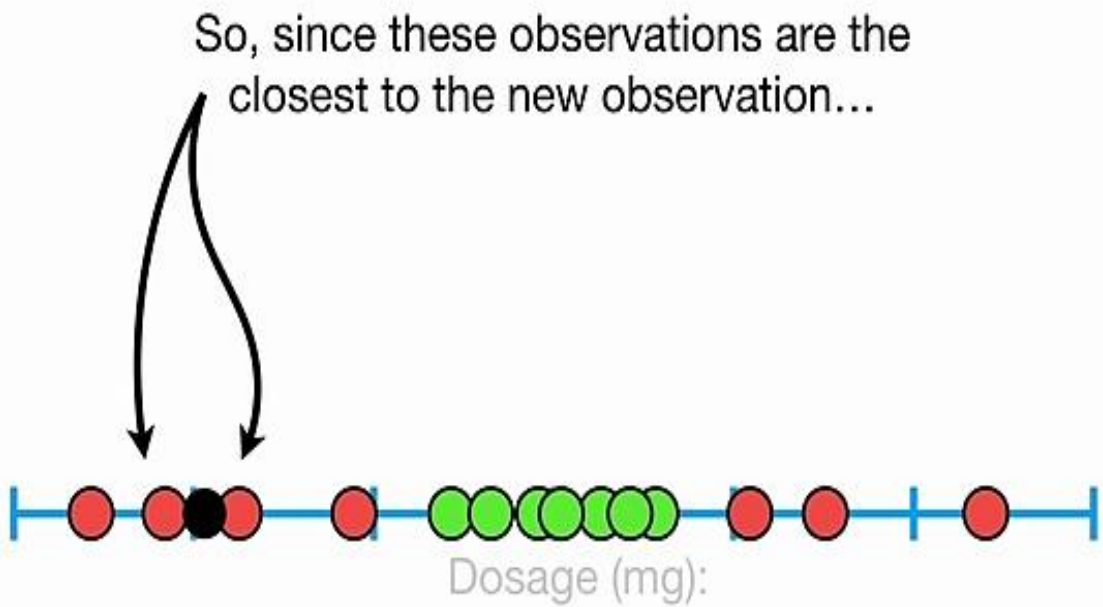

However, when using it on a new observation like this…
Dosage (mg):

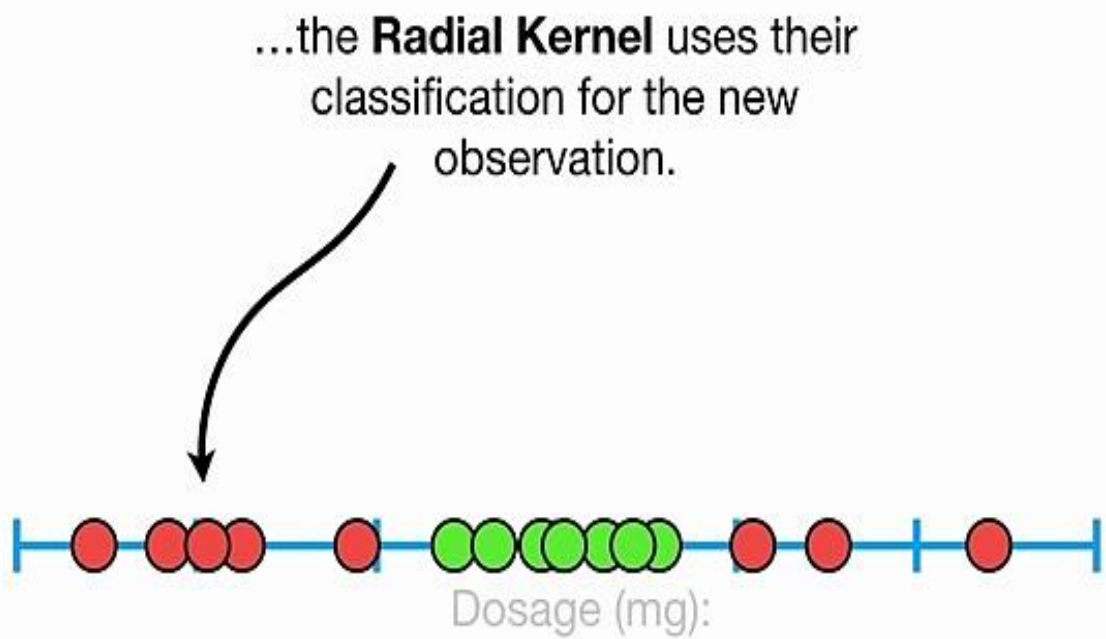
…the **Radial Kernel** behaves like a
Weighted Nearest Neighbor model.

Dosage (mg):

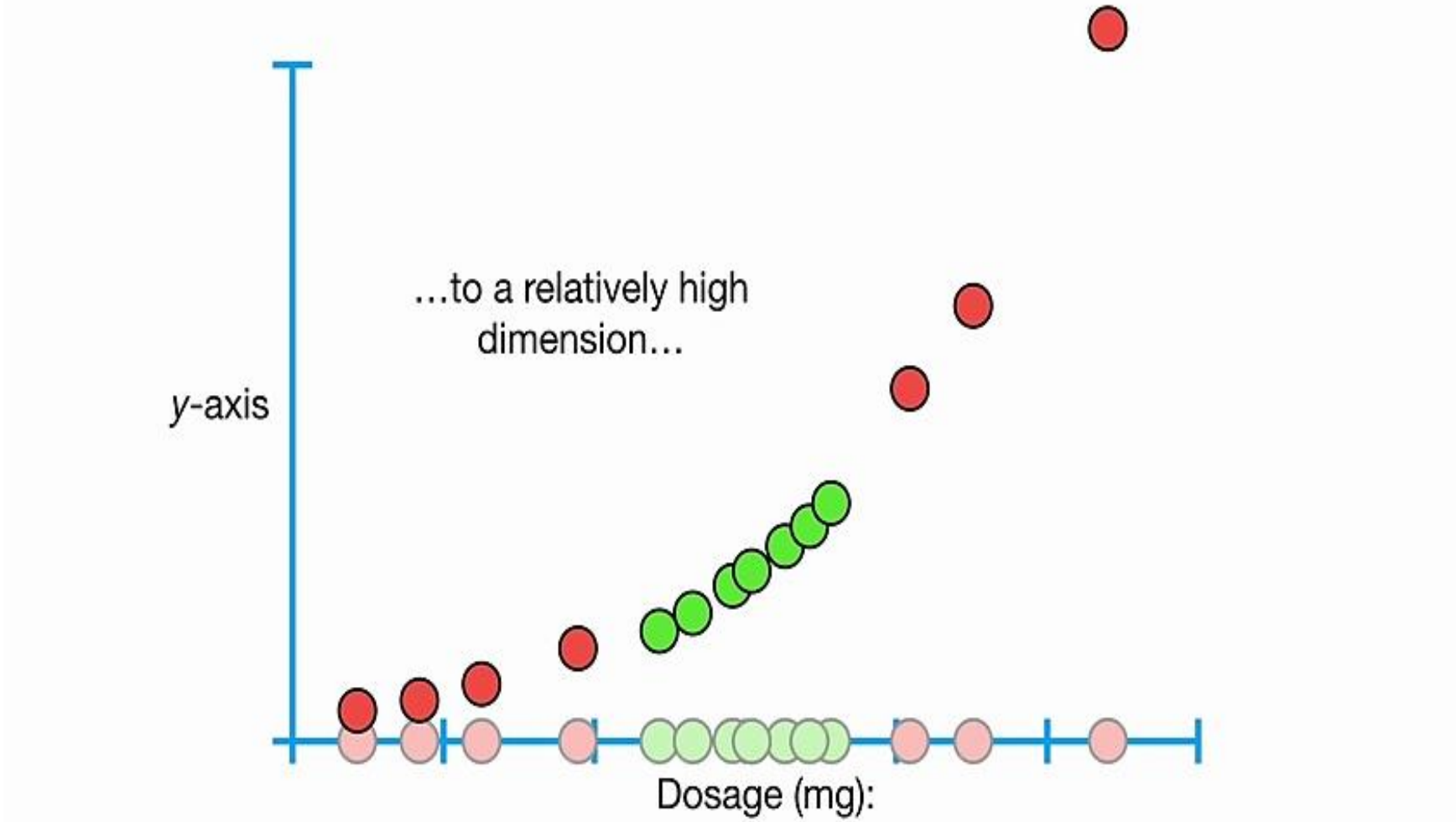

In other words, the closest observations (aka the nearest neighbors) have a lot of influence on how we classify the new observation…
Dosage (mg):

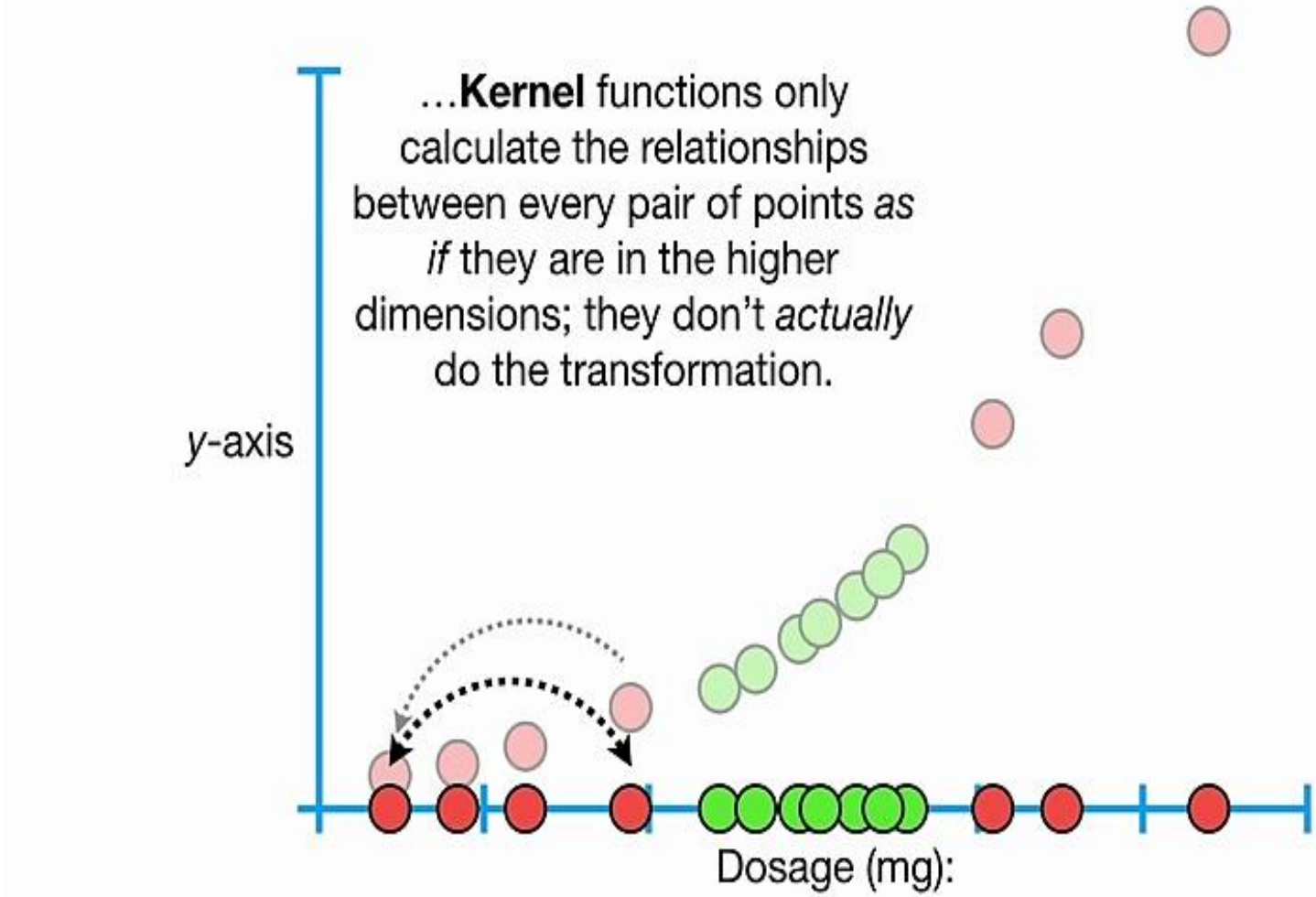

...and observations that are further
away have relatively little influence
on the classification.
Dosage (mg):

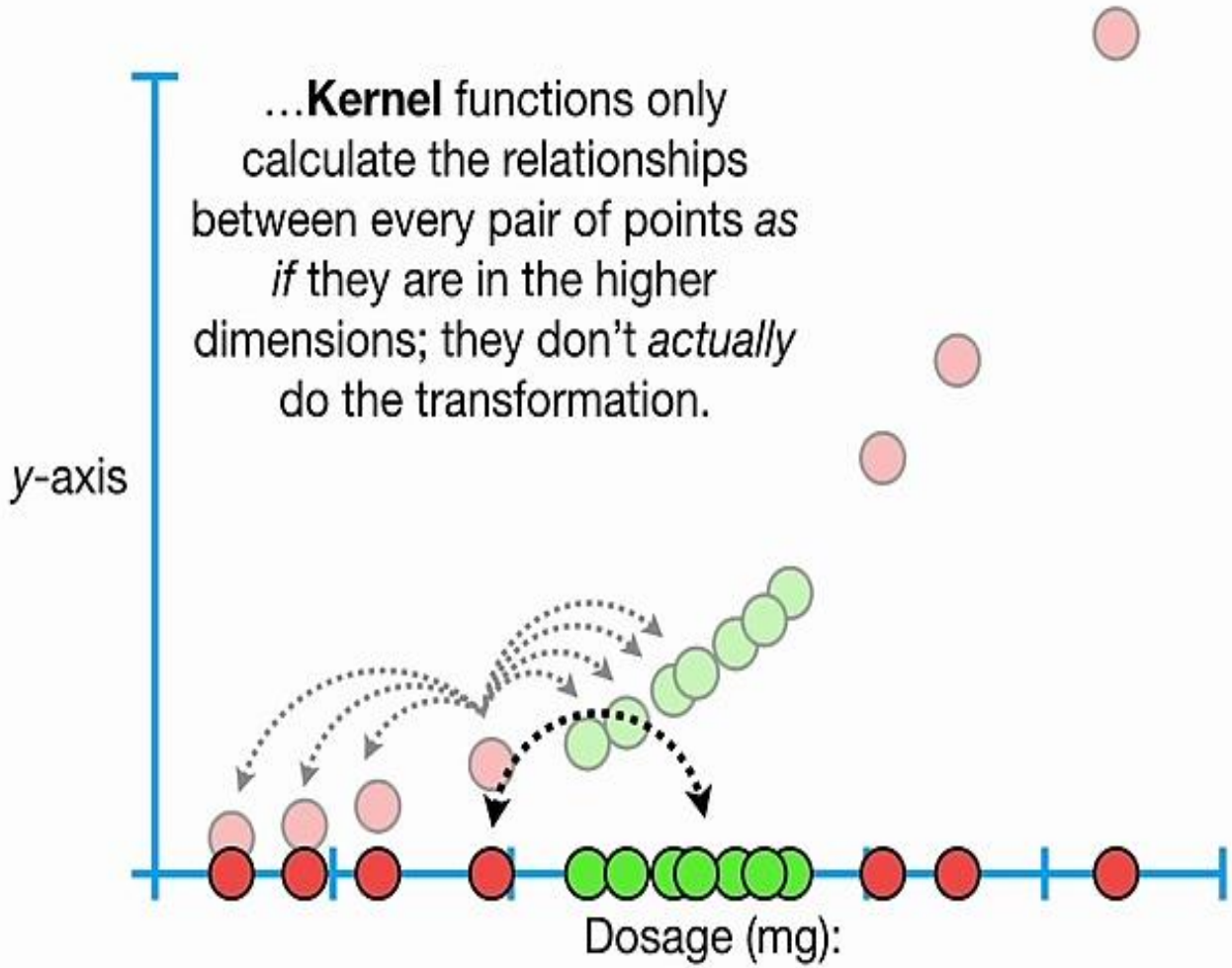

So, since these observations are the closest to the new observation…
Dosage (mg):


...the **Radial Kernel** uses their classification for the new observation.
Dosage (mg):

Although the examples I have given show the data being transformed from a relatively low dimension…


…to a relatively high
dimension…
y-axis
Dosage (mg):


...**Kernel** functions only calculate the relationships between every pair of points *as if* they are in the higher dimensions; they don't *actually* do the transformation.
y-axis
Dosage (mg):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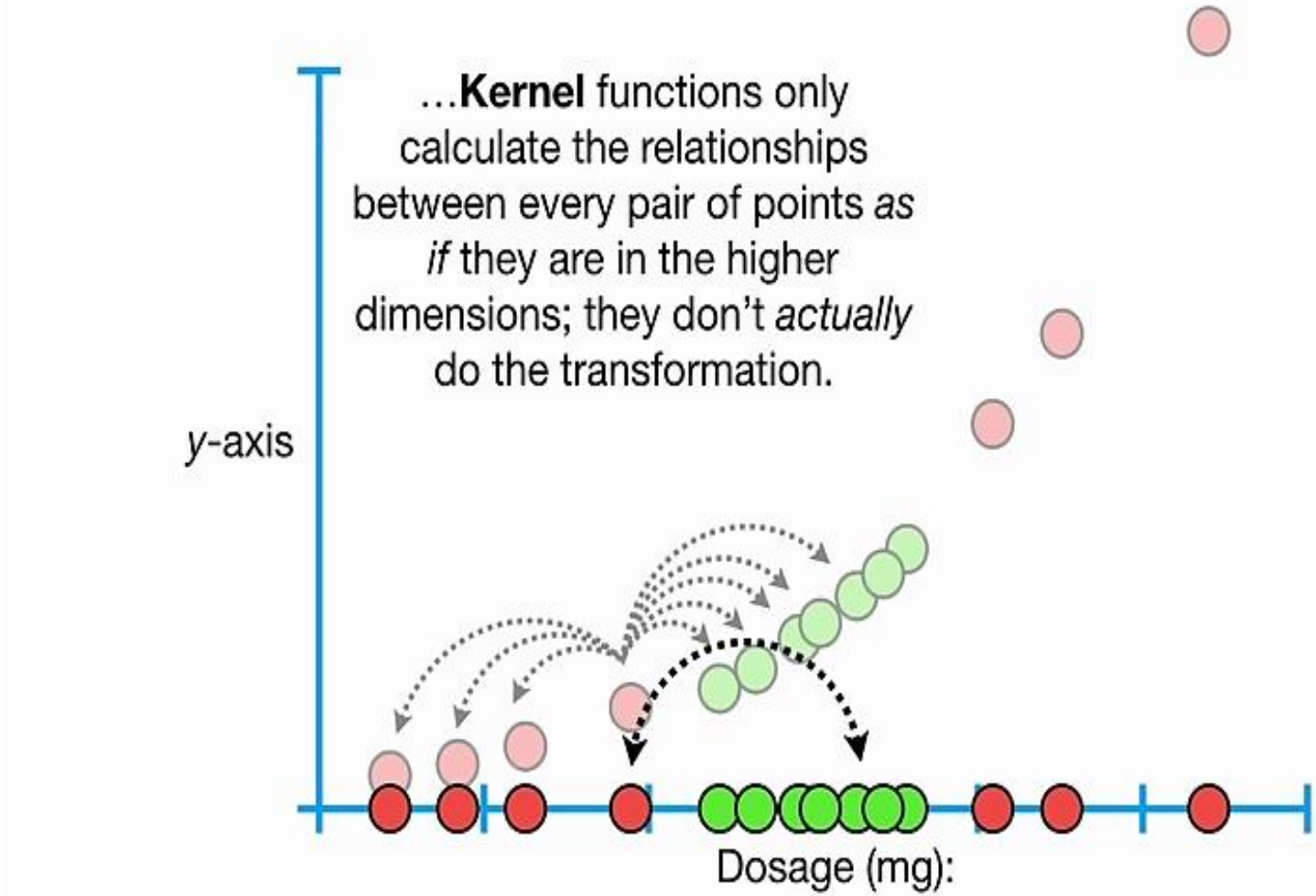
y-axis
Dosage (mg):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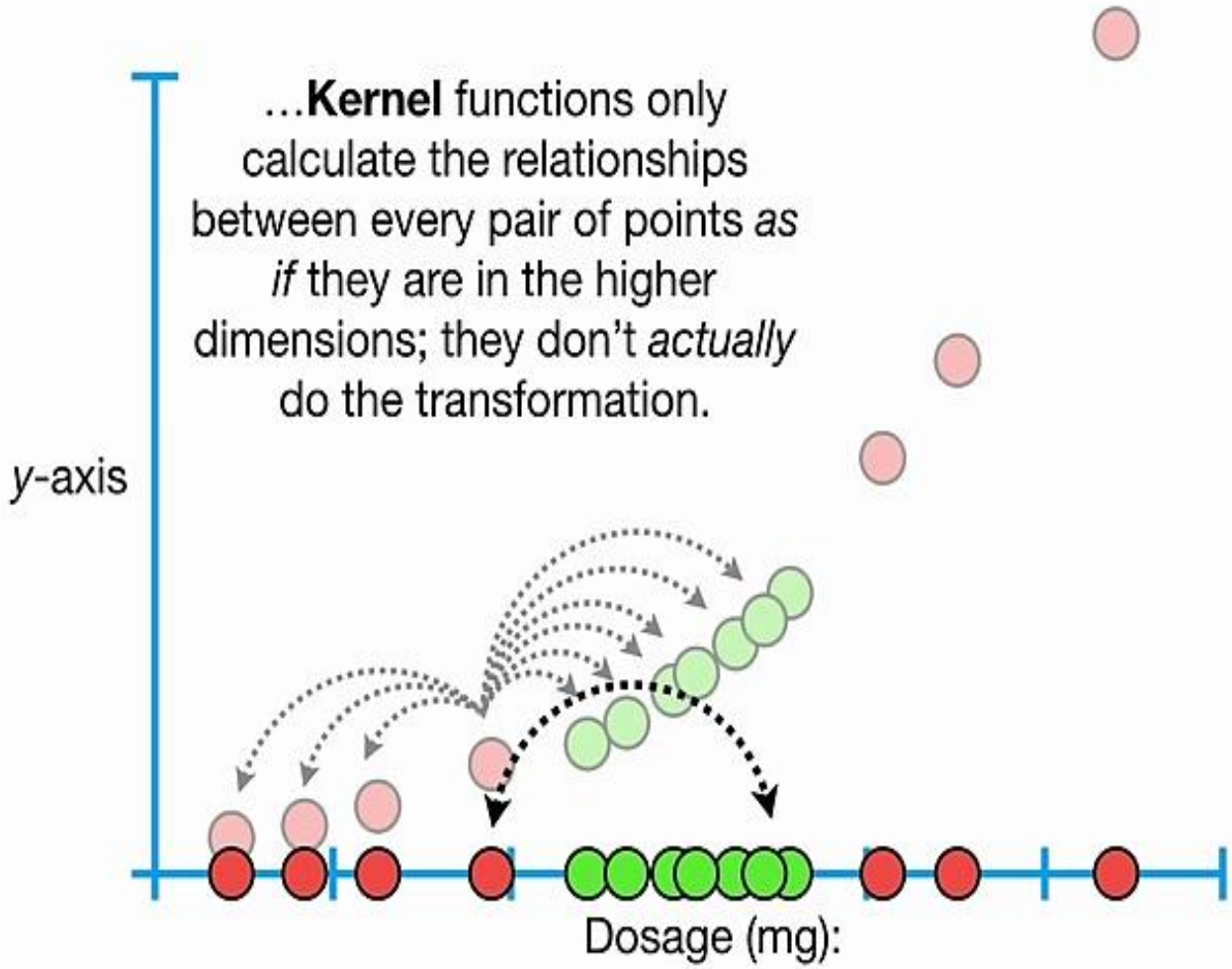
y-axis
Dosage (mg):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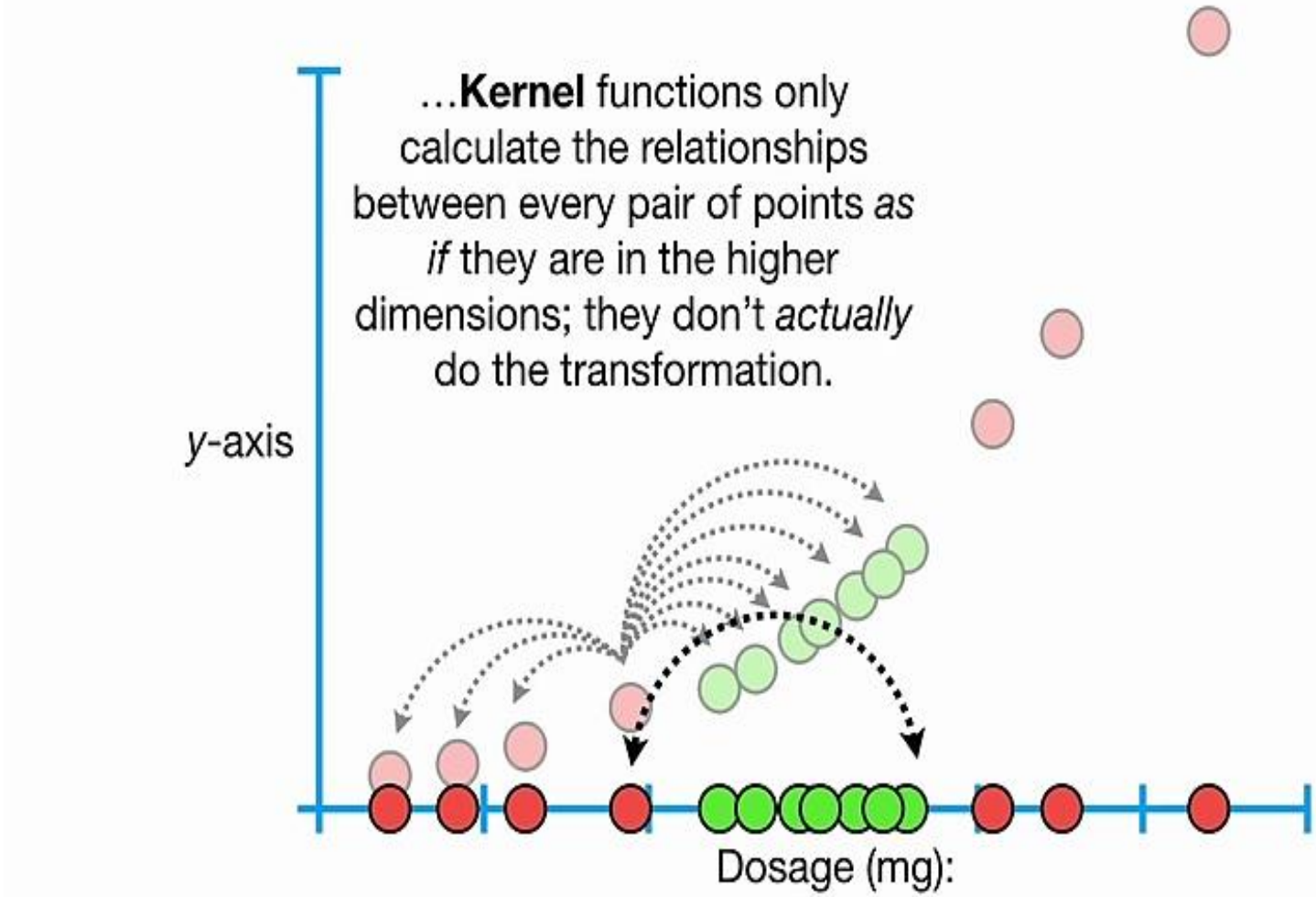
y-axis
Dosage (mg):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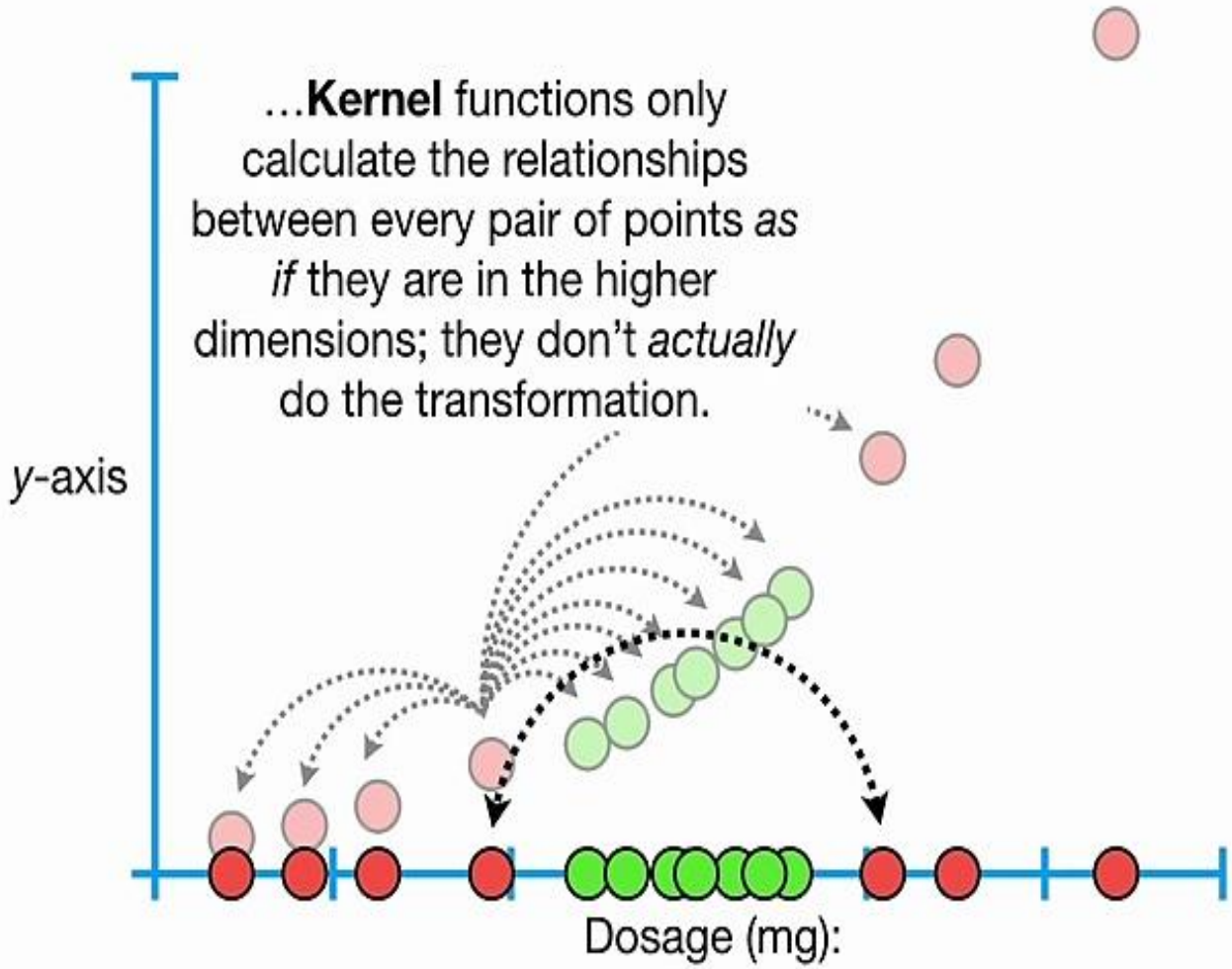
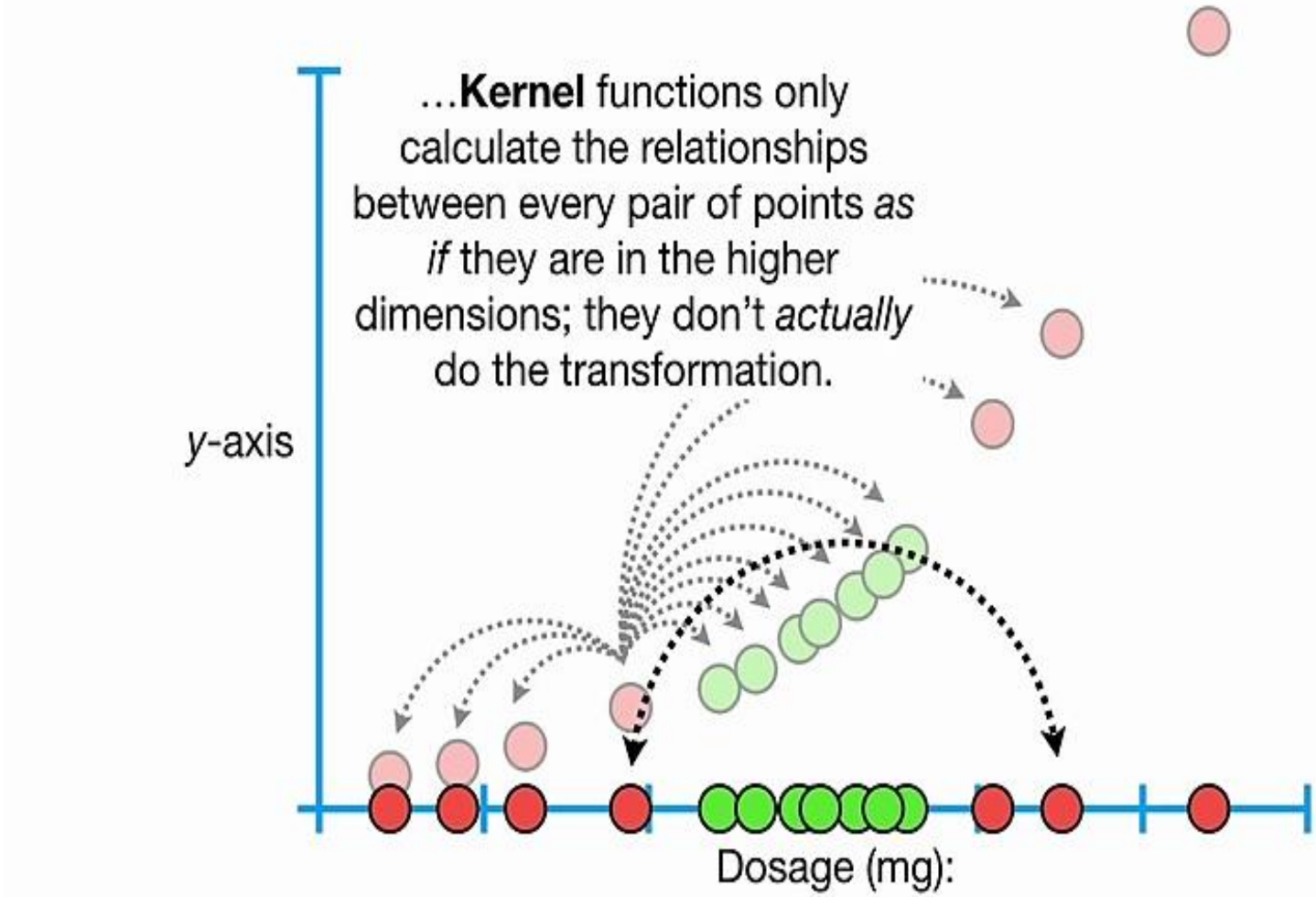
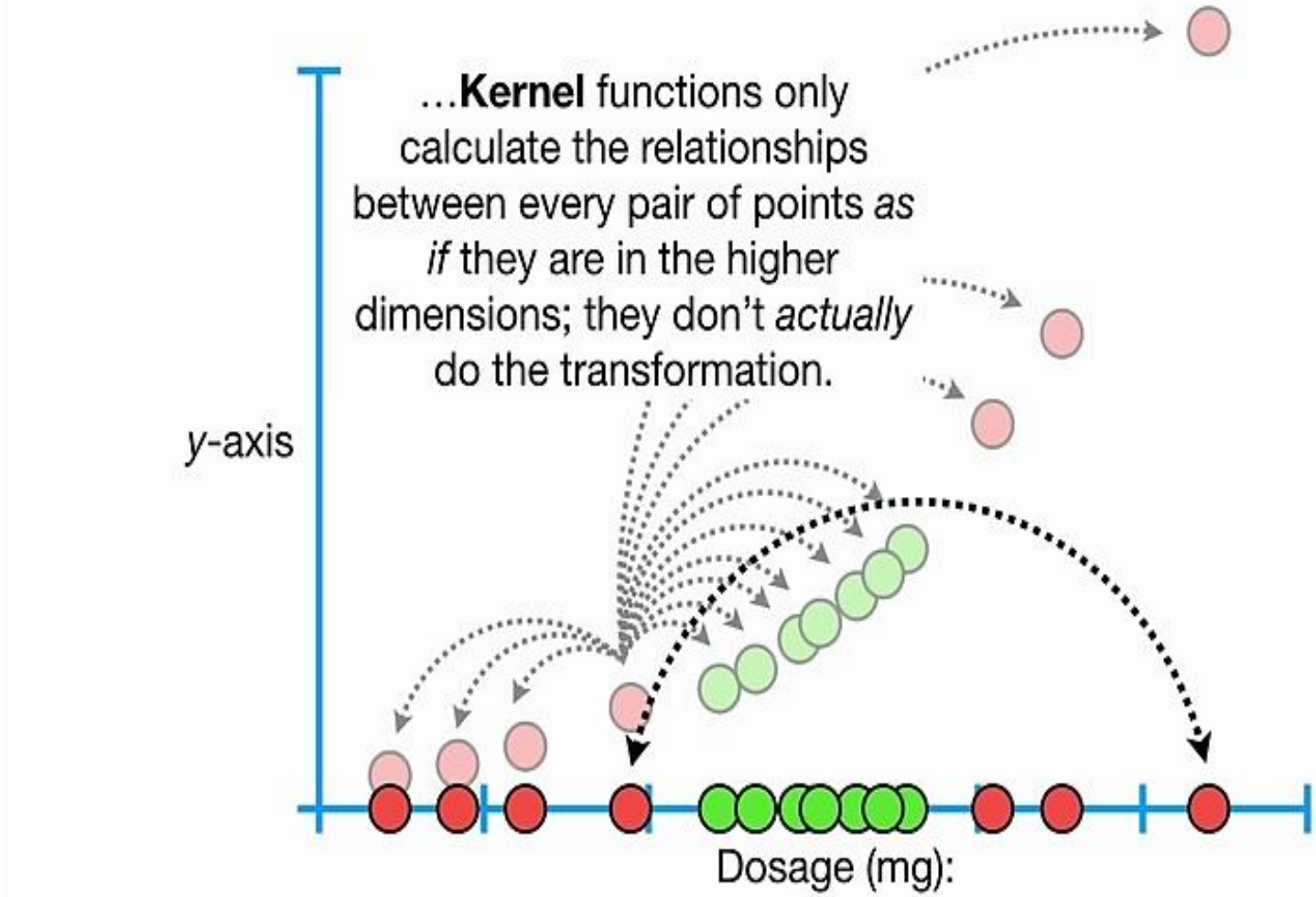
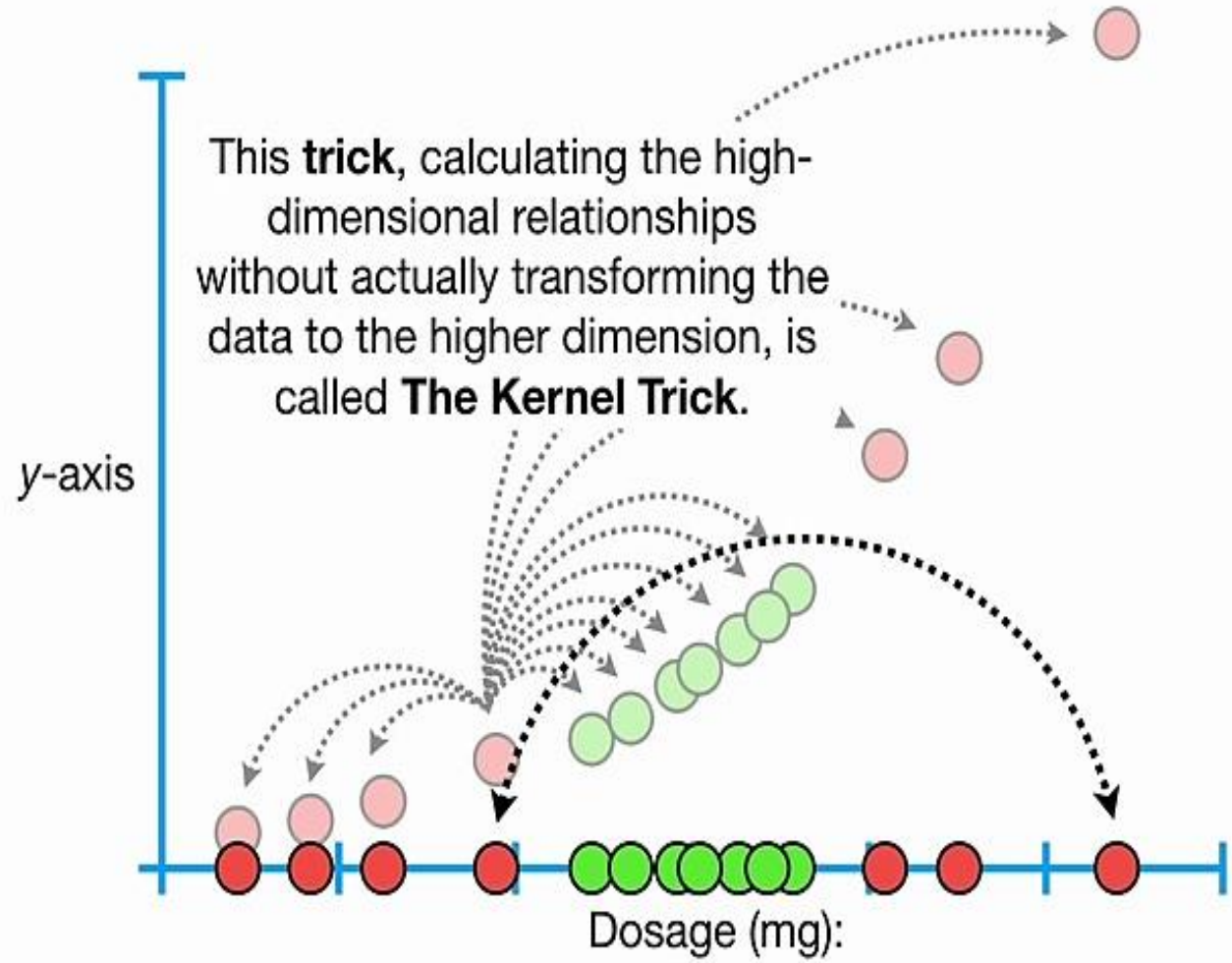
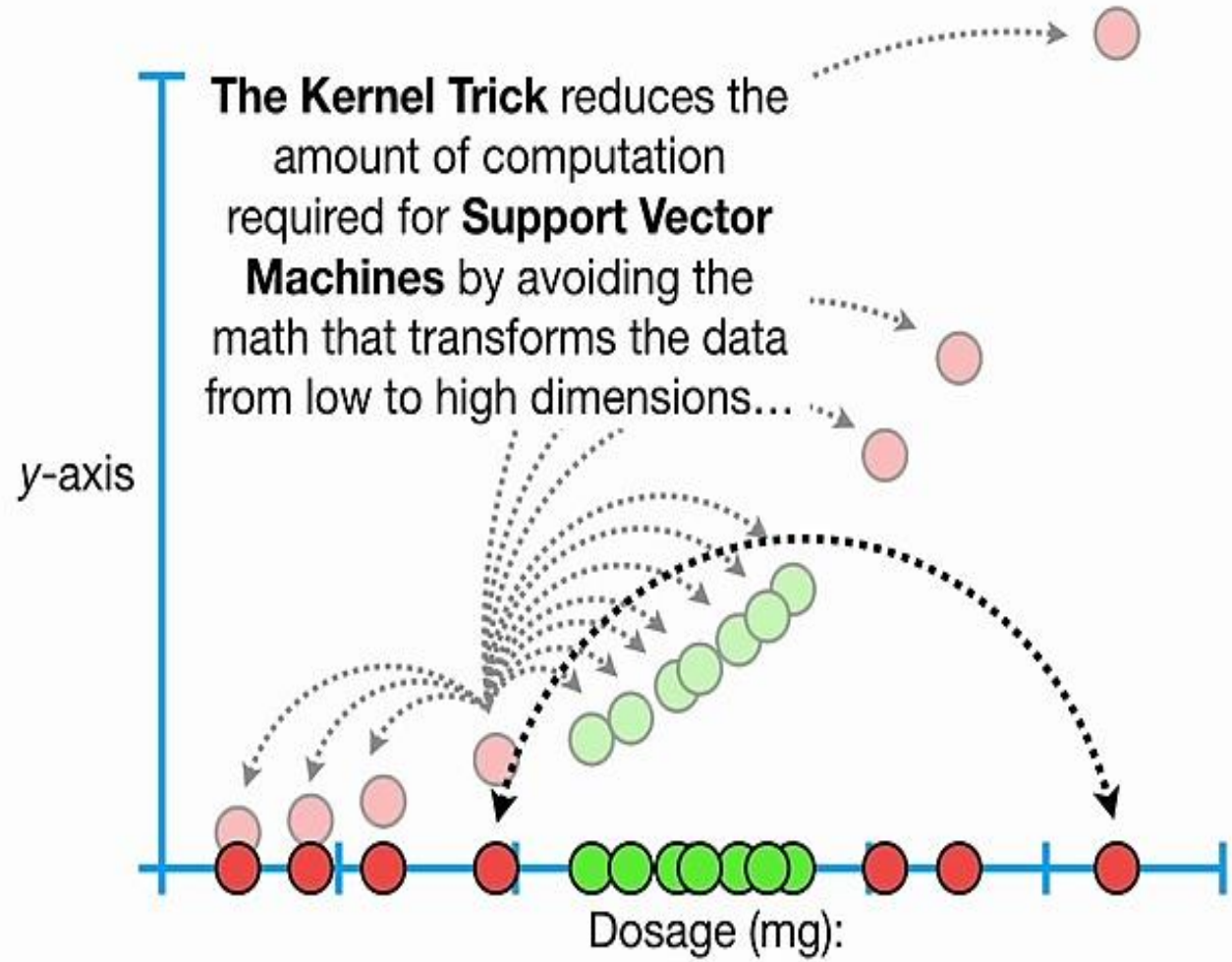
y-axis
Dosage (mg):

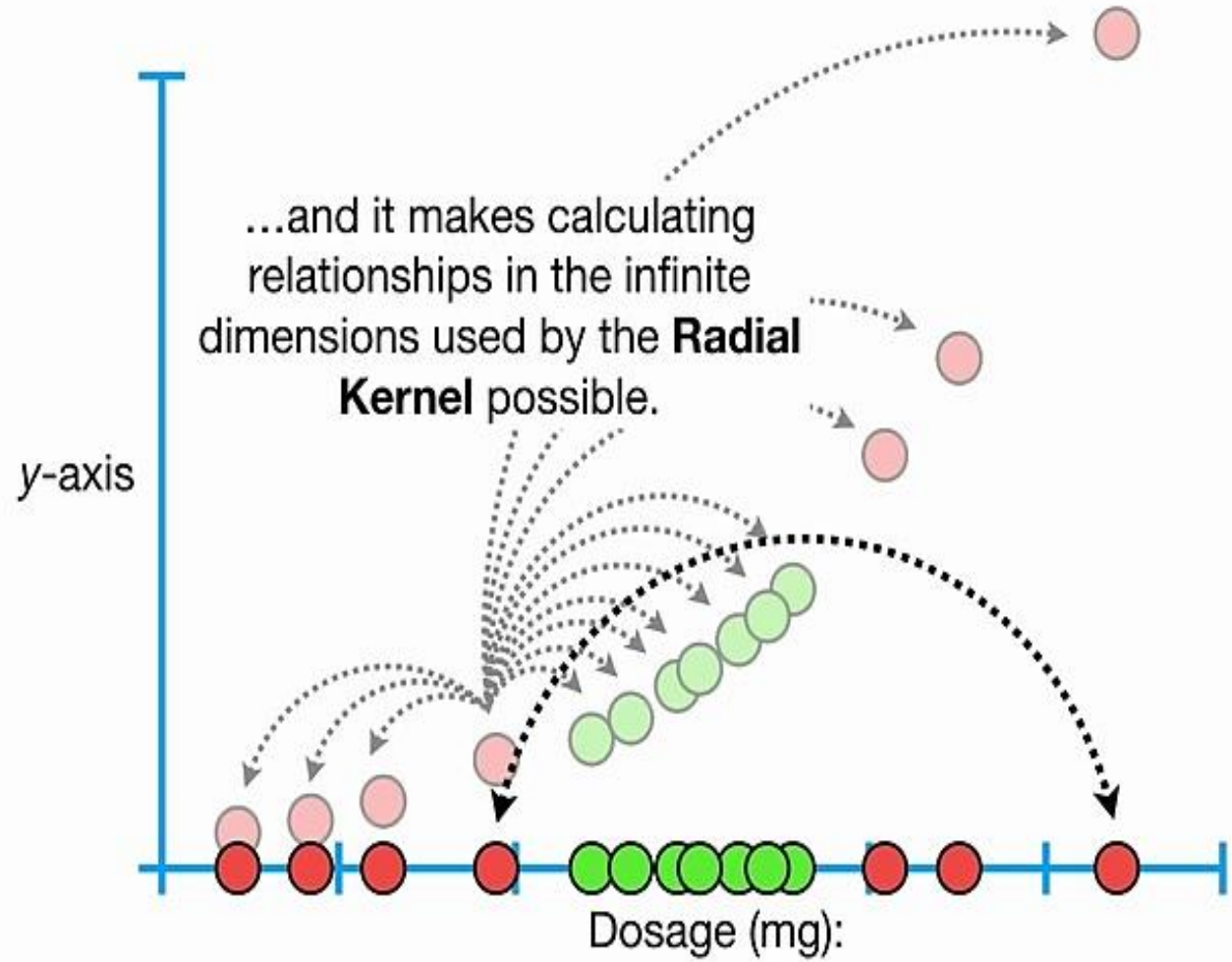

...**Kernel** functions only calculate the relationships between every pair of points *as if* they are in the higher dimensions; they don't *actually* do the transformation.
y-axis
Dosage (mg):


...**Kernel** functions only calculate the relationships between every pair of points *as if* they are in the higher dimensions; they don't *actually* do the transformation.
y-axis
Dosage (mg):


...**Kernel** functions only calculate the relationships between every pair of points *as if* they are in the higher dimensions; they don't *actually* do the transformation.
y-axis
Dosage (mg):

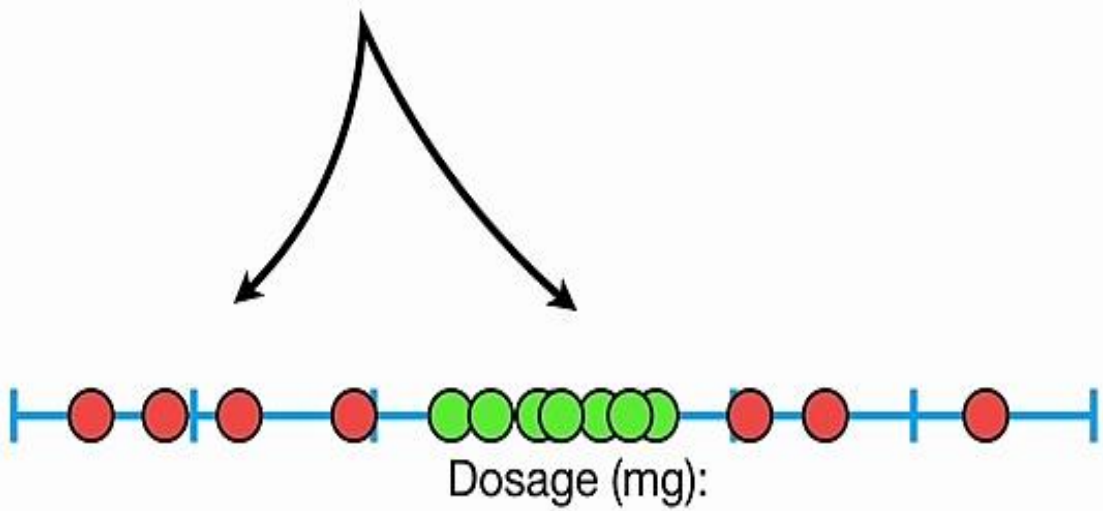

This **trick**, calculating the high-dimensional relationships without actually transforming the data to the higher dimension, is called **The Kernel Trick**.
y-axis
Dosage (mg):

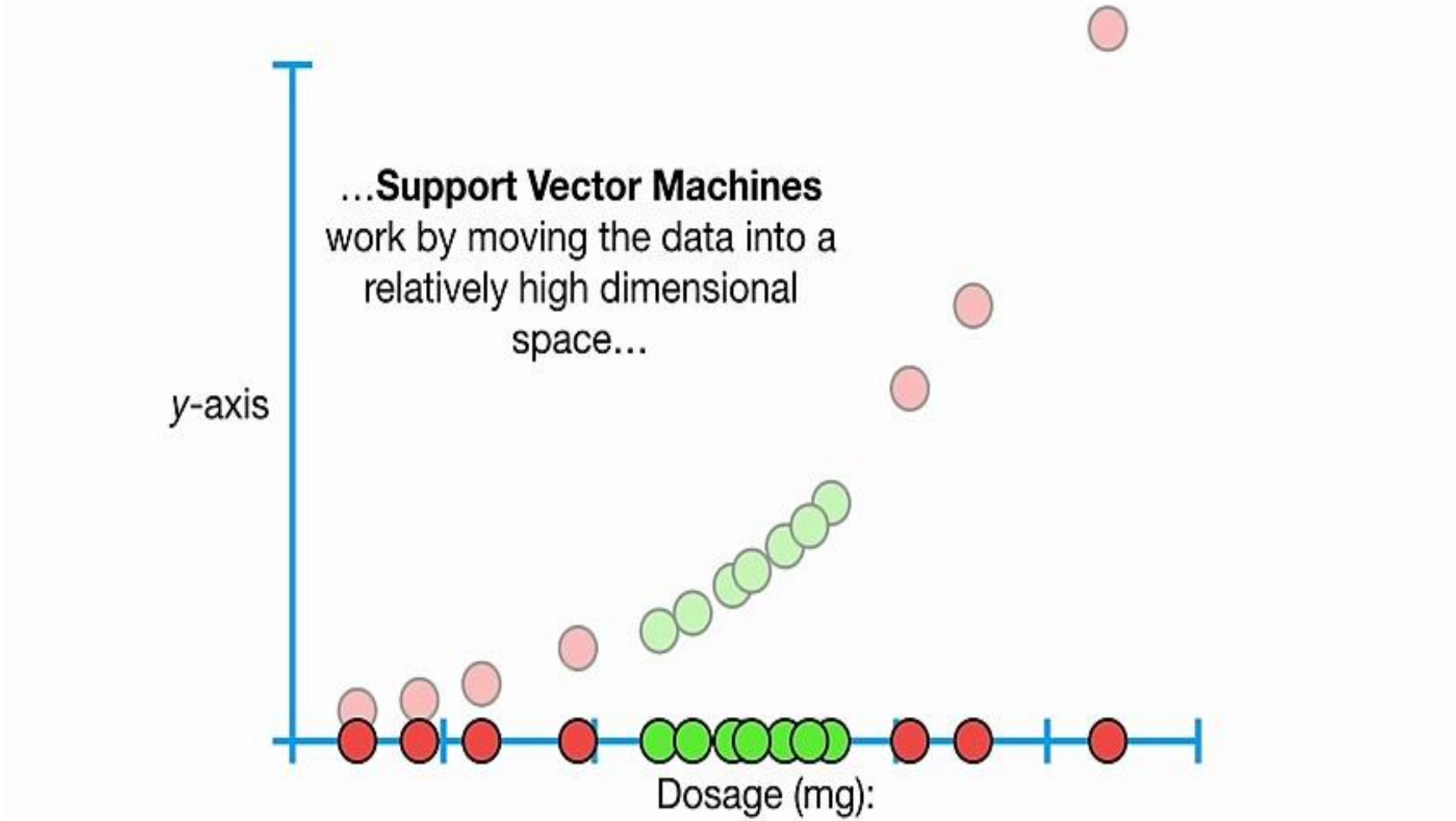

The Kernel Trick reduces the amount of computation required for Support Vector Machines by avoiding the math that transforms the data from low to high dimensions...
y-axis
Dosage (mg):

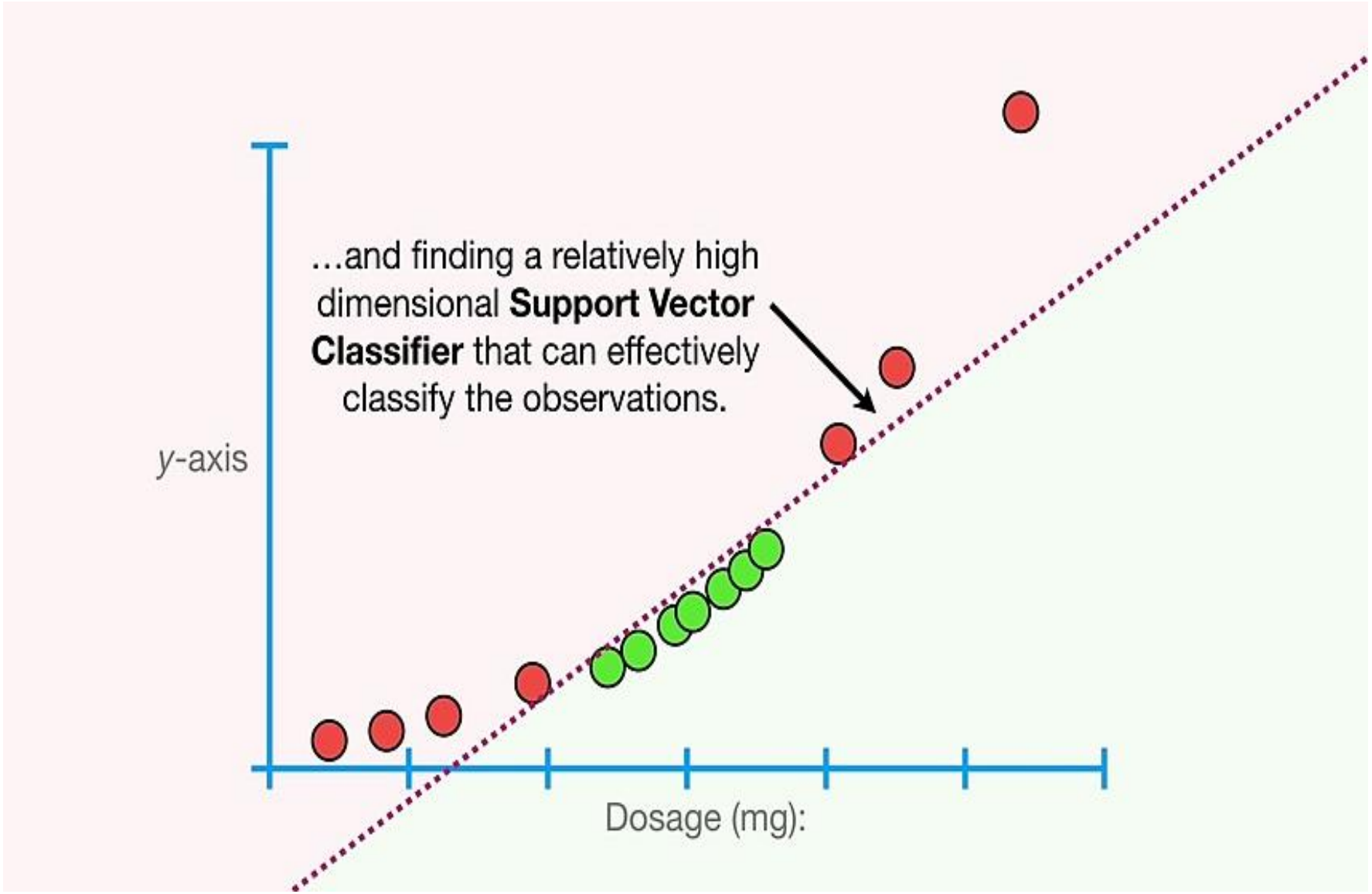

...and it makes calculating relationships in the infinite dimensions used by the **Radial Kernel** possible.
y-axis
Dosage (mg):

However, regardless of how the relationships are calculated, the concepts are the same.

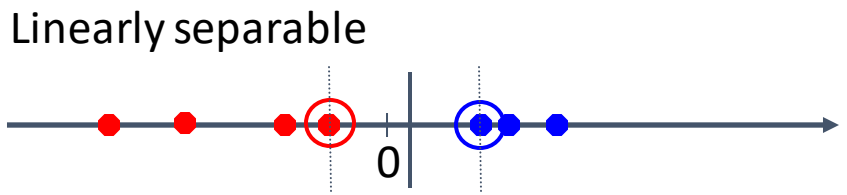
When we have **2** categories, but no obvious linear classifier that separates them in a nice way…




...Support Vector Machines
work by moving the data into a
relatively high dimensional
space...
y-axis
Dosage (mg):

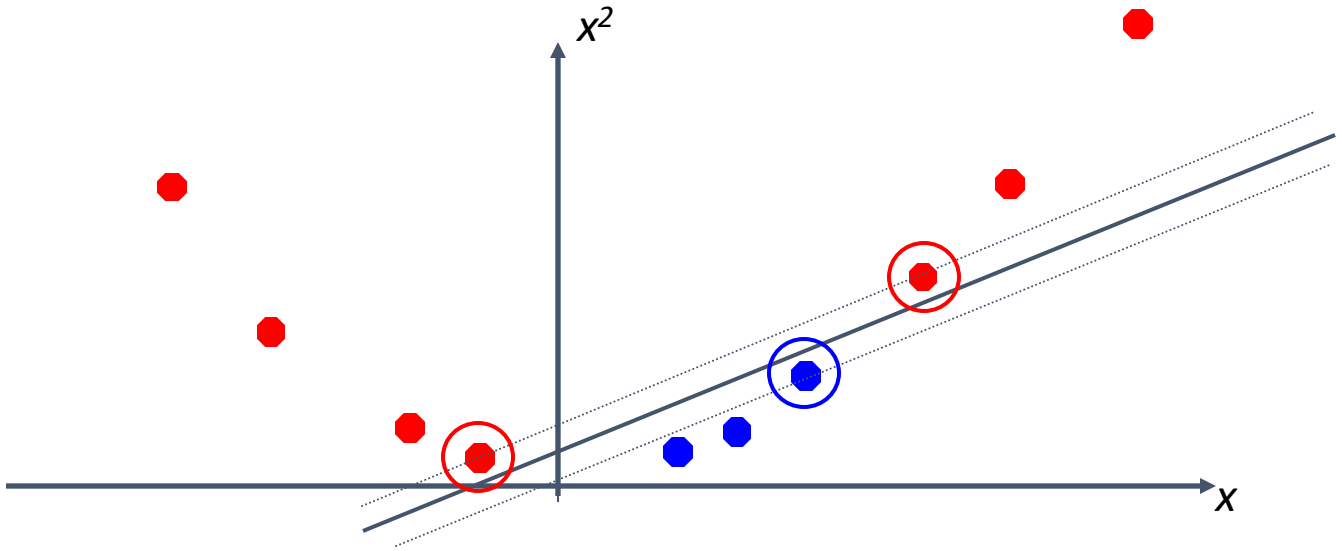

...and finding a relatively high dimensional **Support Vector Classifier** that can effectively classify the observations.
y-axis
Dosage (mg):

Non-linear SVM



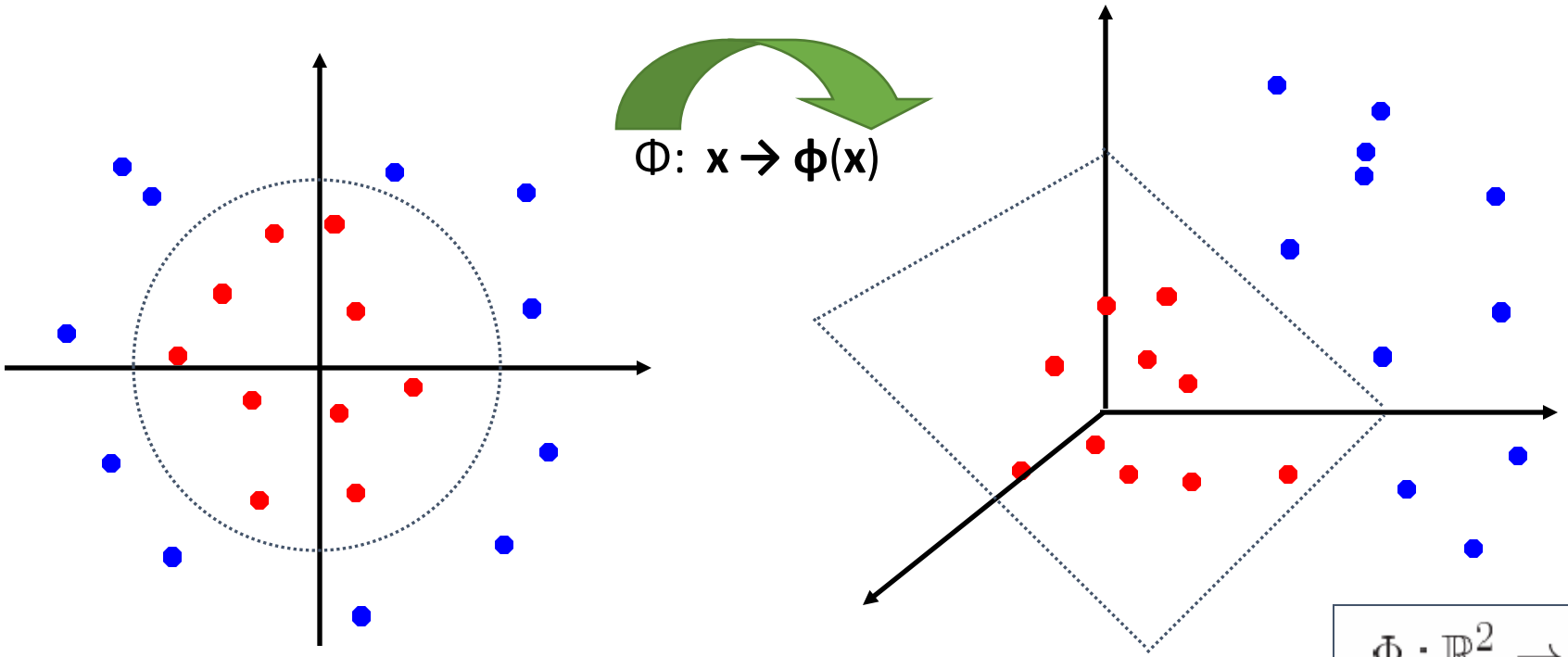
- What if the decision boundary is not linear?

- How about… mapping data to a higher-dimensional space:



Non-linear SVMs: Feature Spaces

Idea: the original feature space can always be mapped to some higher-dimensional feature space where the training set is separable.



$$\Phi : \mathbb{R}^2 \to \mathbb{R}^3$$
$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{2}\, x_1 x_2, x_2^2)$$

Non-linear SVM

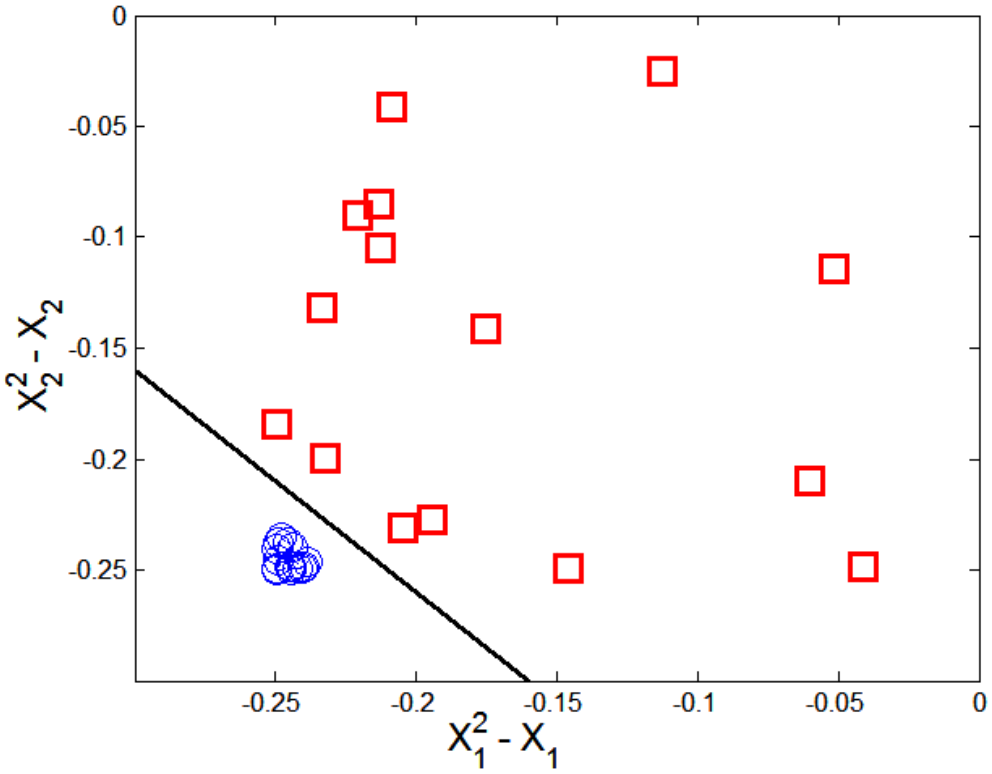
- The trick is to transform the data from its original space x into a new space $\Phi(x)$ (phi) so that a linear decision boundary can be used.

$$x_1^2 - x_1 + x_2^2 - x_2 = -0.46.$$

$$\Phi : (x_1, x_2) \longrightarrow (x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, 1).$$

$$w_4 x_1^2 + w_3 x_2^2 + w_2\sqrt{2}x_1 + w_1\sqrt{2}x_2 + w_0 = 0.$$

- Decision boundary $\vec{w} \bullet \Phi(\vec{x}) + b = 0$



Learning a Nonlinear SVM

- Optimization problem

$$\min_{w} \frac{\|\mathbf{w}\|^2}{2}$$

$$subject\ to \qquad y_i(\boldsymbol{w} \cdot \Phi(x_i) + b) \geq 1,\ \forall\{(x_i, y_i)\}$$

- Which leads to the same set of equations but involve $\Phi(x)$ instead of x.

$$f(\mathbf{z}) = sign(\mathbf{w} \cdot \Phi(\mathbf{z}) + b) = sign(\sum_{i=1}^{n} \lambda_i y_i \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{z}) + b).$$

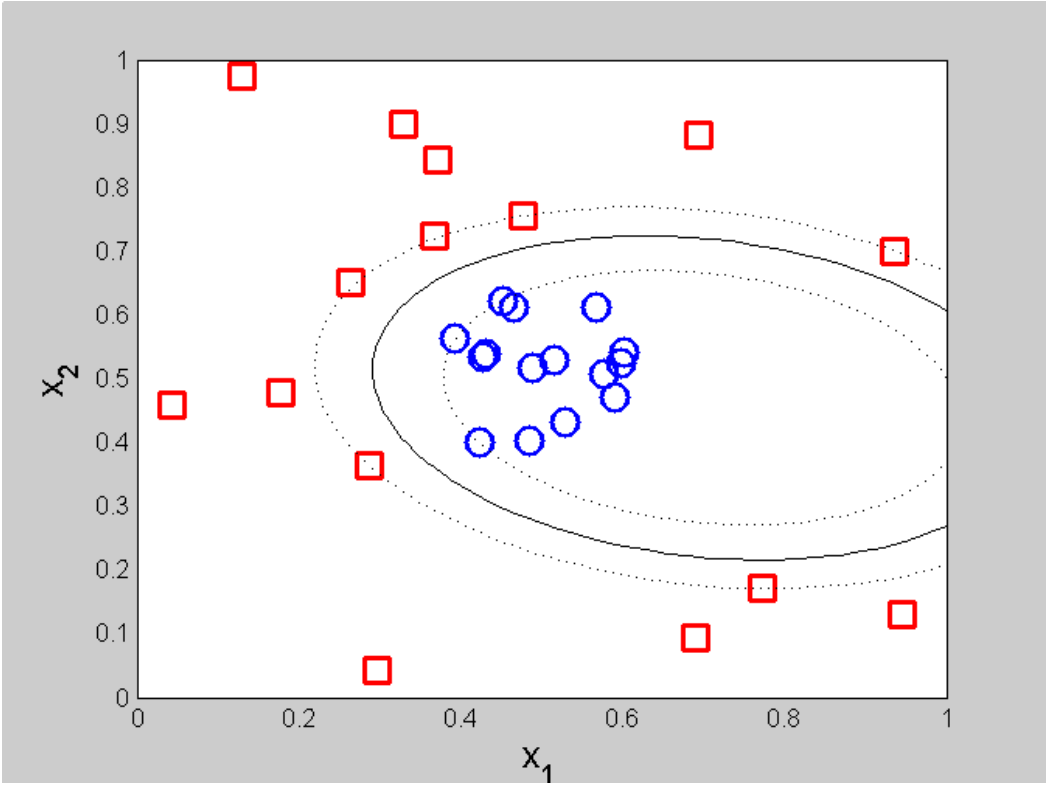
Issues:

- What type of mapping function Φ should be used?
- How to do the computation in high dimensional space?
  - Most computations involve dot product $\Phi(x) \cdot \Phi(x)$
  - Curse of dimensionality?

The Kernel Trick

- $\Phi(x) \cdot \Phi(x) = K(x_i, x_j)$
- $K(x_i, x_j)$ is a kernel function (expressed in terms of the coordinates in the original space)
- Examples:

$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^T\mathbf{y} + 1)^d$$
$$K(\mathbf{x}, \mathbf{y}) = \exp(-||\mathbf{x} - \mathbf{y}||^2/(2\sigma^2))$$
$$K(\mathbf{x}, \mathbf{y}) = \tanh(\kappa\mathbf{x}^T\mathbf{y} + \theta)$$



https://scikit-learn.org/stable/auto_examples/svm/plot_svm_kernels.html#sphx-glr-auto-examples-svm-plot-svm-kernels-py
https://scikit-learn.org/stable/auto_examples/exercises/plot_iris_exercise.html#sphx-glr-auto-examples-exercises-plot-iris-exercise-py

Examples of Kernel Functions

- Polynomial kernel with degree *d*

$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^T\mathbf{y} + 1)^d$$

- Radial basis function kernel with width σ

$$K(\mathbf{x}, \mathbf{y}) = \exp(-||\mathbf{x} - \mathbf{y}||^2/(2\sigma^2))$$

  - Closely related to radial basis function neural networks
  - The feature space is infinite-dimensional

- Sigmoid with parameter κ and θ $\quad K(\mathbf{x}, \mathbf{y}) = \tanh(\kappa\mathbf{x}^T\mathbf{y} + \theta)$
  - It does not satisfy the Mercer condition on all κ and θ

- Choosing the Kernel Function is probably the most tricky part of using SVM.

The Kernel Trick

- The linear classifier relies on inner product between vectors $K(\mathbf{x}_i,\mathbf{x}_j)=\mathbf{x}_i^T\mathbf{x}_j$
- If every datapoint is mapped into high-dimensional space via some transformation Φ: $\mathbf{x} \rightarrow \phi(\mathbf{x})$, the inner product becomes:

$$K(\mathbf{x}_i,\mathbf{x}_j)= \boldsymbol{\phi}(\mathbf{x}_i)^T\boldsymbol{\phi}(\mathbf{x}_j)$$

- A *kernel function* is a function that is equivalent to an inner product in some feature space.
- Example:

  2-dimensional vectors $\mathbf{x}=[x_1 \;\; x_2]$; let $K(\mathbf{x}_i,\mathbf{x}_j)=(1 + \mathbf{x}_i^T\mathbf{x}_j)^2$,

  Need to show that $K(\mathbf{x}_i,\mathbf{x}_j)= \boldsymbol{\phi}(\mathbf{x}_i)^T\boldsymbol{\phi}(\mathbf{x}_j)$:

  $K(\mathbf{x}_i,\mathbf{x}_j)=(1 + \mathbf{x}_i^T\mathbf{x}_j)^2= 1+ x_{i1}^2x_{j1}^2 + 2\, x_{i1}x_{j1}x_{i2}x_{j2}+ x_{i2}^2x_{j2}^2 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2}=$

  $= [1 \;\; x_{i1}^2 \;\; \sqrt{2}\, x_{i1}x_{i2} \;\; x_{i2}^2 \;\; \sqrt{2}x_{i1} \;\; \sqrt{2}x_{i2}]^T [1 \;\; x_{j1}^2 \;\; \sqrt{2}\, x_{j1}x_{j2} \;\; x_{j2}^2 \;\; \sqrt{2}x_{j1} \;\; \sqrt{2}x_{j2}] =$

  $= \boldsymbol{\phi}(\mathbf{x}_i)^T\boldsymbol{\phi}(\mathbf{x}_j)$, where $\boldsymbol{\phi}(\mathbf{x}) = [1, \; x_1^2, \; \sqrt{2}\, x_1x_2, \; x_2^2, \; \sqrt{2}x_1, \; \sqrt{2}x_2]$

- Thus, a kernel function *implicitly* maps data to a high-dimensional space (without the need to compute each $\boldsymbol{\phi}(\mathbf{x})$ explicitly).

The Kernel Trick

$$f(\mathbf{z}) = sign(\mathbf{w} \cdot \Phi(\mathbf{z}) + b) = sign(\sum_{i=1}^{n} \lambda_i y_i \boxed{K(\mathbf{x}_i, \mathbf{z})} + b).$$

Advantages of using kernel:

- Don't have to know the mapping function Φ.
- Computing dot product $\Phi(x) \cdot \Phi(y)$ in the original space avoids curse of dimensionality.

Not all functions can be kernels

- Must make sure there is a corresponding Φ in some high-dimensional space.
- *Mercer's theorem* (see textbook) that ensures that the kernel functions can always be expressed as the dot product in some high dimensional space.

Mercer theorem: the function must be "positive-definite"

This implies that the *n* by *n* kernel matrix, in which the *(i,j)*-th entry is the $K(x_i, x_j)$, is always positive definite

This also means that optimization problem can be solved in polynomial time!

Constrained Optimization Problem with Kernel

Minimize $\| \mathbf{w} \| = \langle \mathbf{w} \cdot \mathbf{w} \rangle$ subject to $y_i(\langle \mathbf{x}_i \cdot \mathbf{w} \rangle + b) \geq 1$ for all i

Lagrangian method : maximize $\inf_{\mathbf{w}} L(\mathbf{w}, b, \alpha)$, where

$$L(\mathbf{w}, b, \alpha) = \frac{1}{2} \| \mathbf{w} \|^2 - \sum_i \alpha_i \left[\left(y_i (\mathbf{x}_i \cdot \mathbf{w}) + b \right) - 1 \right]$$

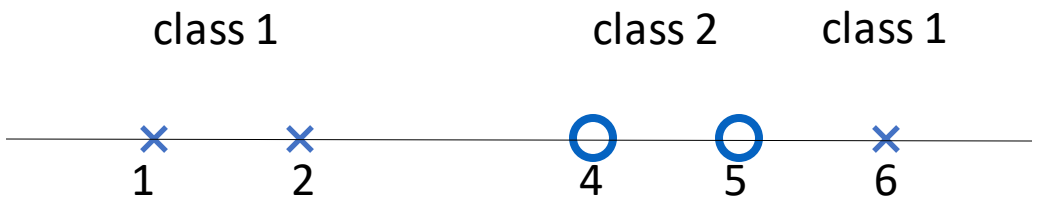
At the extremum, the partial derivative of L with respect both $\mathbf{w}$ and b must be 0. Taking the derivatives, setting them to 0, substituting back into L, and simplifying yields :

Maximize $\sum_i \alpha_i - \frac{1}{2} \sum_{i,j} y_i y_j \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j)$

subject to $\sum_i y_i \alpha_i = 0$ and $\alpha_i \geq 0$

$\lambda = \alpha$

Example



Example

- Suppose we have 5 one-dimensional data points
  - x_1=1, x_2=2, x_3=4, x_4=5, x_5=6, with values 1, 2, 6 as class 1 and 4, 5 as class 2
  - $\Rightarrow$ y_1=1, y_2=1, y_3=-1, y_4=-1, y_5=1
- We use the polynomial kernel of degree 2
  - **K(x,z) = (xz+1)²**
  - C is set to 100
- We first find α_i (*i*=1, …, 5) by

$$\text{max.} \sum_{i=1}^{5} \alpha_i - \frac{1}{2} \sum_{i=1}^{5} \sum_{j=1}^{5} \alpha_i \alpha_j y_i y_j (x_i x_j + 1)^2$$

$$\text{subject to } 100 \geq \alpha_i \geq 0, \sum_{i=1}^{5} \alpha_i y_i = 0$$

Example

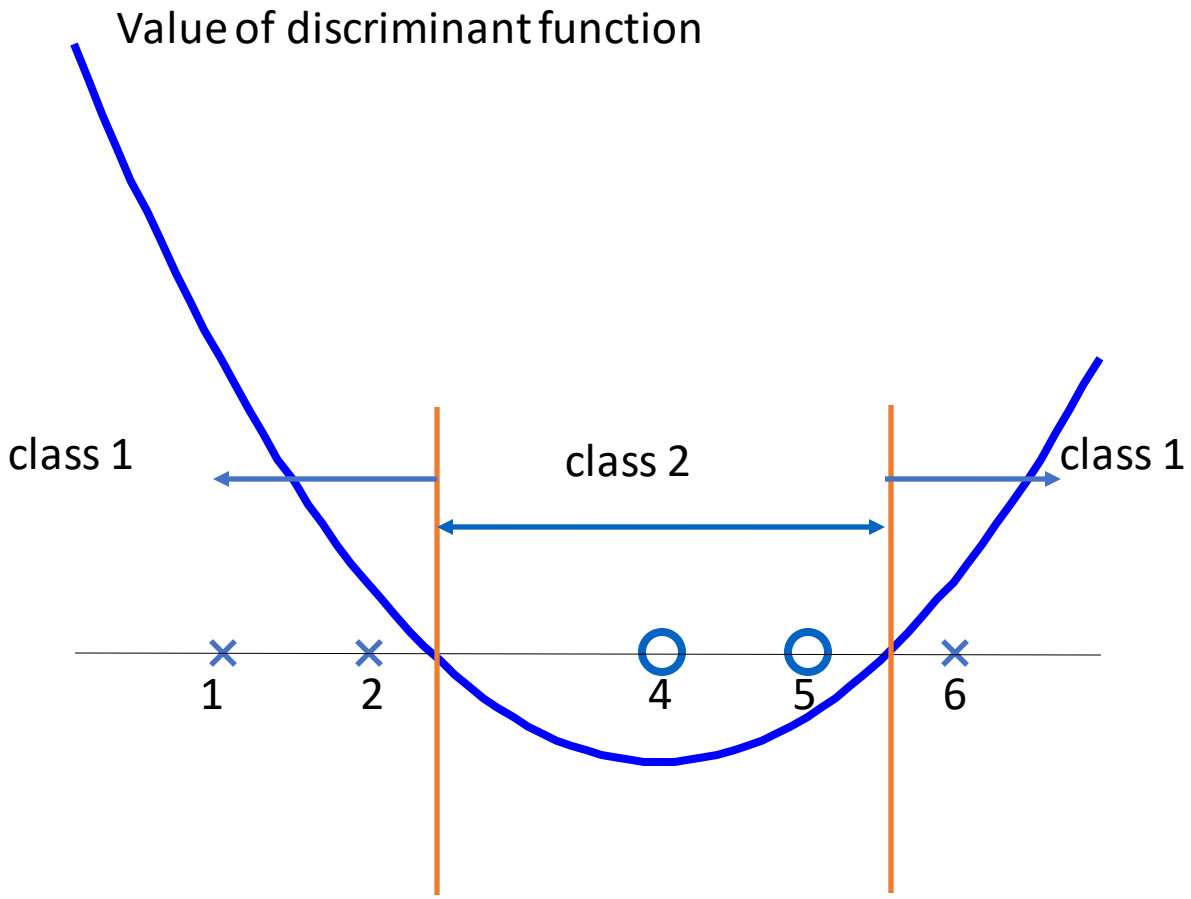
- We get
  - α_1=0, α_2=2.5, α_3=0, α_4=7.333, α_5=4.833
  - Note that the constraints are indeed satisfied
  - The support vectors are {x_2=2, x_4=5, x_5=6}
- The discriminant function is

$$\begin{aligned} f(z) &= 2.5(1)(2z+1)^2 + 7.333(-1)(5z+1)^2 + 4.833(1)(6z+1)^2 + b \\ &= 0.6667z^2 - 5.333z + b \end{aligned}$$

(α_5, y_5, $K(z, x_5)$)

- *b* is recovered by solving f(2)=1 or by f(5)=-1 or by f(6)=1, as x_2 and x_5 lie on the line $\phi(\mathbf{w})^T\phi(\mathbf{x}) + b = 1$ and x_4 lies on the line $\phi(\mathbf{w})^T\phi(\mathbf{x}) + b = -1$
- All three give b=9 $\Rightarrow$ $f(z) = 0.6667z^2 - 5.333z + 9$

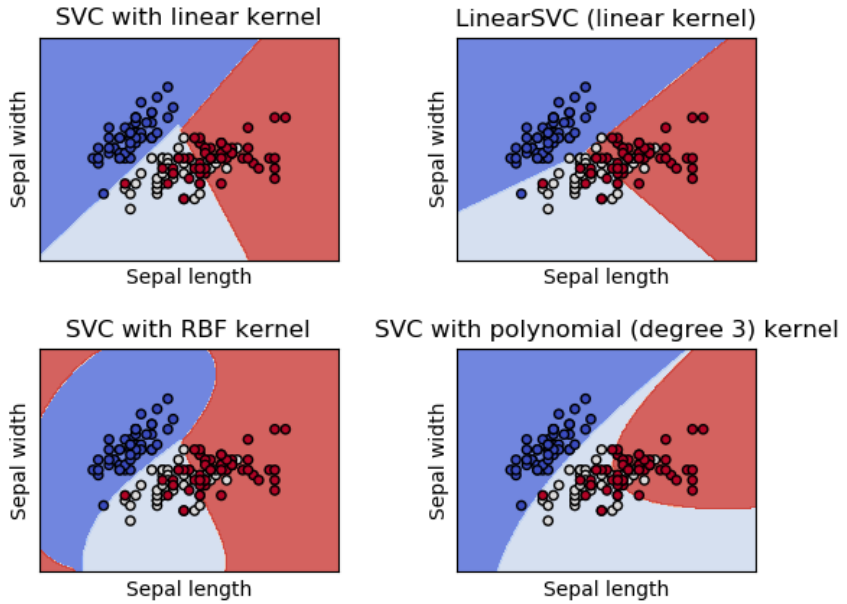
Example


Value of discriminant function
class 1
class 2
class 1
1
2
4
5
6

Support Vector Machine (SVM)

- SVM represents the decision boundary using a subset of the training examples, known as the **support vectors**.

- The basic idea behind SVM lies within the concept of **maximal margin hyperplane.**



Characteristics of SVM

- Since the learning problem is formulated as a convex optimization problem, efficient algorithms are available to find the **global** minima of the objective function (many of the other methods use greedy approaches and find **locally** optimal solutions).
- Overfitting is addressed by maximizing the margin of the decision boundary, but the user still needs to provide the type of kernel function and cost function.
- Difficult to handle missing values.
- Robust to noise.
- High computational complexity for building the model.

Multiclass Classification

Multiclass Classification

- Combining binary classifiers
  - One-vs-all
  - All-vs-all

- Training a single classifier
  - Multiclass SVM
  - Constraint classification

Binary to Multiclass

- Can we use a binary classifier to construct a multiclass classifier?
  - Decompose the prediction into multiple binary decisions

- How to decompose?
  - One-vs-all
  - All-vs-all

One-vs-all Classification

- Assumption: Each class individually separable from ***all*** the others

- Learning: Given a dataset $D = \{\langle \mathbf{x}_i, \mathbf{y}_i \rangle\}$,

  Note: $\mathbf{x}_i \in \mathbb{R}^n$, $\mathbf{y}_i \in \{1, 2, \cdots, K\}$

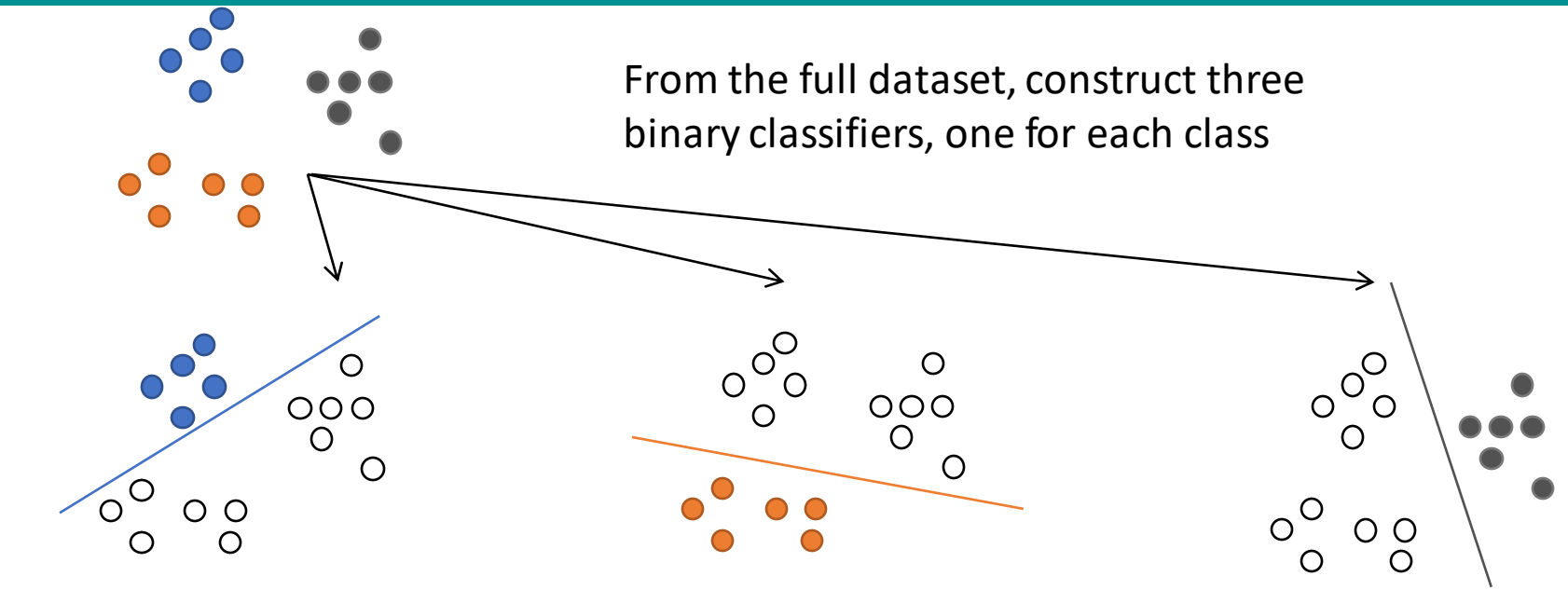
  - Decompose into K binary classification tasks
  - For class k, construct a binary classification task as:
    - Positive examples: Elements of D with label k
    - Negative examples: All other elements of D
  - Train K binary classifiers $\mathbf{w}_1, \mathbf{w}_2, \cdots \mathbf{w}_K$ using any learning algorithm we have seen

- Prediction: "*Winner Takes All*"

$$\text{argmax}_i \ \mathbf{w}_i^T \mathbf{x}$$

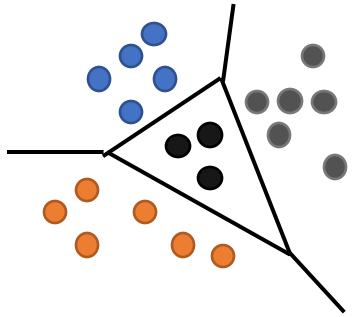
Question: What is the dimensionality of each $\mathbf{w}_i$?

Visualizing One-vs-All



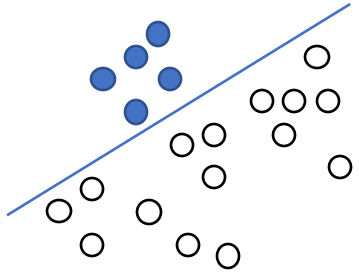
Winner Take All will predict the right answer. Only the correct label will have a positive score

One-vs-All May not Always Work

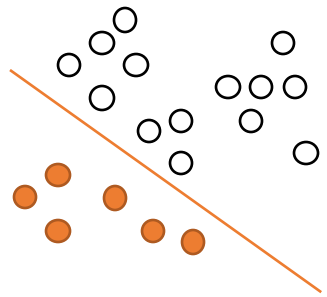


Black points are not separable with a single binary classifier

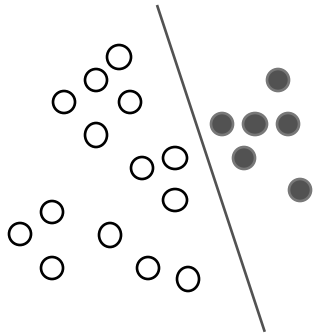
The decomposition will not work for these cases!



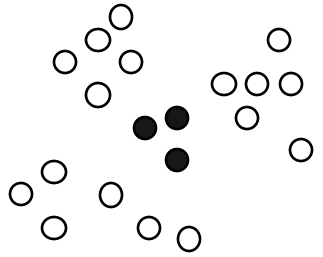
$\mathbf{w}_{blue}^T\mathbf{x} > 0$ for **blue inputs**



$\mathbf{w}_{red}^T\mathbf{x} > 0$ for **red inputs**



$\mathbf{w}_{green}^T\mathbf{x} > 0$ for **green inputs**



???

One-vs-All Classification: Summary

- Easy to learn
  - Use any binary classifier learning algorithm
- Problems
  - No theoretical justification
  - Calibration issues
    - We are comparing scores produced by K classifiers trained independently. No reason for the scores to be in the same numerical range!
  - Might not always work
    - Yet, works fairly well in many cases, especially if the underlying binary classifiers are tuned, regularized

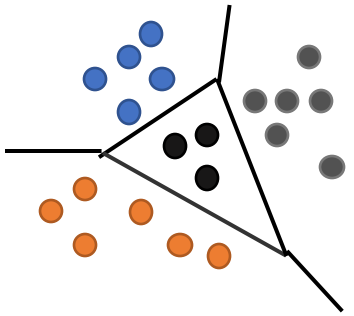
All-vs-All Classification

Sometimes called one-vs-one, used by sklearn

- Assumption: *Every* pair of classes is separable
- Learning: Given a dataset D = {<$\mathbf{x}_i$, $\mathbf{y}_i$>},

  Note: $\mathbf{x}_i \in \mathbb{R}^n$, $\mathbf{y}_i \in \{1, 2, \cdots, K\}$
  - For every pair of labels (j, k), create a binary classifier with:
    - Positive examples: All examples with label j
    - Negative examples: All examples with label k
  - Train $\binom{K}{2} = \frac{K(K-1)}{2}$ classifiers in all
- Prediction: More complex, each label get K-1 votes
  - How to combine the votes? Many methods
    - Majority: Pick the label with maximum votes
    - Organize a tournament between the labels

All-vs-All Classification



- Every pair of labels is linearly separable here
  - When a pair of labels is considered, all others are ignored
- Problems
  1. $O(K^2)$ weight vectors to train and store
  2. Size of training set for a pair of labels could be very small, leading to overfitting
  3. Prediction is often ad-hoc and might be unstable

     Eg: What if two classes get the same number of votes? For a tournament, what is the sequence in which the labels compete?

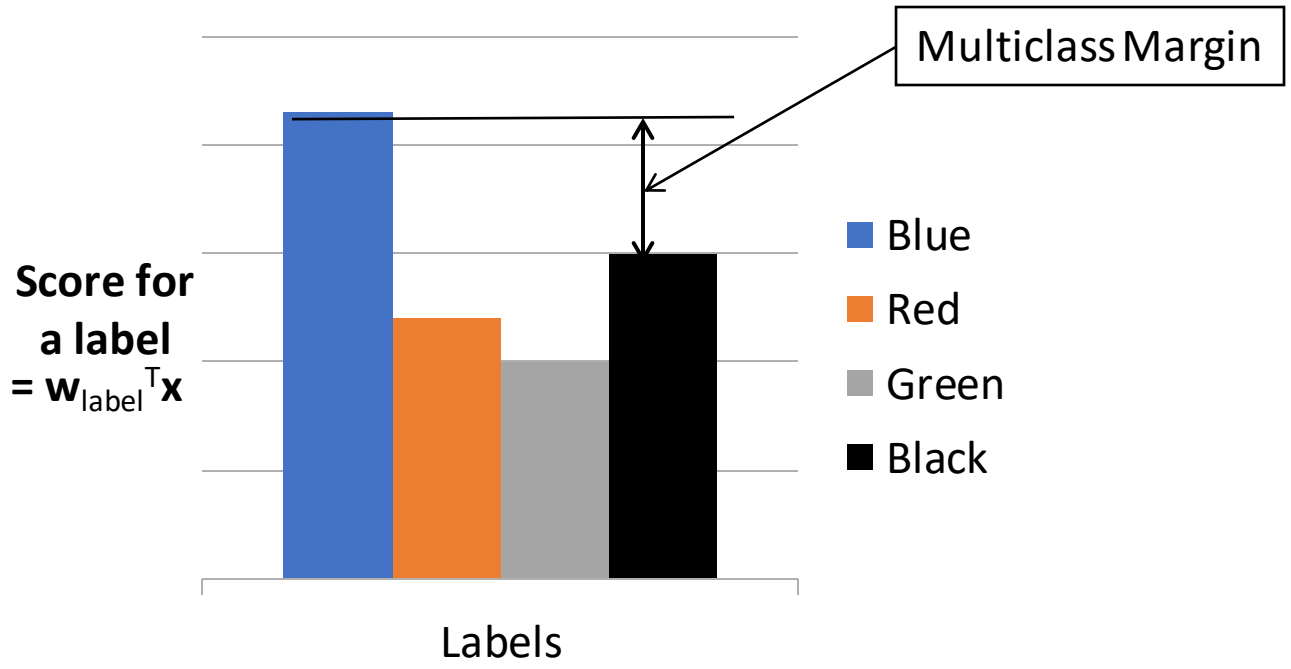
Training a Single Classifier: Motivation

- Decomposition methods
  - Do not account for how the final predictor will be used
  - Do not optimize any global measure of correctness

- Goal: To train a multiclass classifier that is “global”

Multiclass Margin

Defined as the score difference between the highest scoring label and the second one



Multiclass SVM (Intuition)

- Recall: Binary SVM
  - Maximize margin
  - Equivalently,

    Minimize norm of weights such that the closest points to the hyperplane have a score §1

- Multiclass SVM
  - Each label has a different weight vector (like one-vs-all)
  - Maximize multiclass margin
  - Equivalently,

    Minimize total norm of the weights such that the true label is scored at least 1 more than the second best one

References

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- http://www.kernel-machines.org/
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- An Introduction to Support Vector Machines. N. Cristianini and J. Shawe-Taylor.
- C.J.C. Burges: A tutorial on Support Vector Machines. Data Mining and Knowledge Discovery 2:121-167, 1998.