Classification and clustering

Neural data science with Python

Heike Stein

01/12/2023

Classification and Clustering: Overview

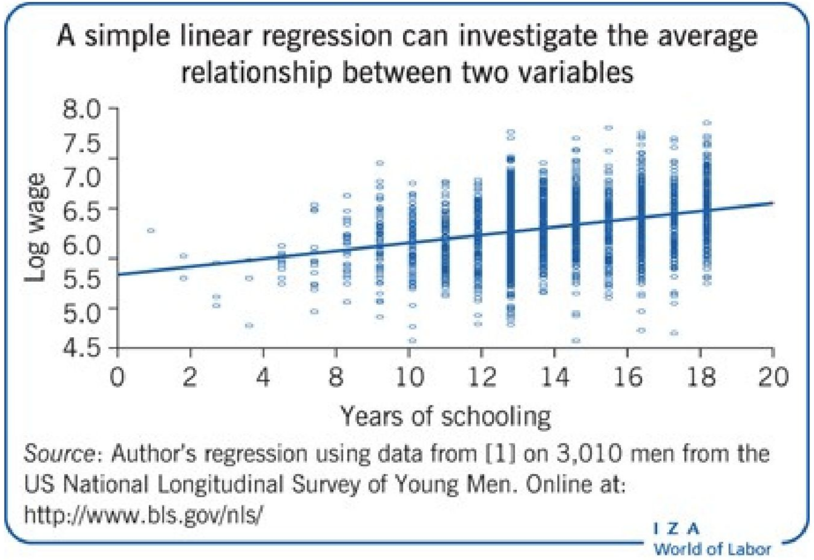
Classification

- Logistic regression
- Support vector machines

Clustering

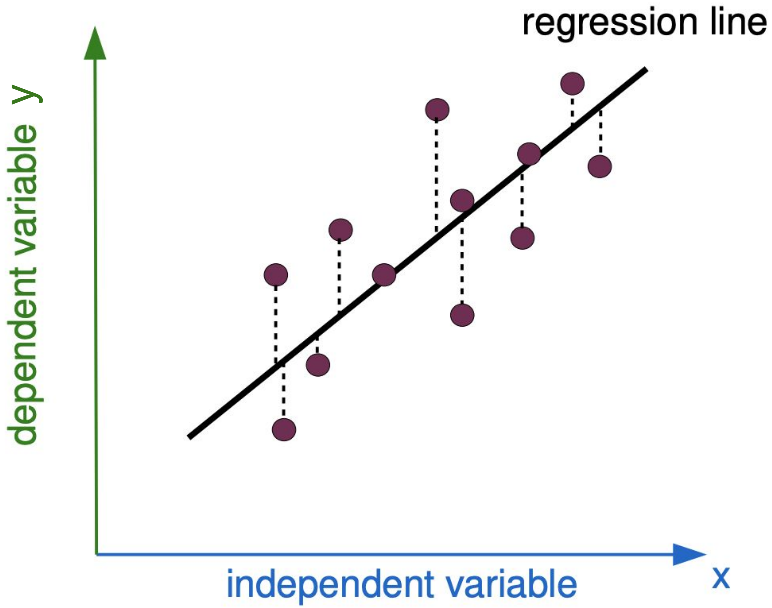
- k-means

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



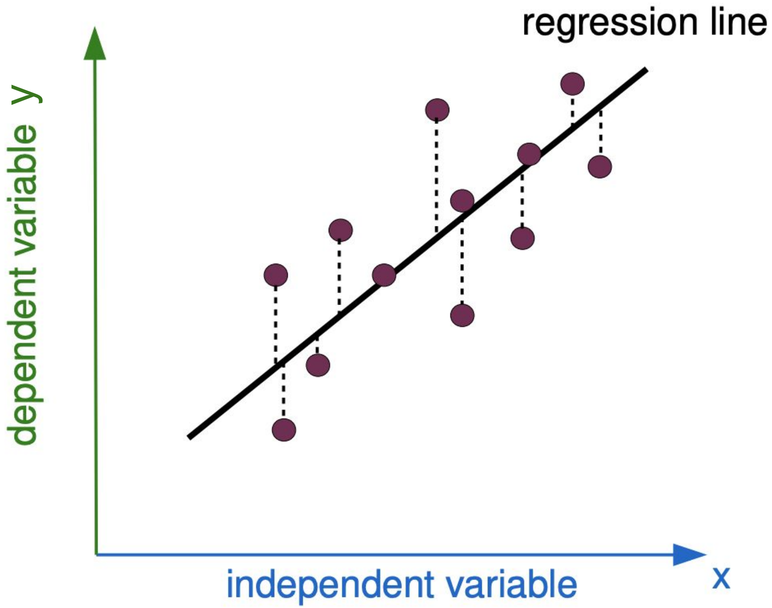
→ linear mapping from predictor (“independent”) variable(s) x (e.g. years of schooling) to outcome (“dependent”) variable y (e.g. wage)

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

weights (“parameters”)

errors (“residuals”)

Regression analysis



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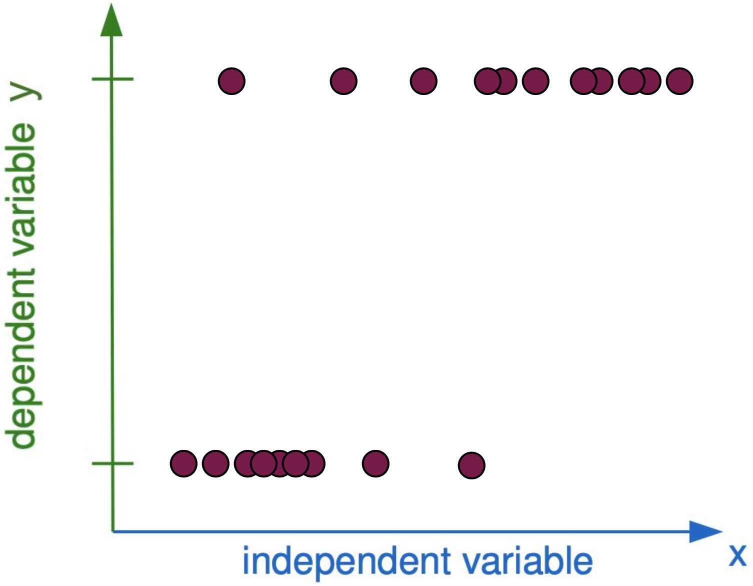
$$y = \boxed{\beta_0} + \boxed{\beta_1} x_1 + \boxed{\varepsilon}$$

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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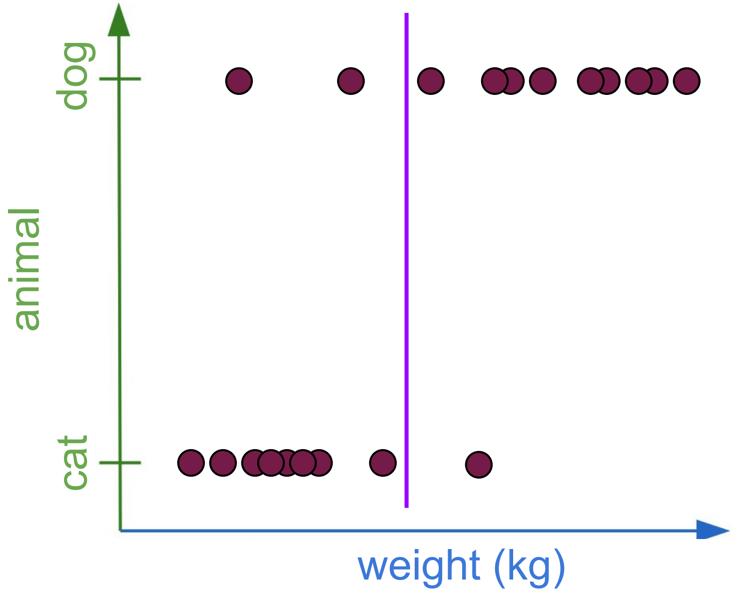
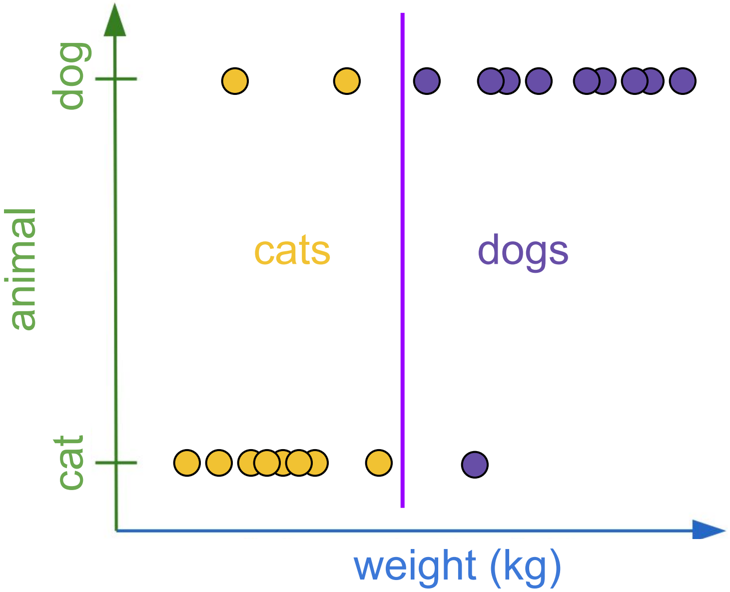


Given knowledge of x, what is the most likely category of y?

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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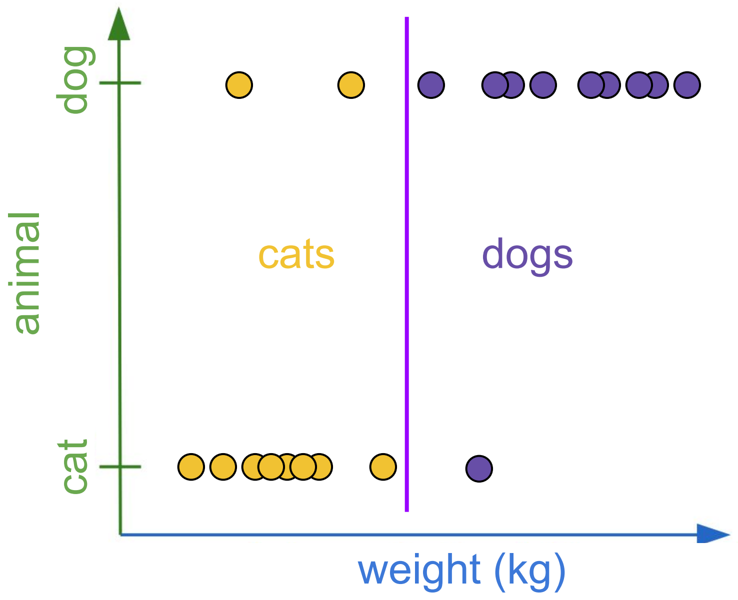
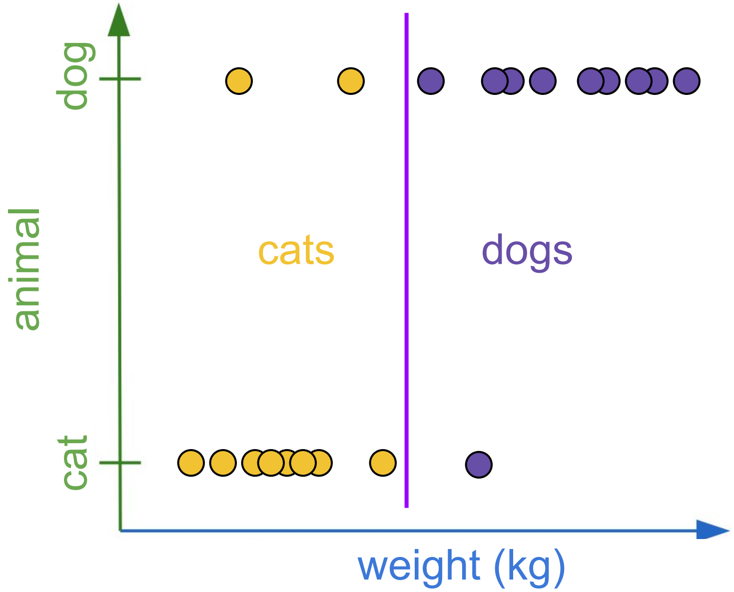


How do we find a good decision boundary?

Classification: Predicting categorical values



How do we find a good decision boundary?

It should minimize the number of misclassifications.

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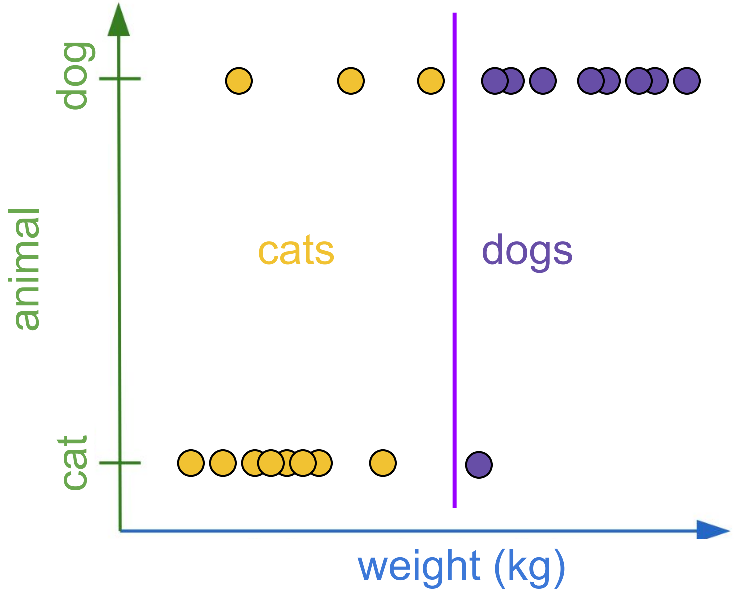

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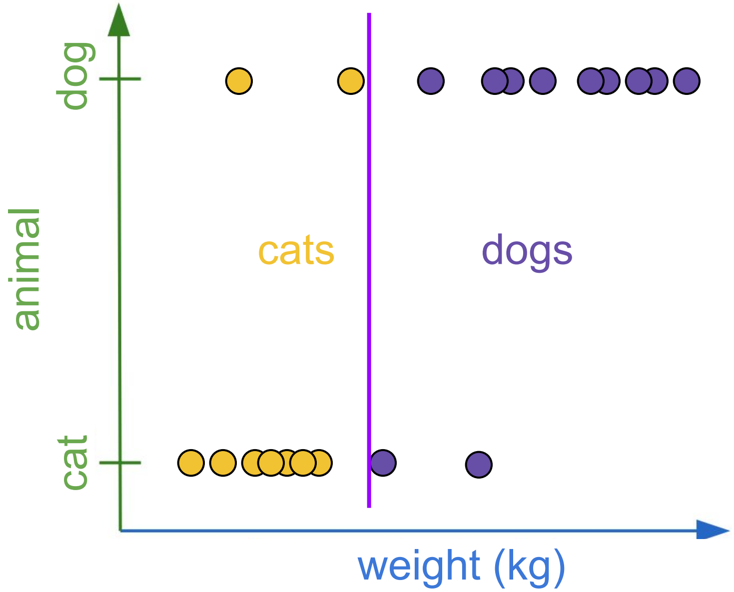

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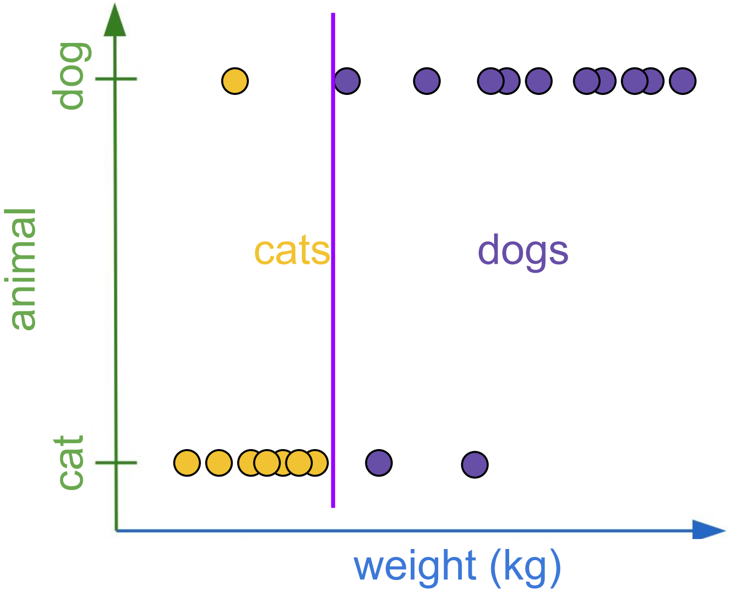

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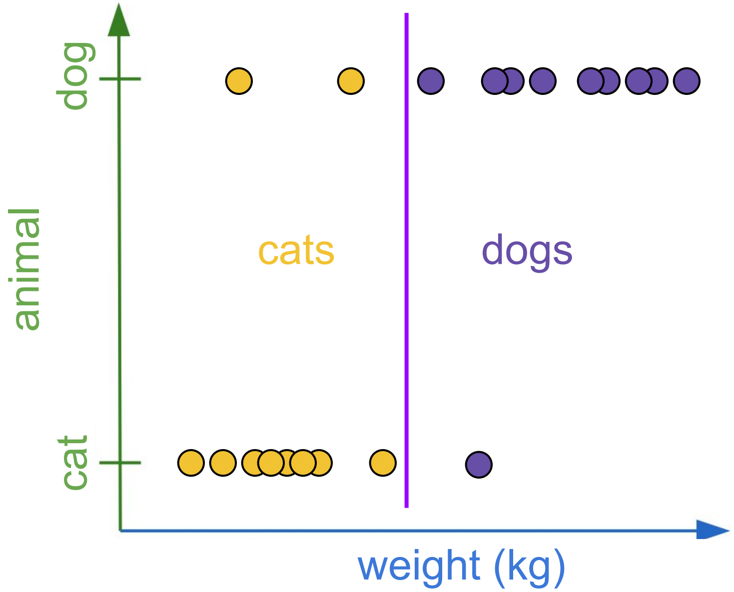


How do we find a good decision boundary?

It should minimize the number of misclassifications.

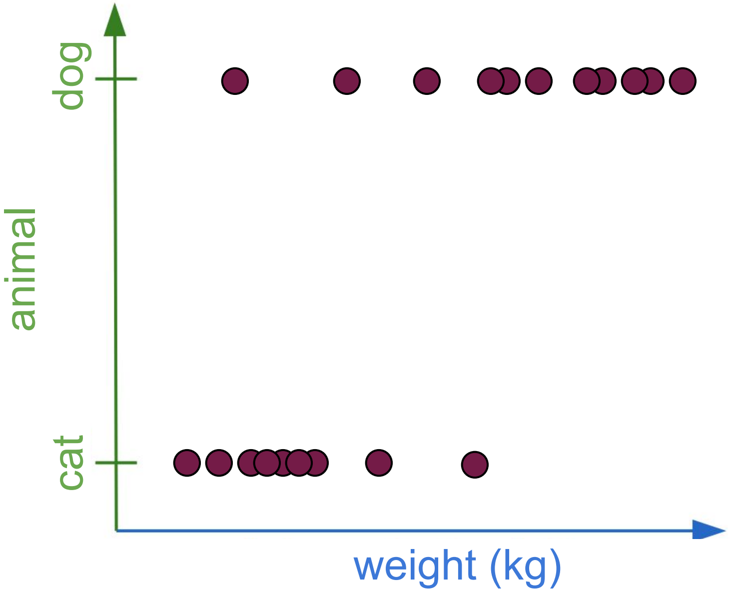
Which solution is found depends on the classification method.

Classification and Clustering: Overview

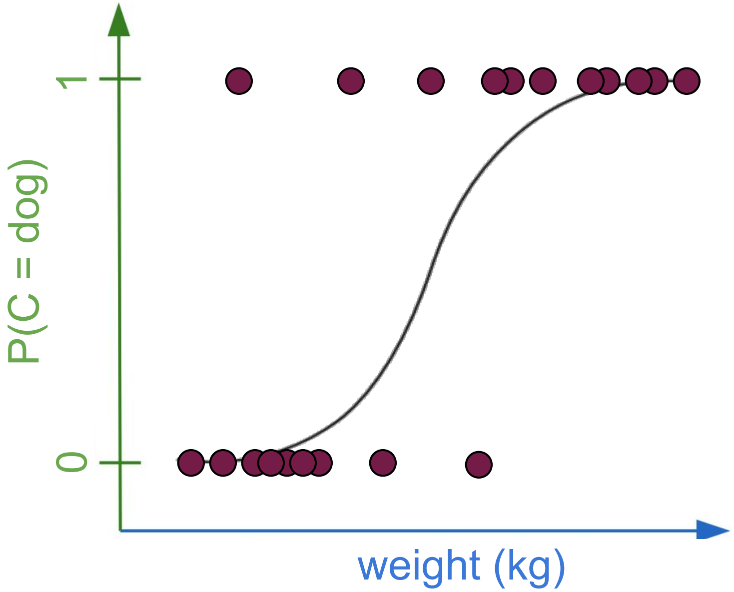
Classification

1. Logistic regression
2. Support vector machines

Classification: Logistic regression



Classification: Logistic regression

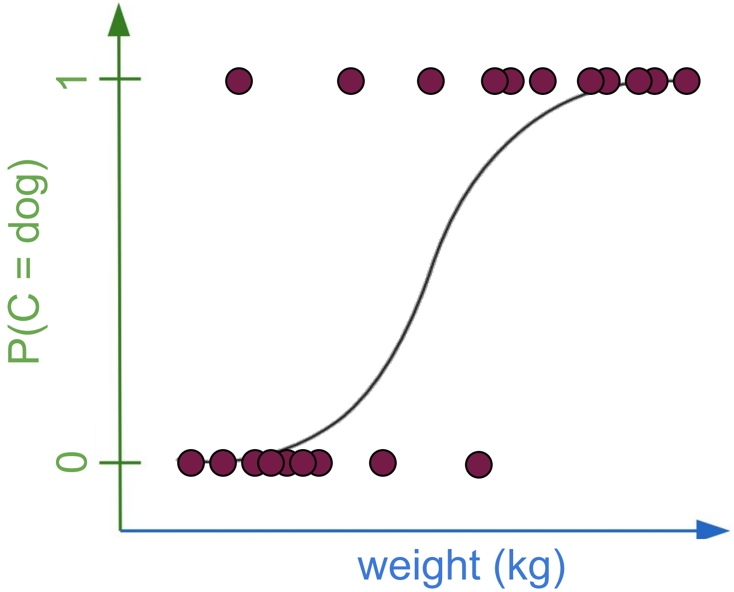


Logistic regression fits the weights of a generalized linear model:

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

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

Classification: Logistic regression



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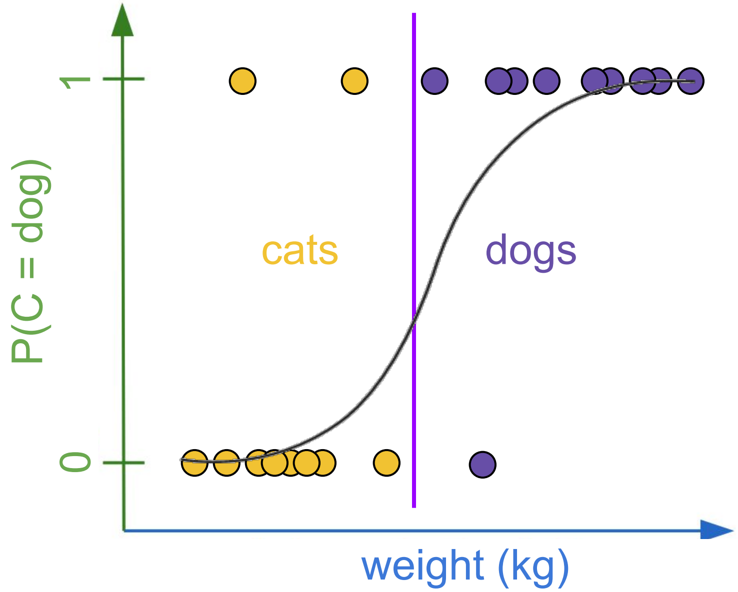
$$\Leftrightarrow \quad P(C = \text{"dog"}) = \frac{e^{(\beta_0 + \beta_1 x_1)}}{1 + e^{(\beta_0 + \beta_1 x_1)}}$$

Classification: Logistic regression



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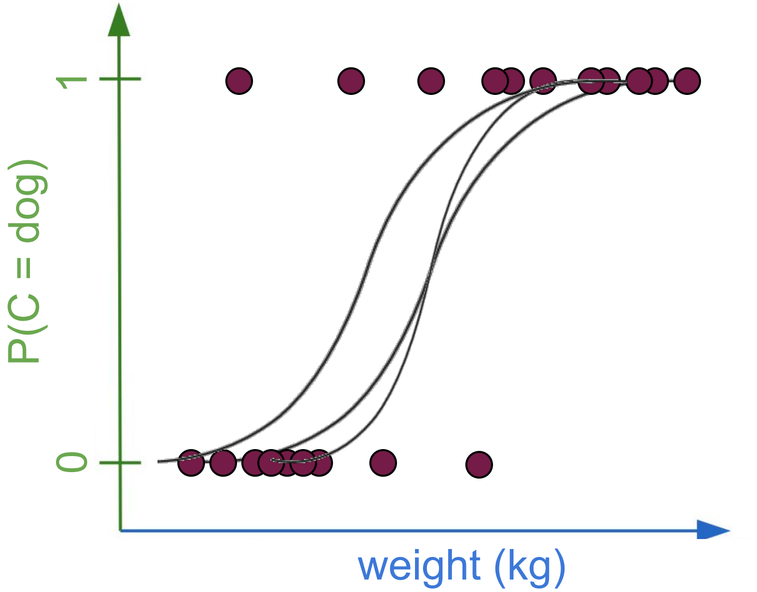
The decision boundary is the value of x for which P(C = “dog”) = 0.5

Classification: Logistic regression



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

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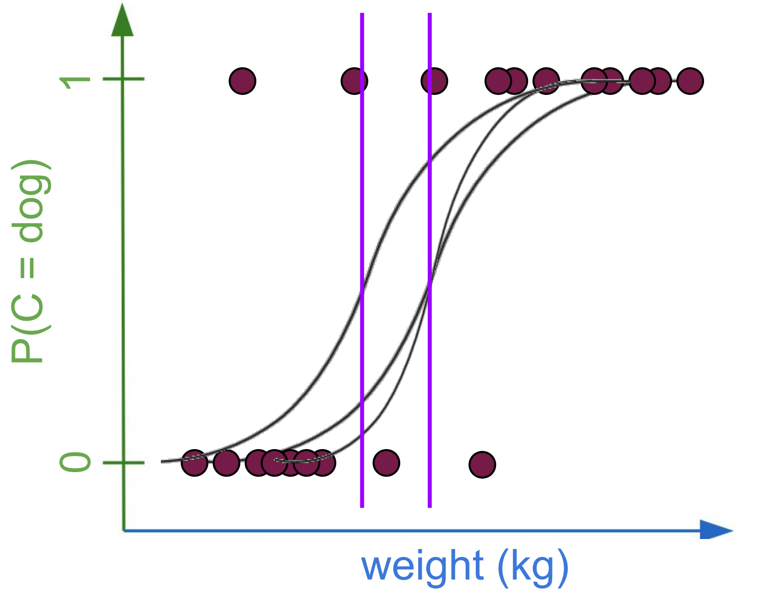

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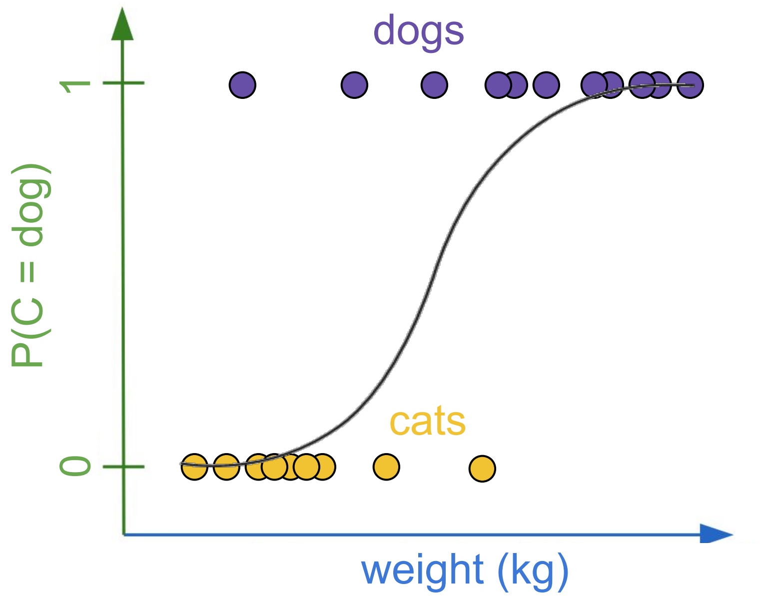

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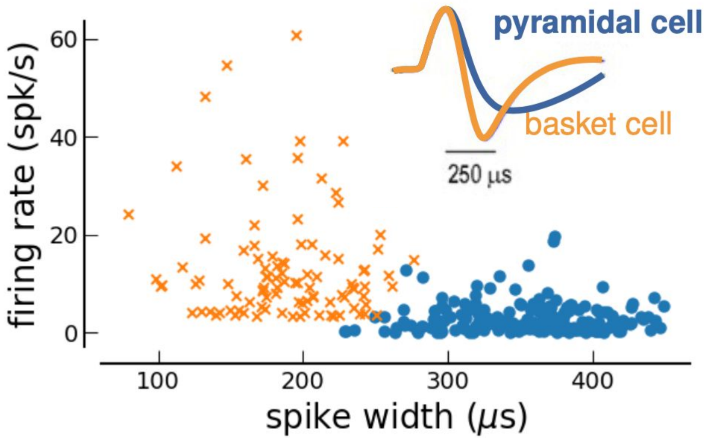
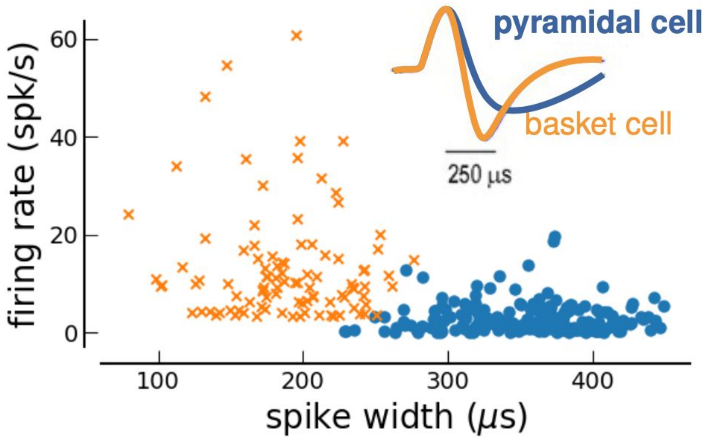
Weights are fitted by minimizing an error function between P(C = dog) and true labels: t = 1 if dog, t = 0 if cat

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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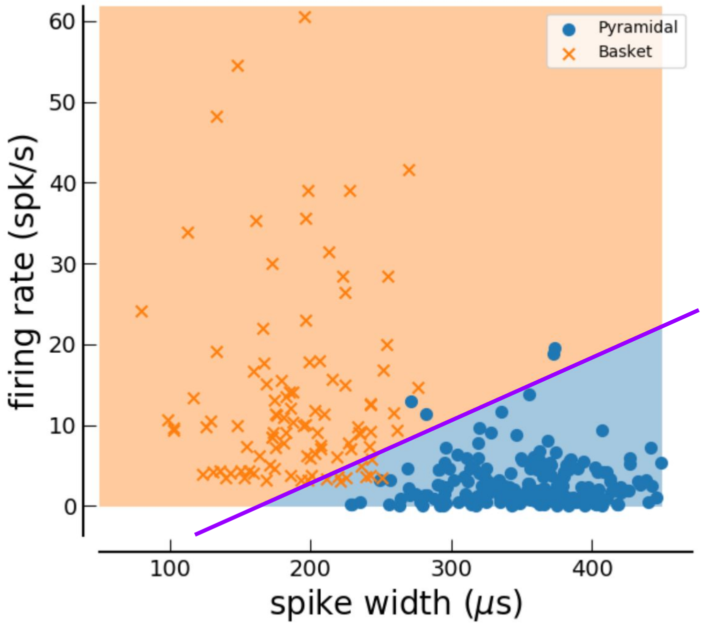

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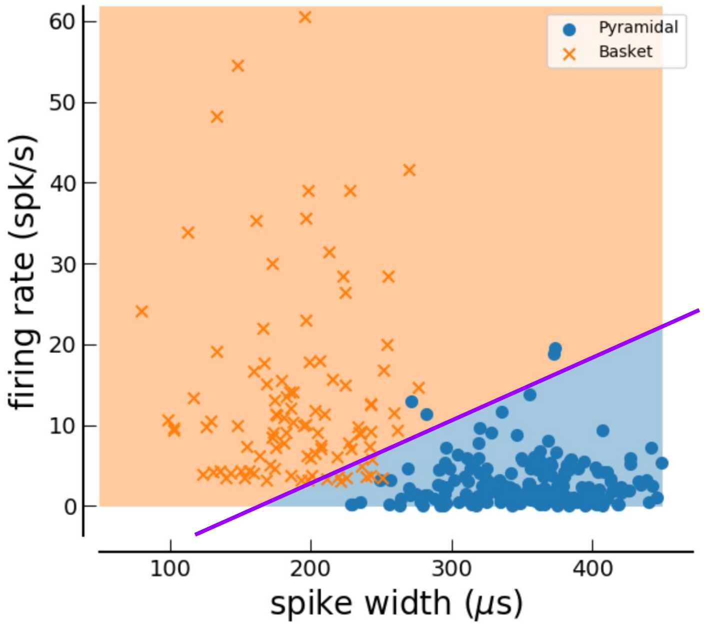
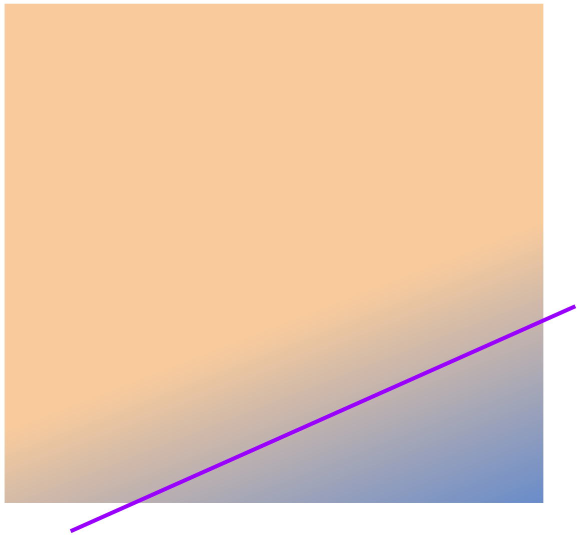
with sigmoidal function $\quad f(x) = \dfrac{e^x}{1 + e^x}$

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

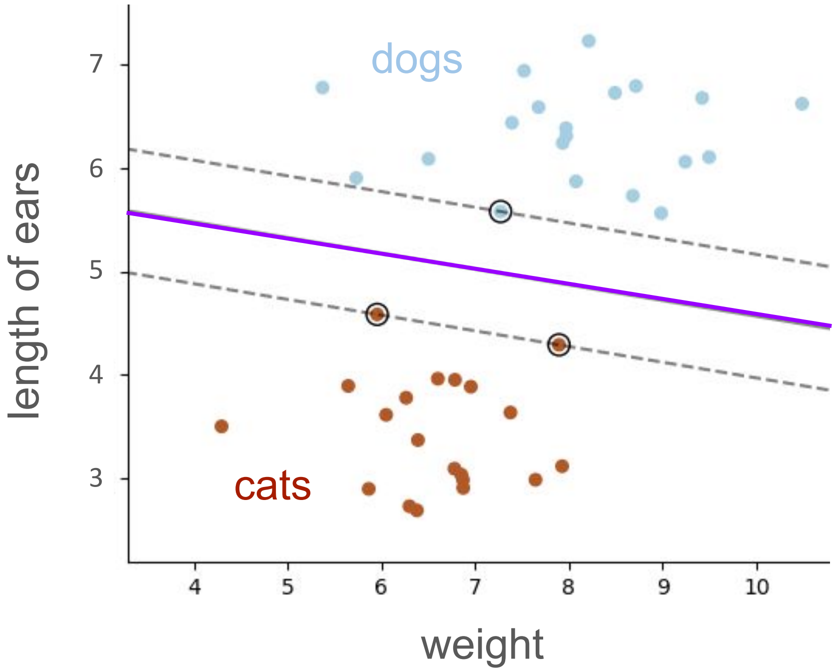
Classification: Logistic regression in 2D



Sigmoidal function in 2D



Classification: Support vector machines (SVM)



Again, we're looking for a decision boundary

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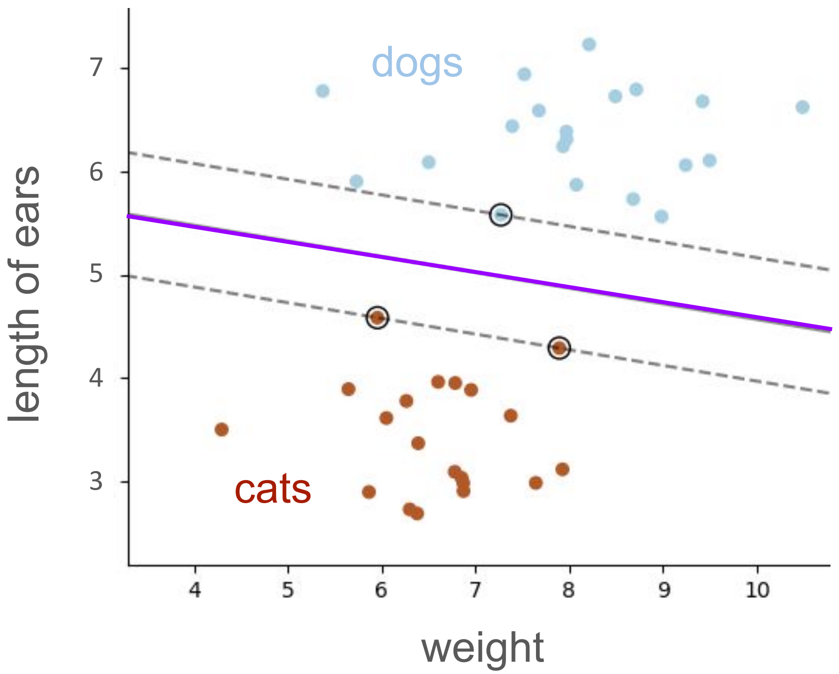

Again, we're looking for a decision boundary

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

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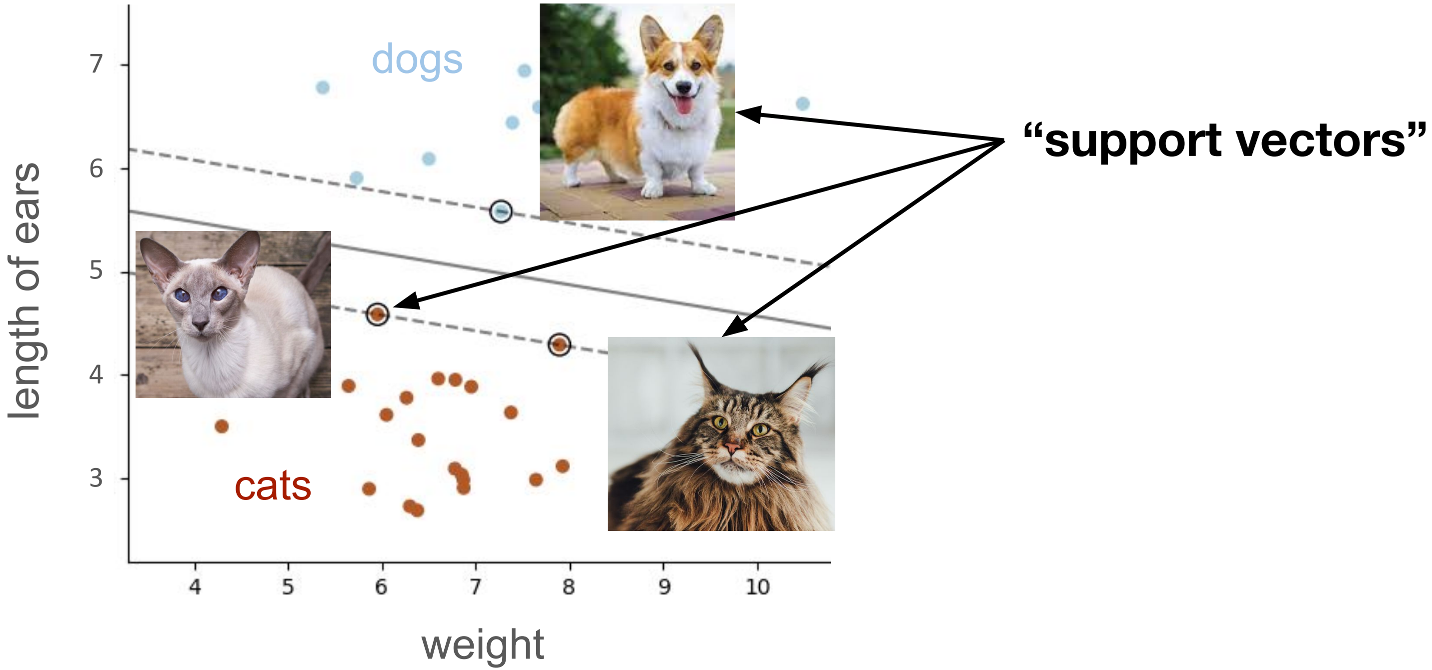

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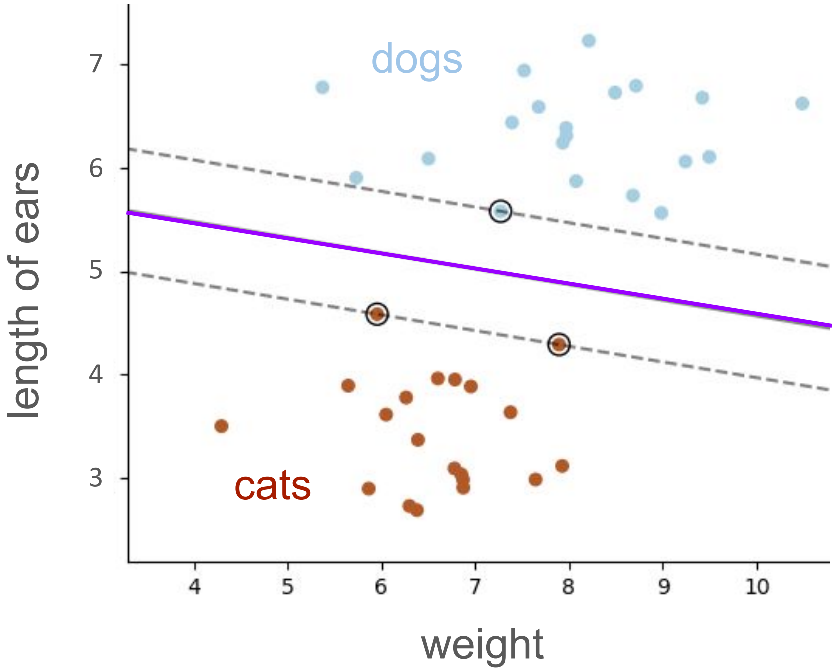

The decision boundary is the line that is equally far away from “support vectors” of each class

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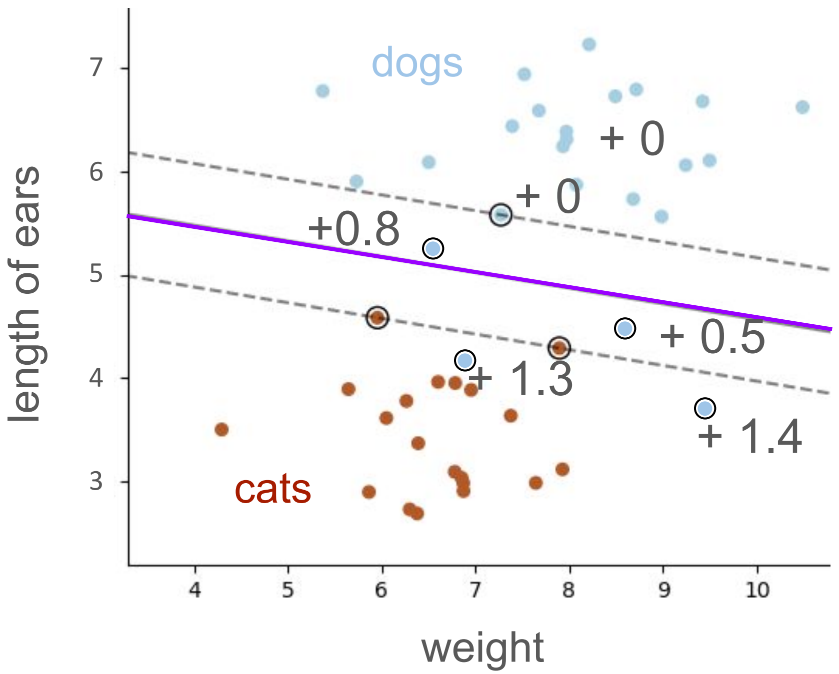
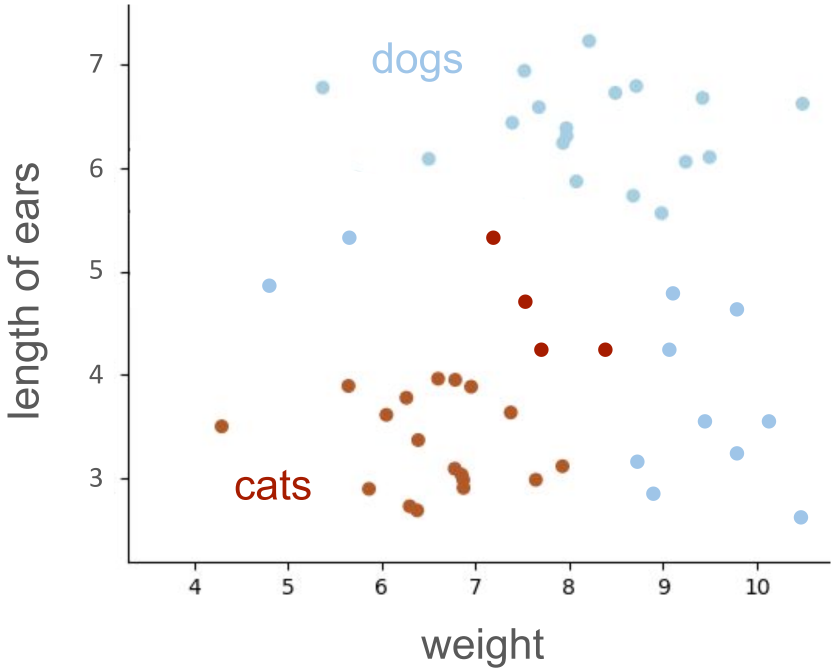


The decision boundary is the line that is equally far away from “support vectors” of each class

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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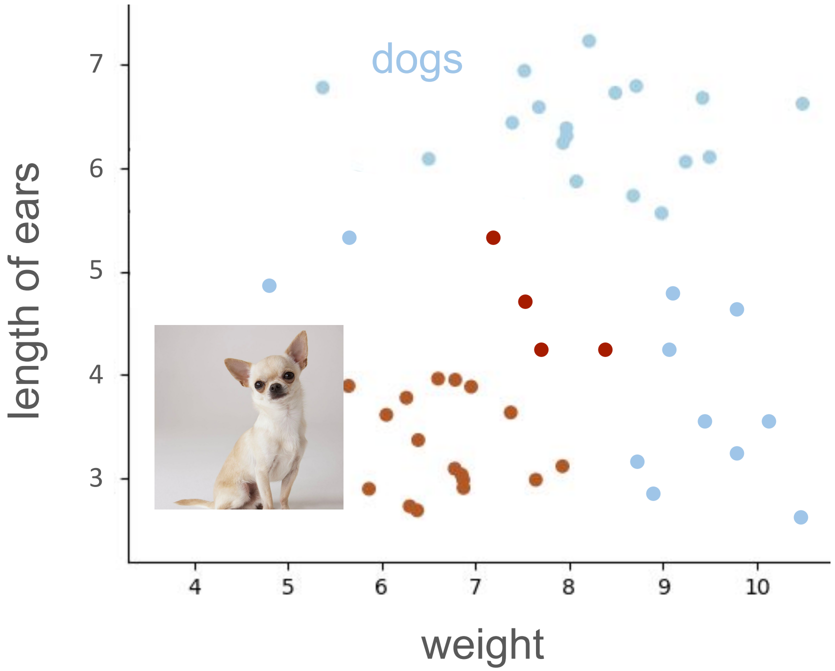

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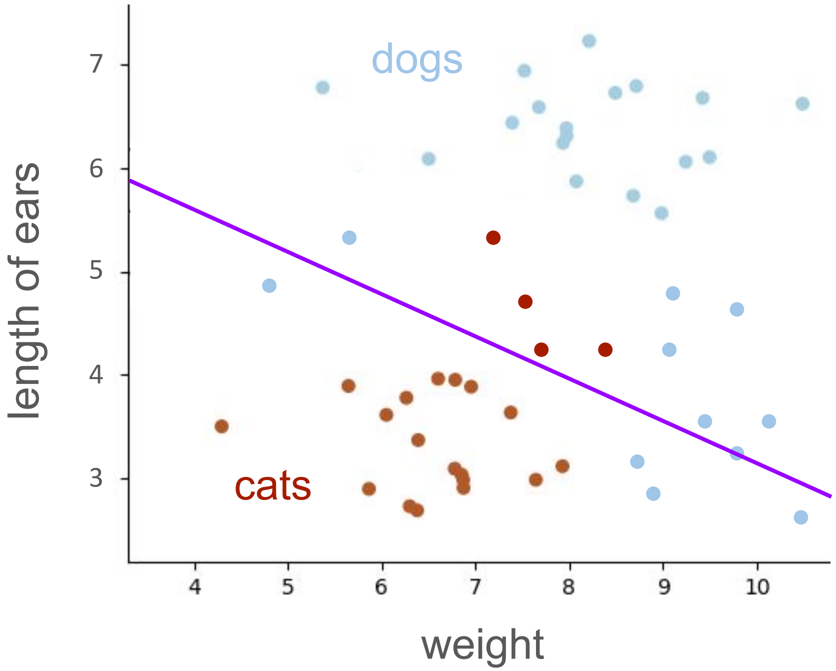
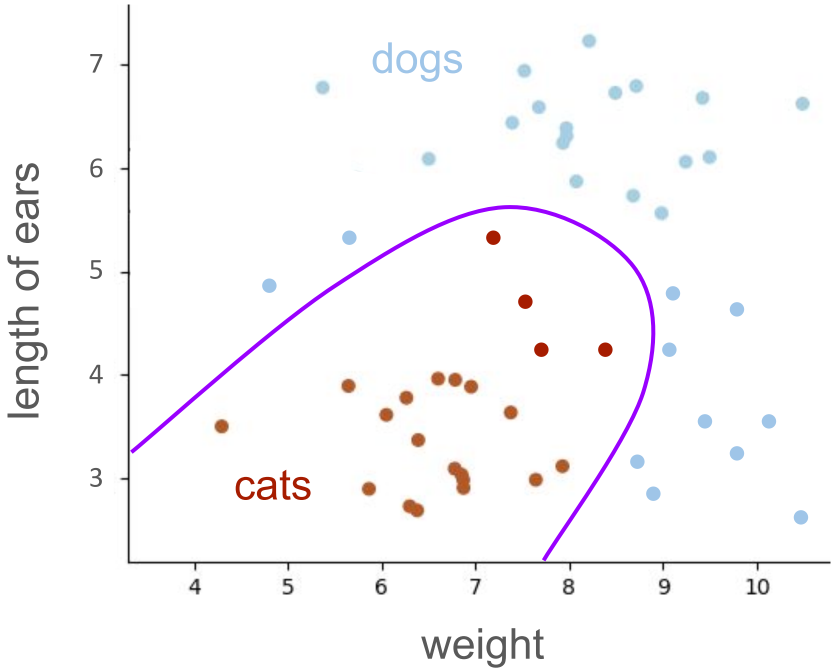


Some problems are not linearly separable

Classification: Support vector machines (SVM)



Some problems are not linearly separable, but they might be nonlinearly separable.

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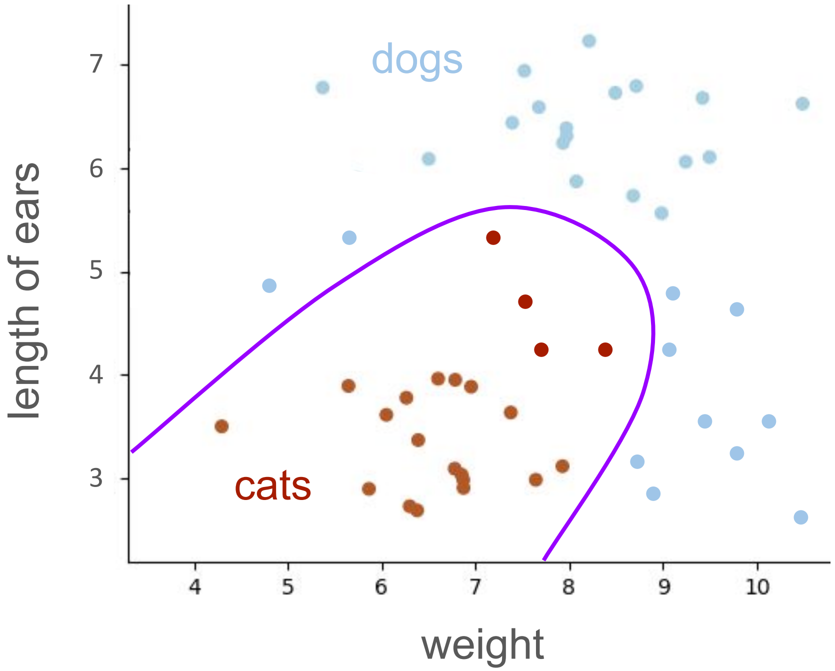

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SVMs use **"kernels"** to transform predictor variables nonlinearly. This can give us nonlinear decision boundaries.

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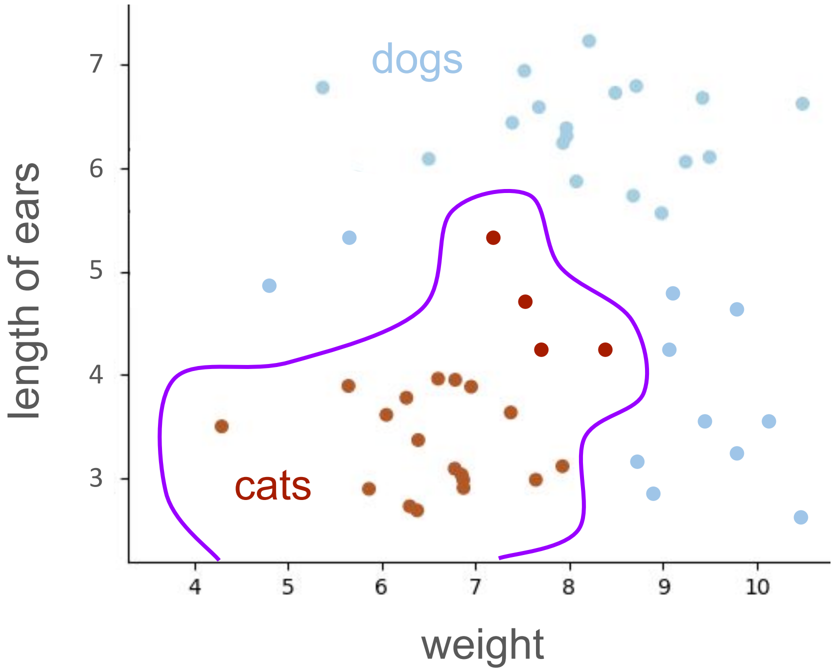

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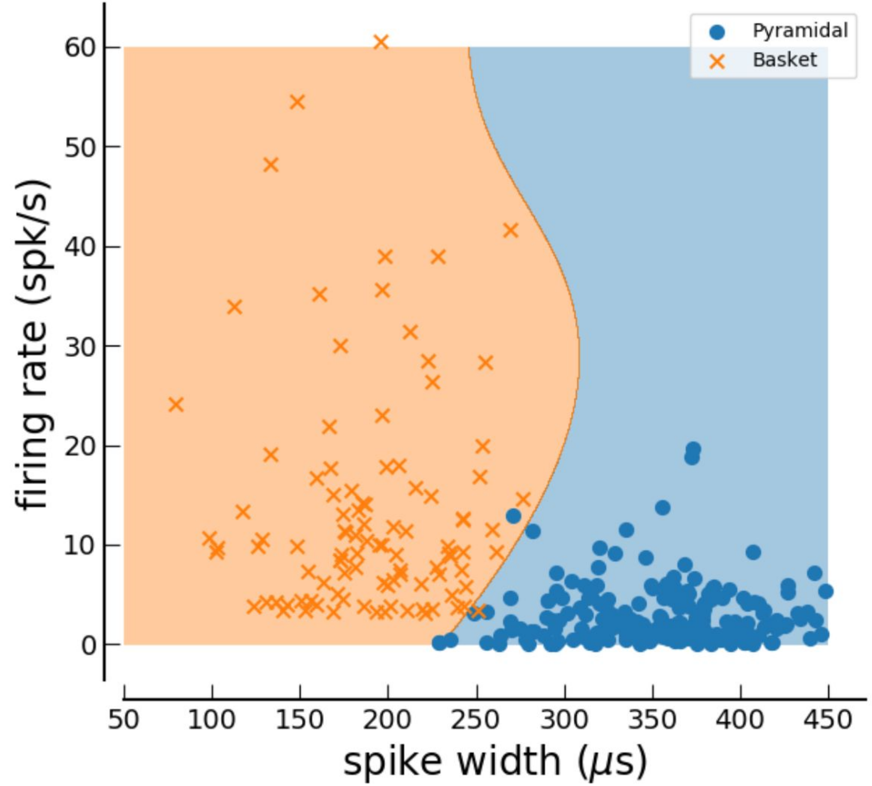
SVMs use **“kernels”** to transform predictor variables nonlinearly. This can give us nonlinear decision boundaries.

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

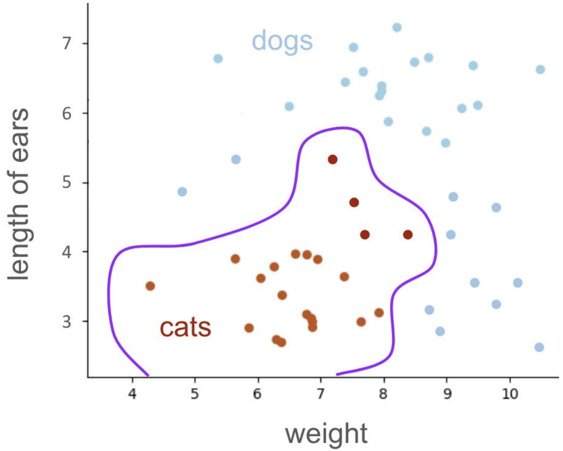
Classification: Support vector machines (SVM)



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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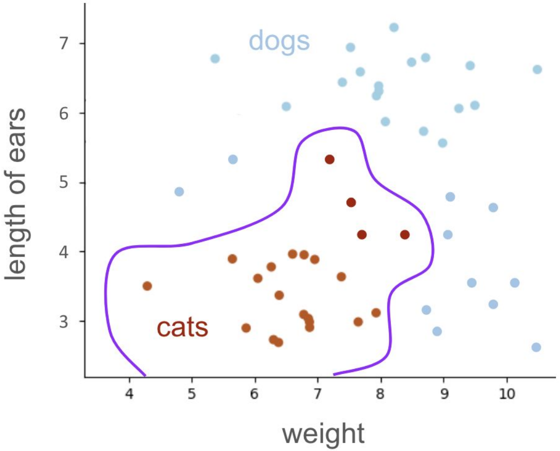

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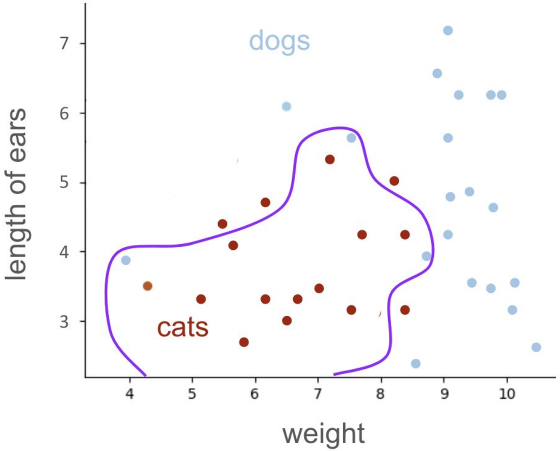
Test set: new data, “old” model.

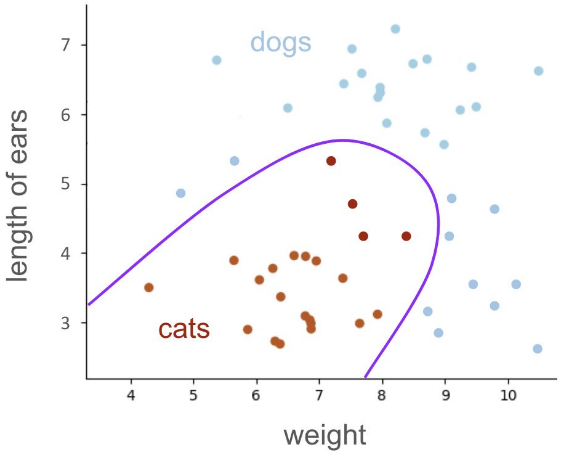


~90 % classification performance

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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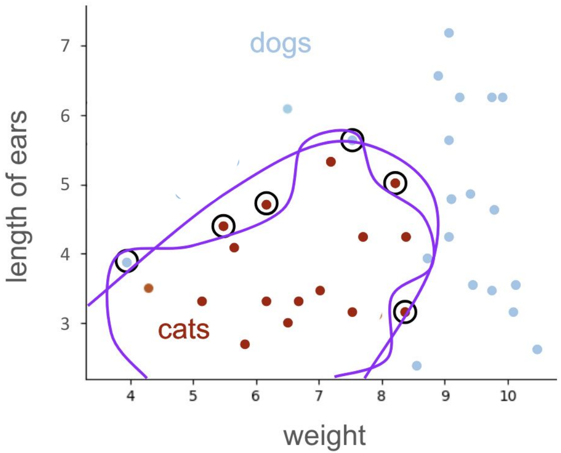
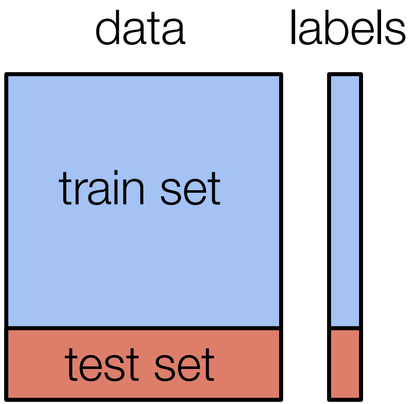


~98 % classification performance

Classification: Cross-validation



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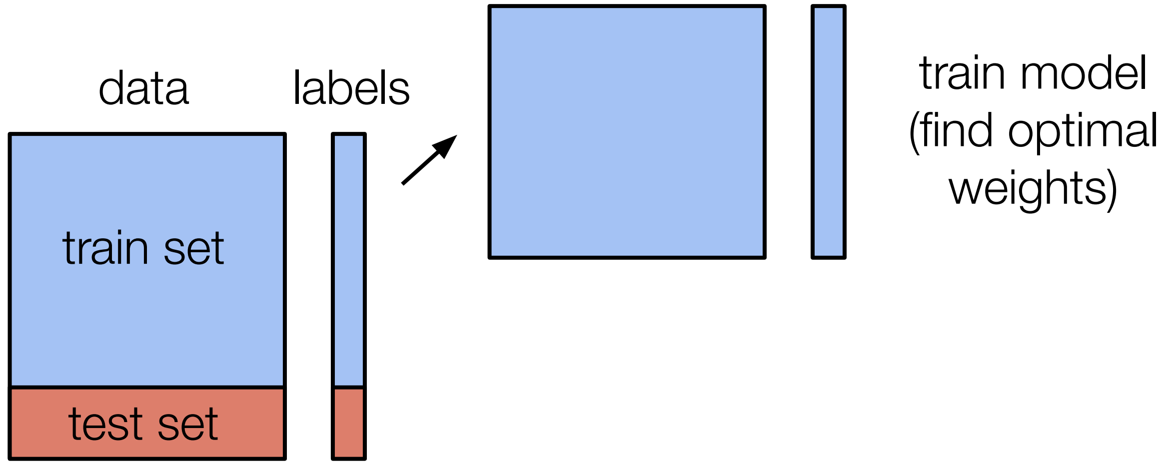

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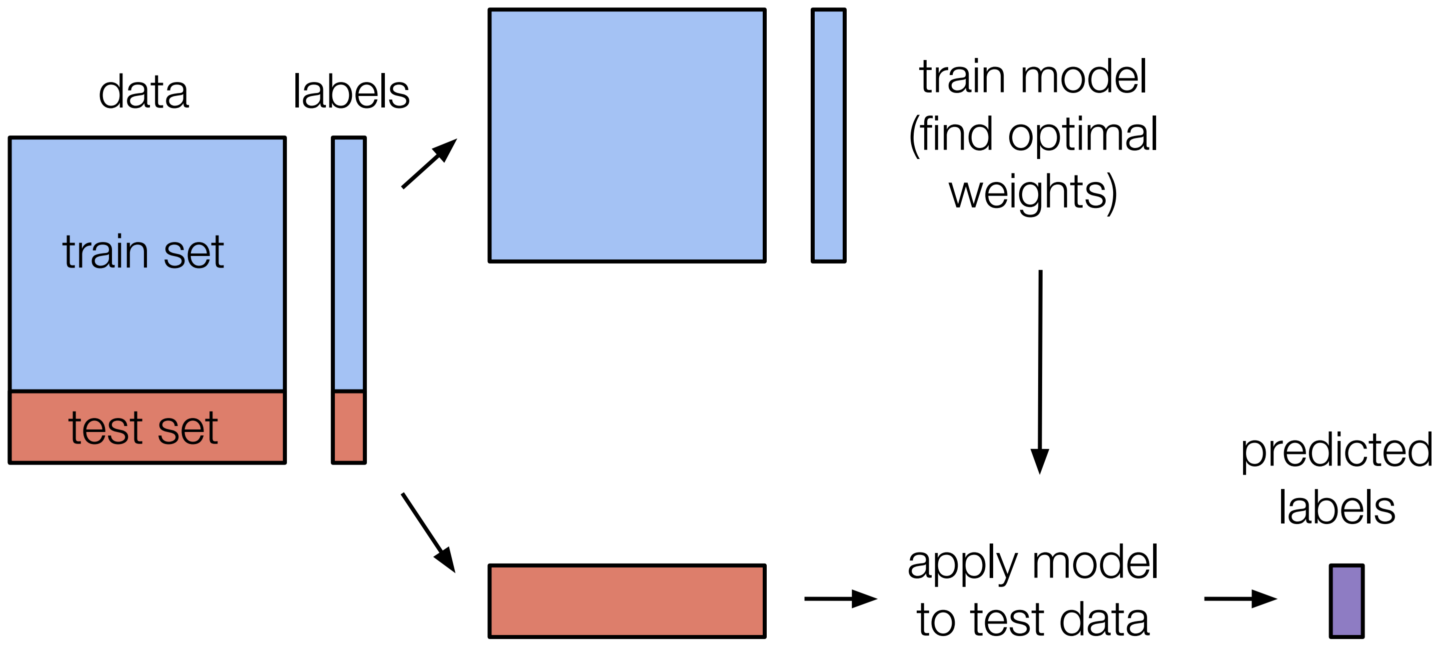

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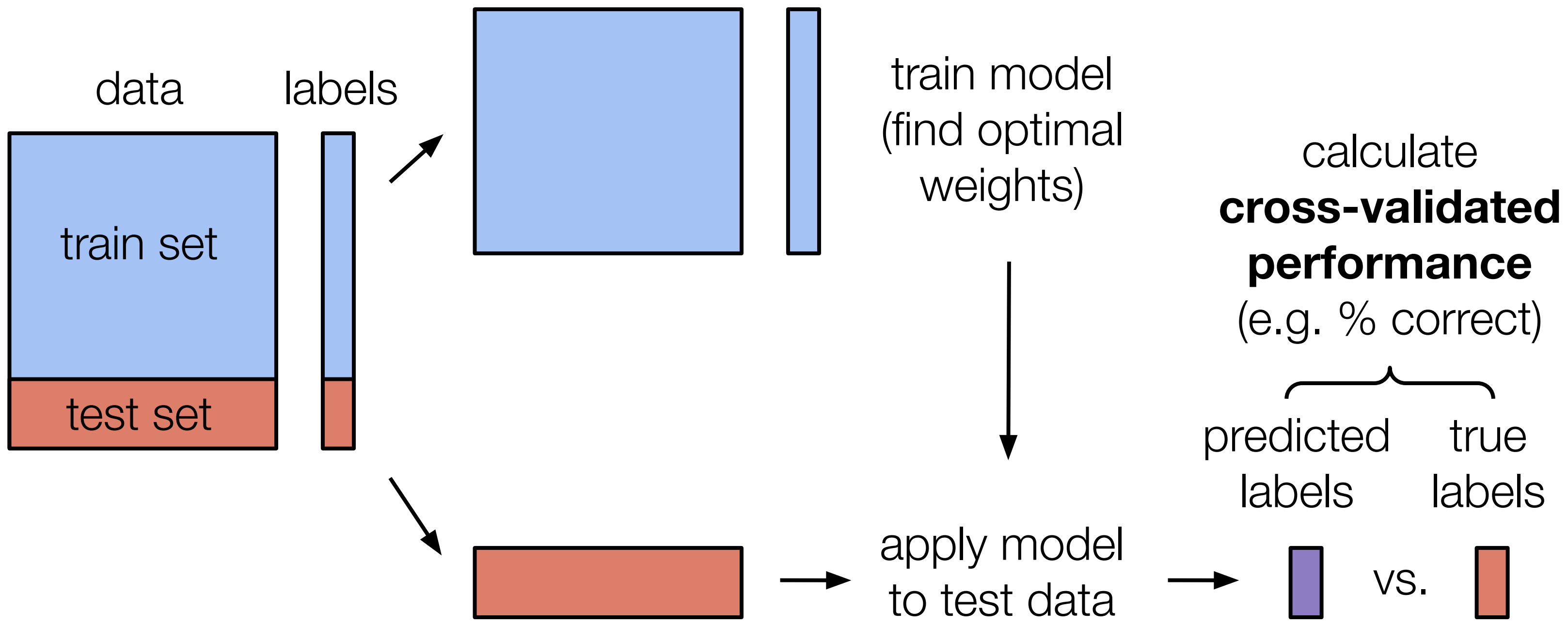

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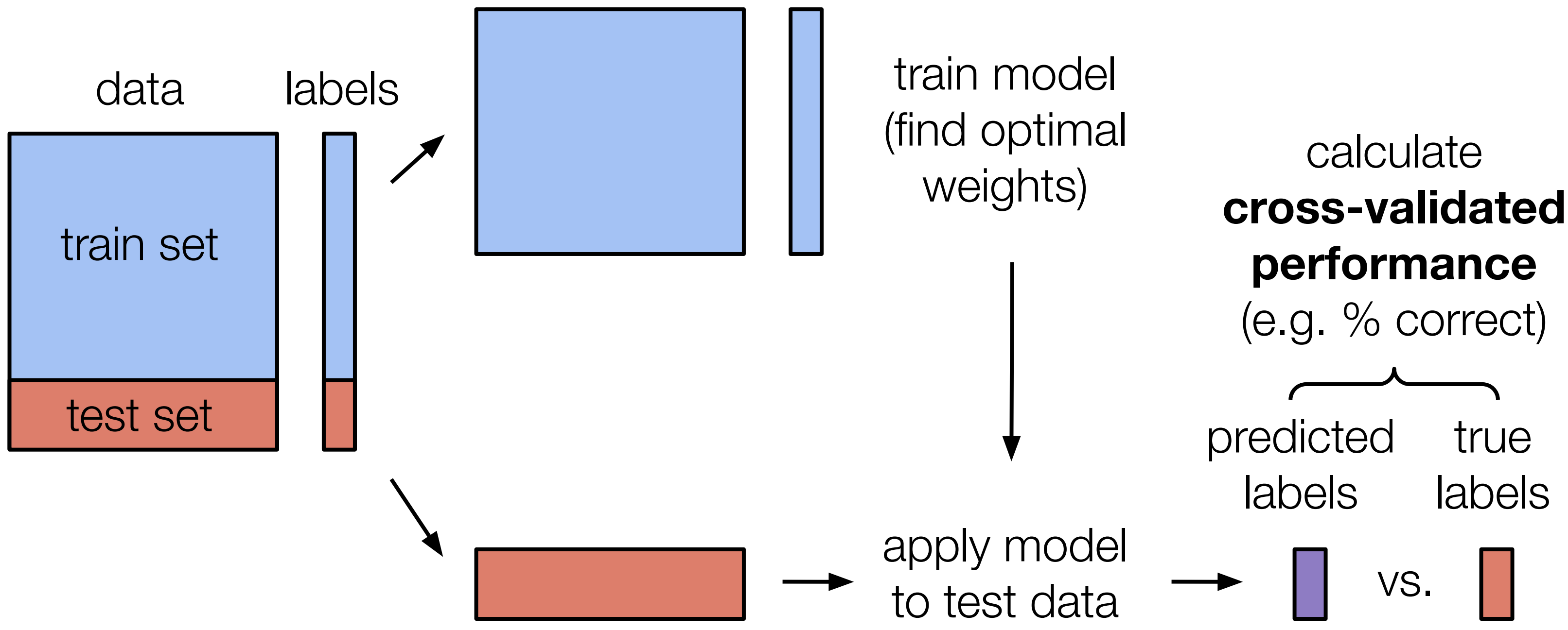

→ Repeat with many train/test splits. Is **perf. better than expected by chance**?

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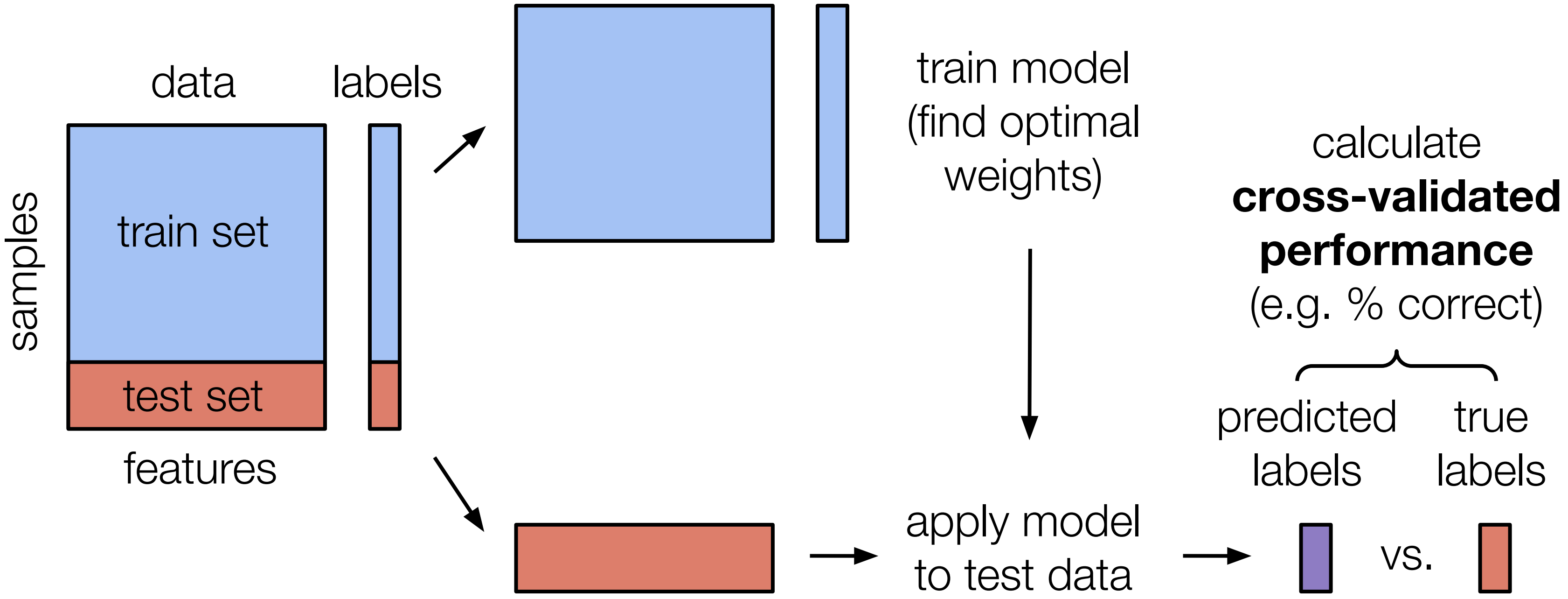
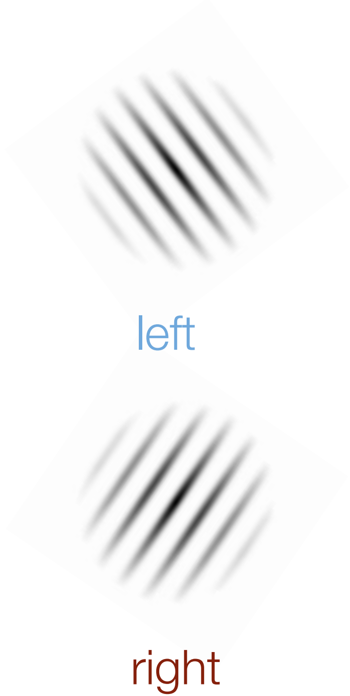
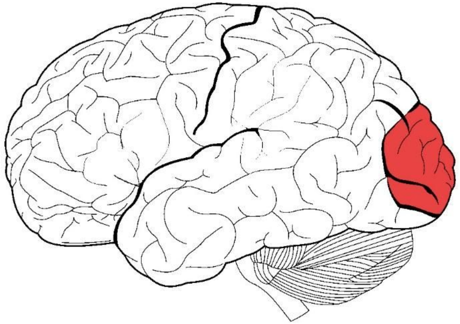


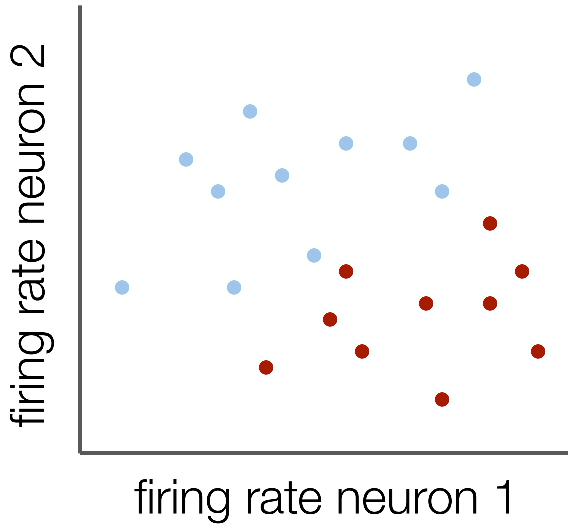
Classification: What can we learn about the brain?

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





recordings from V1



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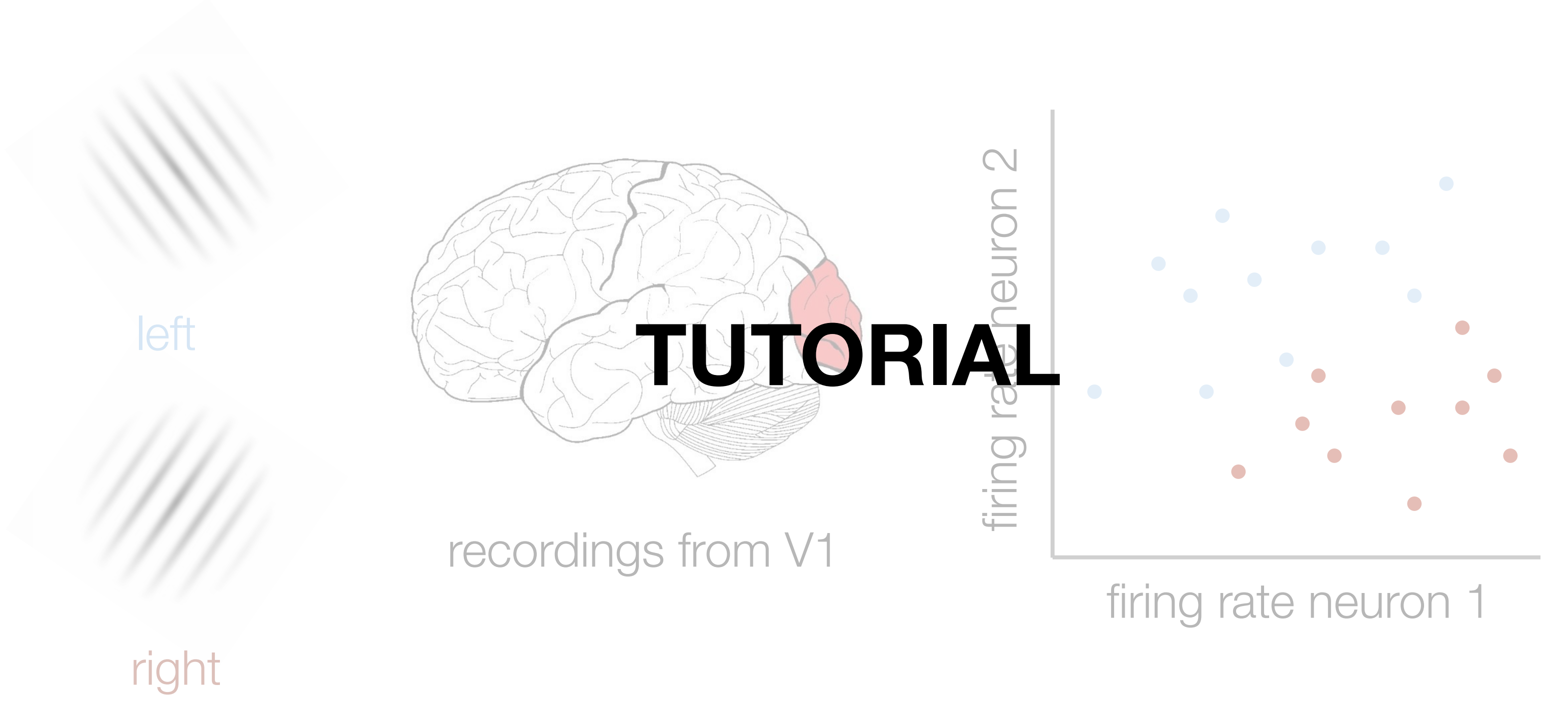
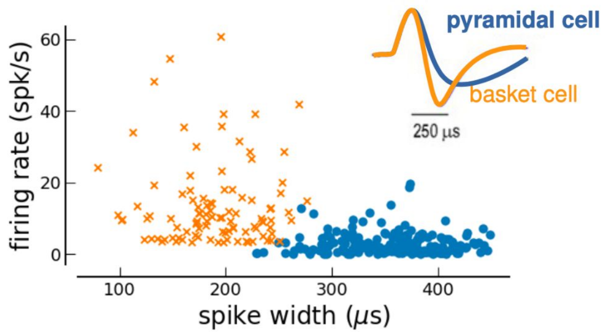


Classification and Clustering: Overview

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).



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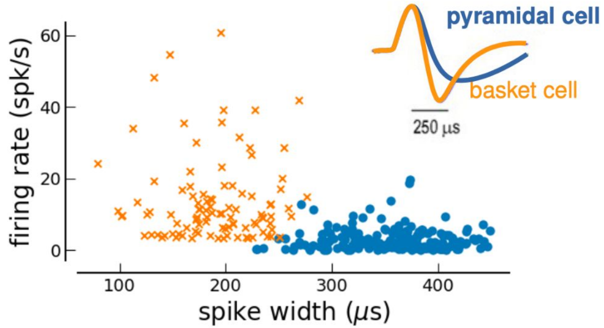
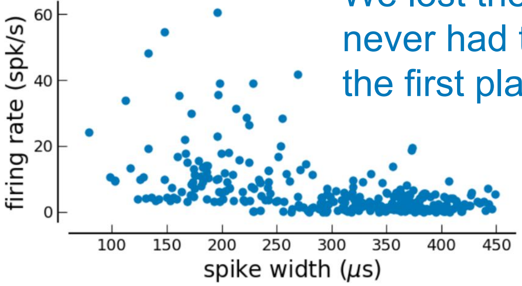
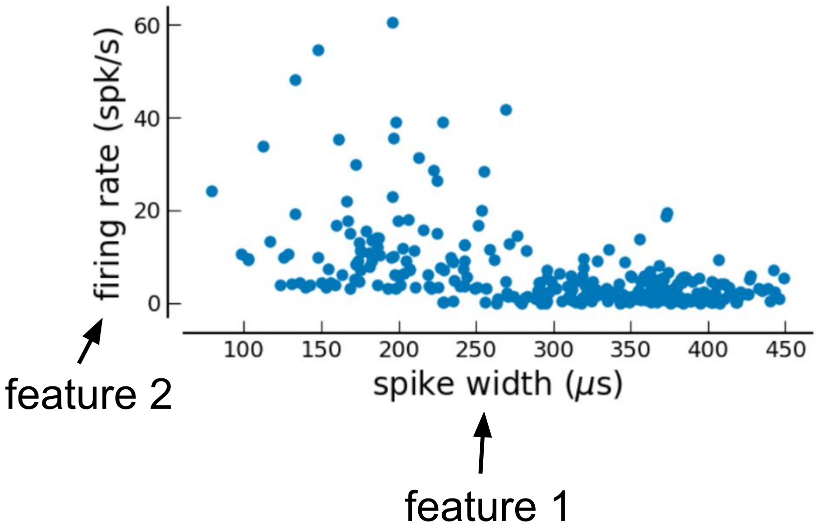
Clustering: We see **patterns** in the data that **suggest multiple categories**, but we don’t know which data point belongs to which category. Clustering is an “**unsupervised**” method (unknown ground truth).





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

Clustering: Guessing categories from patterns in the feature space

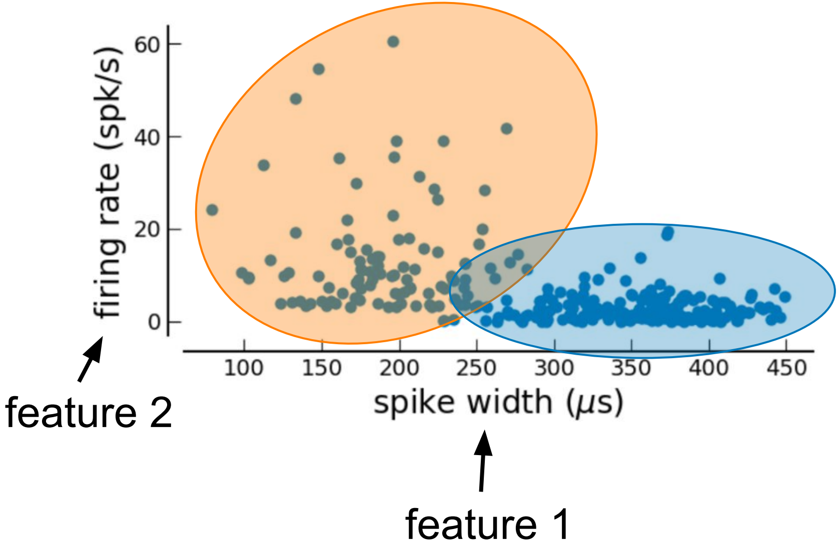


Let's assume that we know that there are two different cell types.

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**?

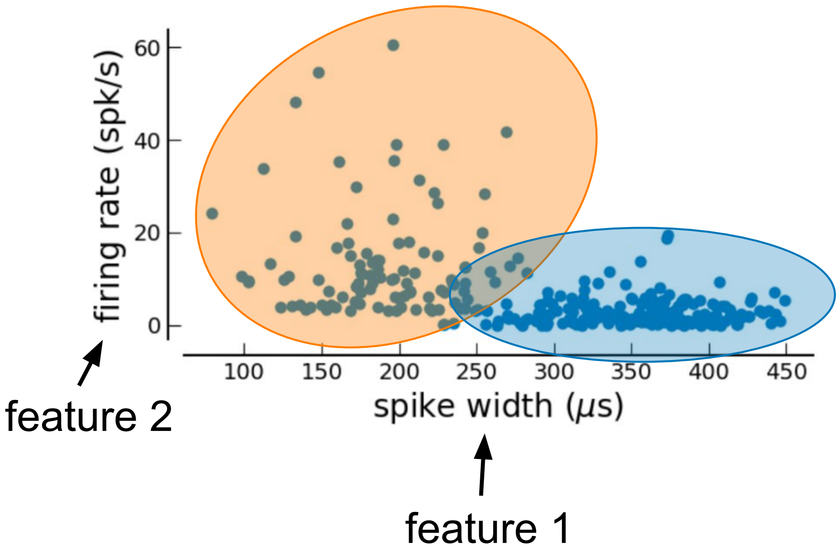
Clustering: Guessing categories from patterns in the feature space



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

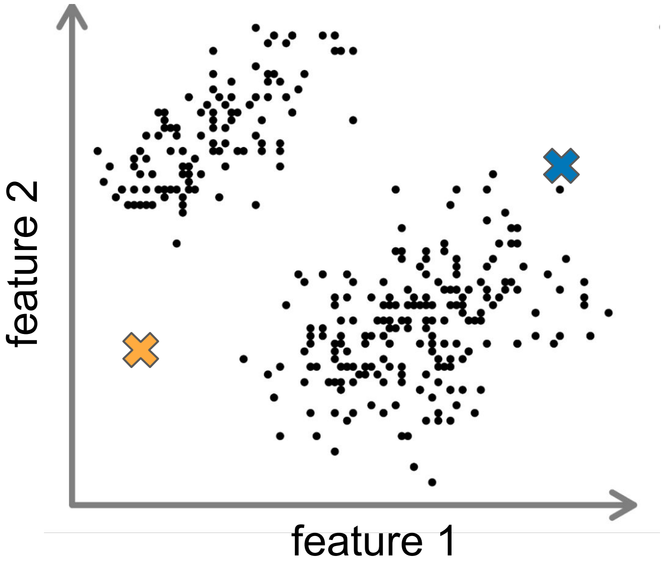


Can we guess which are the points belonging to one vs. the other class?

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

But how?

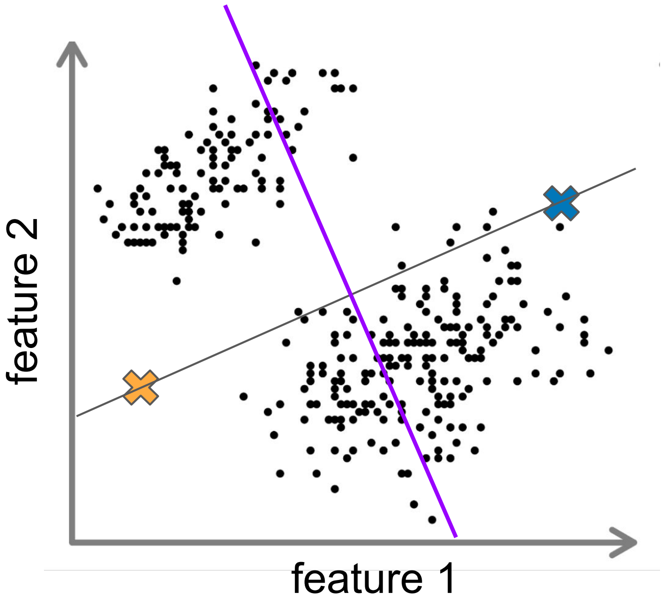
Clustering: k-means



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

1. Pick two random values (“initialization”).

Clustering: k-means



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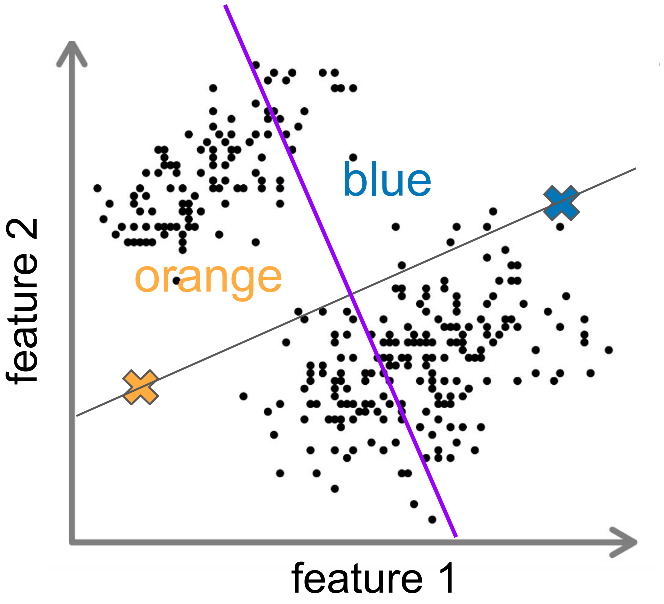

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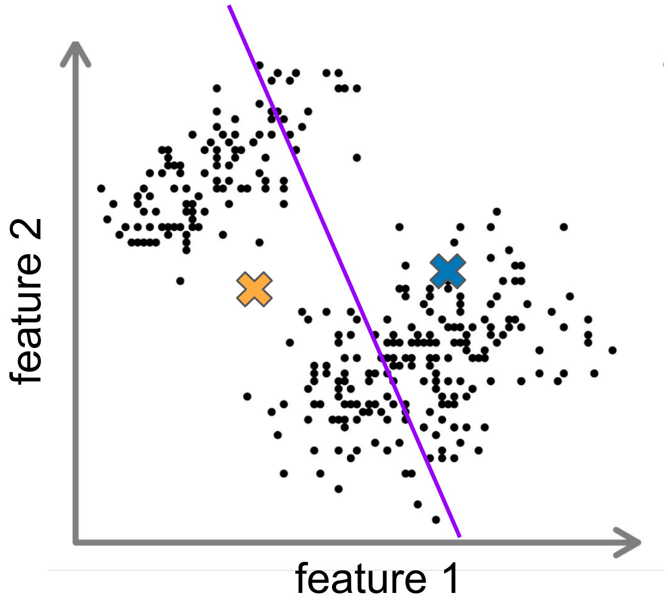

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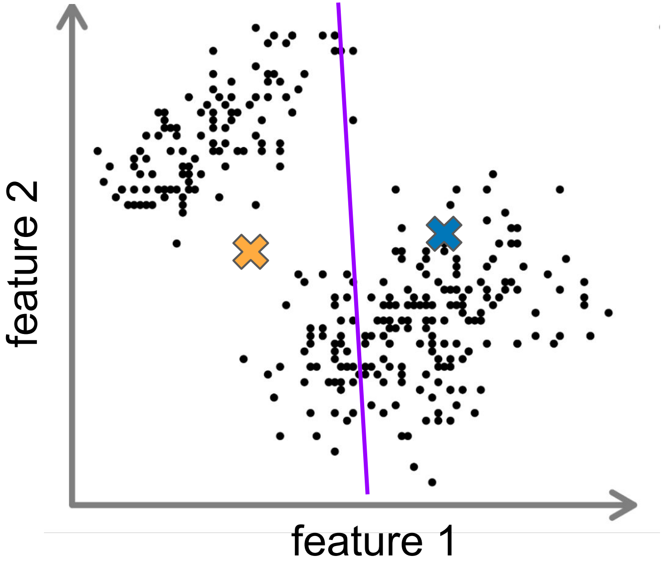
3. Recalculate cluster means

Clustering: k-means



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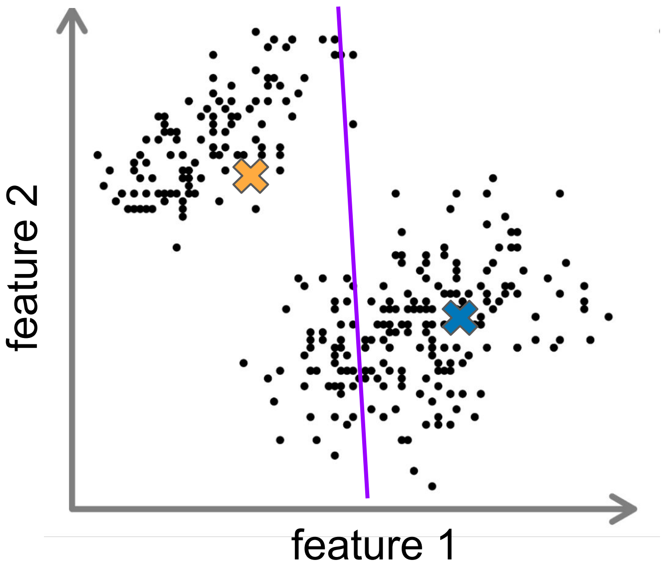

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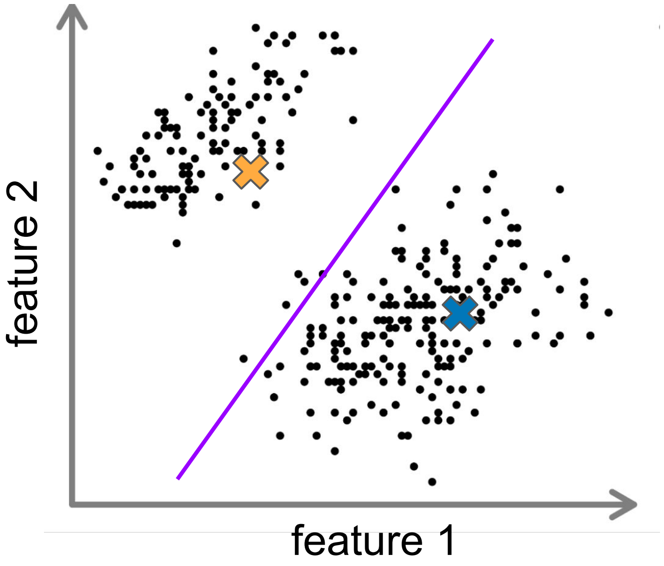

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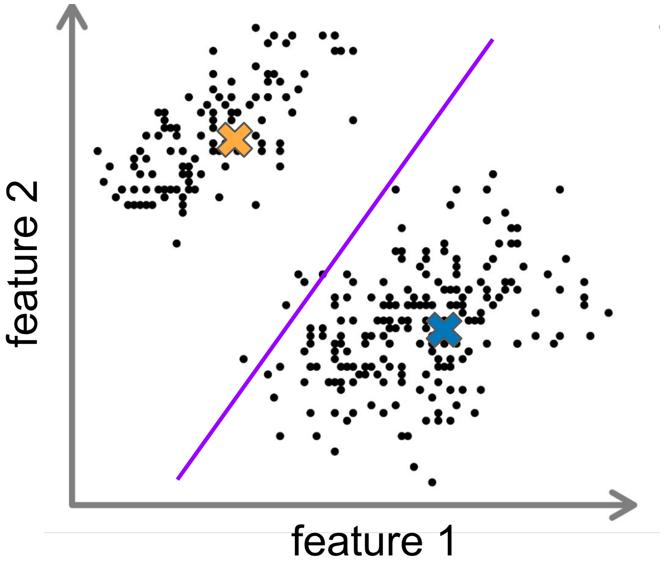

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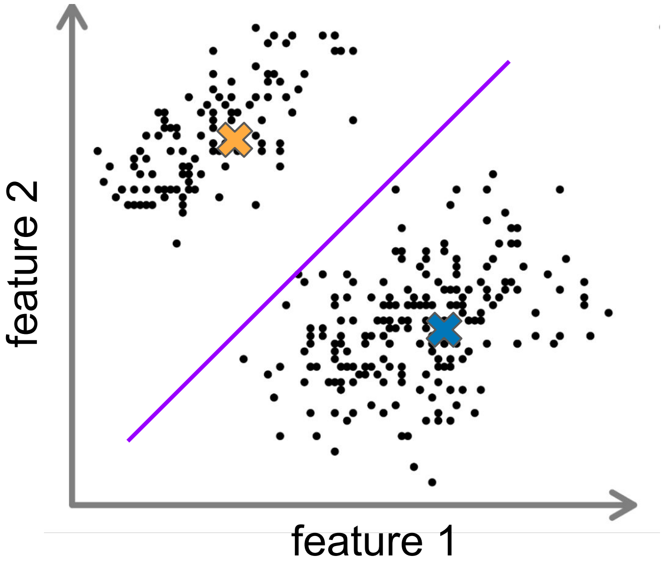

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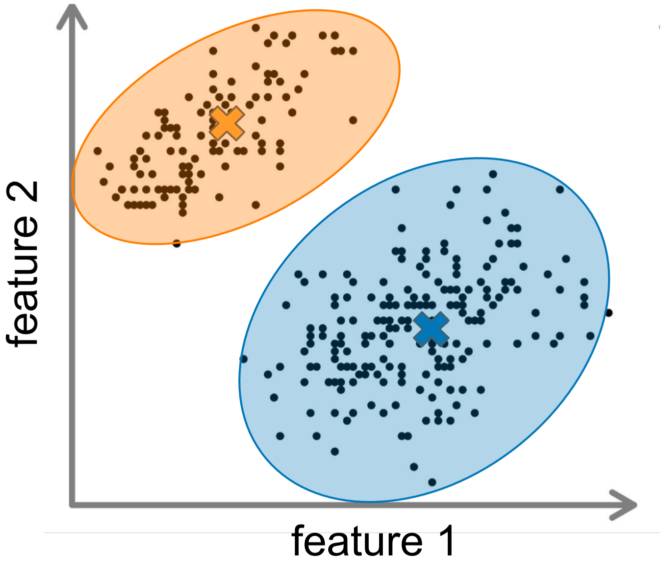

Assuming two clusters, we try to find
k = 2 cluster means (“centroids”).

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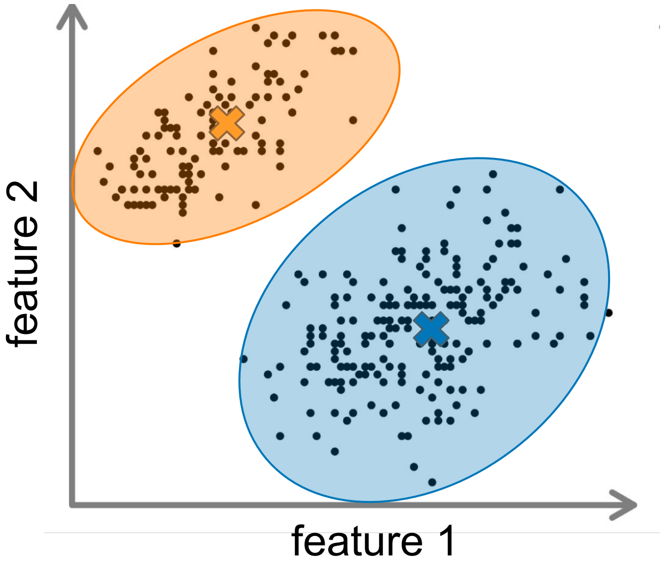
3. Recalculate cluster means.

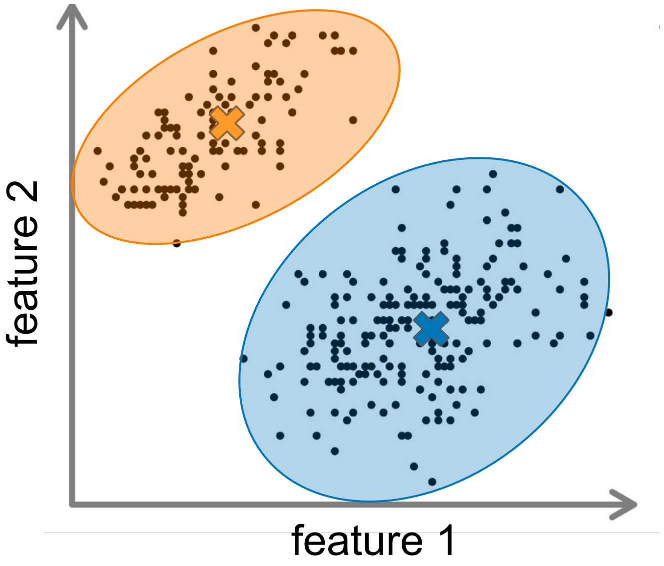
Repeat 2.-3. until cluster means are stable (they “converged”).

Clustering: k-means



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

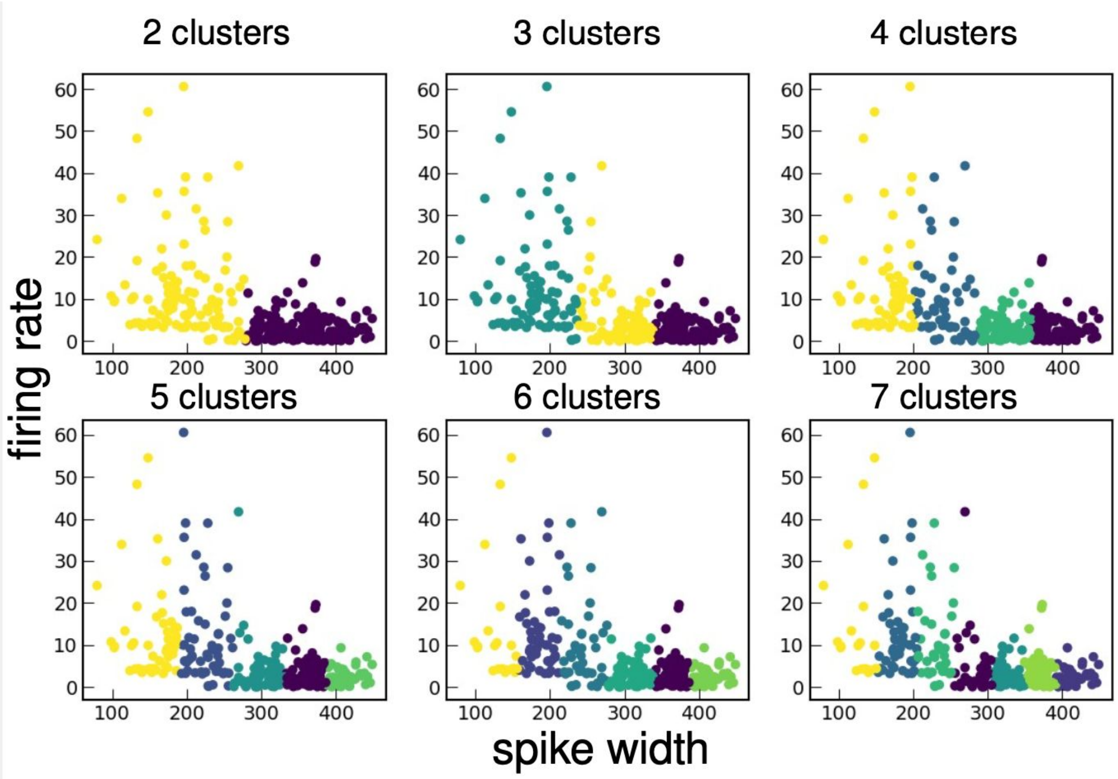
Clustering: k-means



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 = ?)



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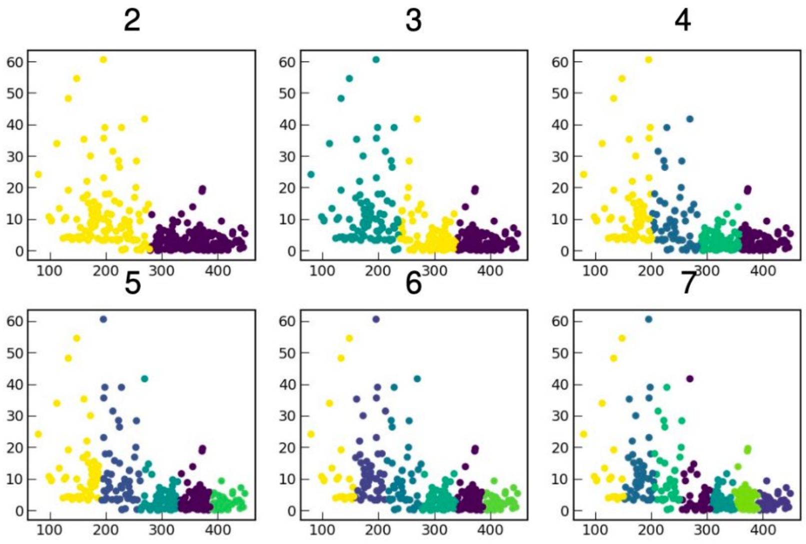
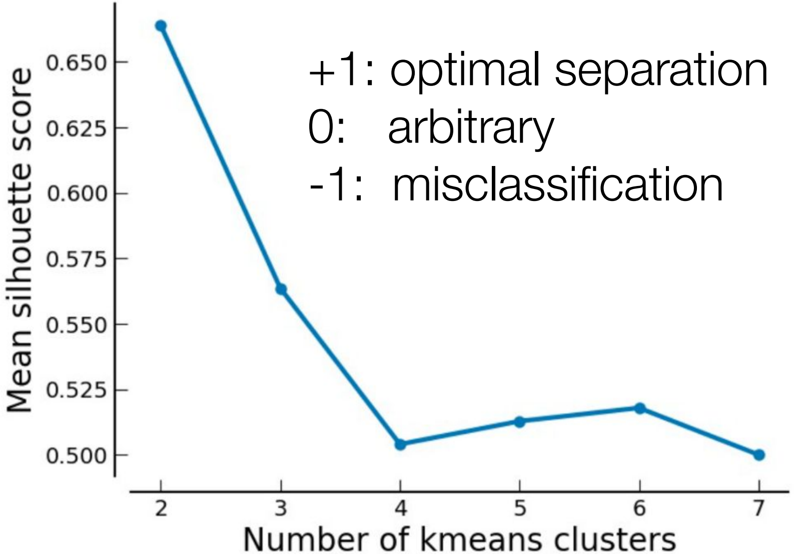


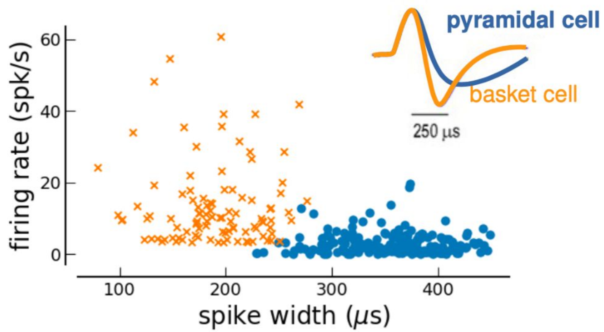


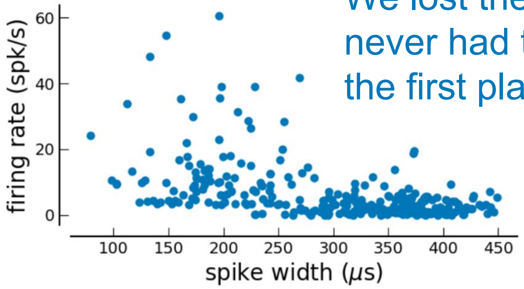
The **Silhouette score** for each point measures the distance to points in the same cluster vs. to points in the neighboring cluster

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