Classification and clustering

Neural data science with Python

Heike Stein
17/11/2025

Classification and Clustering: Overview

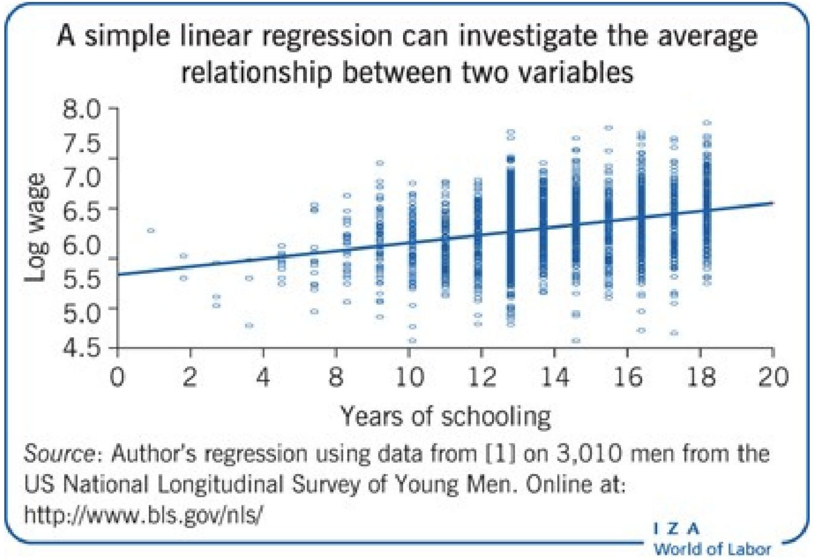
Classification

- Logistic regression
- Support vector machines

Clustering

- k-means

Regression analysis

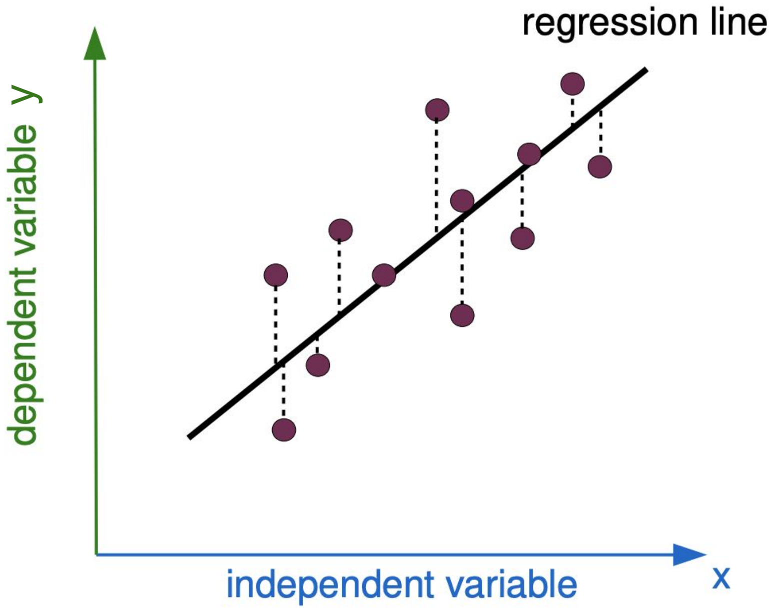

A simple linear regression can investigate the average relationship between two variables

Source: Author's regression using data from [1] on 3,010 men from the US National Longitudinal Survey of Young Men. Online at: http://www.bls.gov/nls/

I Z A World of Labor

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

Regression analysis



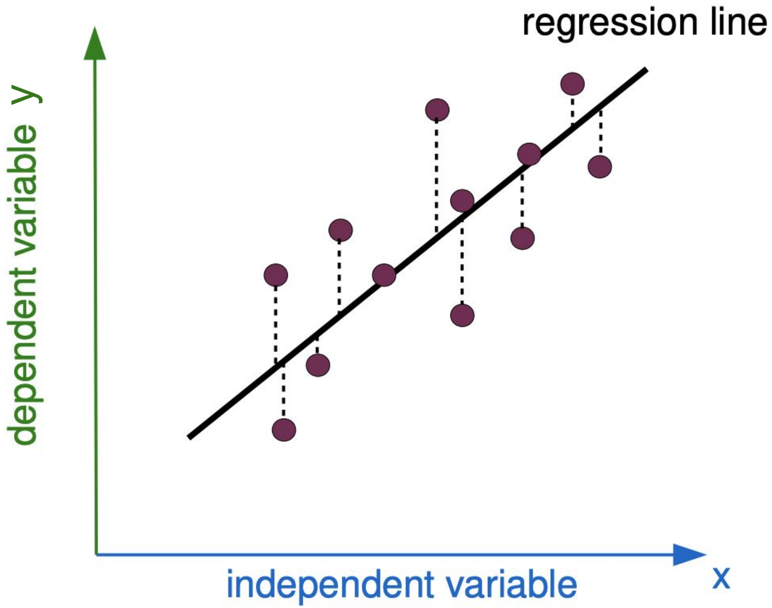
→ linear mapping from predictor (“independent”) variable(s) x (e.g. years of schooling) to outcome (“dependent”) variable y (e.g. wage)

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

weights (“parameters”)

errors (“residuals”)

Regression analysis



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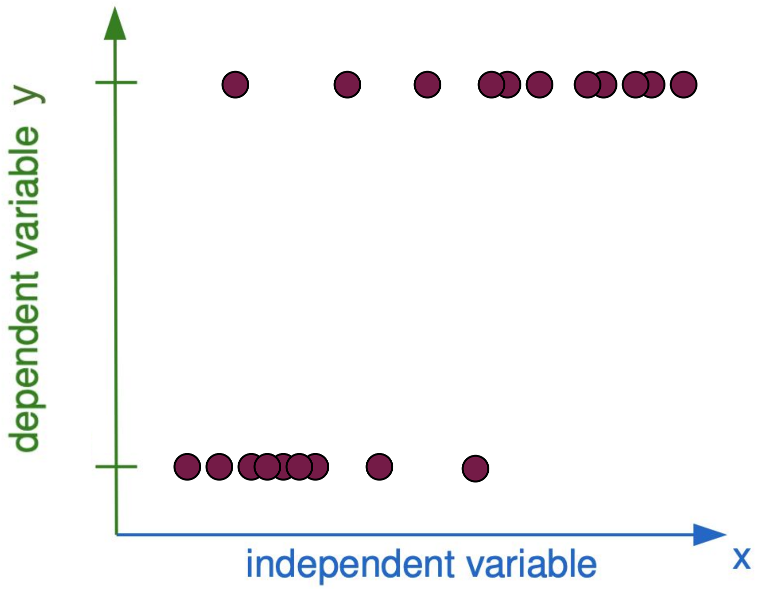
$$y = \boxed{\beta_0} + \boxed{\beta_1} x_1 + \boxed{\varepsilon}$$

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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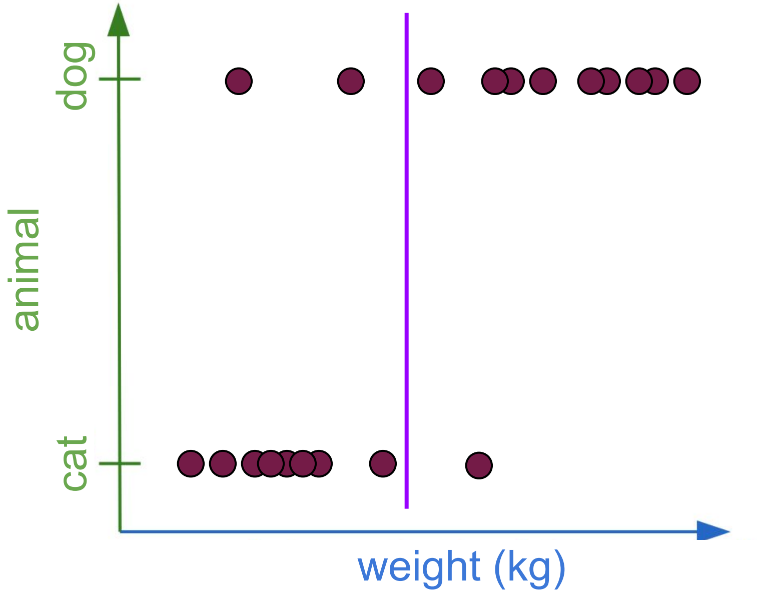
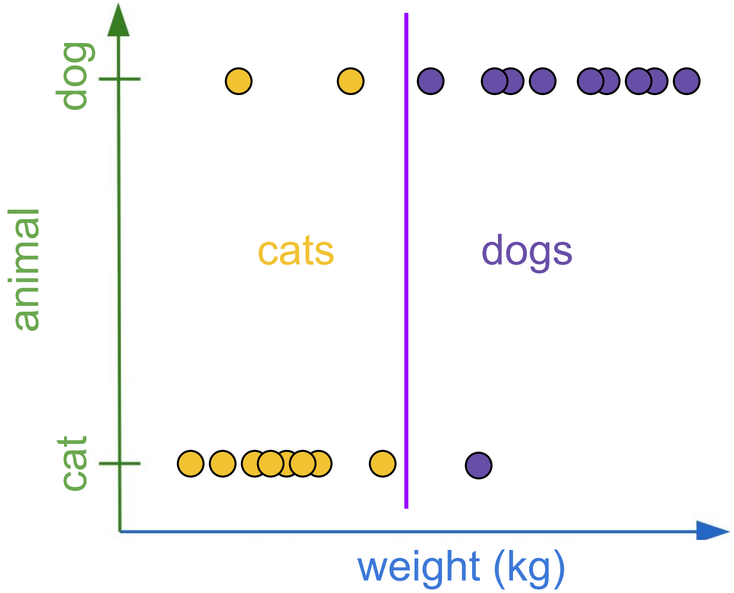


Given knowledge of x, what is the most likely category of y?

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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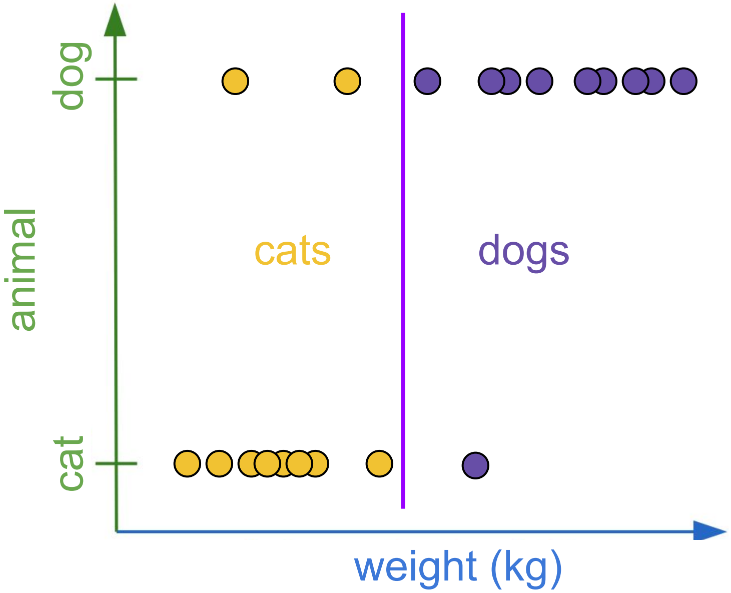
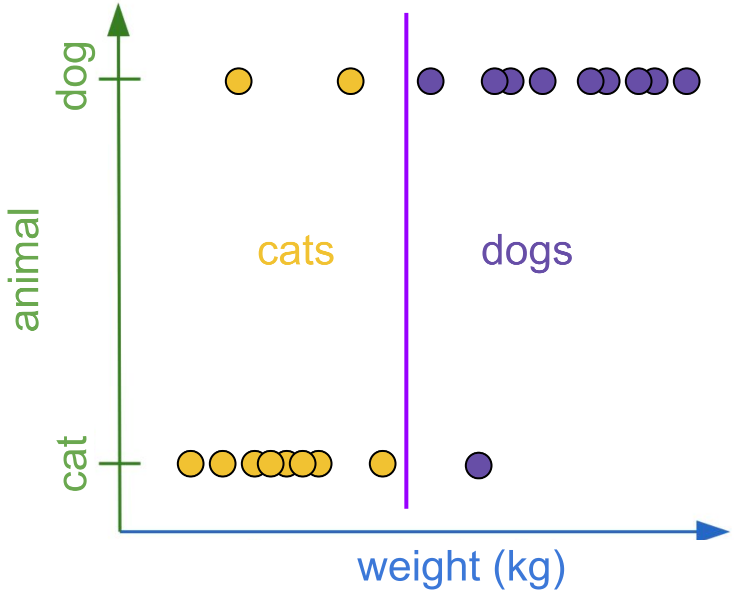


How do we find a good decision boundary?

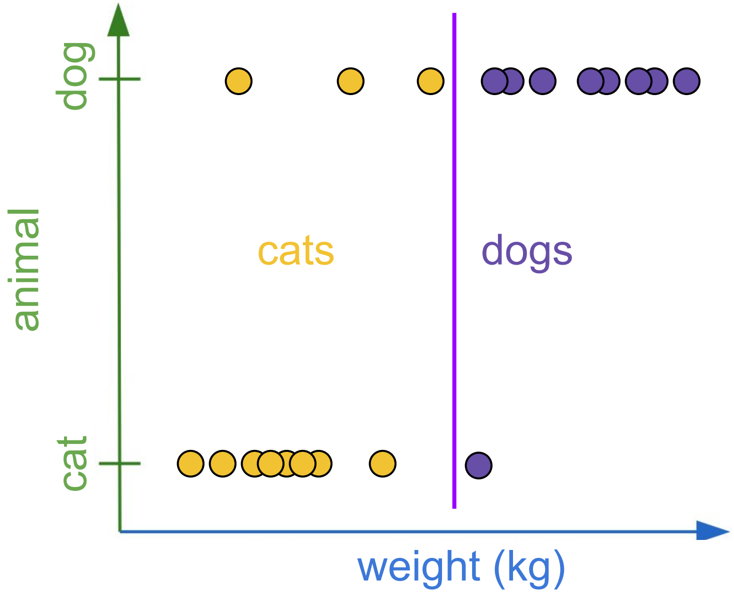
Classification: Predicting categorical values



How do we find a good decision boundary?

It should minimize the number of misclassifications.

Classification: Predicting categorical values



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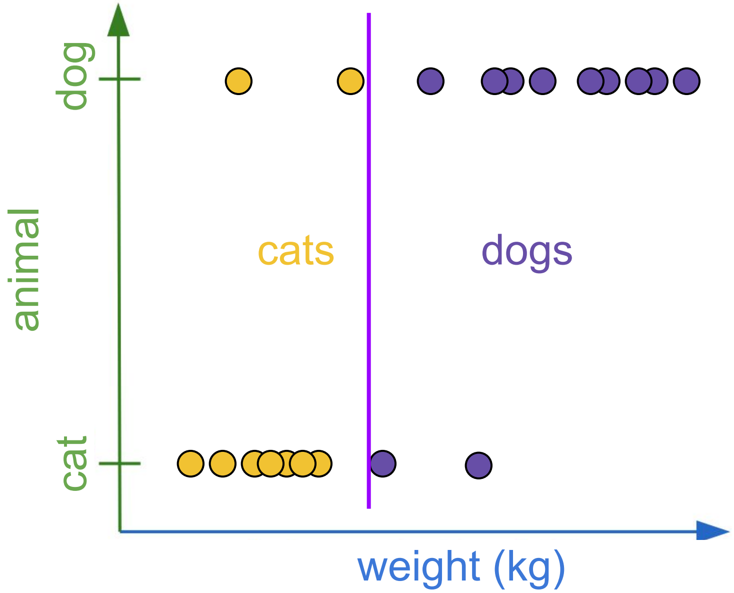

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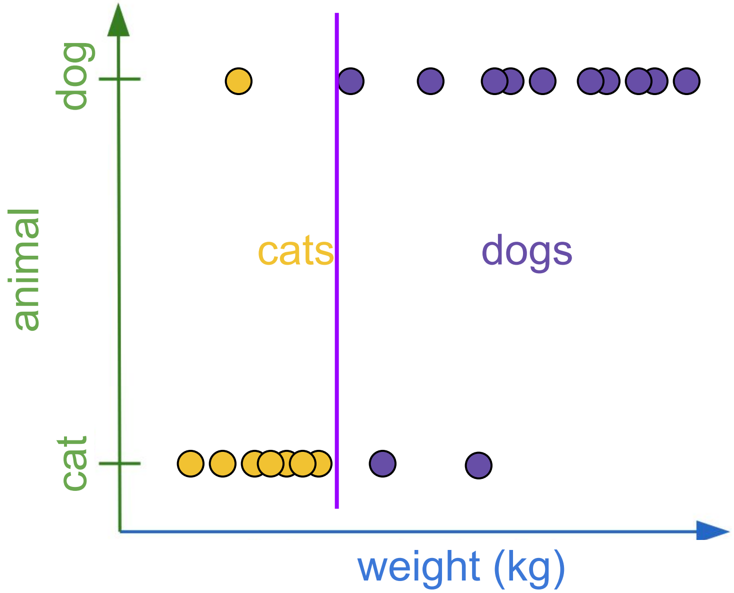

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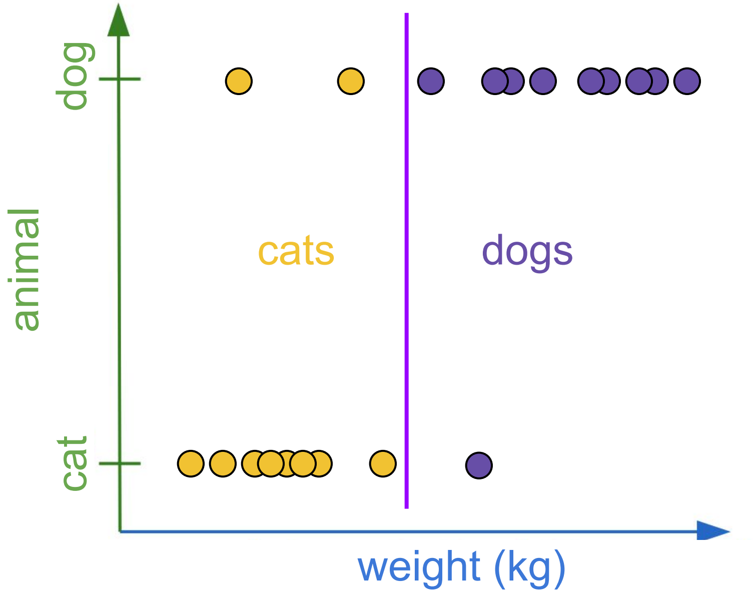


How do we find a good decision boundary?

It should minimize the number of misclassifications.

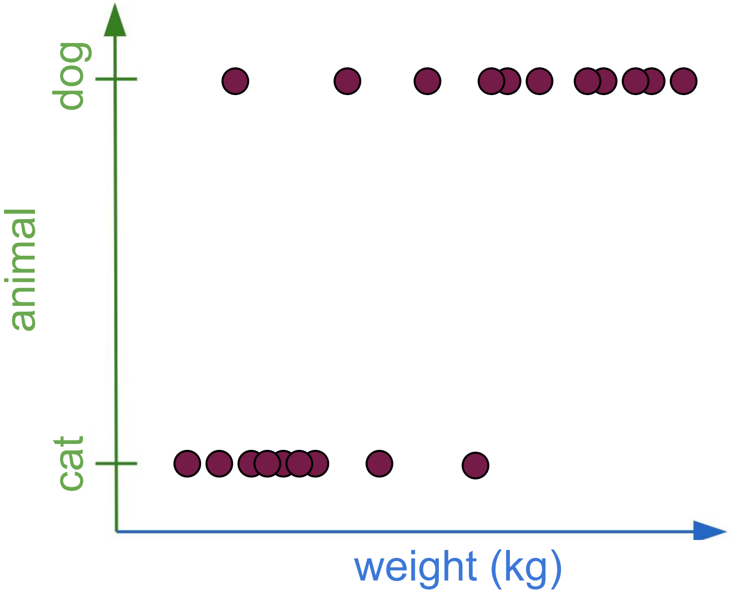
Which solution is found depends on the classification method.

Classification and Clustering: Overview

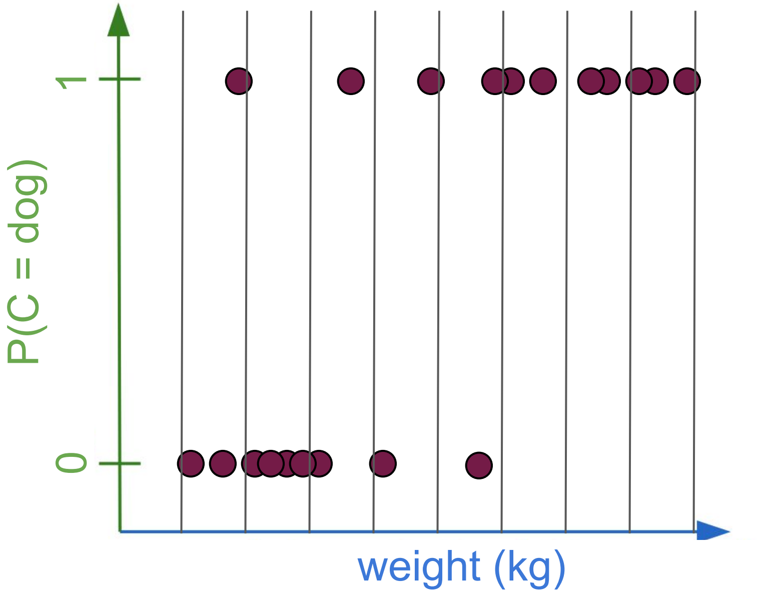
Classification

1. Logistic regression
2. Support vector machines

Classification: Logistic regression

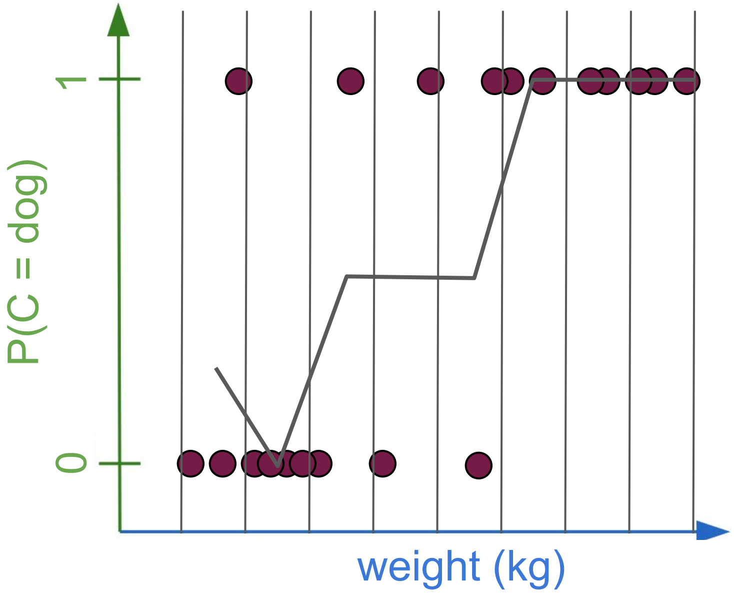


Classification: Logistic regression



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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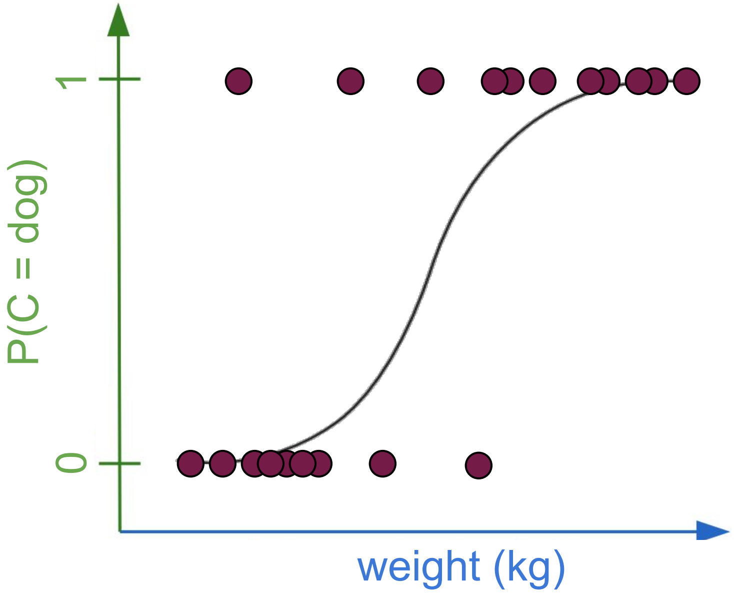
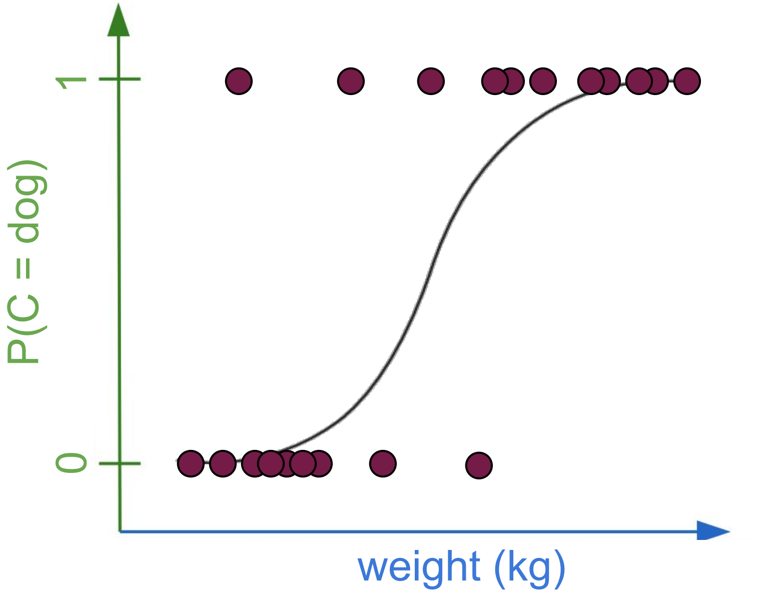


Logistic regression fits the weights of a generalized linear model:

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

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

Classification: Logistic regression



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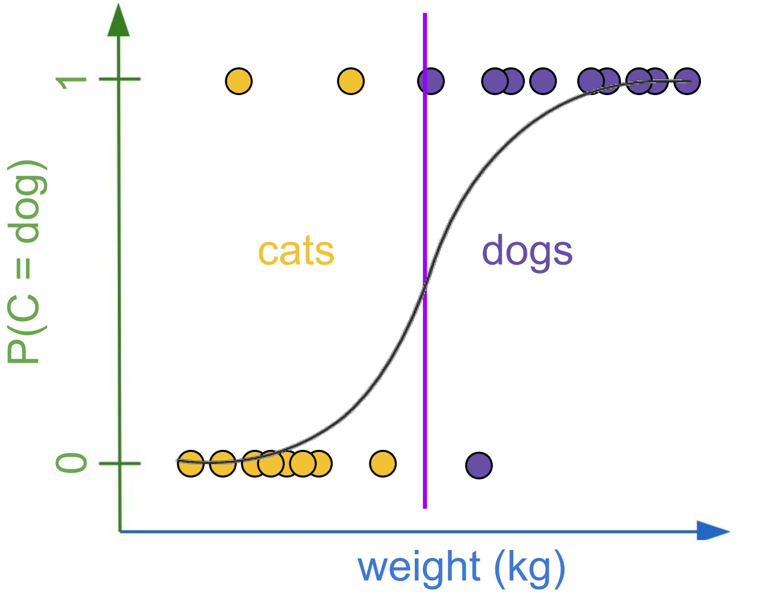
$$\Leftrightarrow \quad P(C = \text{"dog"}) = \frac{e^{(\beta_0 + \beta_1 x_1)}}{1 + e^{(\beta_0 + \beta_1 x_1)}}$$

Classification: Logistic regression



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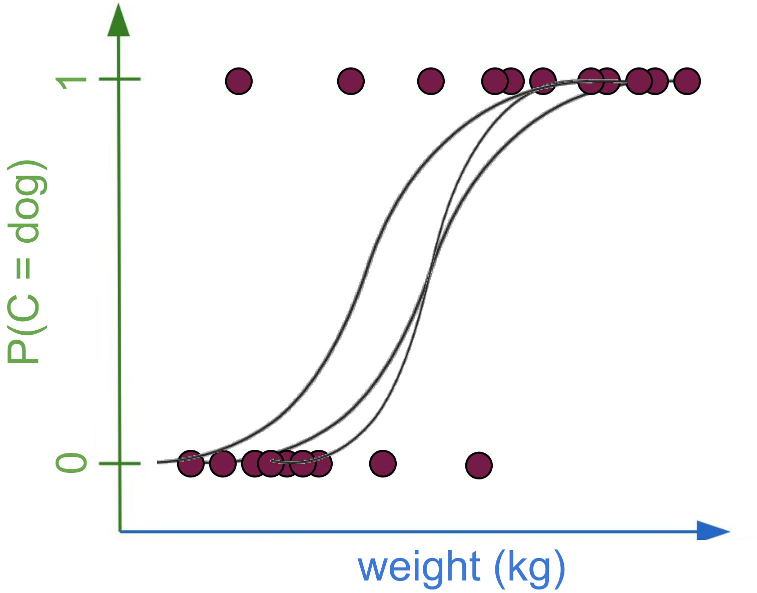
$$P(C = \text{"dog"}) = f(\beta_0 + \beta_1 x_1)$$

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

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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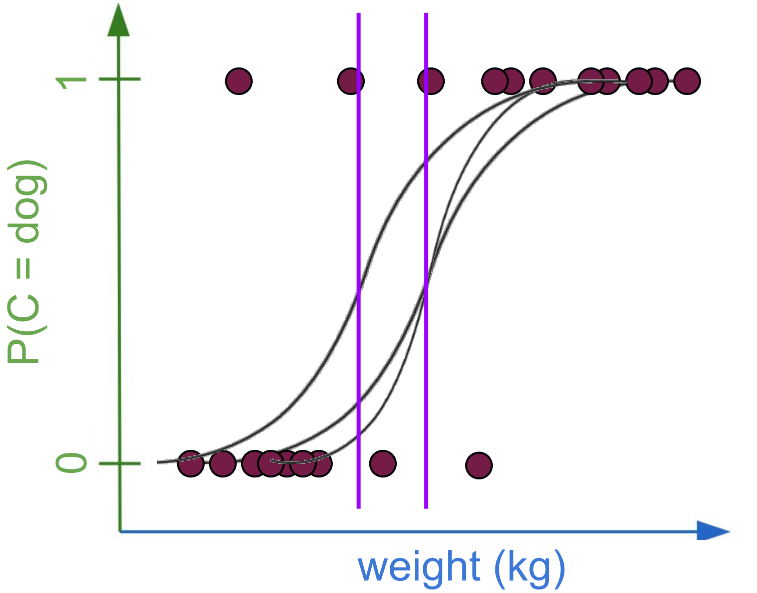

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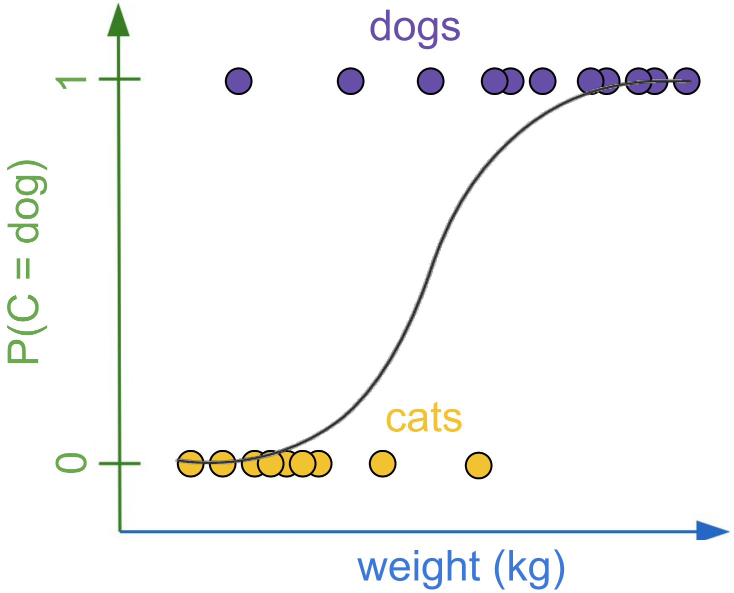
Weights affect slope and x-offset of the sigmoidal function. They thereby affect the decision boundary.

Classification: Logistic regression



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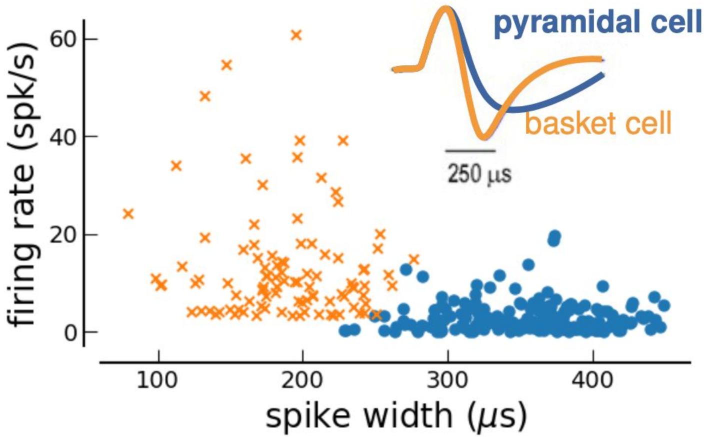
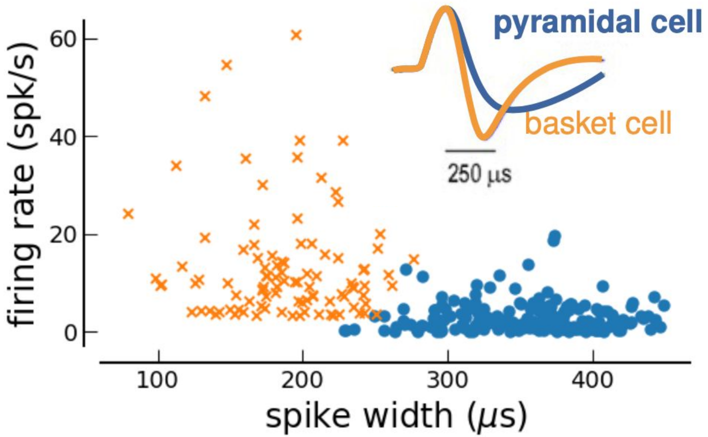
Weights are fitted by minimizing an error function between P(C = dog) and true labels: t = 1 if dog, t = 0 if cat

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



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"))?

Logistic regression fits the weights of a generalized linear model:

$$P(C = \text{"basket cell"}) = f(\boxed{\beta_0} + \boxed{\beta_1} x_1 + \boxed{\beta_2} x_2)$$

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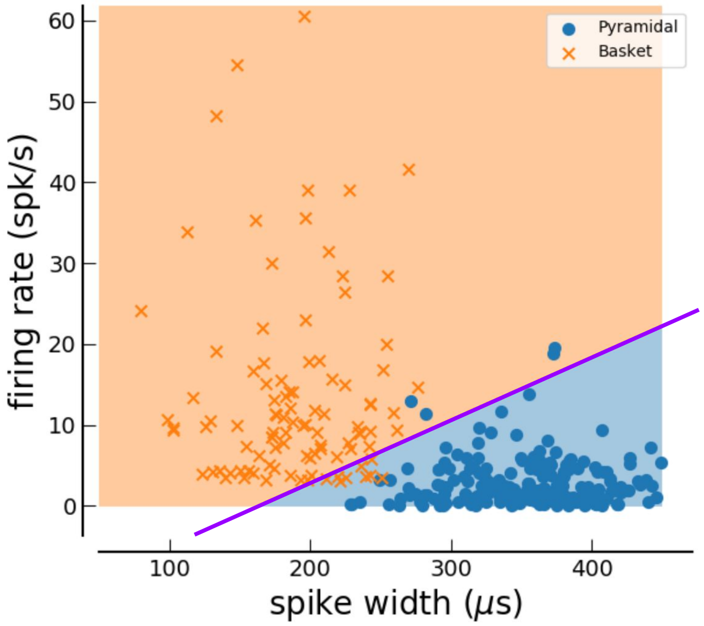

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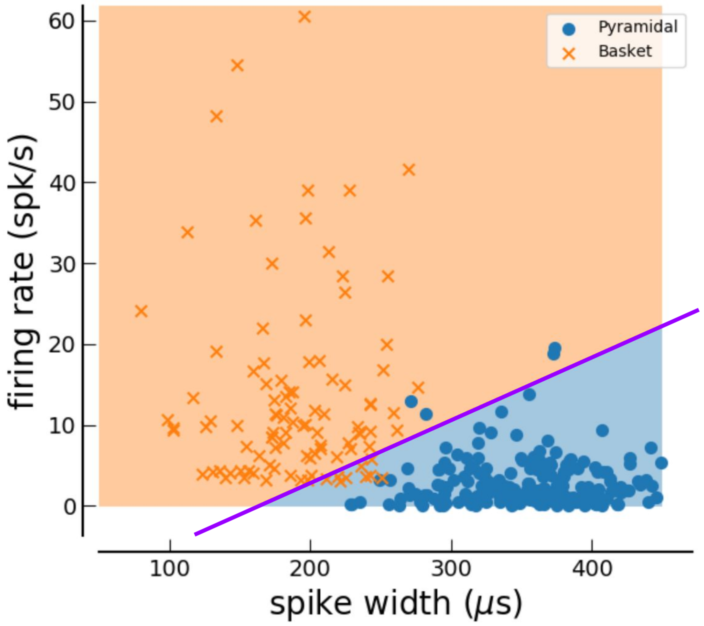
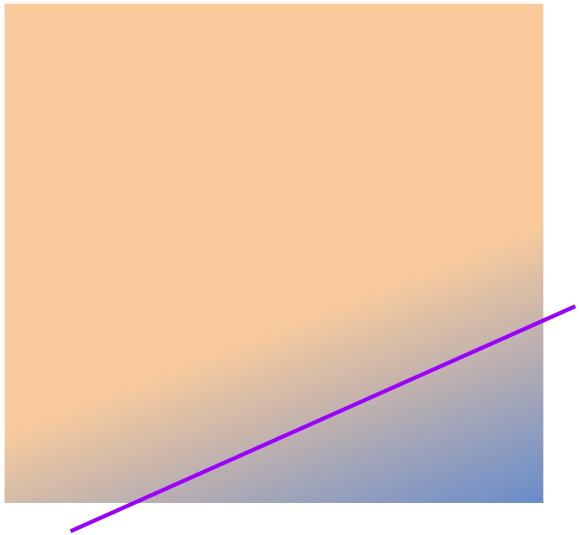
The decision boundary is now a 1D line in the 2D space for which P(C = “basket cell”) = 0.5

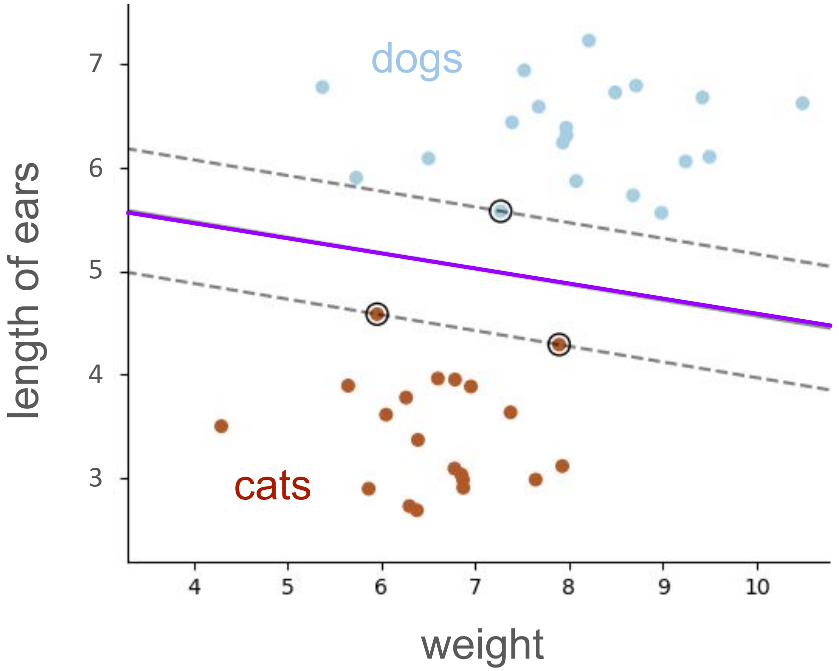
Classification: Logistic regression in 2D



Sigmoidal function in 2D

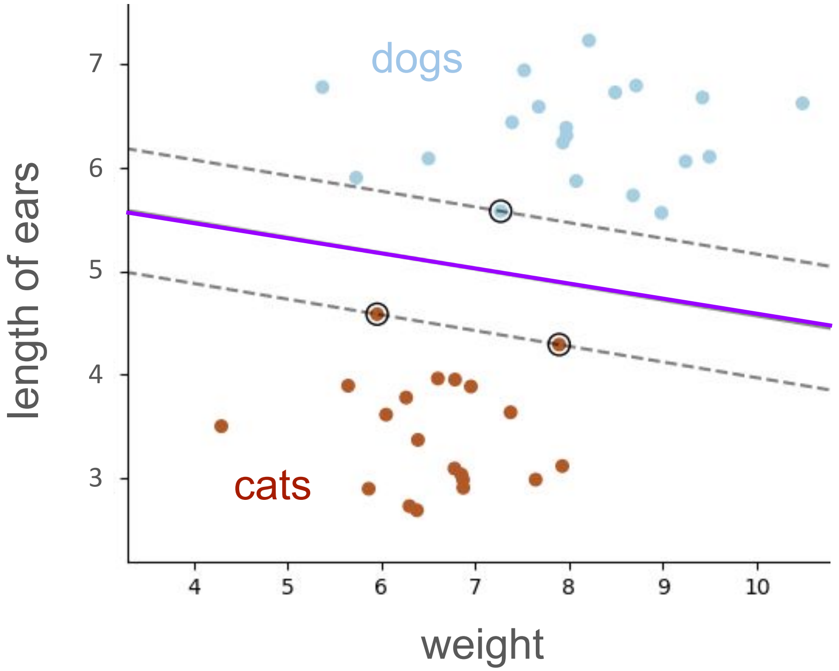


Classification: Support vector machines (SVM)



Again, we're looking for a decision boundary

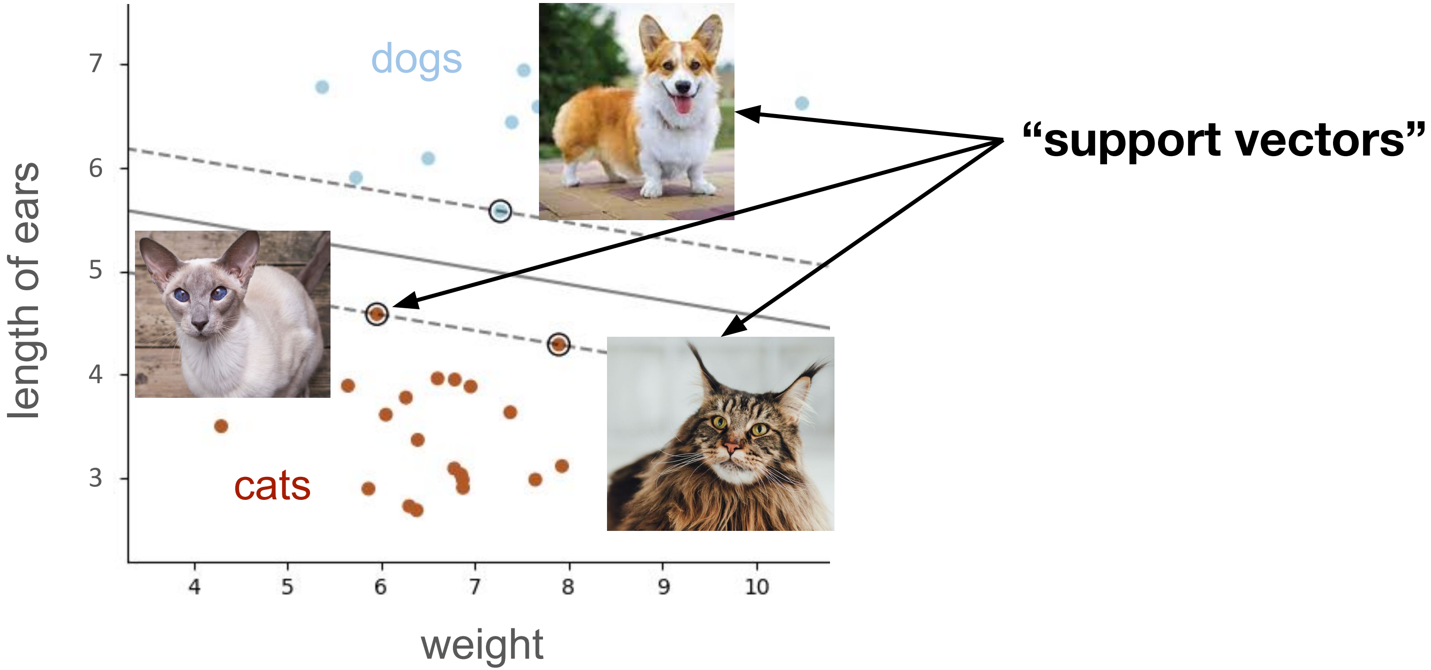
Classification: Support vector machines (SVM)



Again, we're looking for a decision boundary

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

Classification: Support vector machines (SVM)



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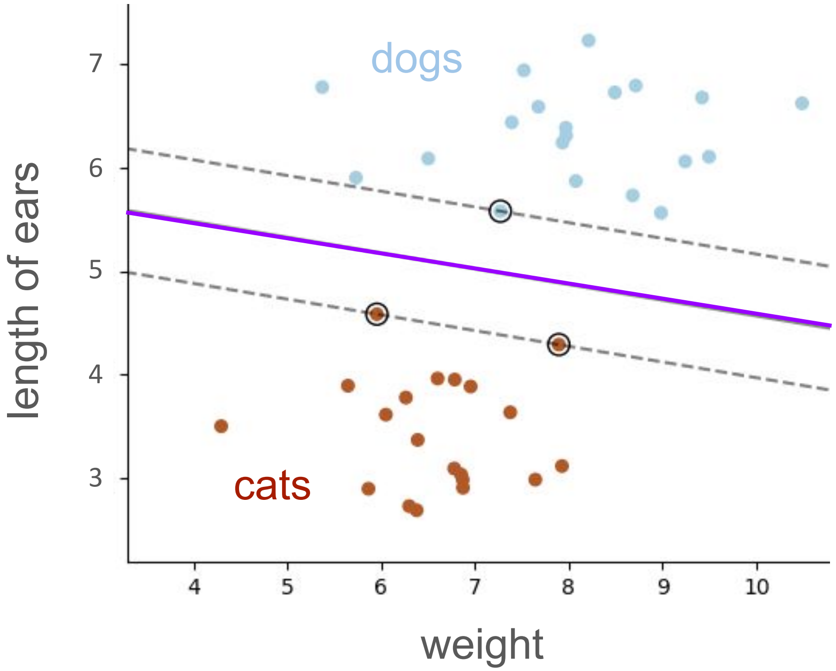
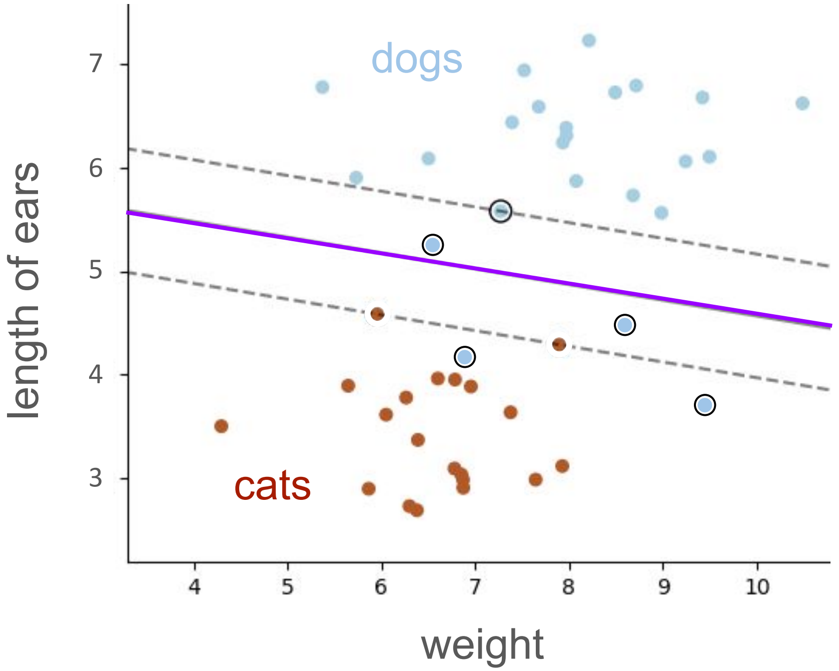


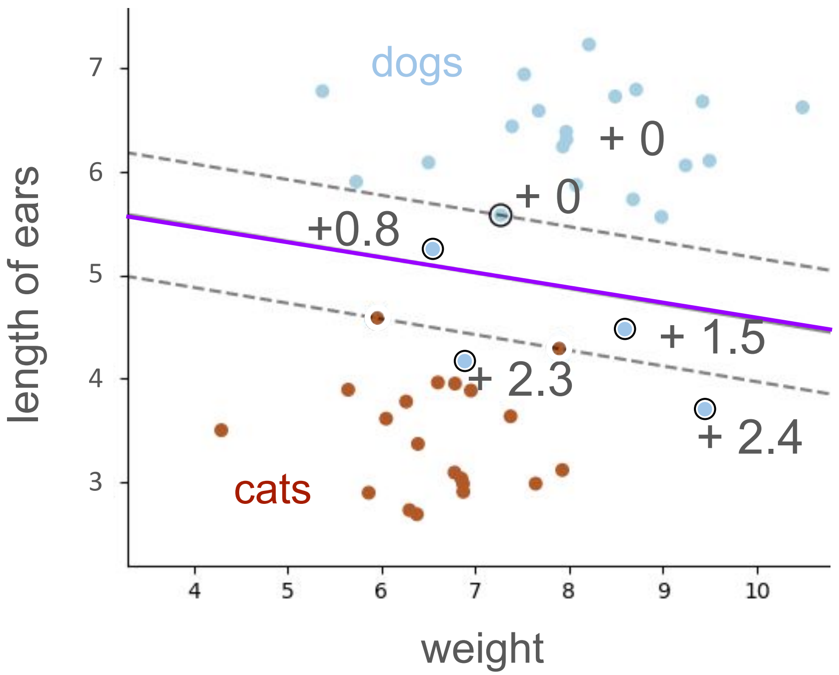
The decision boundary is the line that is equally far away from “support vectors” of each class

Classification: Support vector machines (SVM)



What to do if classes are not separable?

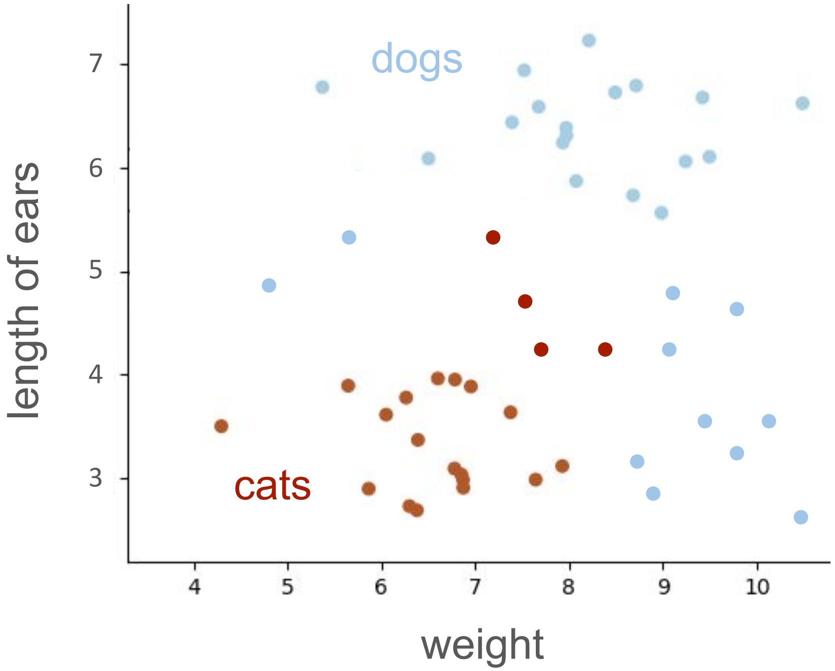
Classification: Support vector machines (SVM)



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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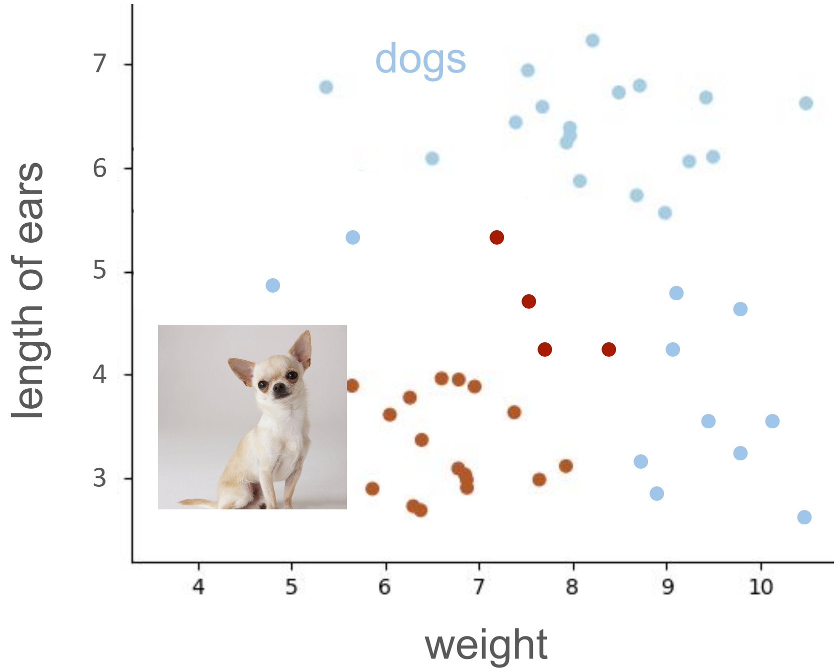

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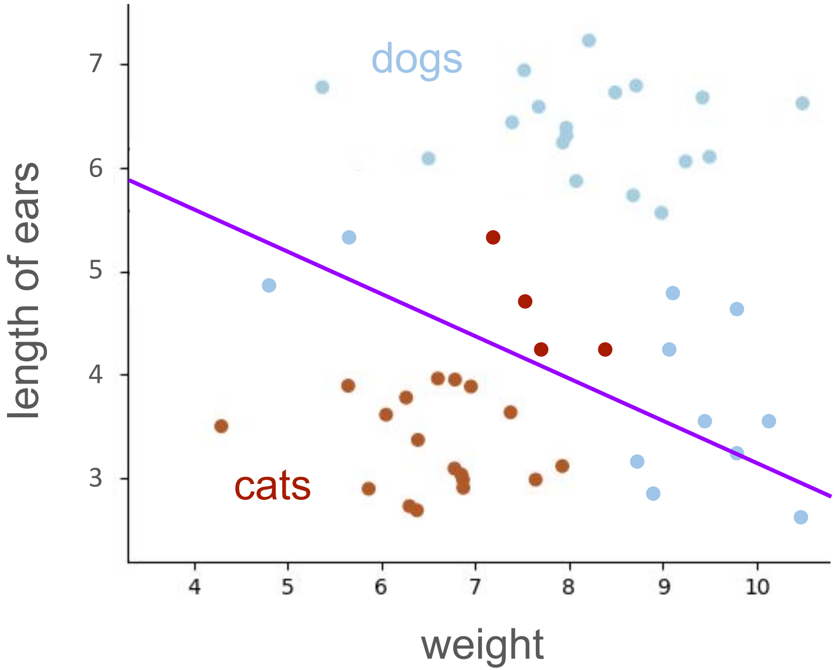
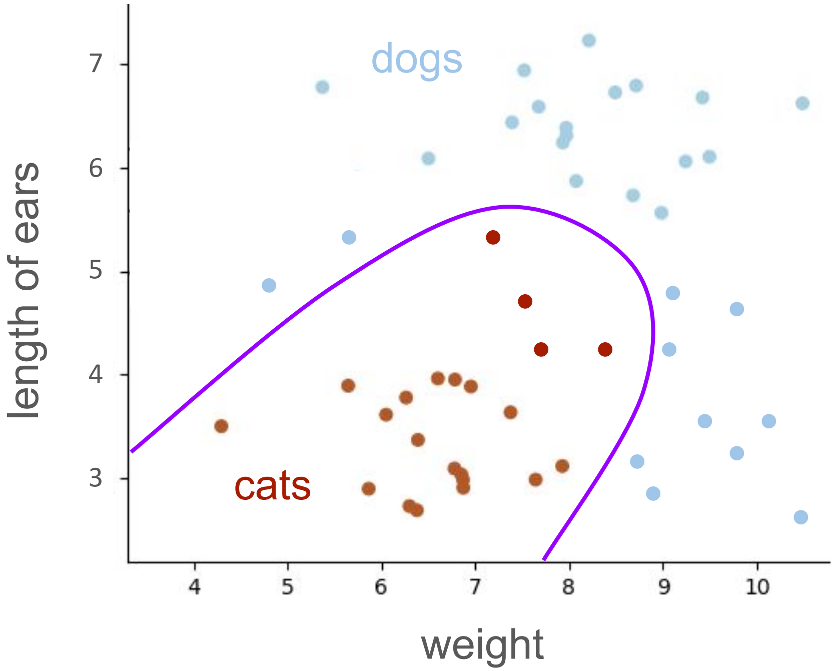


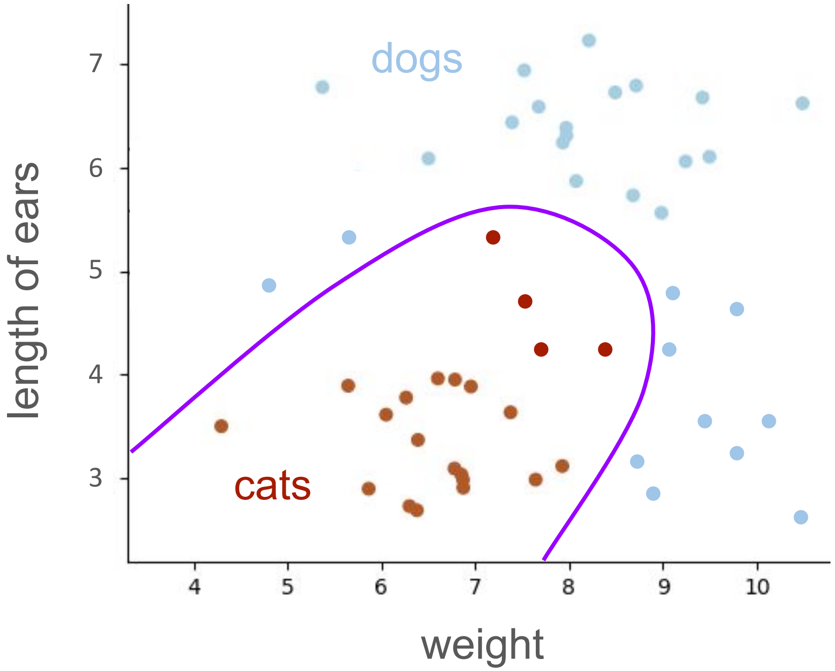
Some problems are not linearly separable

Classification: Support vector machines (SVM)



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

Classification: Support vector machines (SVM)



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

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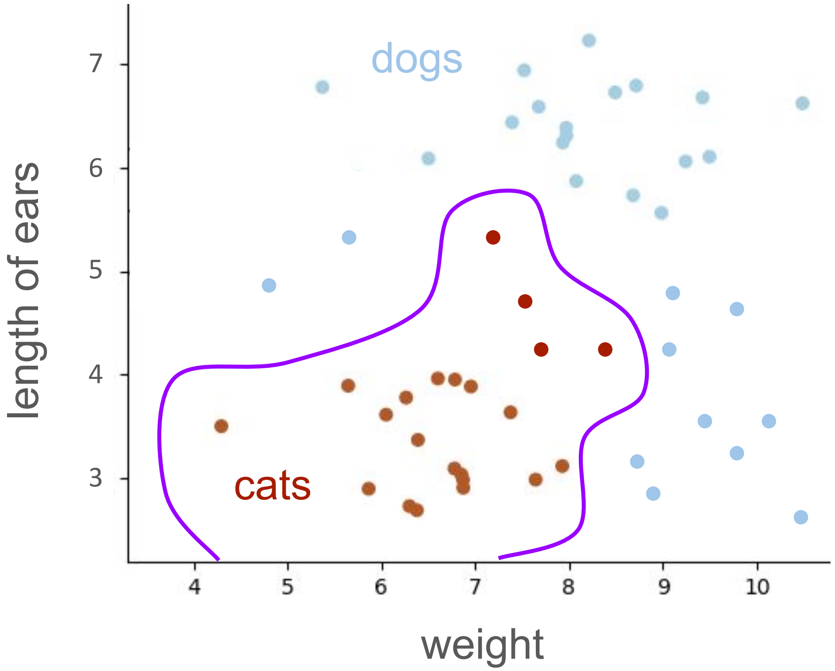

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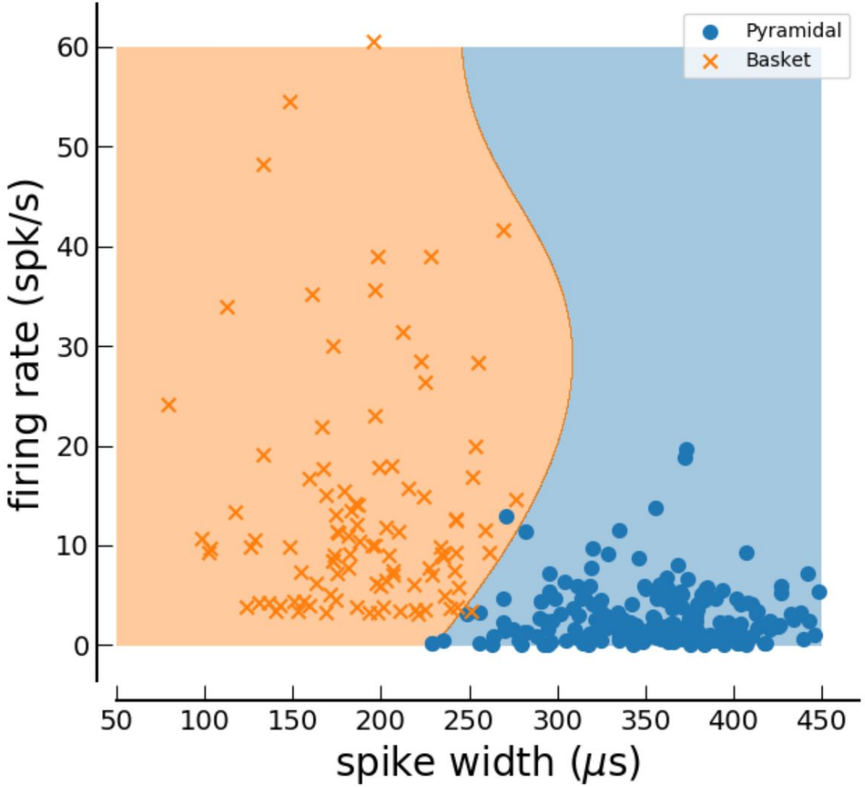
E.g. polynomial kernels of increasing degree create increasing nonlinearity.

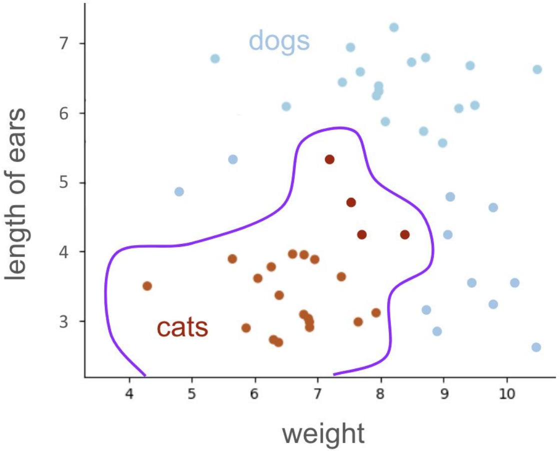
Classification: Support vector machines (SVM)



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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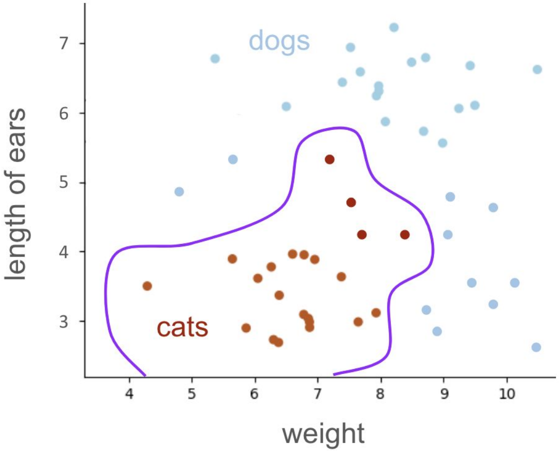
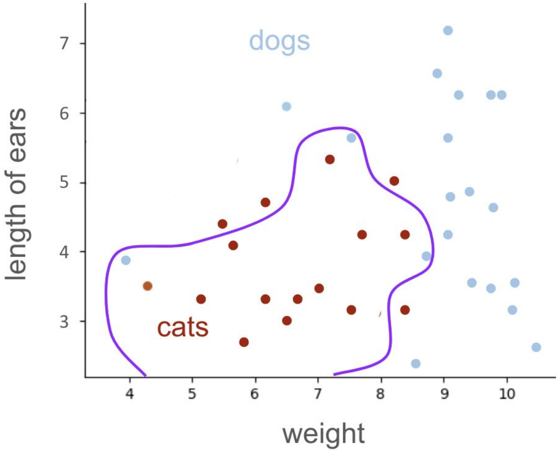


100 % classification performance

Test set: new data, “old” model.

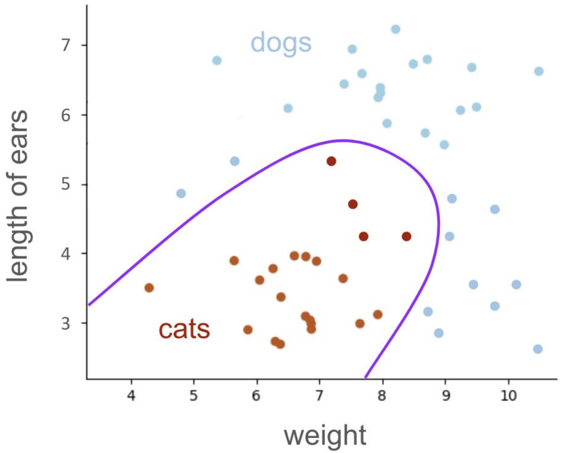


~90 % classification performance

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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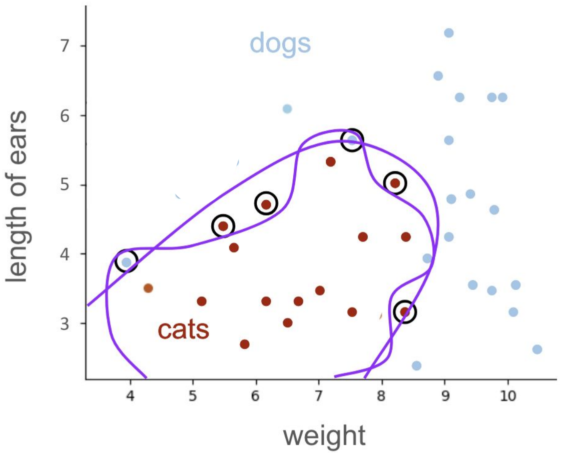
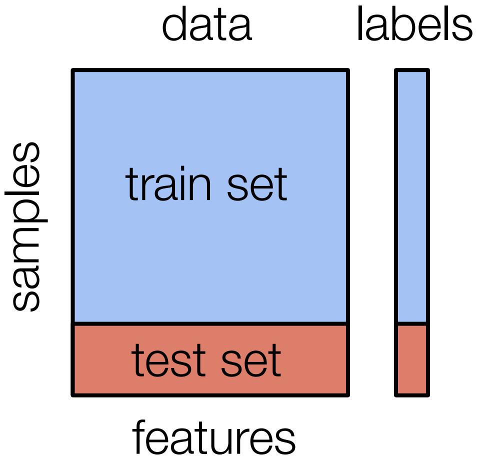


~98 % classification performance

Classification: Cross-validation



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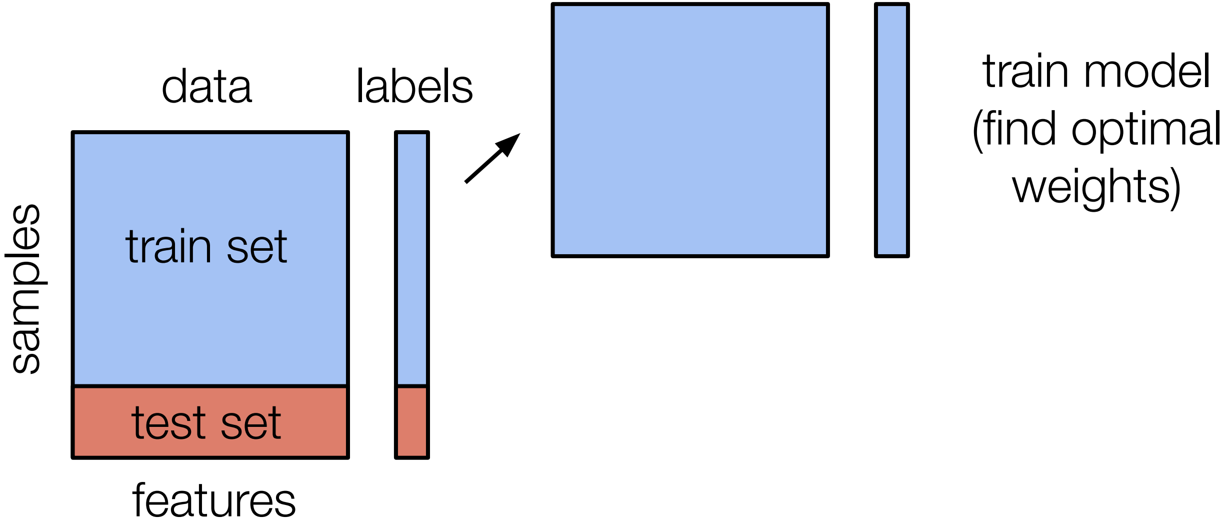

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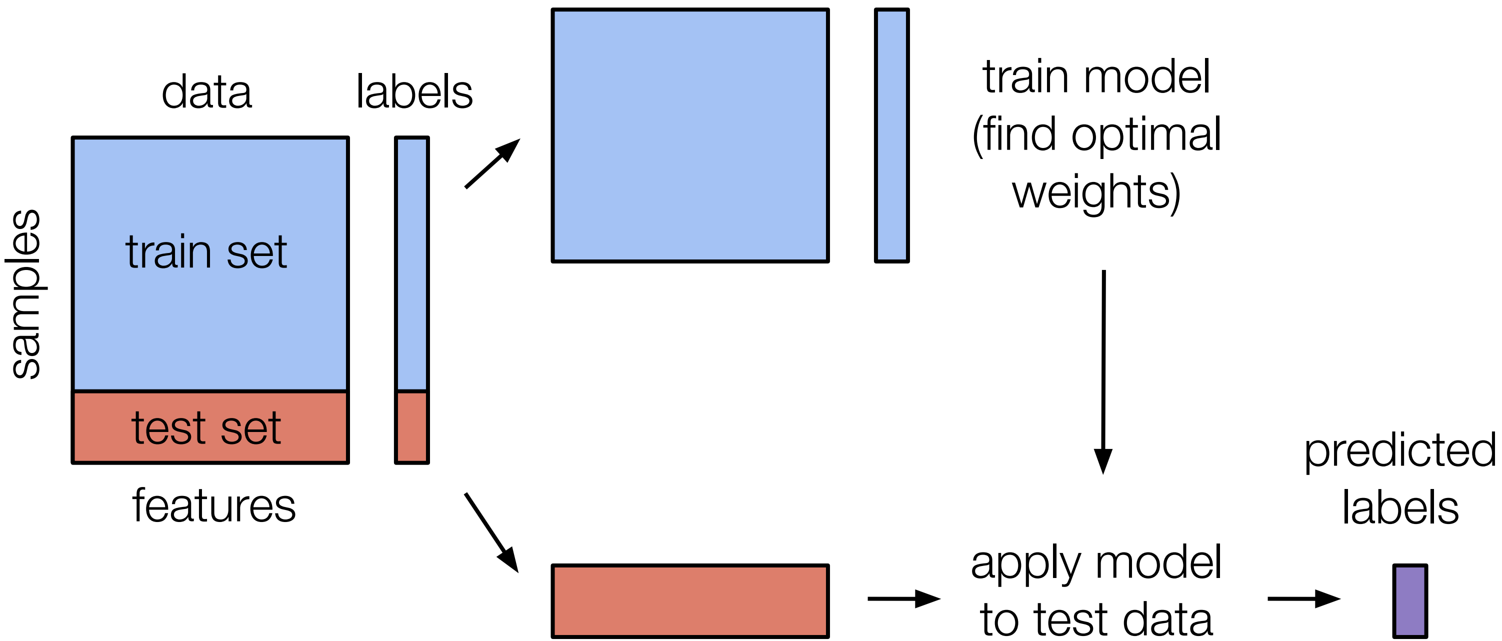

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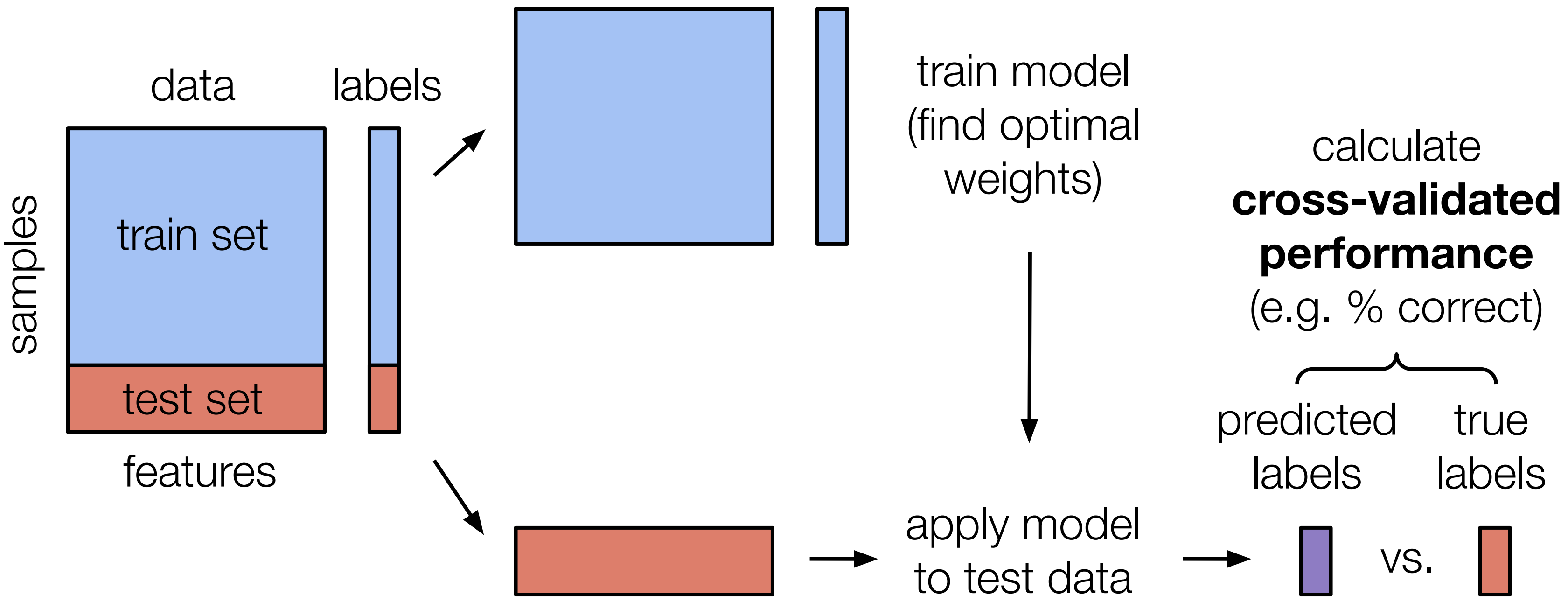

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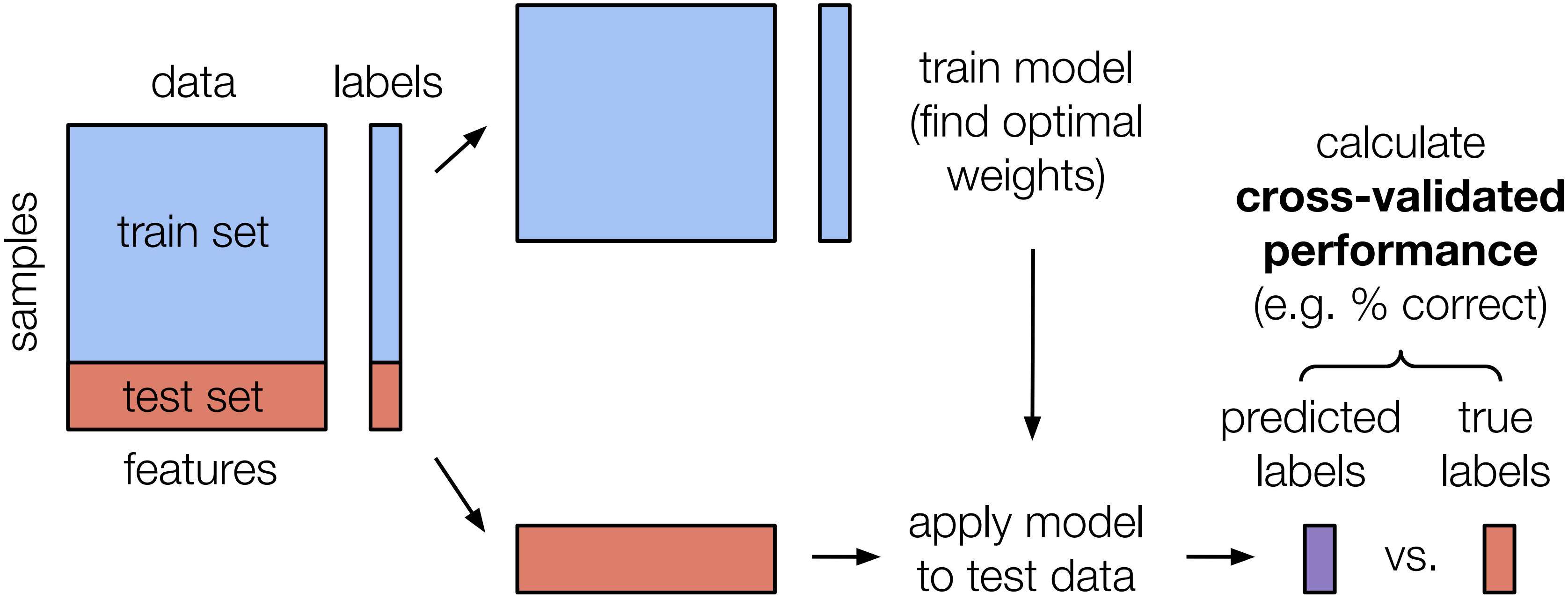
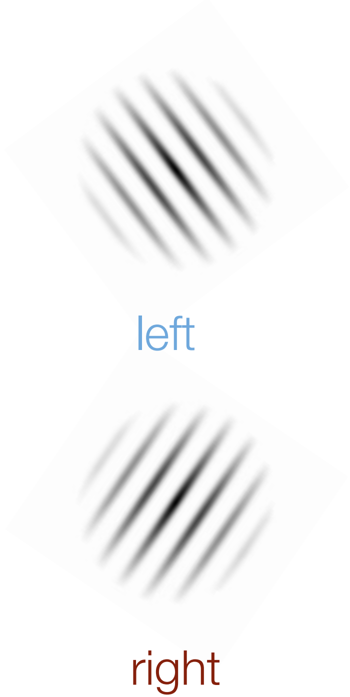
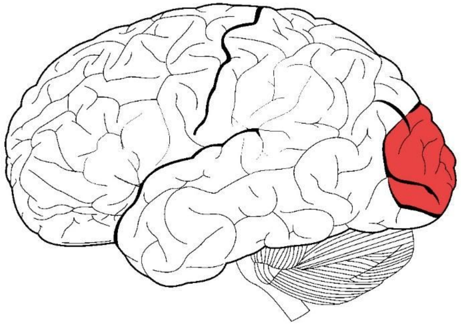


→ Repeat with many train/test splits. Is **perf. better than expected by chance**?

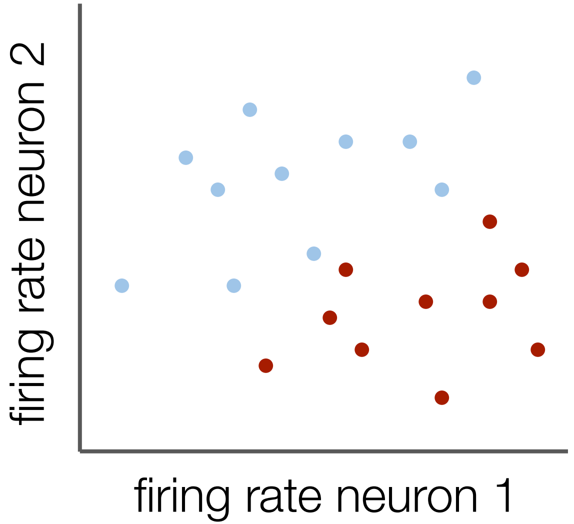
Classification: What can we learn about the brain?

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





recordings from V1



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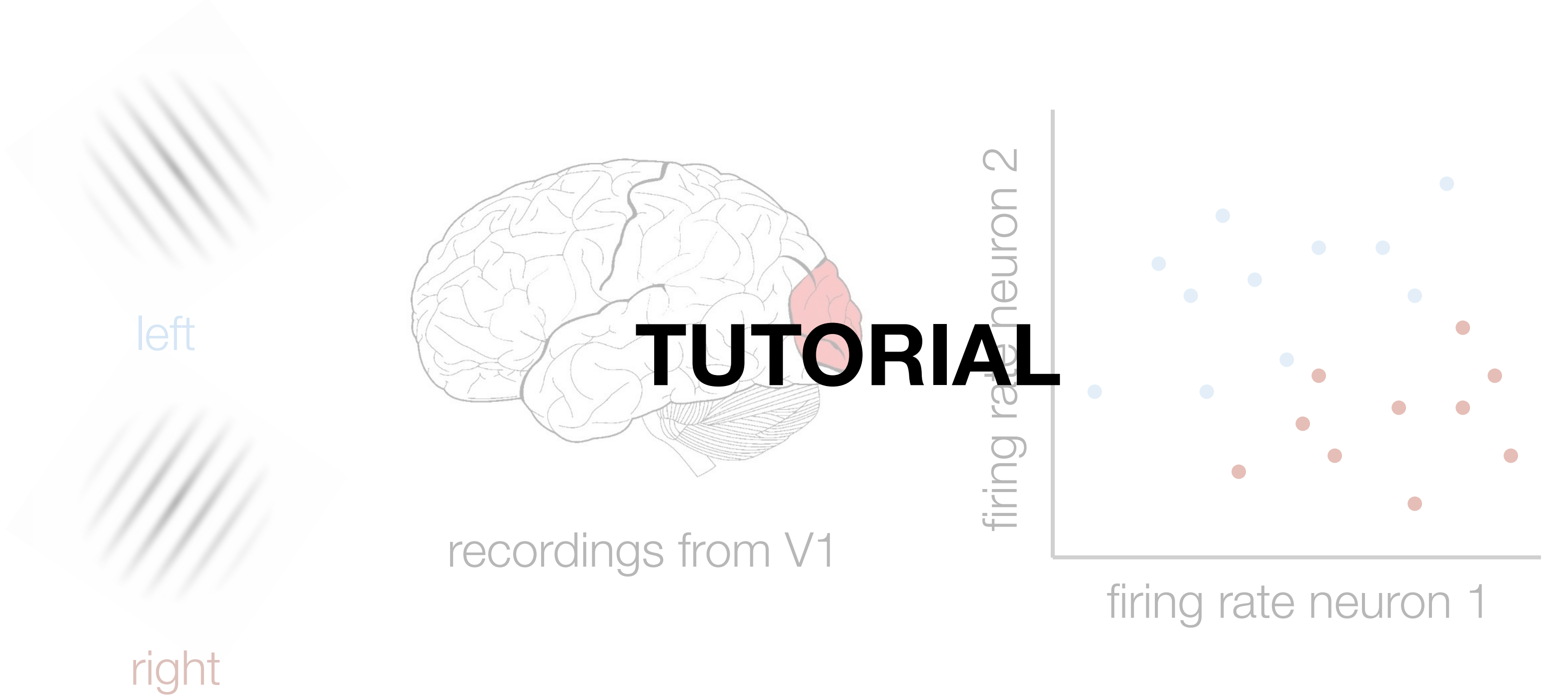
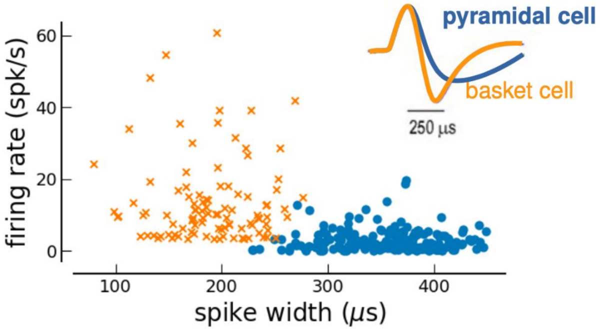


TUTORIAL

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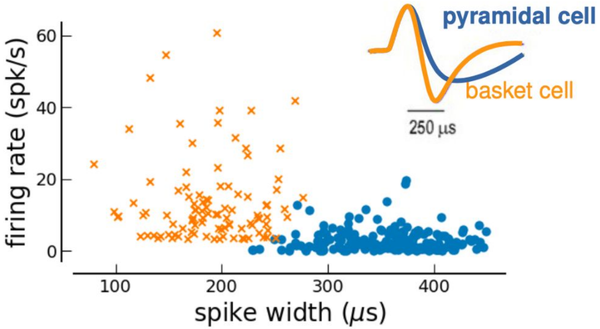
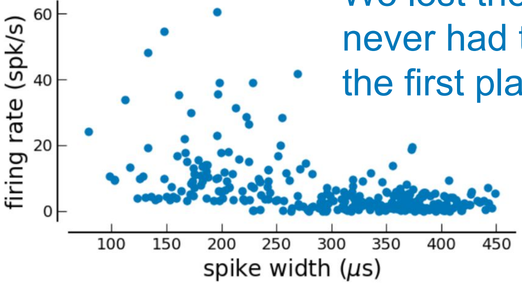
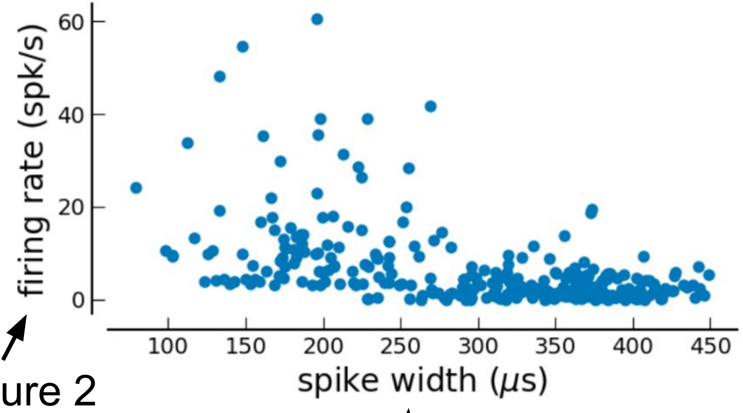
Clustering: We see **patterns** in the data that **suggest multiple categories**, but we don't know which data point belongs to which category. Clustering is an "**unsupervised**" method (unknown ground truth).





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

Clustering: Guessing categories from patterns in the feature space



feature 2

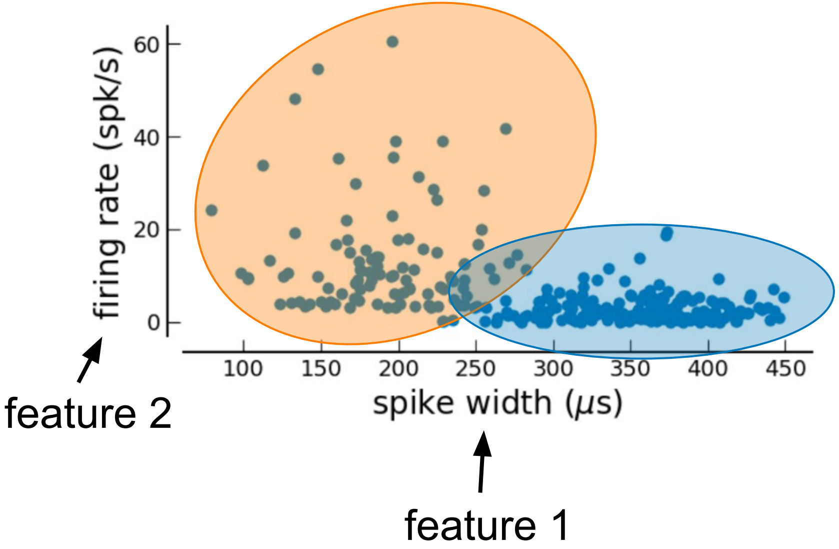
feature 1

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**?

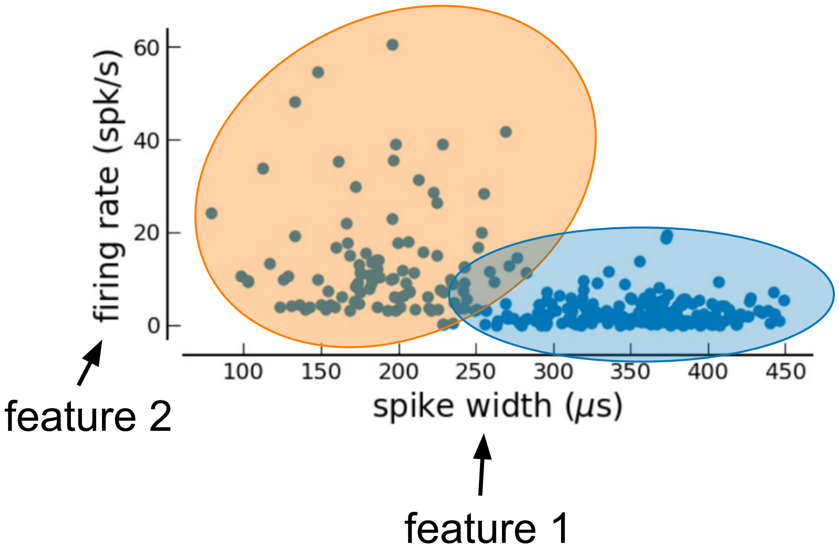
Clustering: Guessing categories from patterns in the feature space



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?

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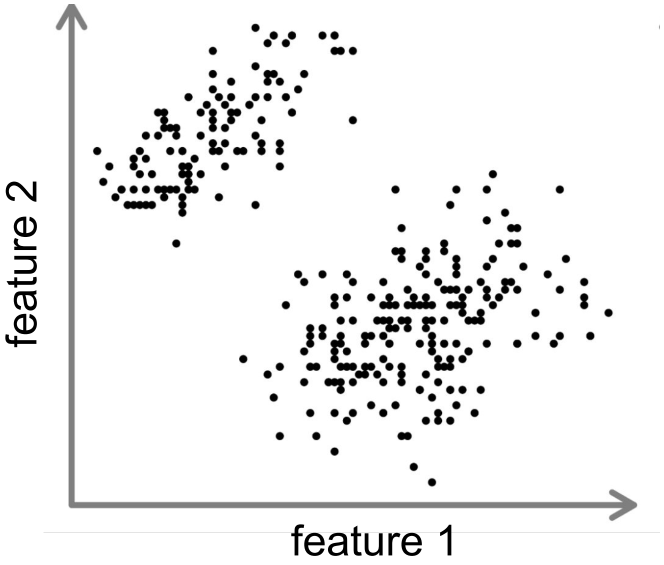
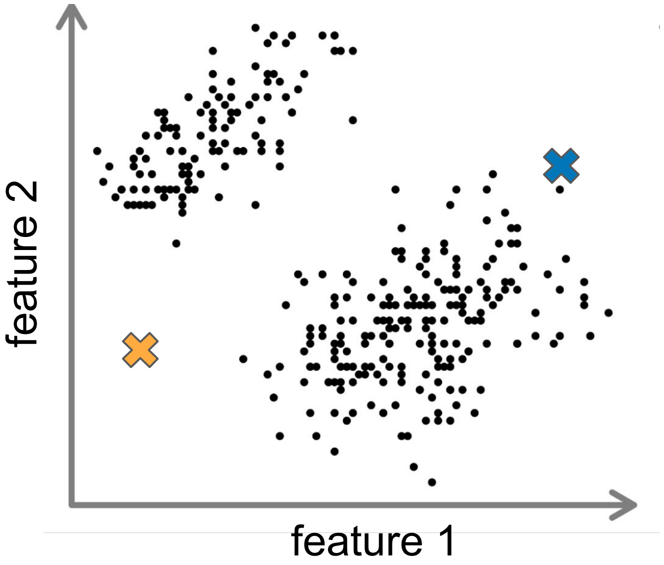
But how?

Clustering: k-means



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

Clustering: k-means



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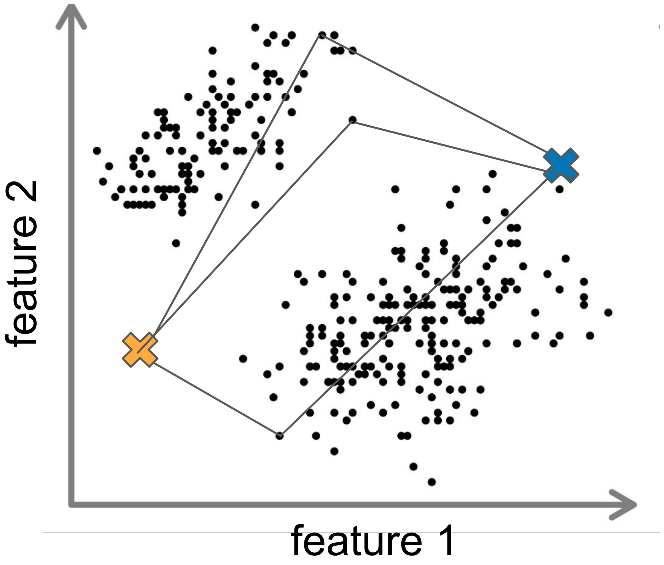
1. Pick two random values (“initialization”).

Clustering: k-means



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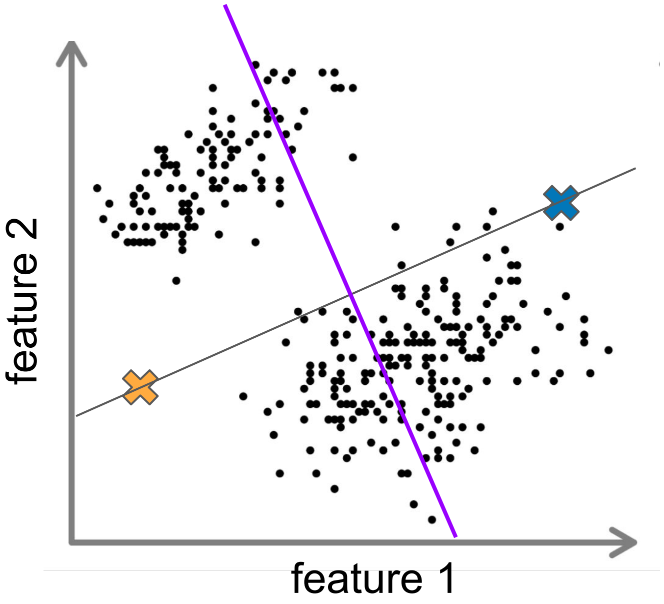

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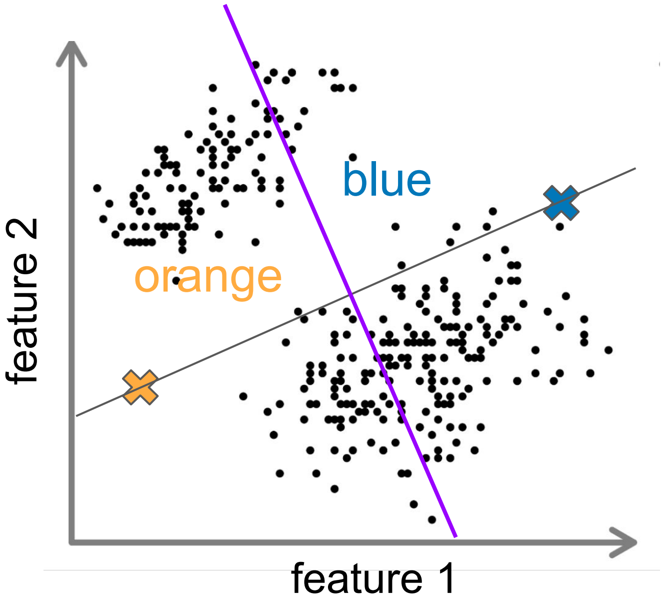

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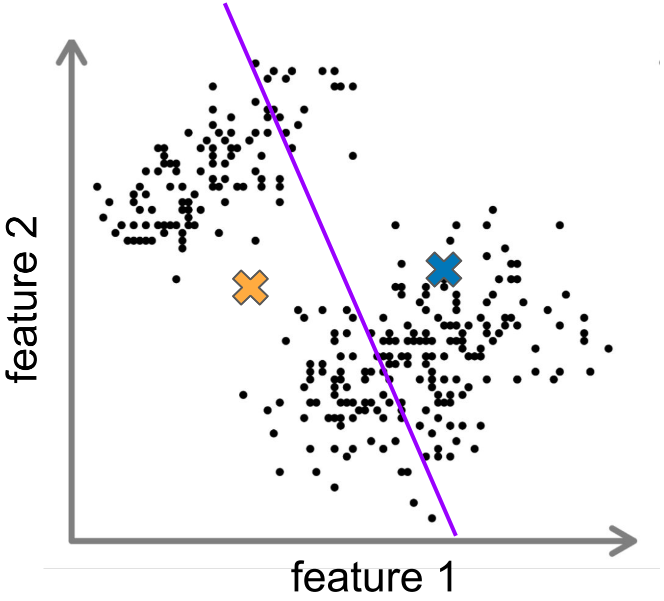

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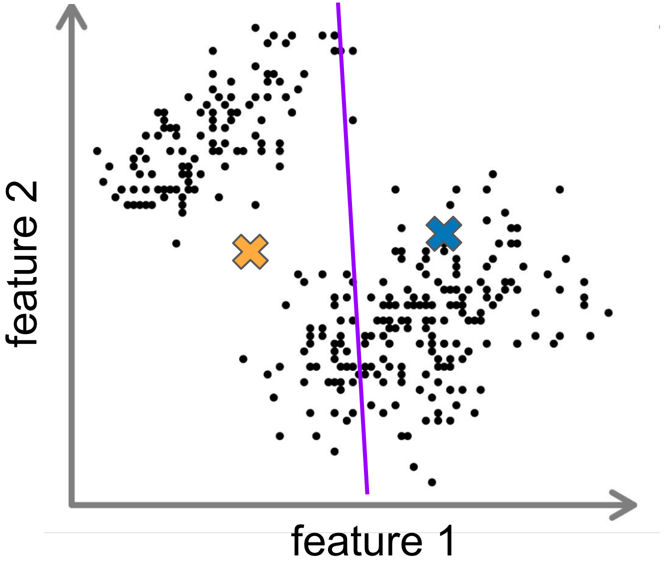

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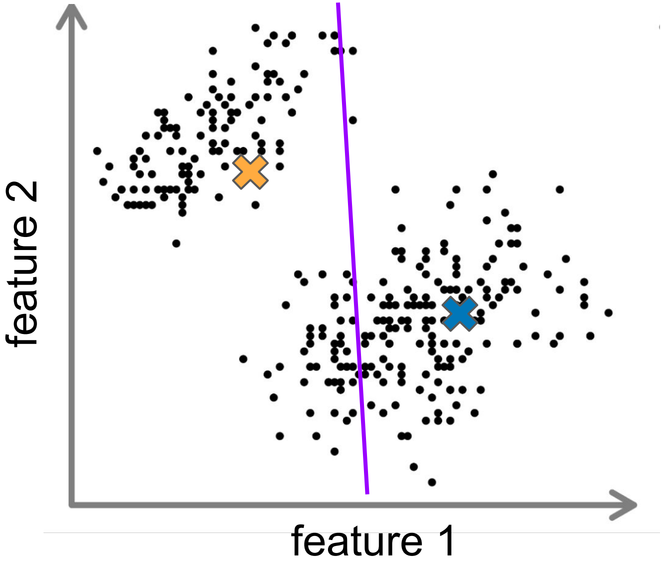

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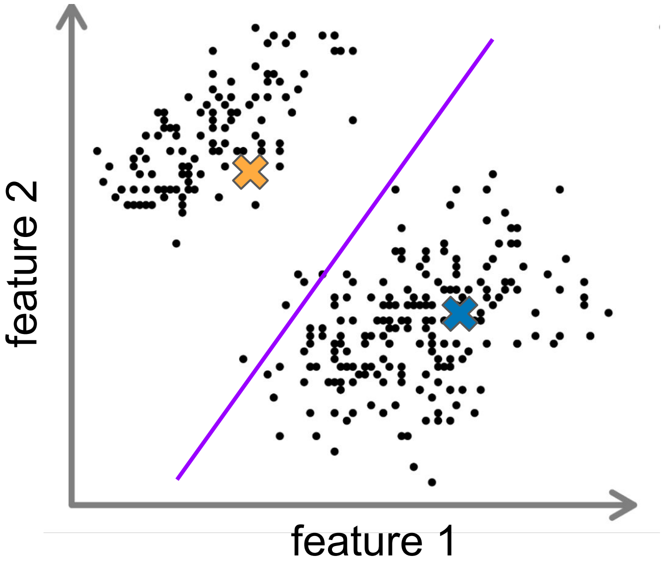

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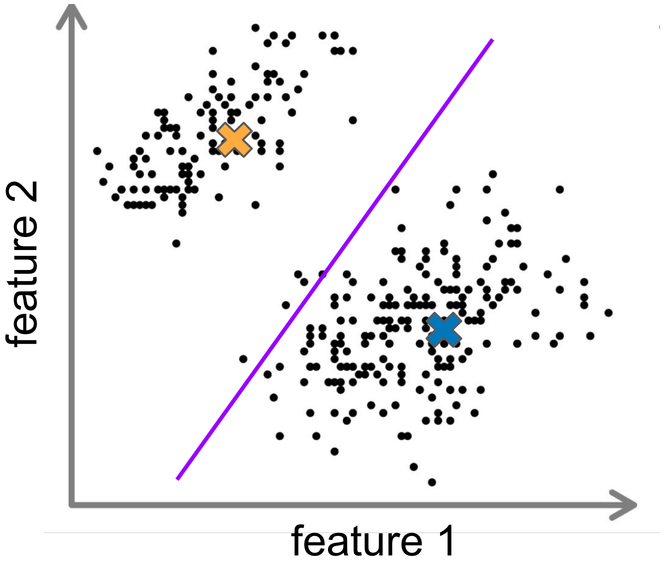

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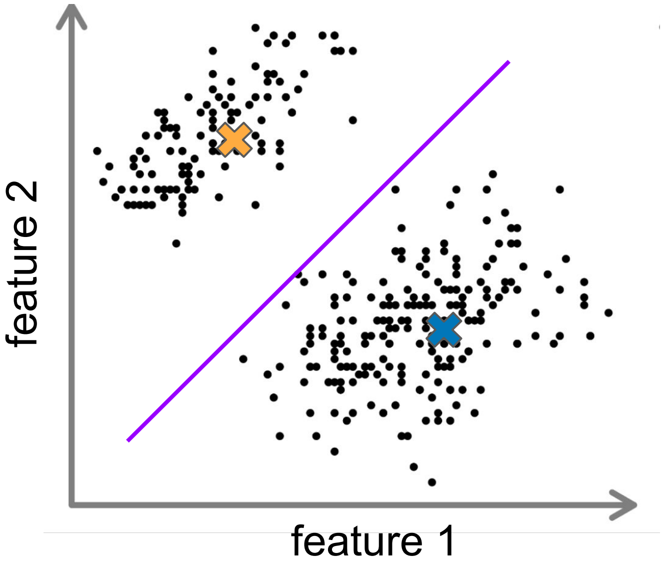

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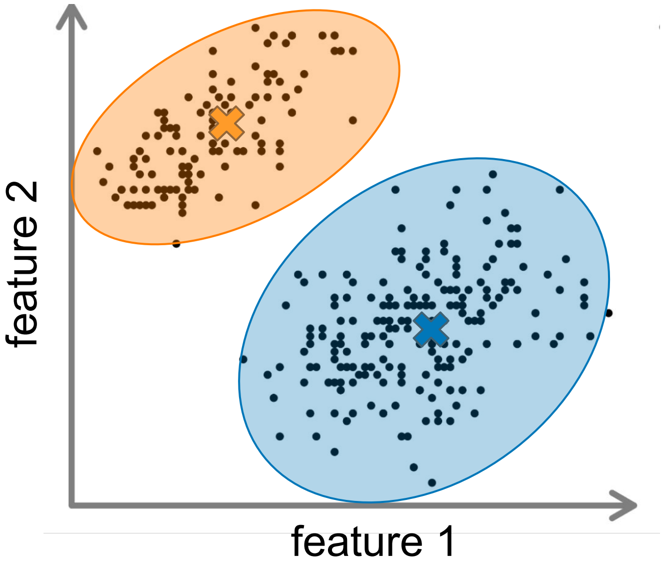

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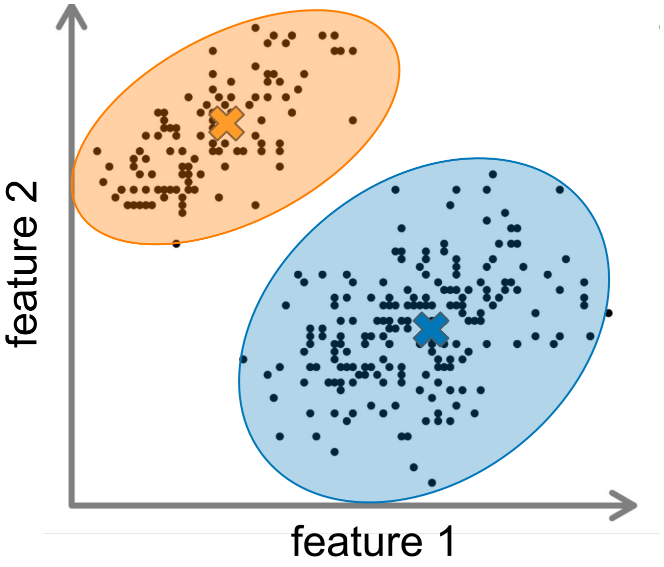
Repeat 2.-3. until cluster means are stable (they “converged”).

Clustering: k-means



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

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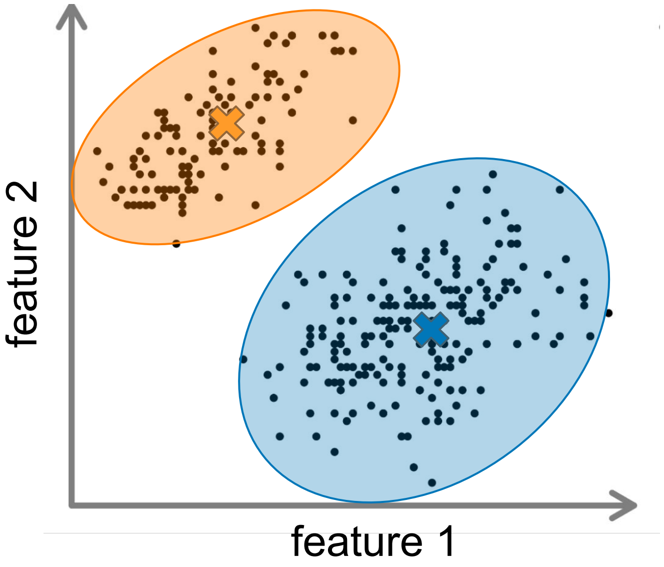
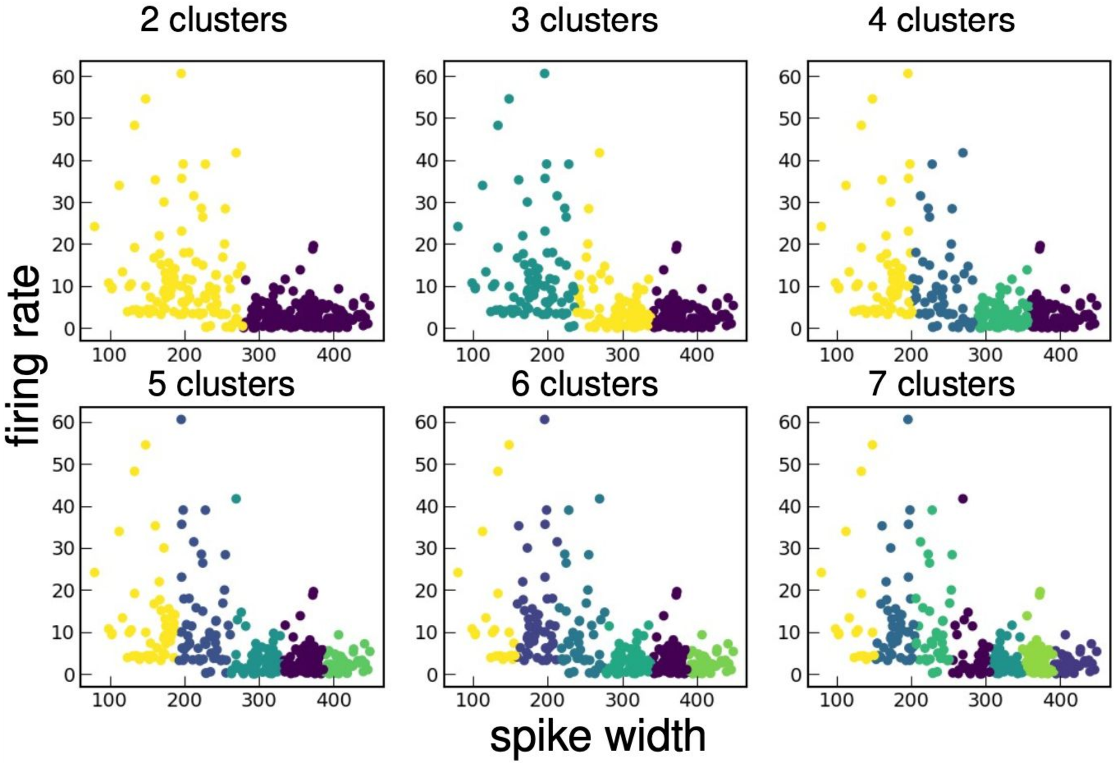


Clustering is **iterative** (repeat steps until convergence).

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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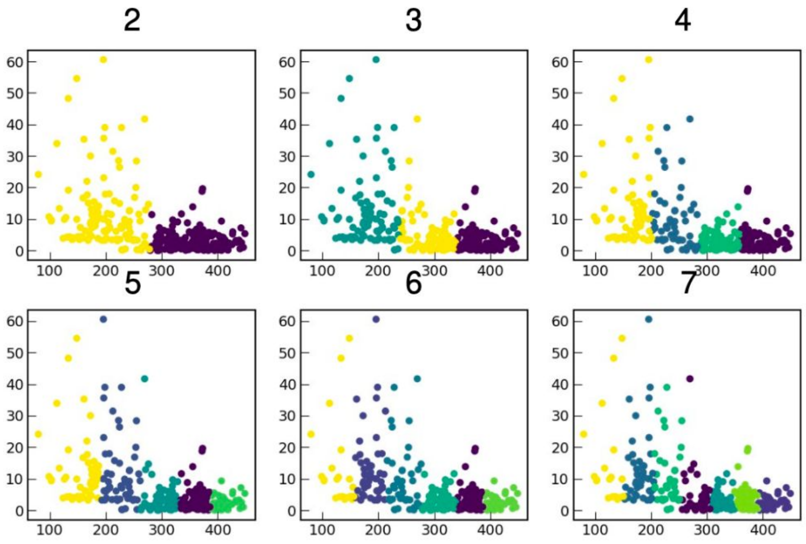

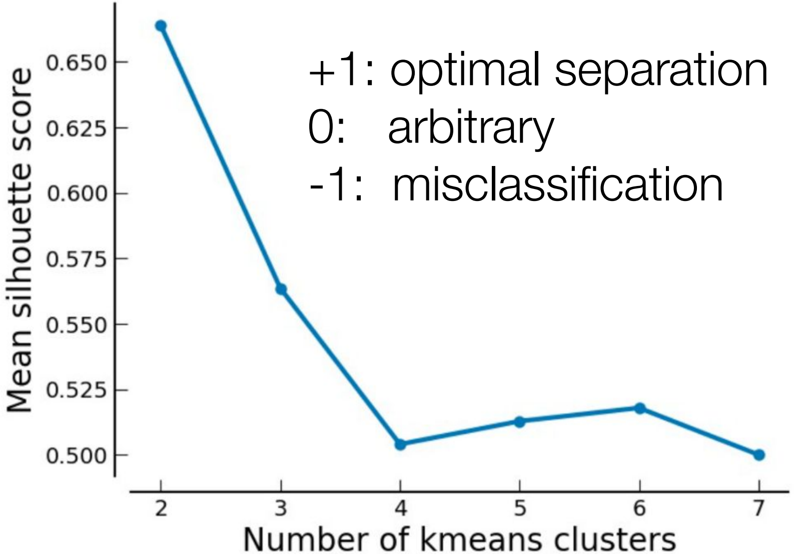

+1: optimal separation

0: arbitrary

-1: misclassification

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

$$S = \frac{1}{N} \boxed{\sum_{i=1}^{N}} \frac{\boxed{b(i)} - \boxed{a(i)}}{\max(a(i),\, b(i))}$$

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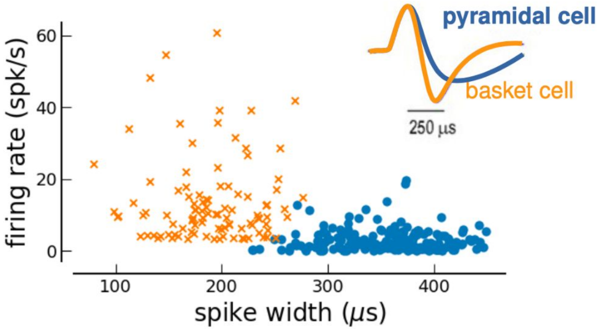

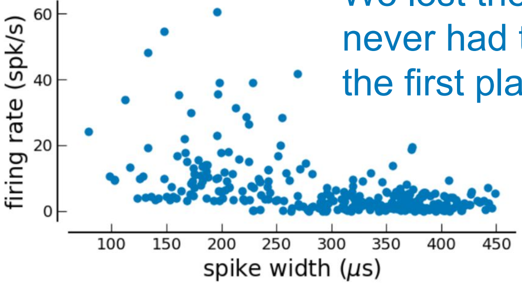

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Classification and Clustering: Overview

Classification

- Logistic regression
- Support vector machines

Clustering

- k-means