# Classification and clustering

Neural data science with Python

Heike Stein

01/12/2023

# Classification and Clustering: Overview

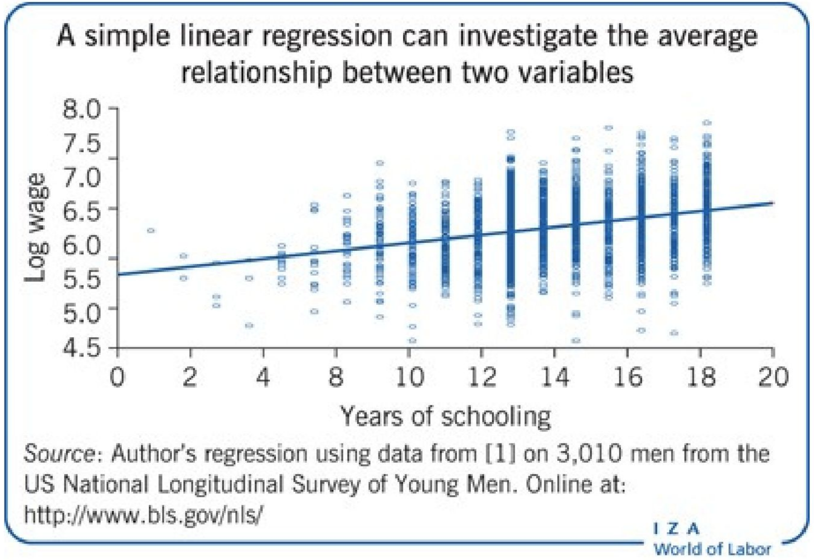
**Classification**

- Logistic regression
- Support vector machines

**Clustering**

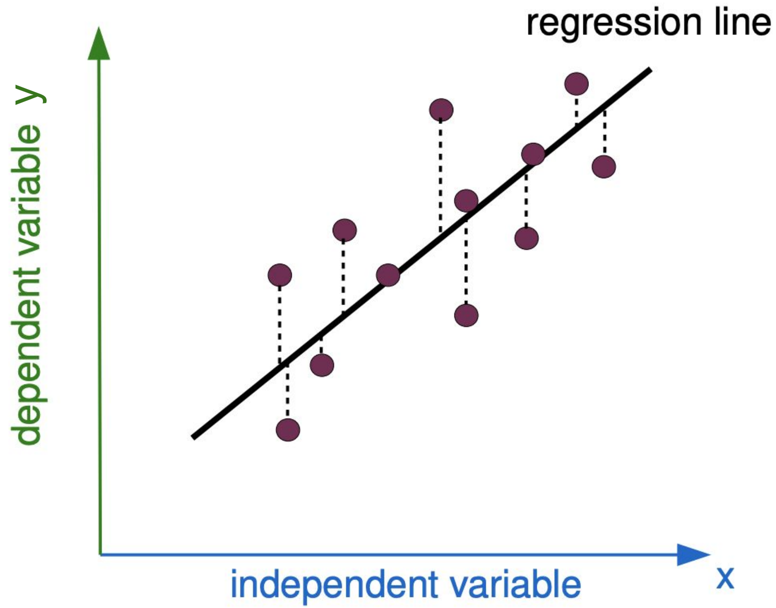
- k-means

# Regression analysis




→ linear mapping from predictor ("independent") variable(s) x (e.g. years of schooling) to outcome ("dependent") variable y (e.g. wage)

# Regression analysis



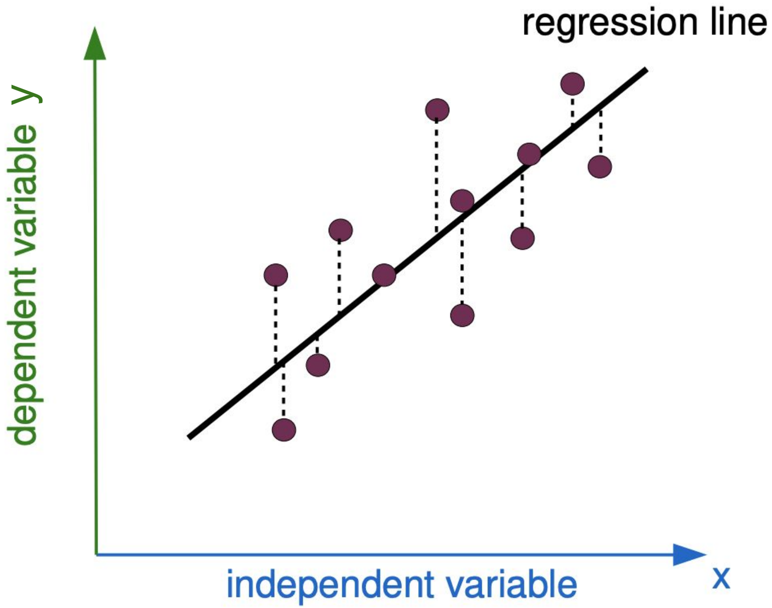

→ linear mapping from predictor ("independent") variable(s) x (e.g. years of schooling) to outcome ("dependent") variable y (e.g. wage)

$$y = \boxed{\beta_0} + \boxed{\beta_1} x_1 + \boxed{\varepsilon}$$

weights ("parameters")

errors ("residuals")

# Regression analysis

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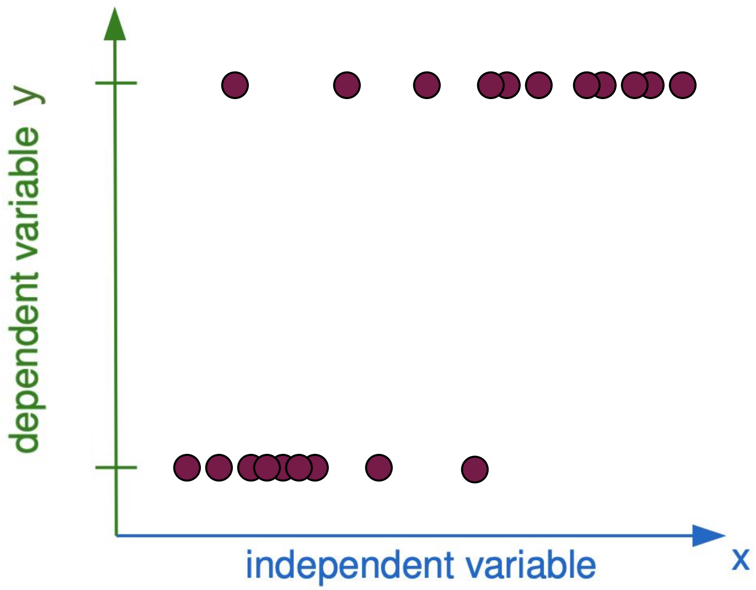
$$y = \boxed{\beta_0} + \boxed{\beta_1} x_1 + \boxed{\varepsilon}$$

Weights are chosen so as to minimize errors (model fitting)

# Sometimes, outcomes are categorical




Given knowledge of x, what is the most likely category of y?

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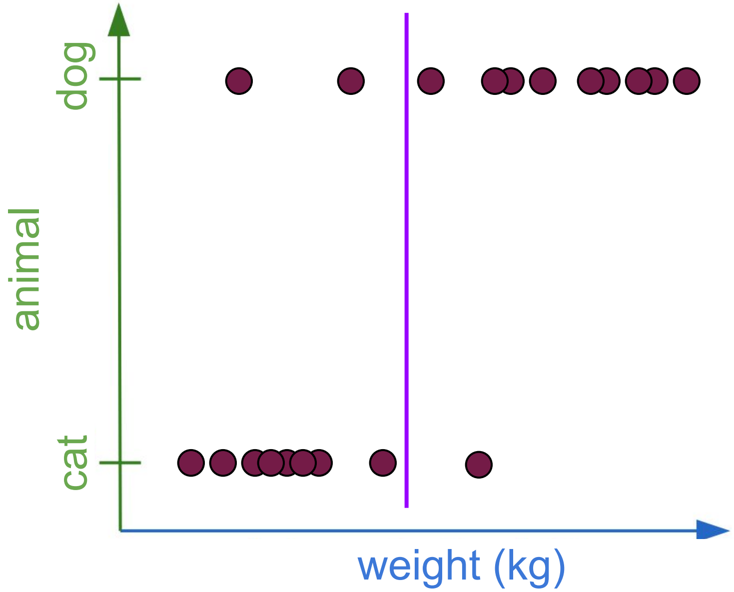
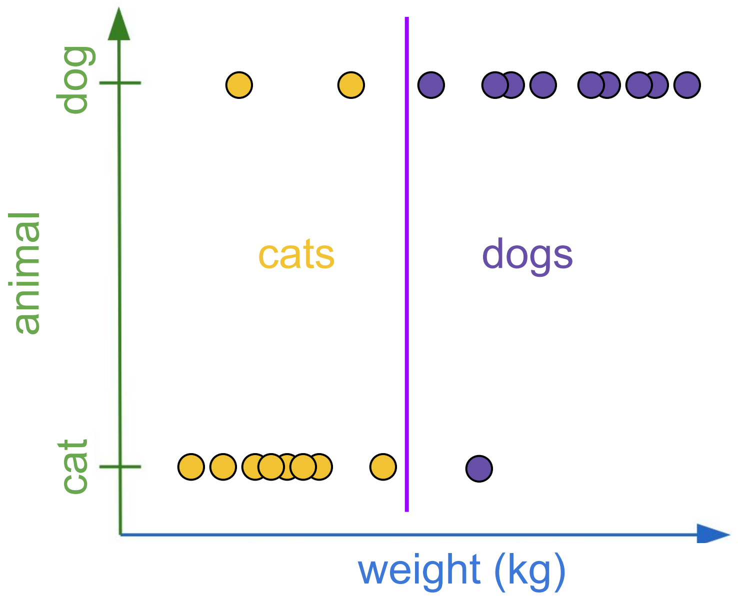



Given knowledge of x, what is the most likely category of y?

We want to find the value of x that best separates cats vs. dogs:
The decision boundary

# Classification: Predicting categorical values

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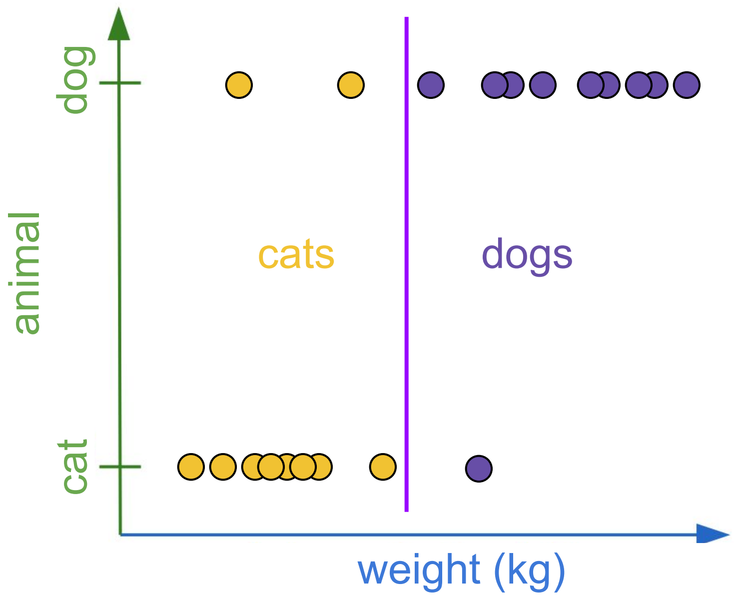


**How do we find a good decision boundary?**

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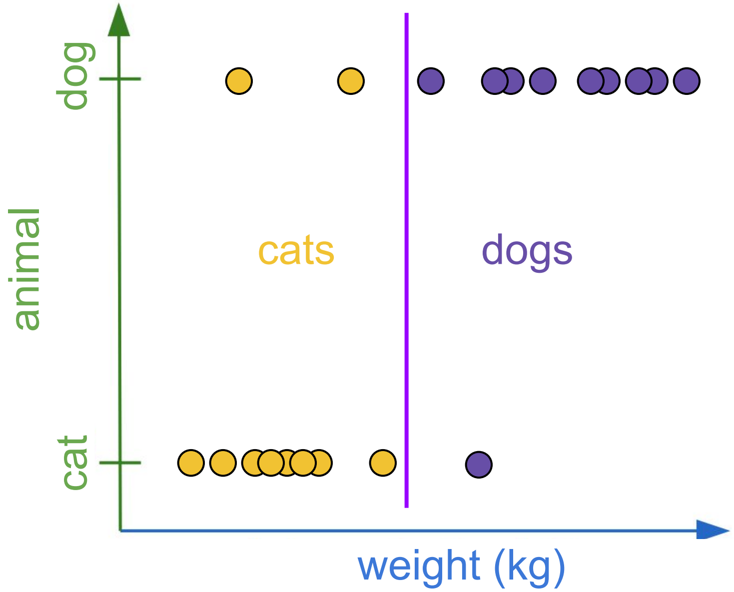


**How do we find a good decision boundary?**

It should minimize the number of misclassifications.

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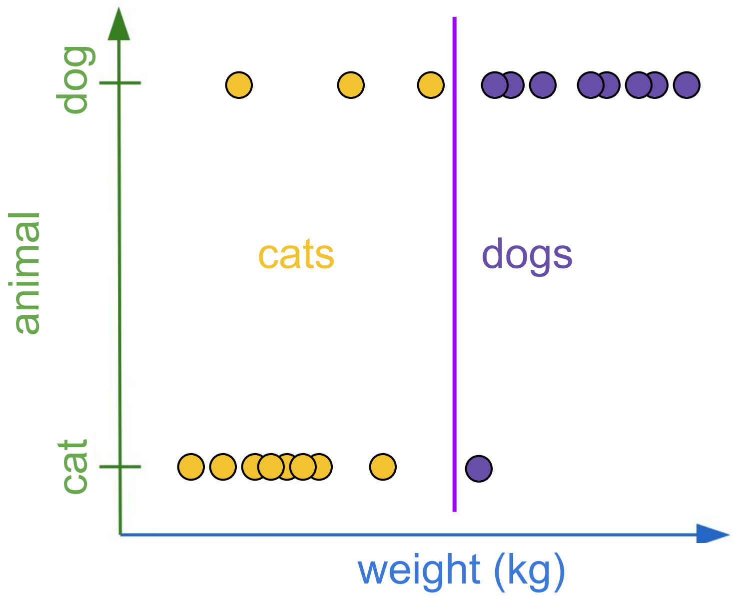


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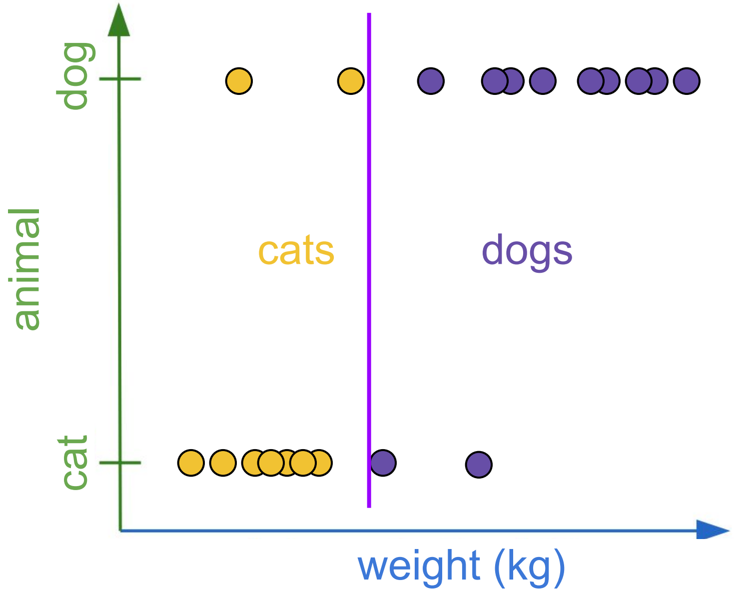


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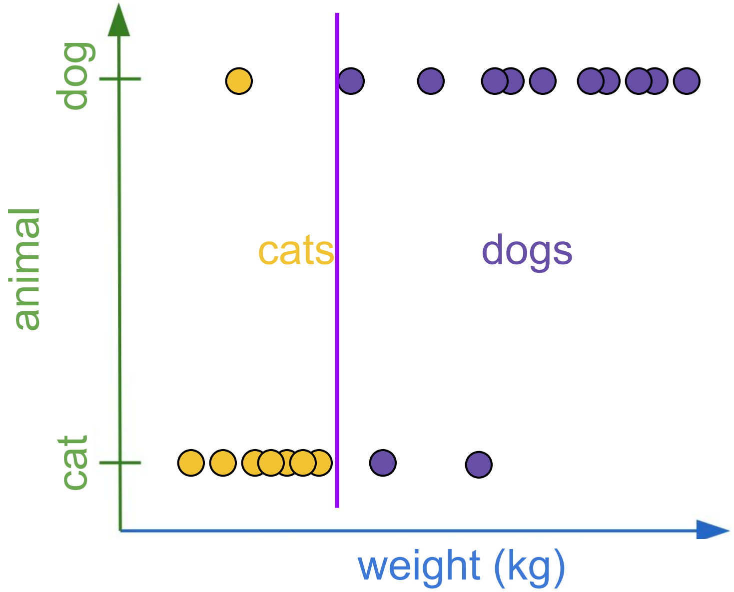


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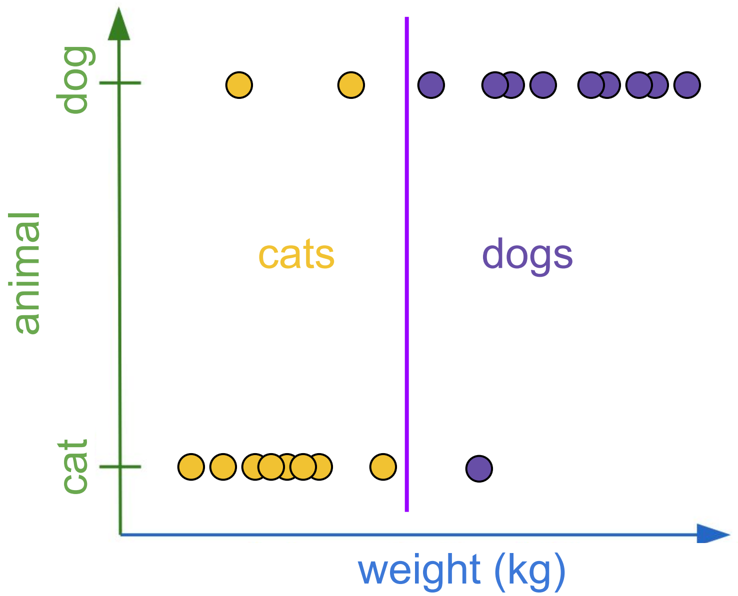



**How do we find a good decision boundary?**

It should minimize the number of misclassifications.

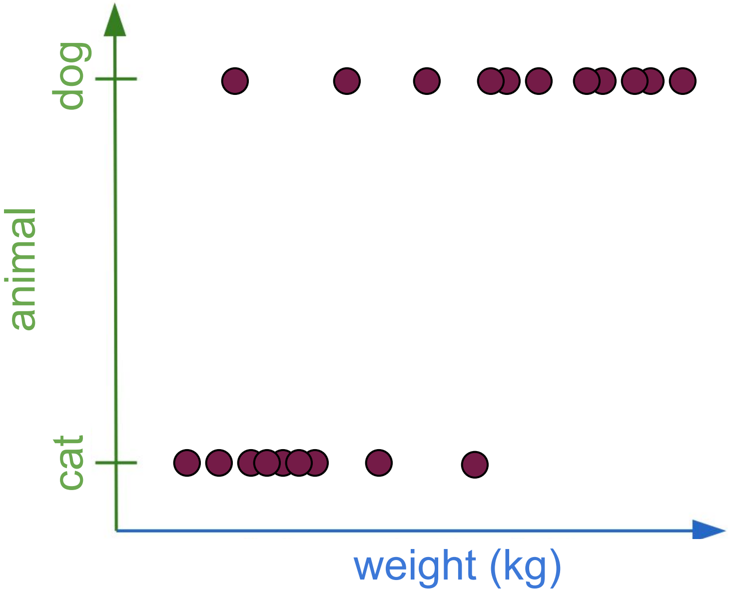
Which solution is found depends on the classification method.

# Classification and Clustering: Overview

**Classification**

1. Logistic regression
2. Support vector machines

# Classification: Logistic regression



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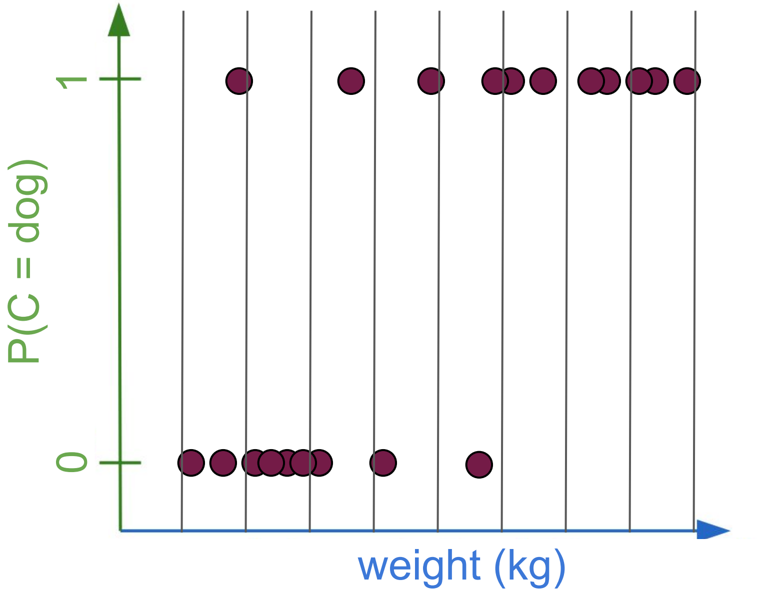
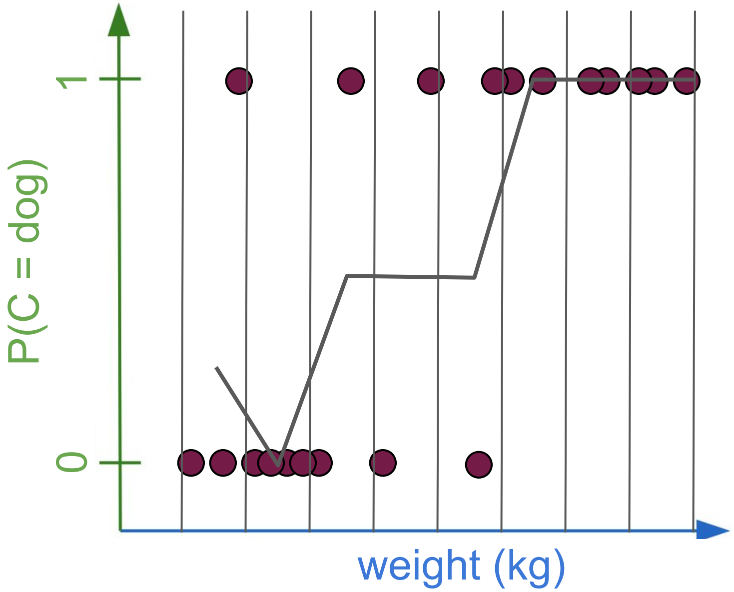



Idea: For each value on x, we can calculate the probability that the animal is a dog: $P(C = \text{"dog"})$

# Classification: Logistic regression

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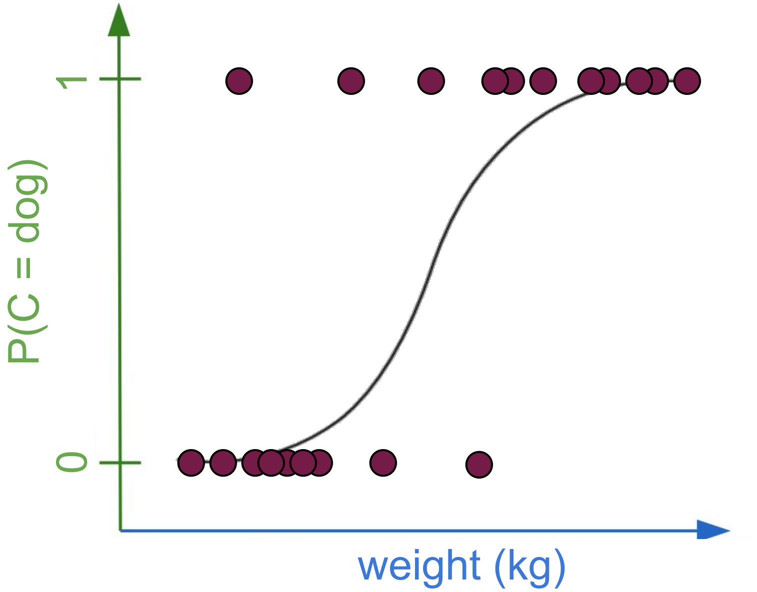


Logistic regression fits the weights of a generalized linear model:

$$P(C = \text{"dog"}) = f(\beta_0 + \beta_1 x_1)$$

with sigmoidal link function $f(x) = \dfrac{e^x}{1 + e^x}$

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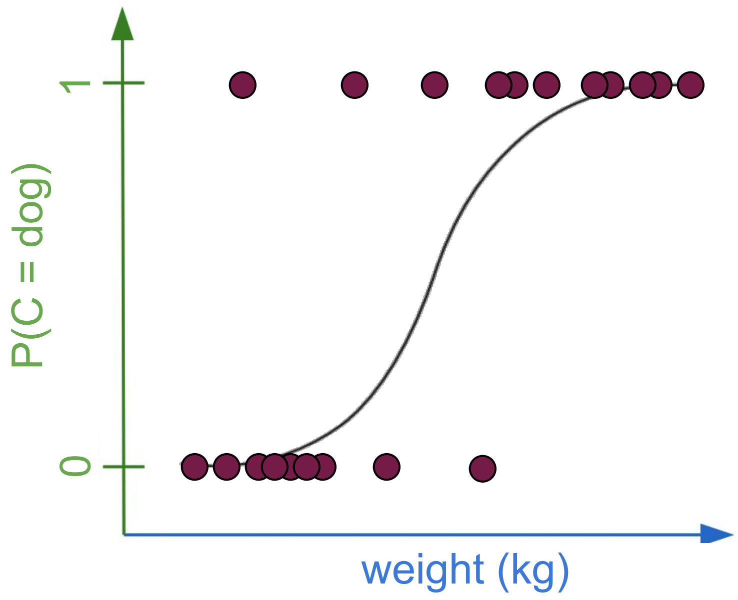


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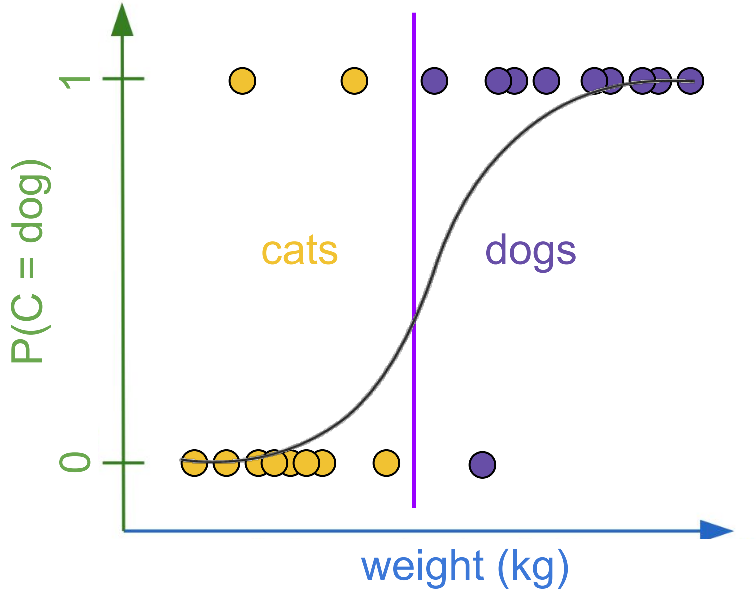
$$\Leftrightarrow \quad P(C = \text{"dog"}) = \frac{e^{(\beta_0 + \beta_1 x_1)}}{1 + e^{(\beta_0 + \beta_1 x_1)}}$$

# Classification: Logistic regression

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$$P(C = \text{"dog"}) = f(\beta_0 + \beta_1 x_1)$$

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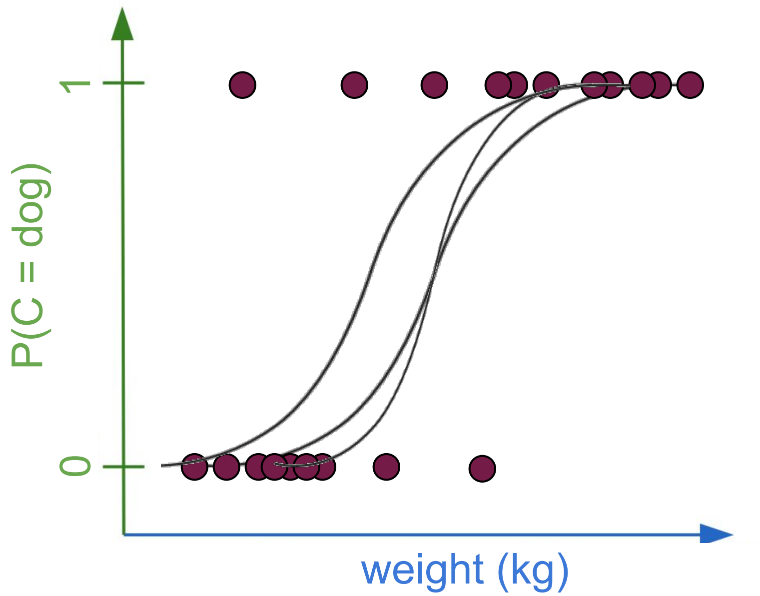
The decision boundary is the value of x for which P(C = “dog”) = 0.5

# Classification: Logistic regression

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Weights affect slope and x-offset of the sigmoidal function.

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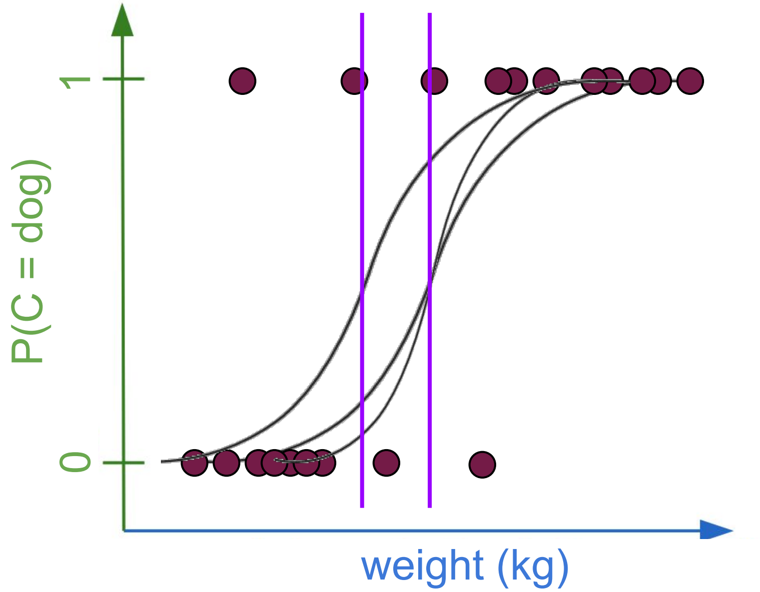


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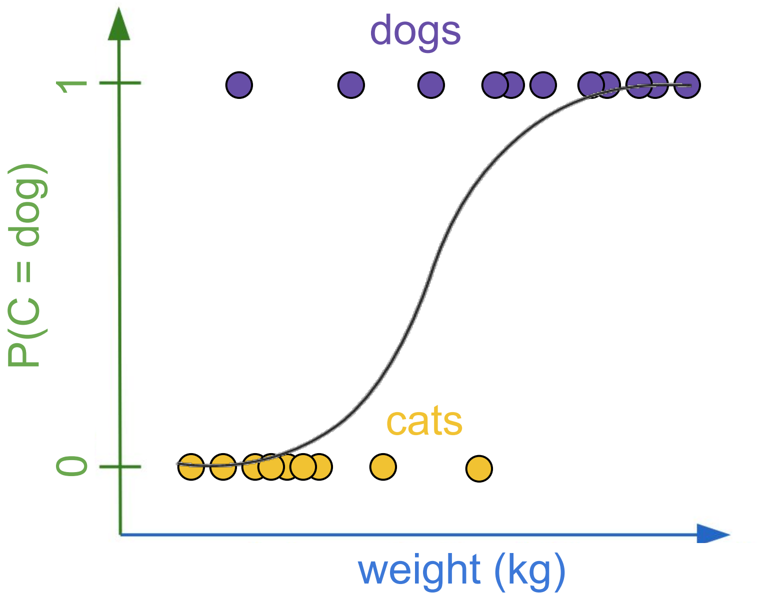
# Classification: Logistic regression

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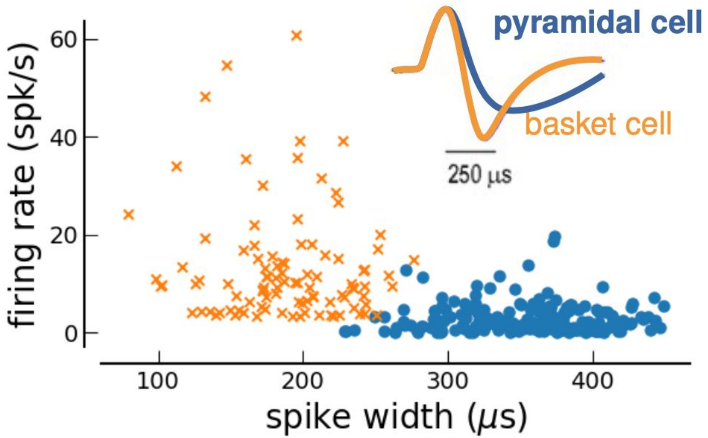
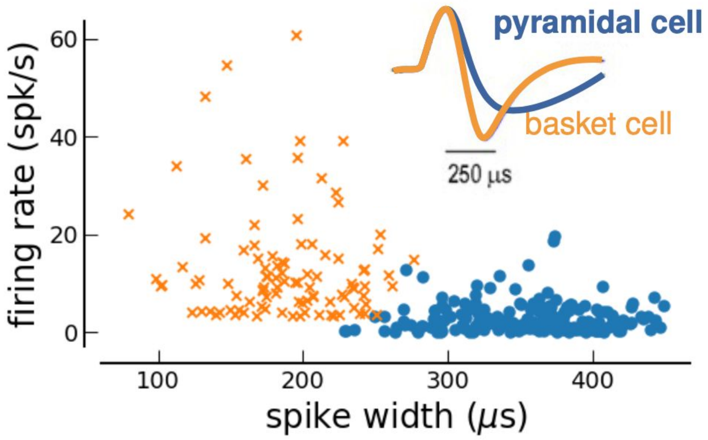
Weights are fitted by minimizing an error function between P(C = dog) and true labels: t = 1 if dog, t = 0 if cat

# Classification: Logistic regression in 2D




Given the predictor variables $x_1$: spike width and $x_2$ : firing rate, what is the probability that we are looking at a basket cell ($y$: P(C = "basket cell"))?

# Classification: Logistic regression in 2D

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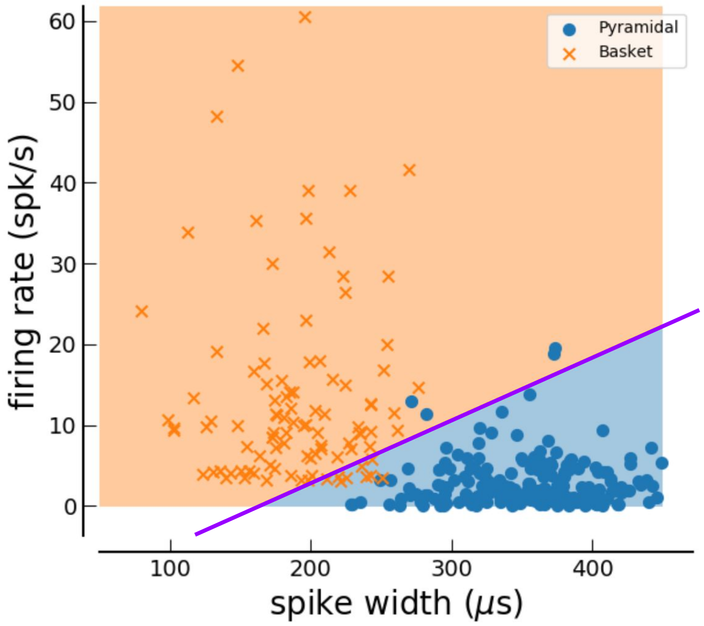


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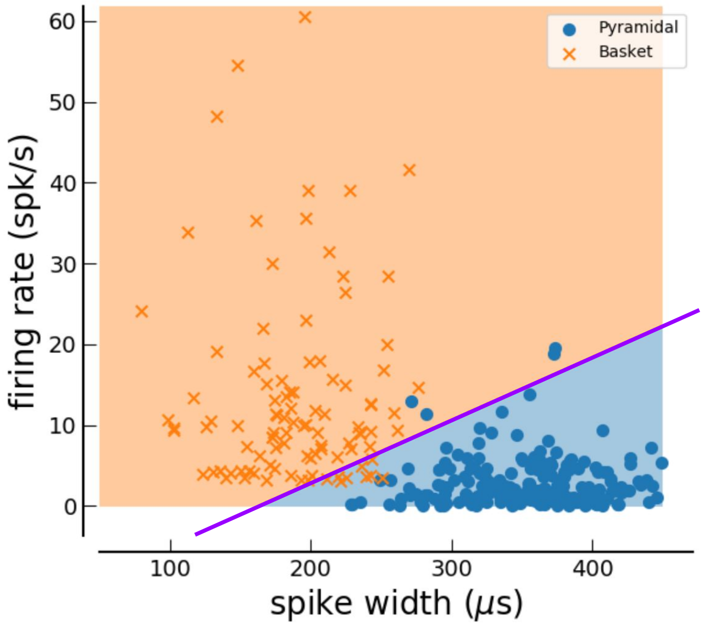
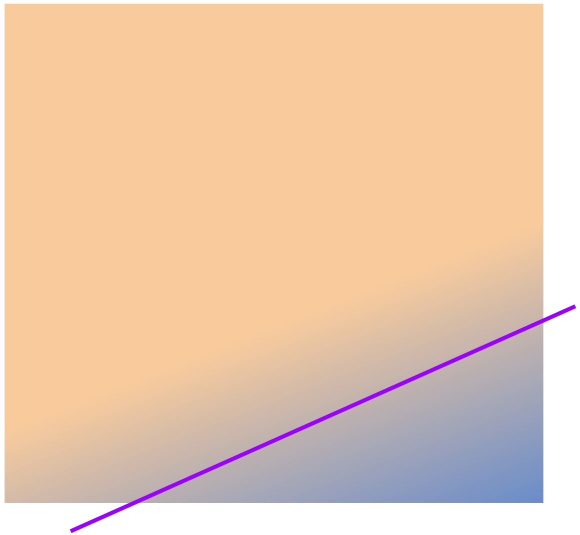
The decision boundary is now a 1D line in the 2D space for which P(C = “basket cell”) = 0.5

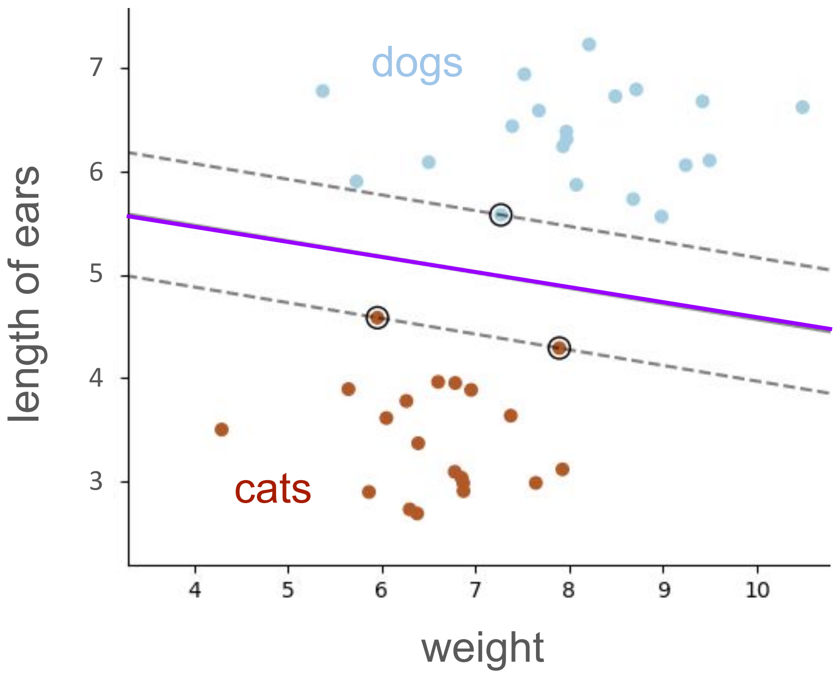
# Classification: Logistic regression in 2D




Sigmoidal function in 2D



# Classification: Support vector machines (SVM)




Again, we're looking for a decision boundary

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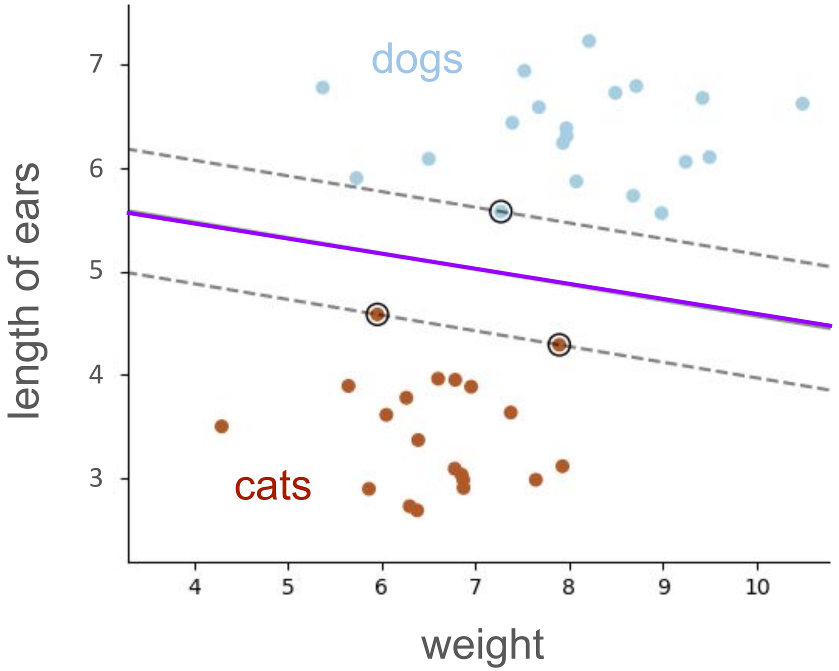
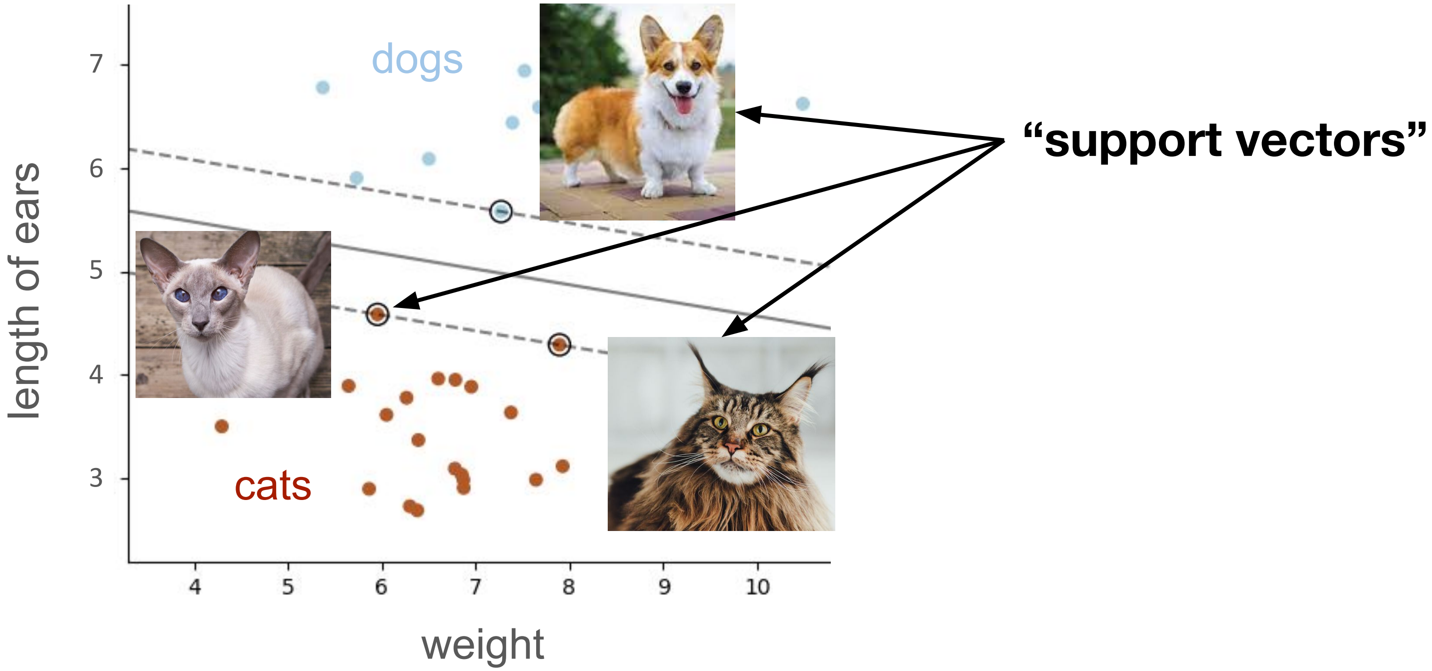



Again, we're looking for a decision boundary

This time, we define it as the line that is equally far away from the nearest exemplars of each class: the **"support vectors"**

# Classification: Support vector machines (SVM)



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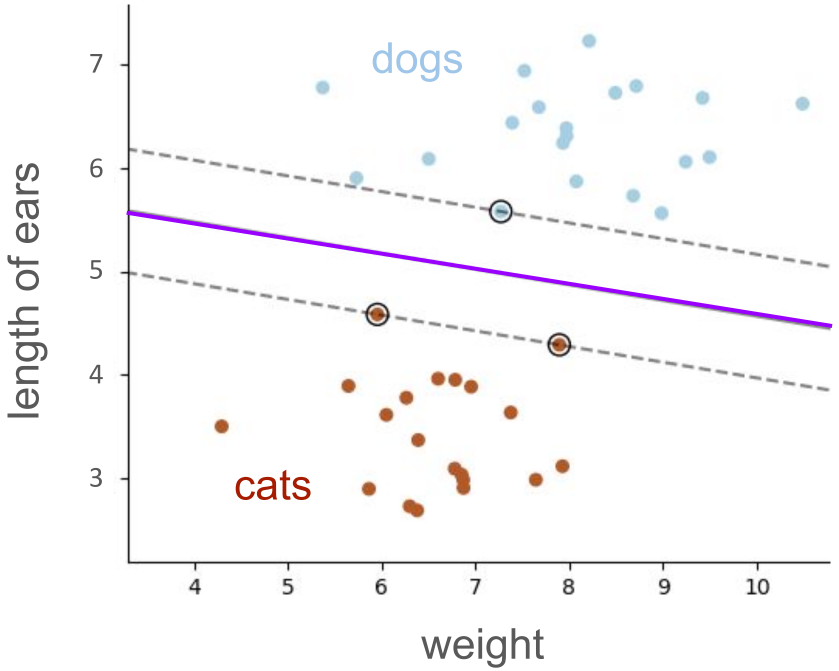


The decision boundary is the line that is equally far away from “support vectors” of each class

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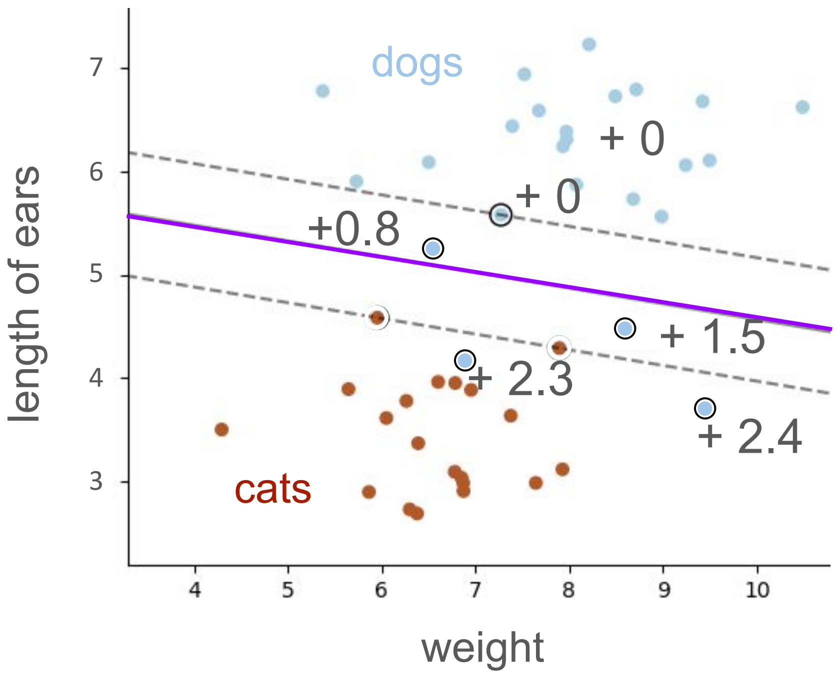
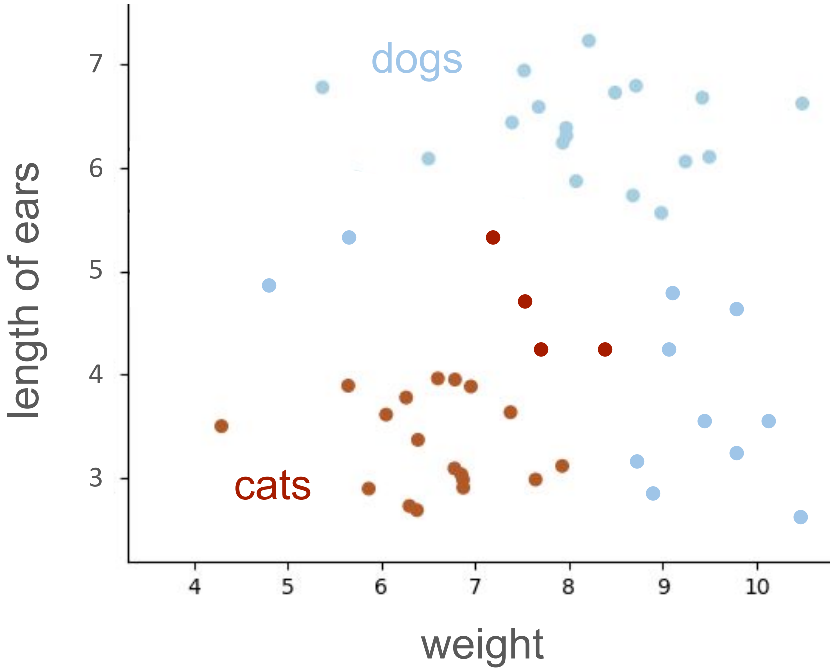



The decision boundary is the line that is equally far away from “support vectors” of each class

What to do if classes are not separable?
→ We penalize misclassifications with a point system that depends on the distance from boundary and margin.

Fitting an SVM means maximizing the margin while minimizing penalties.

# Classification: Support vector machines (SVM)



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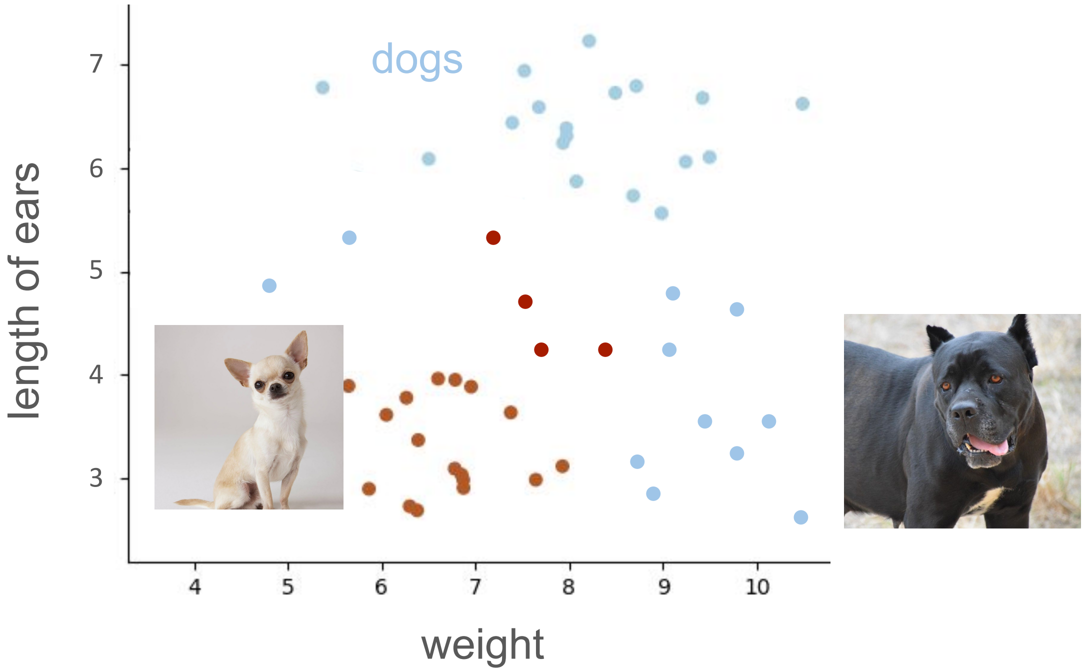

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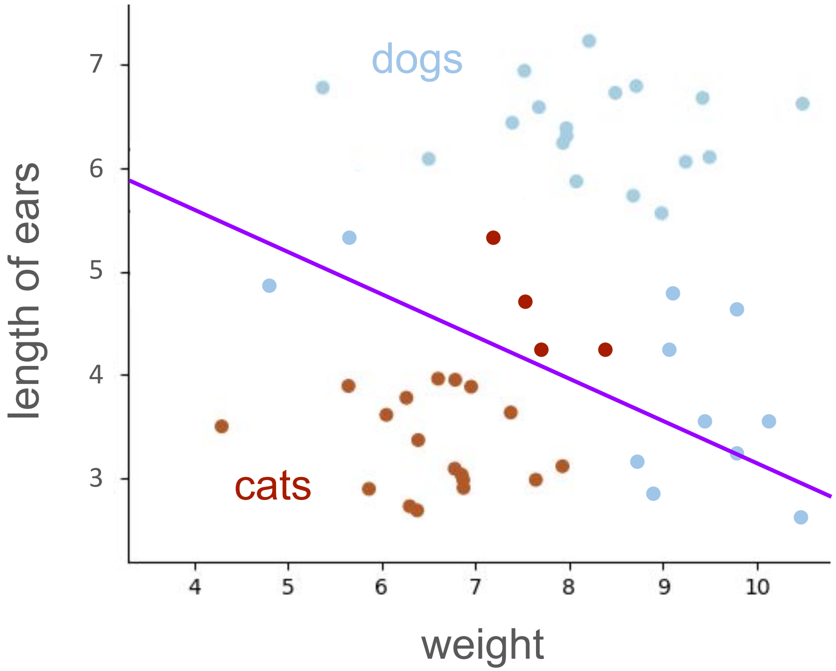
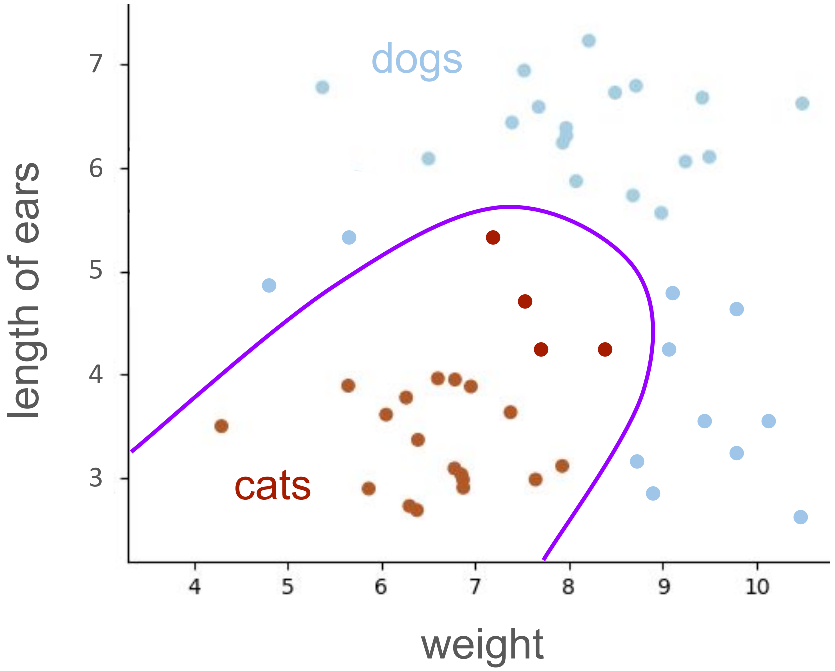



Some problems are not linearly separable

# Classification: Support vector machines (SVM)

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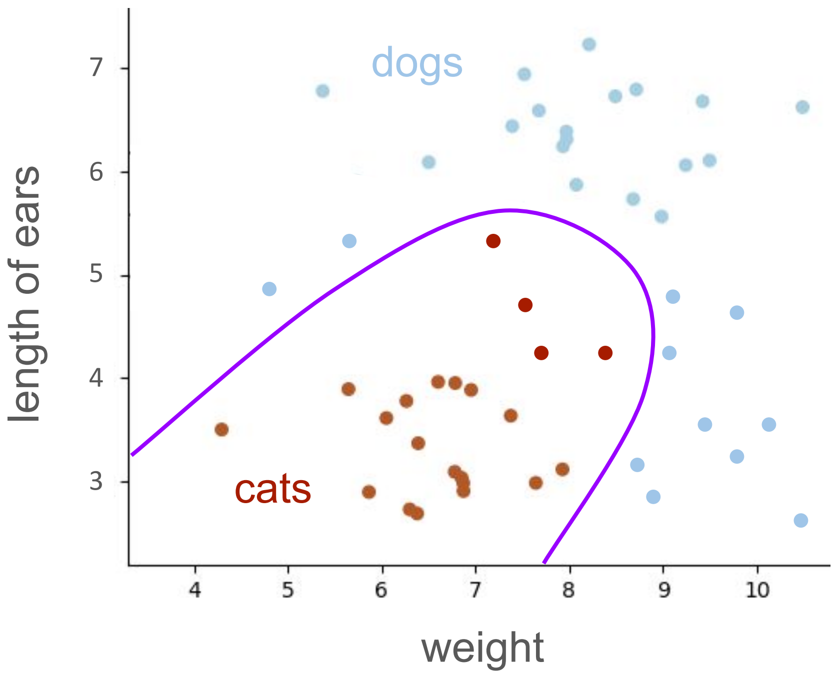


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SVMs use **“kernels”** to transform predictor variables nonlinearly. This can give us nonlinear decision boundaries.

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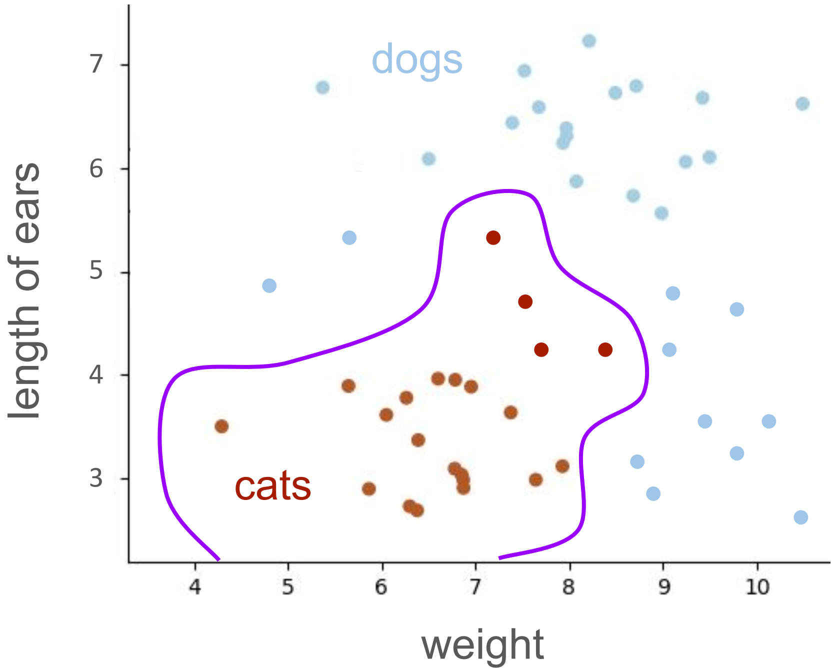


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E.g. polynomial kernels of increasing degree create increasing nonlinearity.

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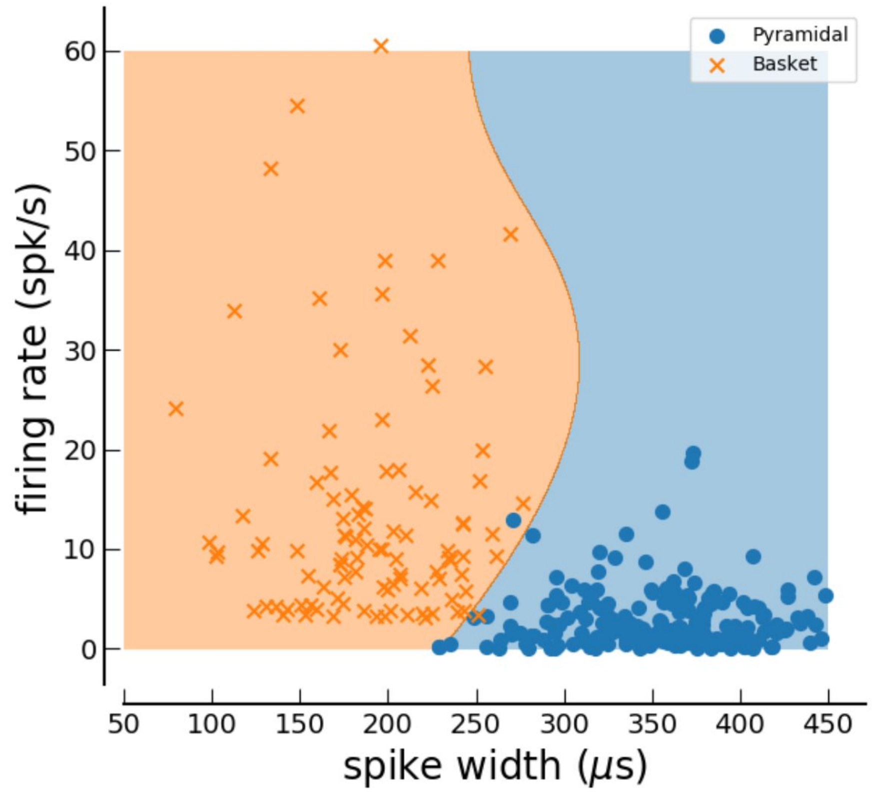
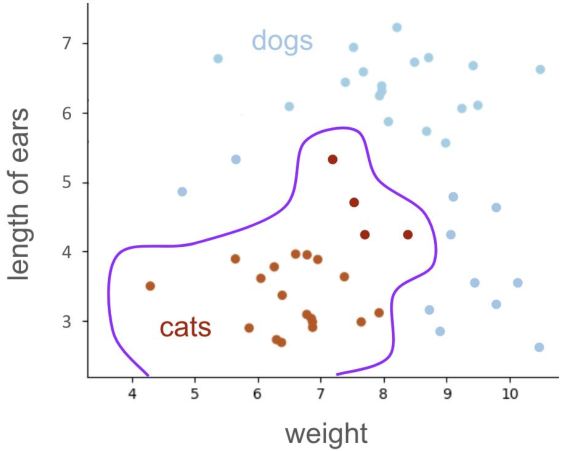


# Classification: Overfitting and classification performance

The more flexible our boundary, the more likely we are to "**overfit**": Classification performance is good on the original dataset, but bad on a new sample

**Train set**: data used to fit the classifier




100 % classification performance

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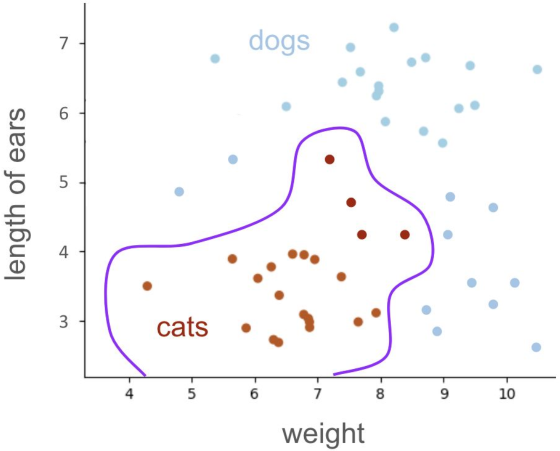


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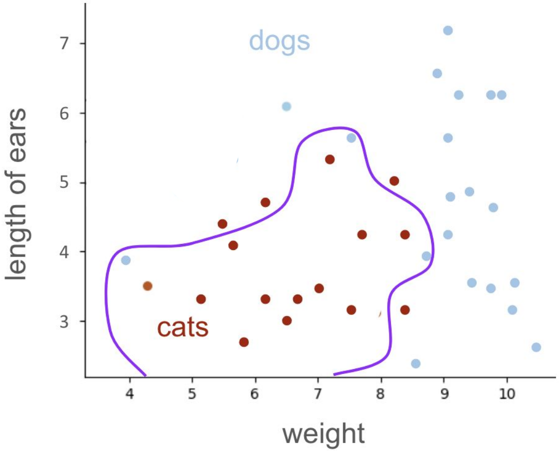
**Test set**: new data, “old” model.

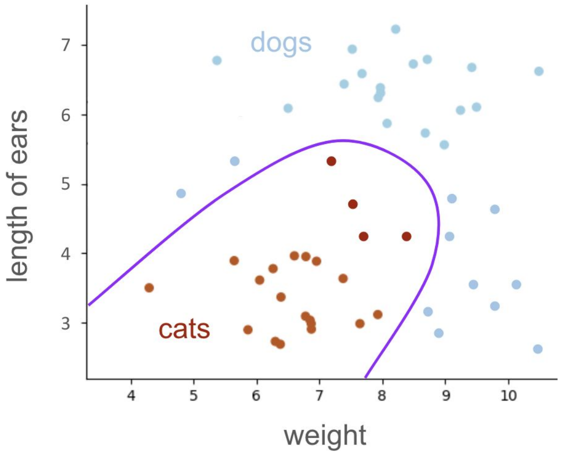



~90 % classification performance

# Classification: Overfitting and classification performance

Simpler models tend to **generalize** better ( = less overfitting ): Less discrepancy between performance on train and test set.

**Train set**: data used to fit the classifier

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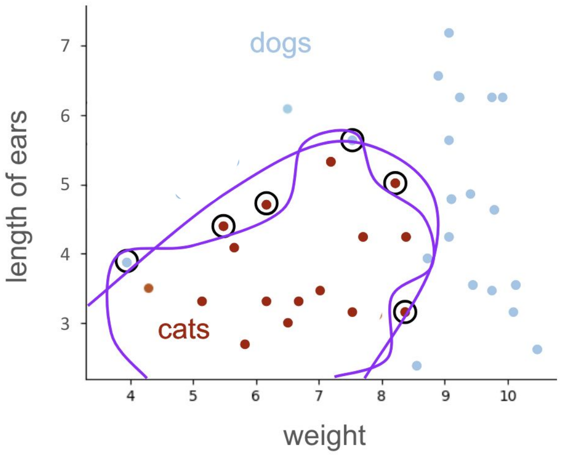
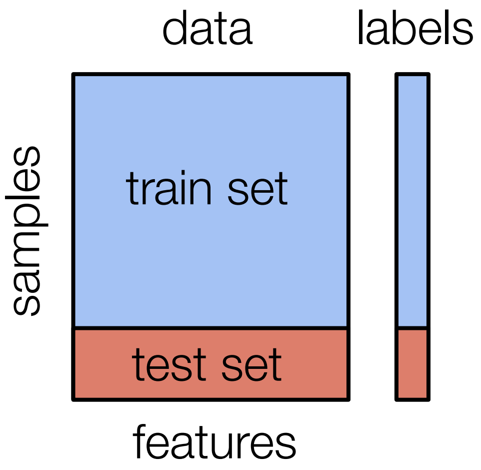



~98 % classification performance

# Classification: Cross-validation



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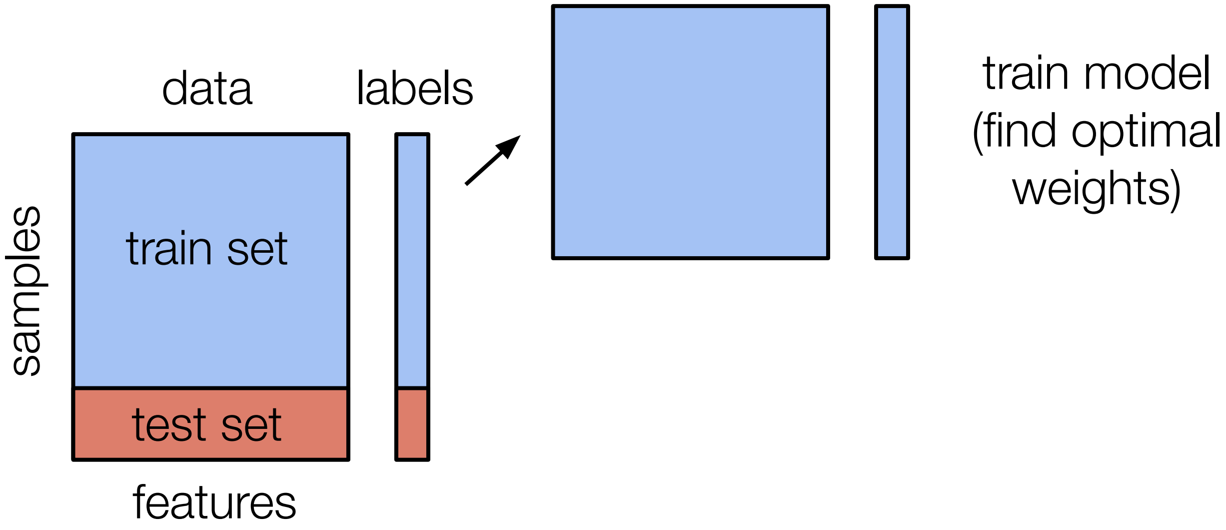

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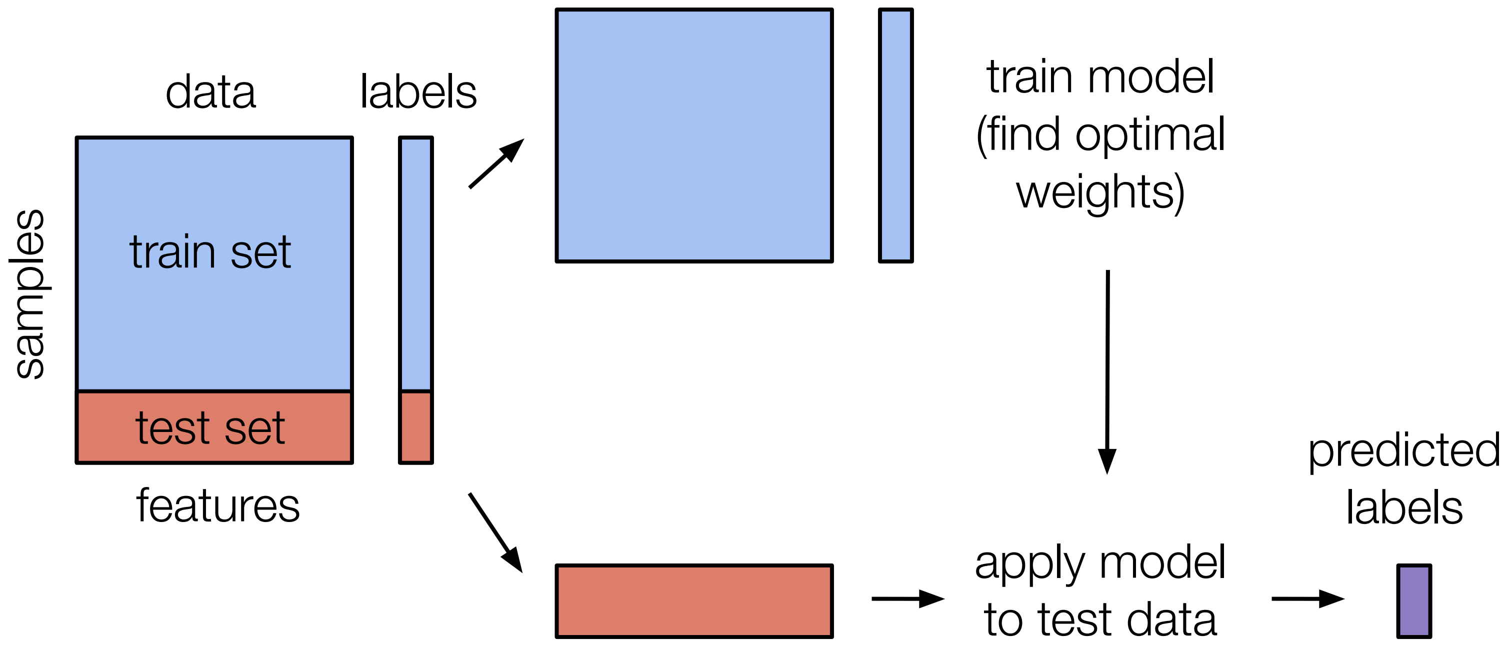

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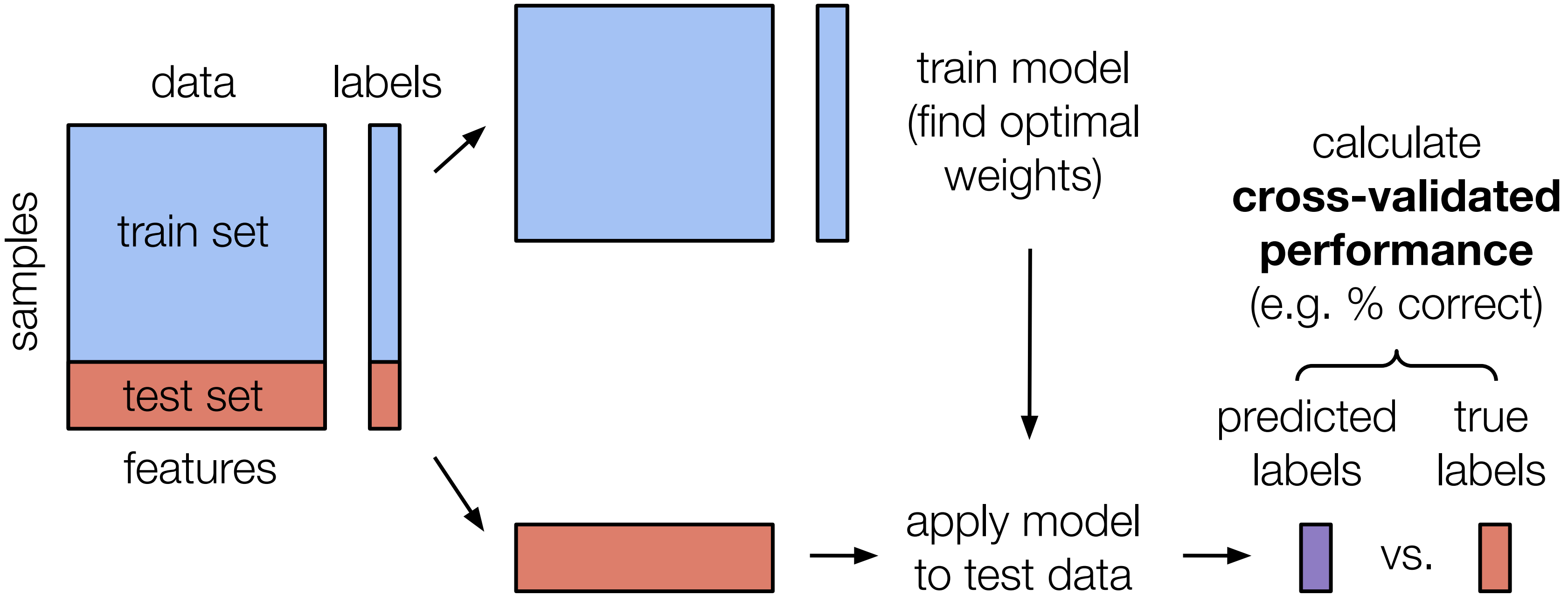

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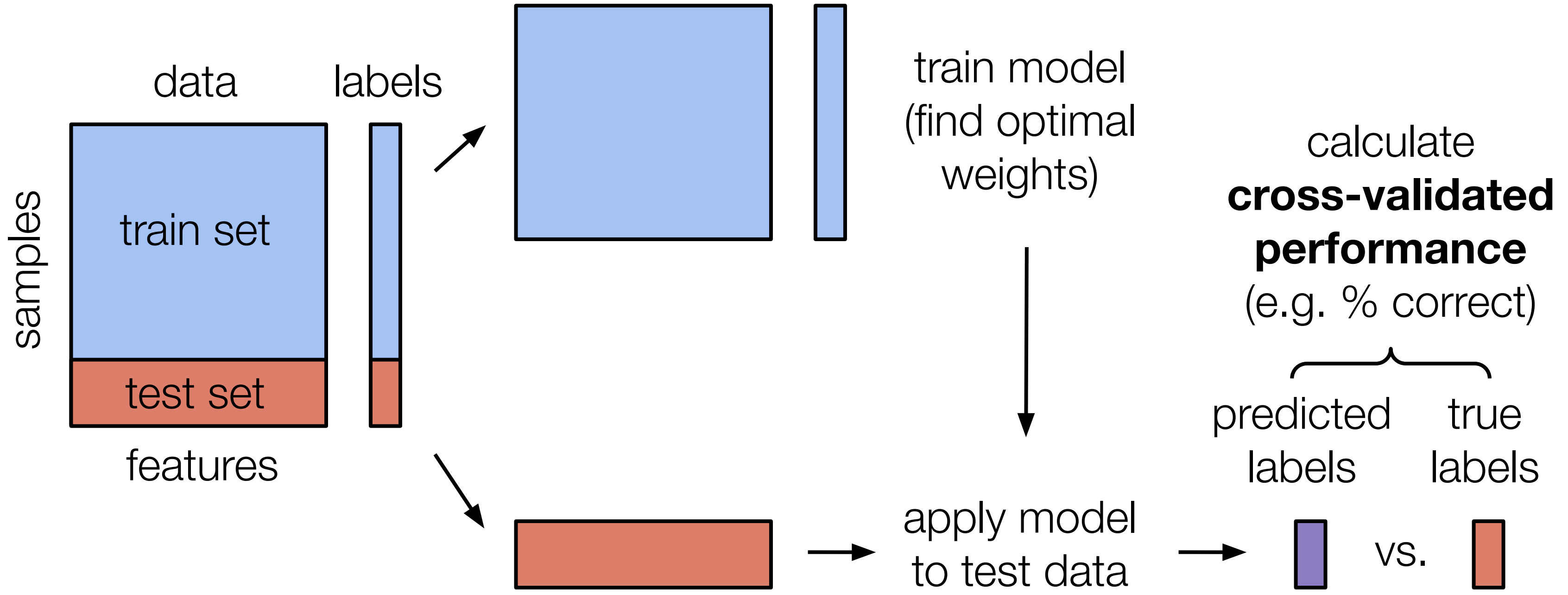


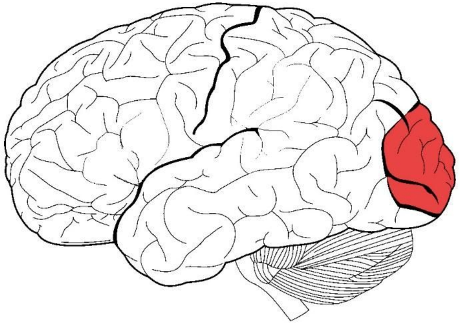

→ Repeat with many train/test splits. Is **perf. better than expected by chance**?

# Classification: What can we learn about the brain?

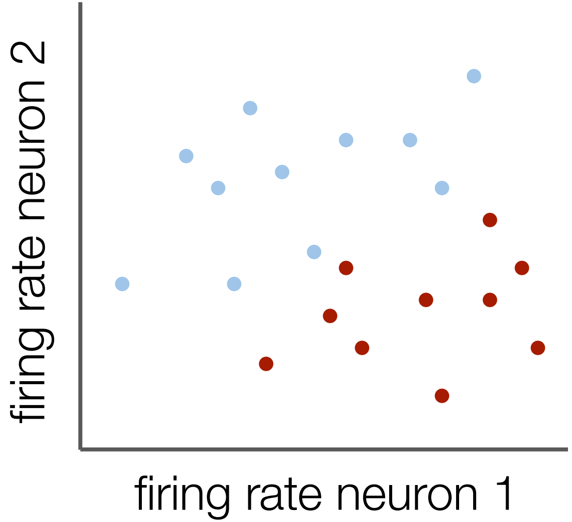
We can test whether a group of neurons encodes stimulus information in its activity

left

right



recordings from V1



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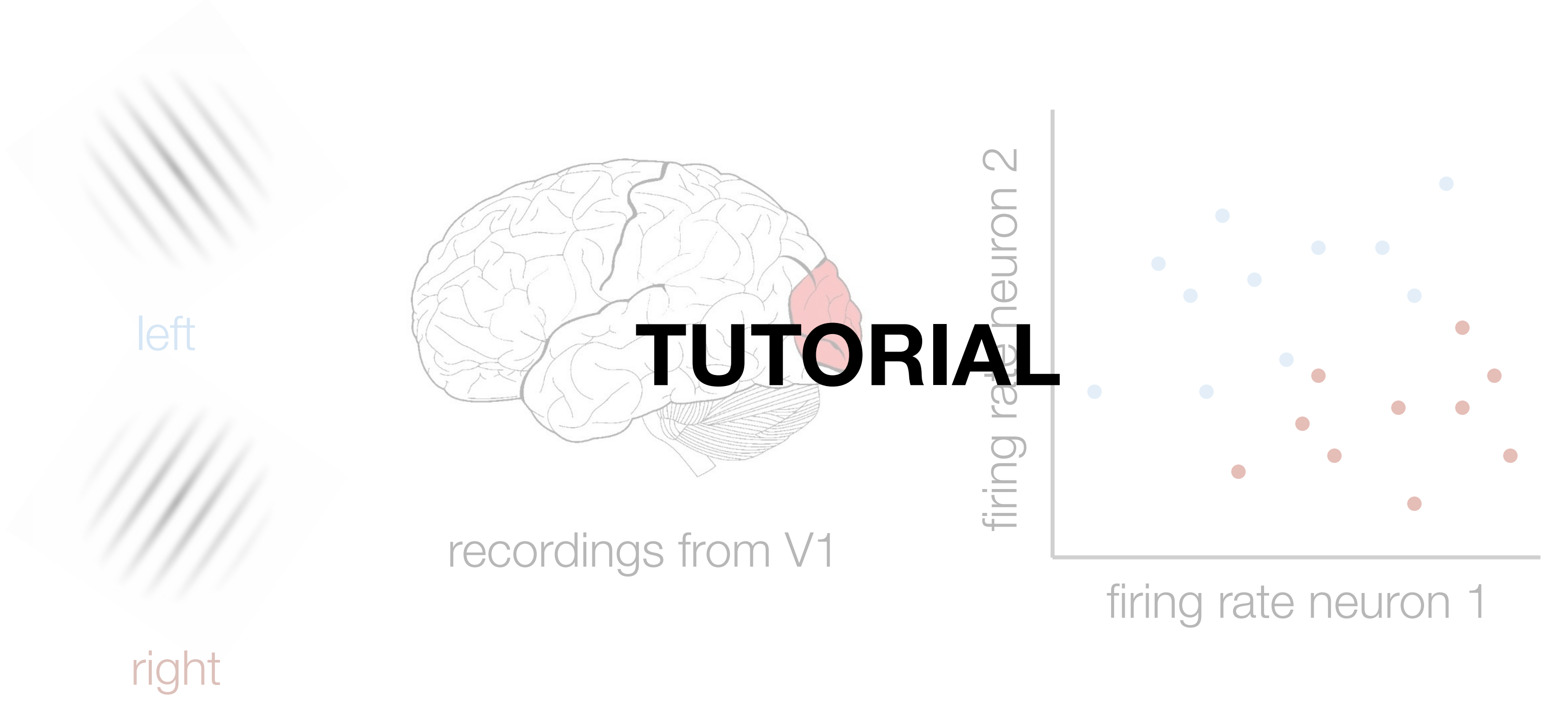

# Classification and Clustering: Overview

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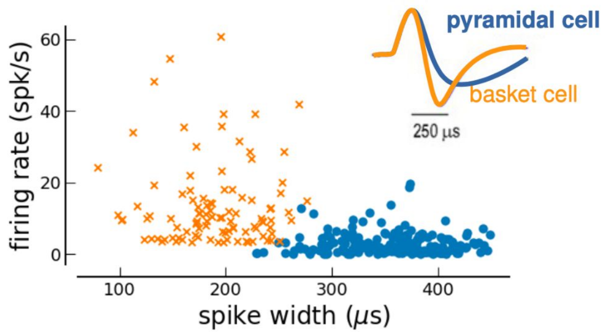

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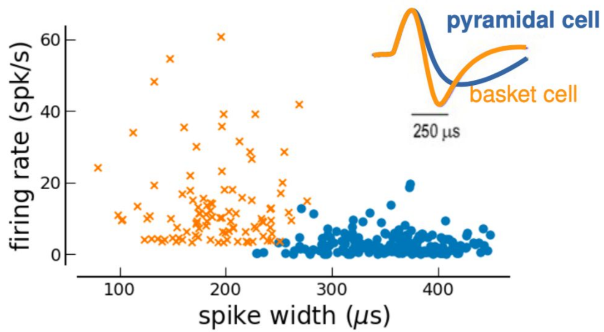
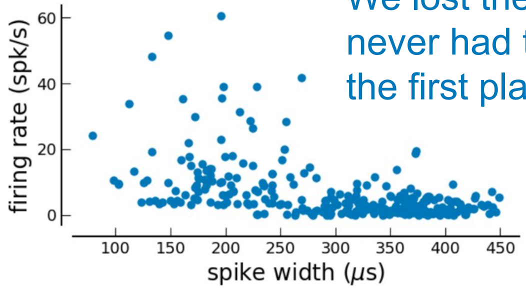
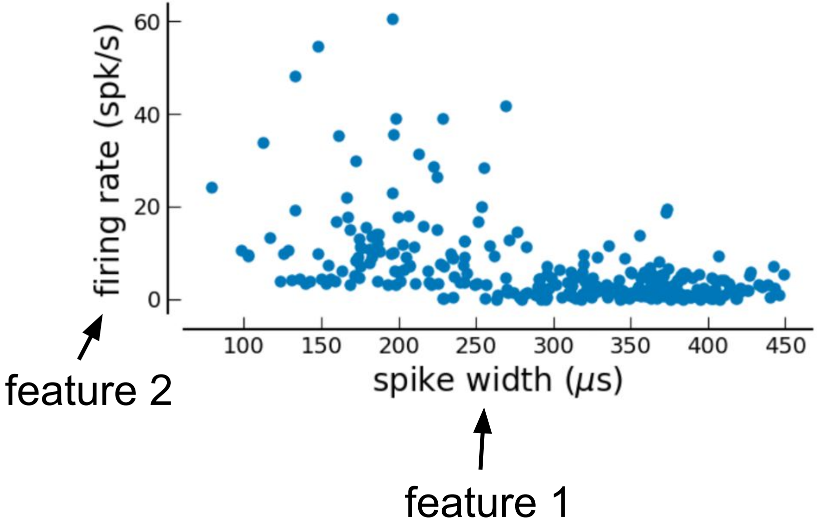
**Clustering**: We see **patterns** in the data that **suggest multiple categories**, but we don't know which data point belongs to which category. Clustering is an "**unsupervised**" method (unknown ground truth).




We lost the labels or never had them in the first place.

# Clustering: Guessing categories from patterns in the feature space

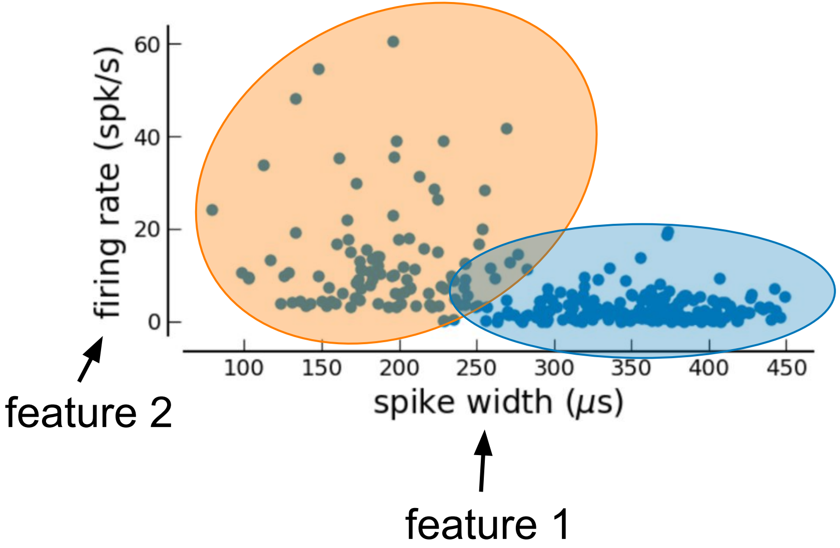



Let's assume that we know that there are two different cell types.

However, we don't have the label for each cell (we cannot classify).

Can we **guess which are the points belonging to one vs. the other class**?

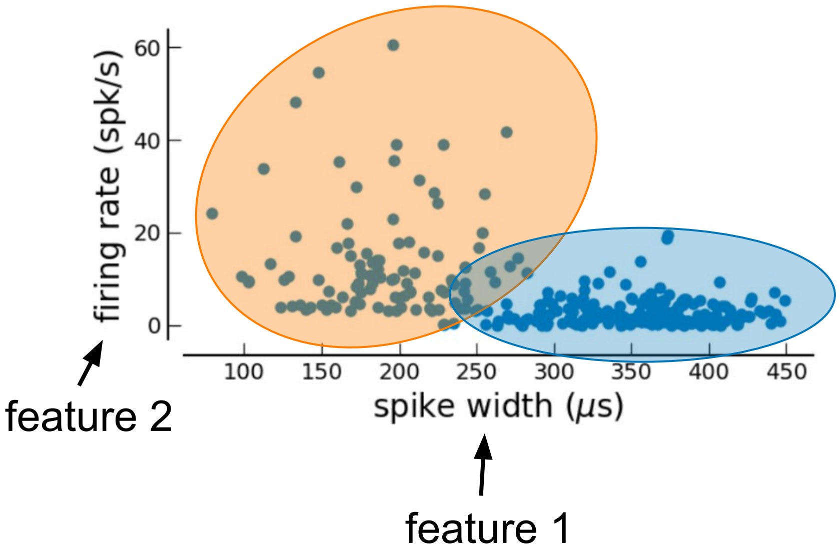
# Clustering: Guessing categories from patterns in the feature space




Can we guess which are the points belonging to one vs. the other class?

We do this by defining **regions of the feature space**.

# Clustering: Guessing categories from patterns in the feature space

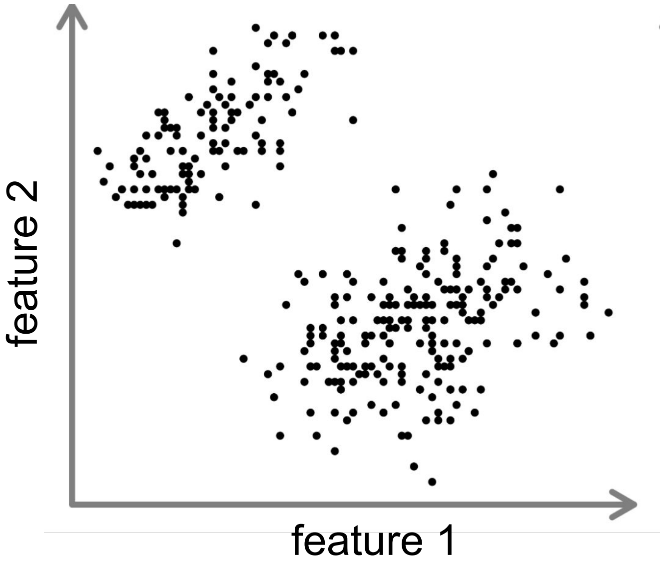



Can we guess which are the points belonging to one vs. the other class?

We do this by defining **regions of the feature space**.

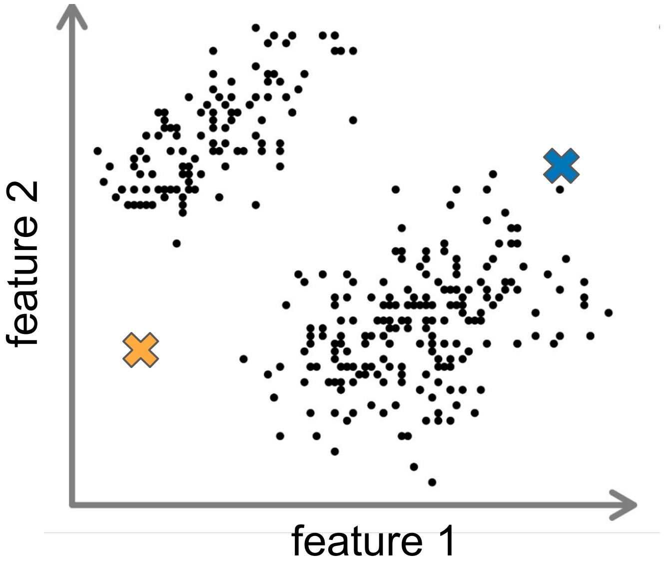
But how?

# Clustering: k-means




Assuming two clusters, we try to find k = 2 cluster means (“centroids”).

# Clustering: k-means




Assuming two clusters, we try to find
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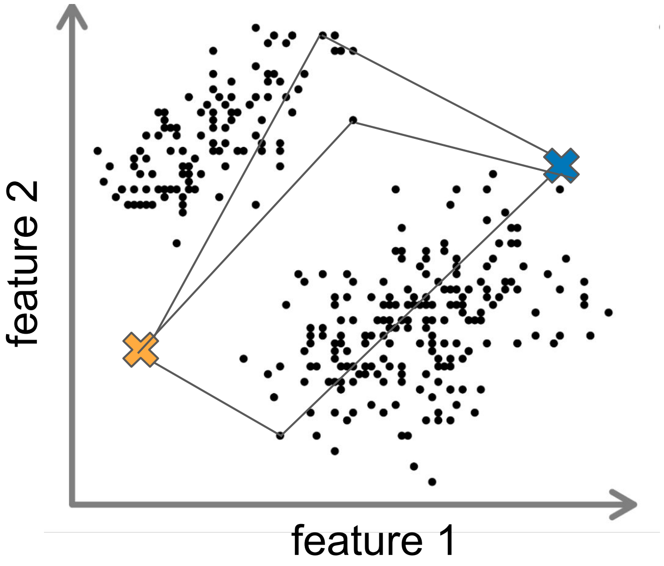
1. Pick two random values (“initialization”).

# Clustering: k-means

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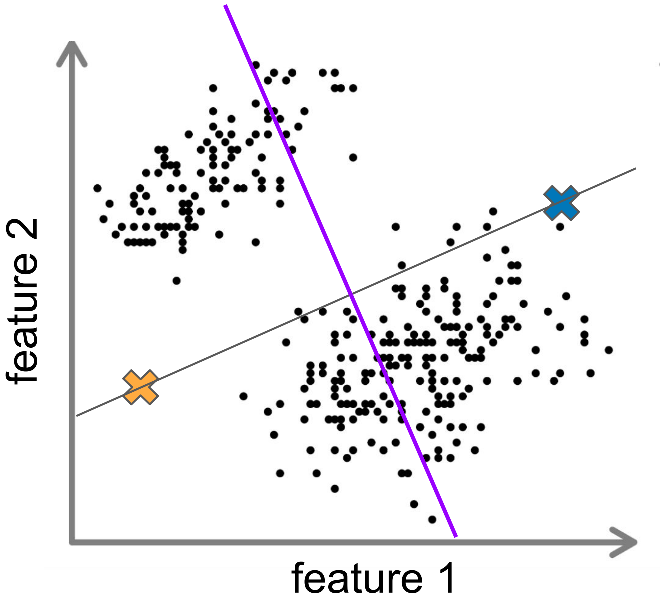
2. Assign each data point to closest cluster.

# Clustering: k-means

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   (note: there is effectively a decision boundary!).

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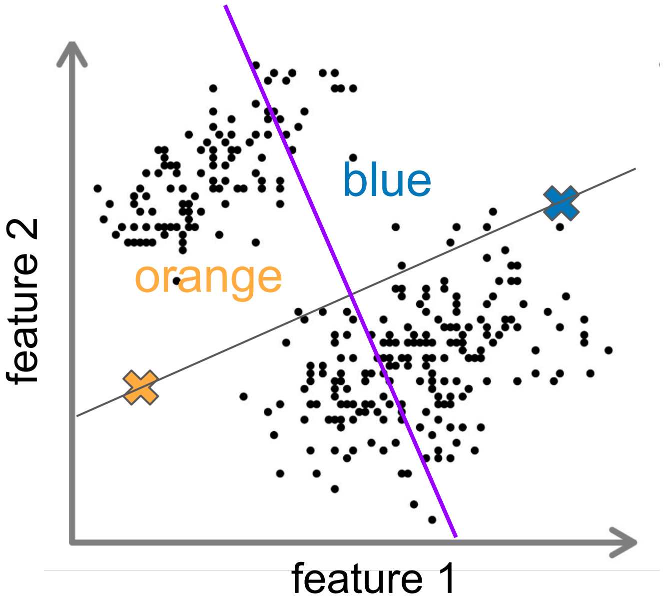


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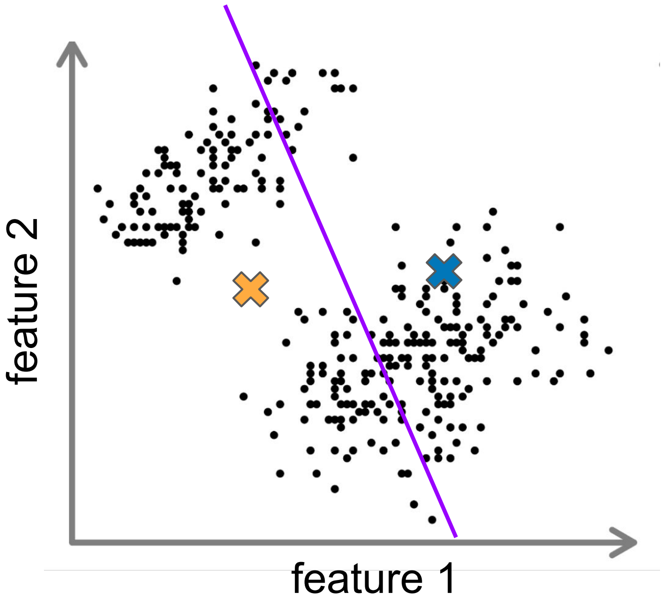


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3. Recalculate cluster means

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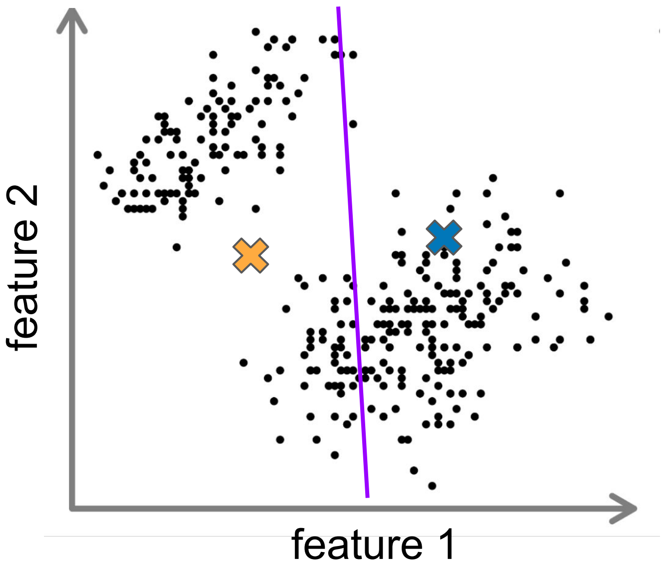


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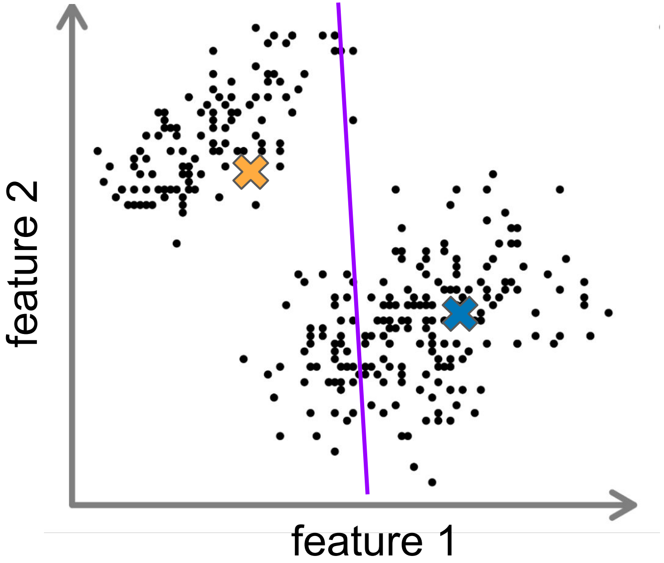


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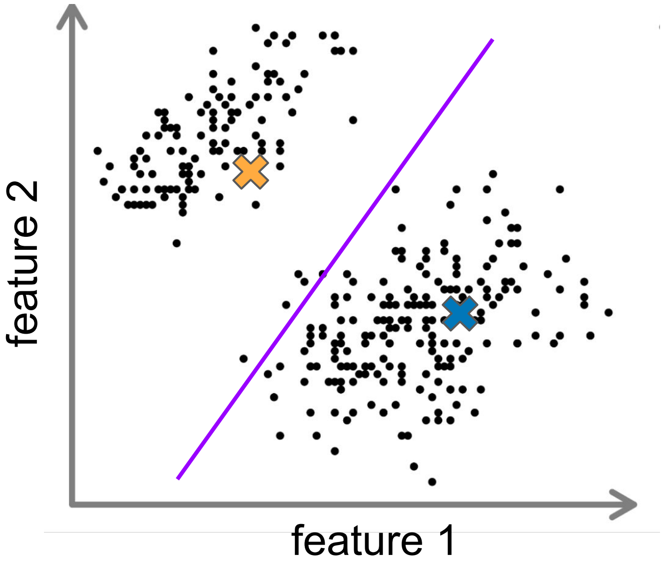


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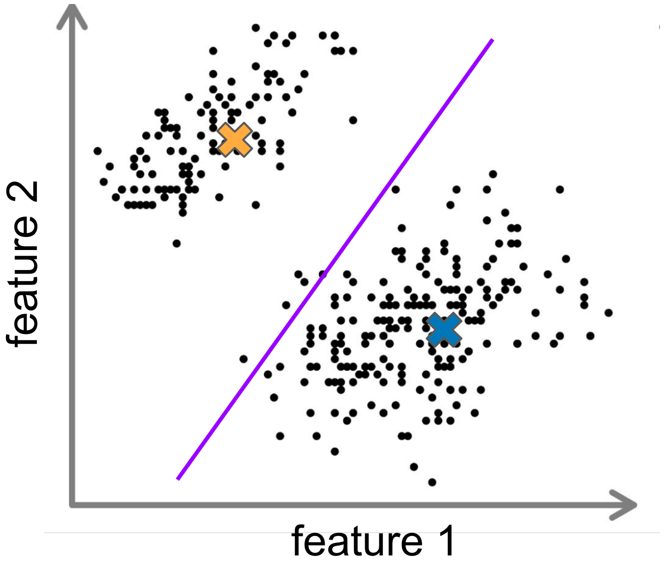


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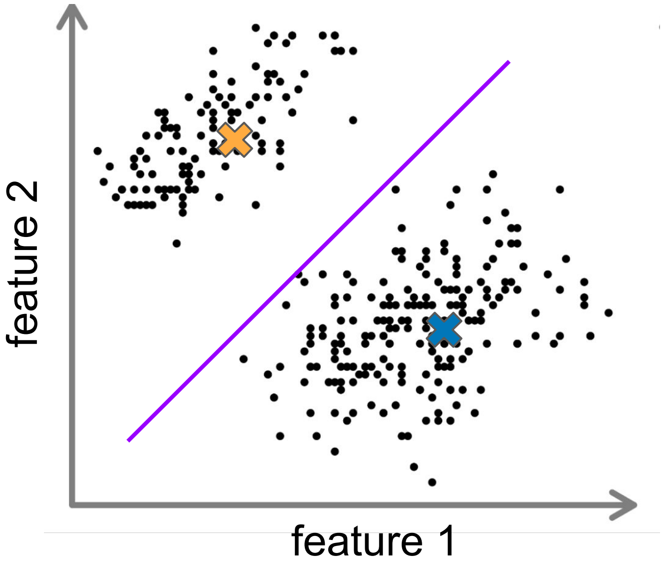


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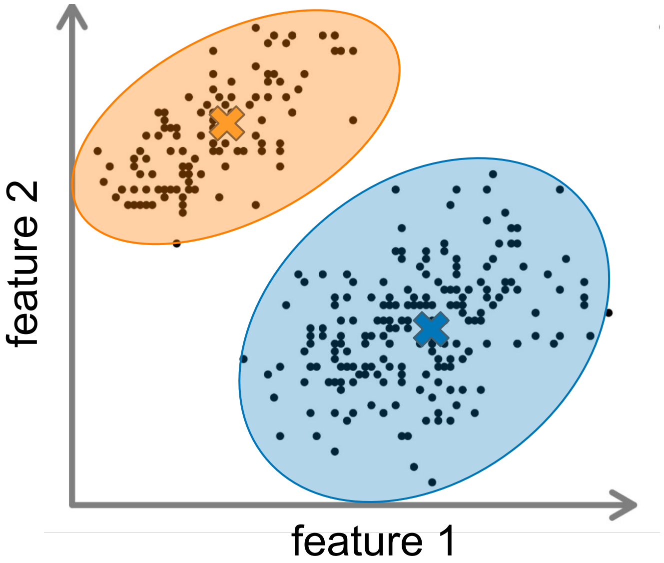


Assuming two clusters, we try to find
k = 2 cluster means (“centroids”).

1. Pick two random values (“initialization”).
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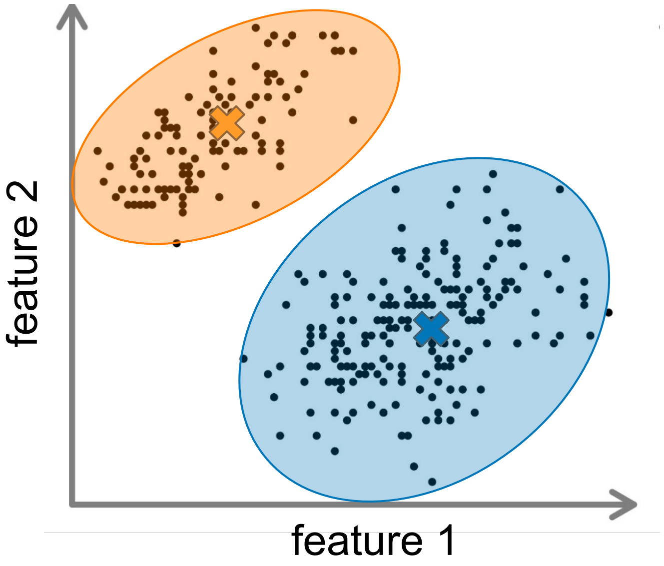
3. Recalculate cluster means.

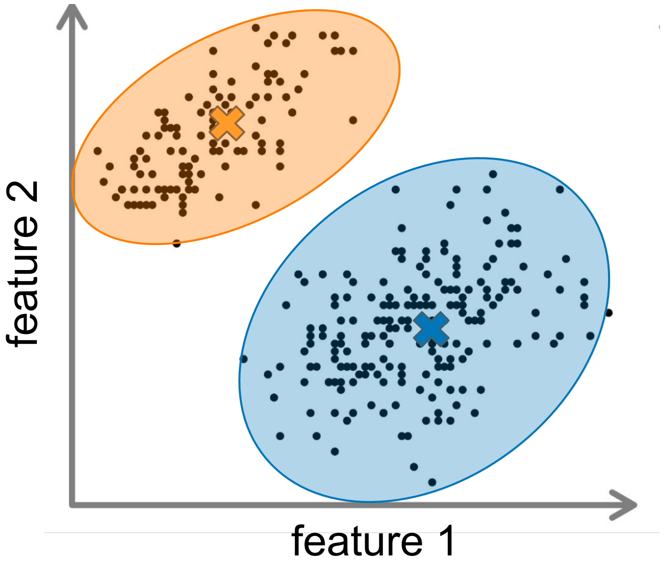
Repeat 2.-3. until cluster means are stable (they “converged”).

# Clustering: k-means




Clustering is **iterative** (repeat steps until convergence).

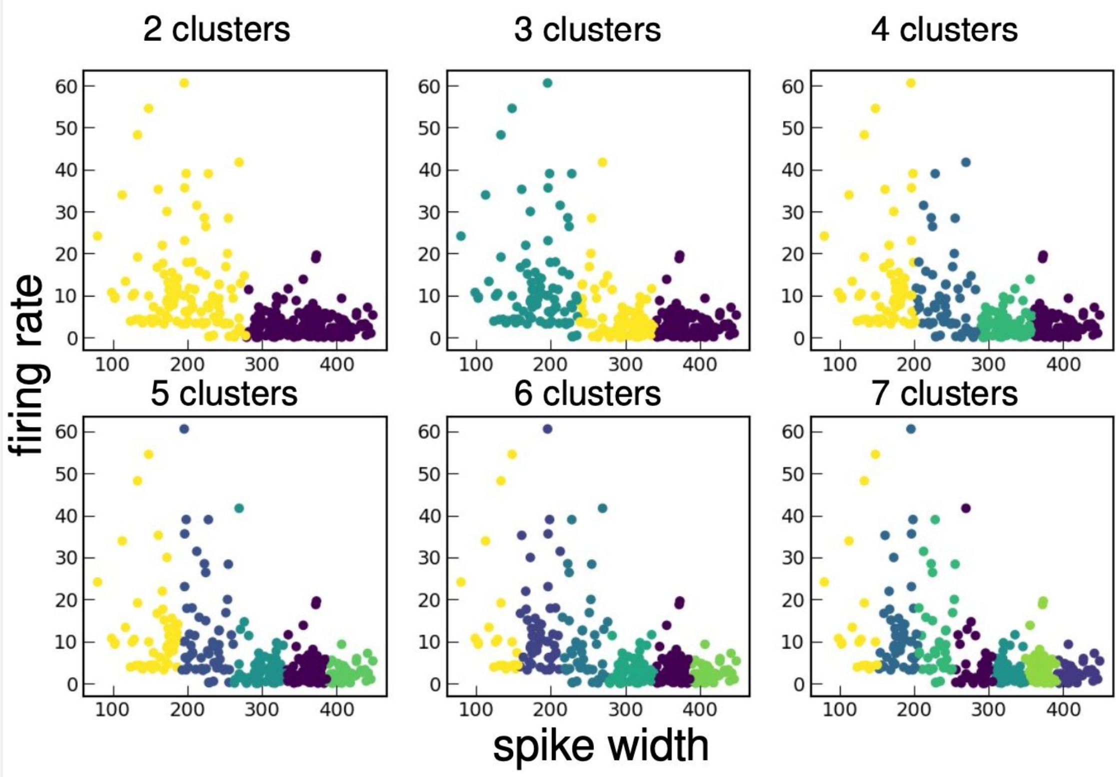
# Clustering: k-means



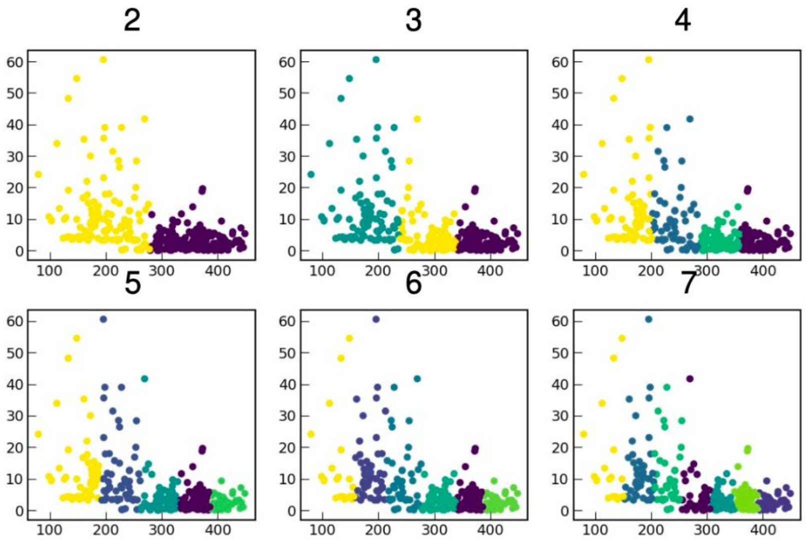

Clustering is **iterative** (repeat steps until convergence).

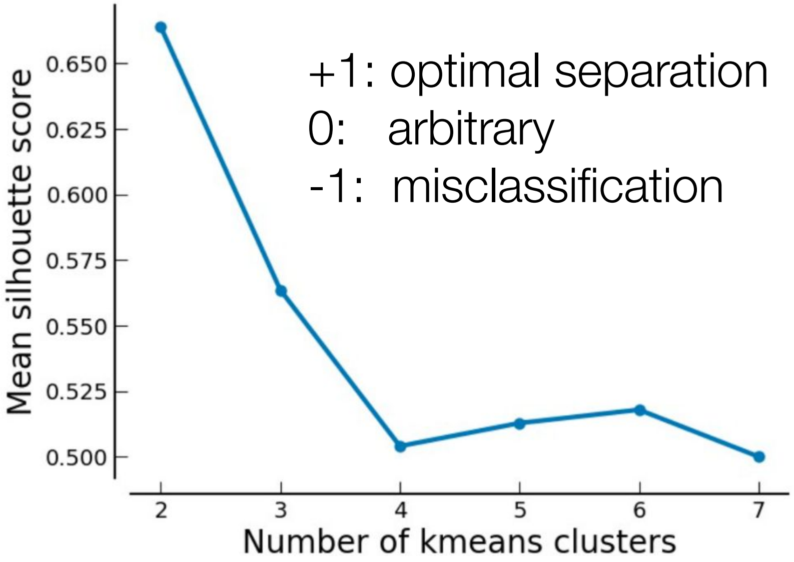
The **optimal number of clusters is not always obvious**: We therefore often repeat clustering for different values of “hyperparameter” k and compare a “goodness of fit” measure (in k-means: “Silhouette score”).

# Clustering: hyperparameter selection (k = ?)



# Clustering: hyperparameter selection (k = ?)



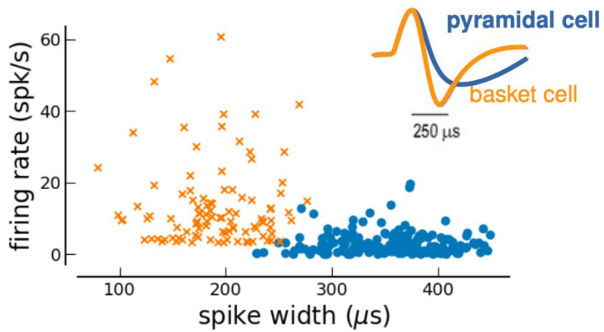



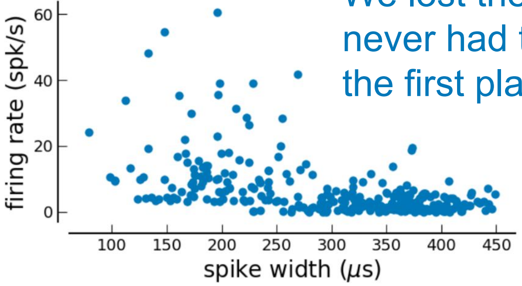

The **Silhouette score** for each point measures the distance to points in the same cluster vs. to points in the neighboring cluster

# Classification and Clustering: Overview

**Classification**: We **know the true categories** and want to know whether there is a reliable relationship between data and categories. Classification methods are also called “**supervised**” (known ground truth).

**Clustering**: We see **patterns** in the data that **suggest multiple categories**, but we don’t know which data point belongs to which category. Clustering is an “**unsupervised**” method (unknown ground truth).




We lost the labels or never had them in the first place.

# Classification and Clustering: Overview

**Classification**

- Logistic regression
- Support vector machines

**Clustering**

- k-means