



# Neural Data Science with **Python**

## L10 : Classification and Clustering

*Michael Graupner*

*SPPIN – Saint-Pères Institute for the Neurosciences*

*Université Paris Cité, CNRS*

# Free tutorial suggestions (next week)

1) Program a game in python : “Rock, Paper, Scissors”



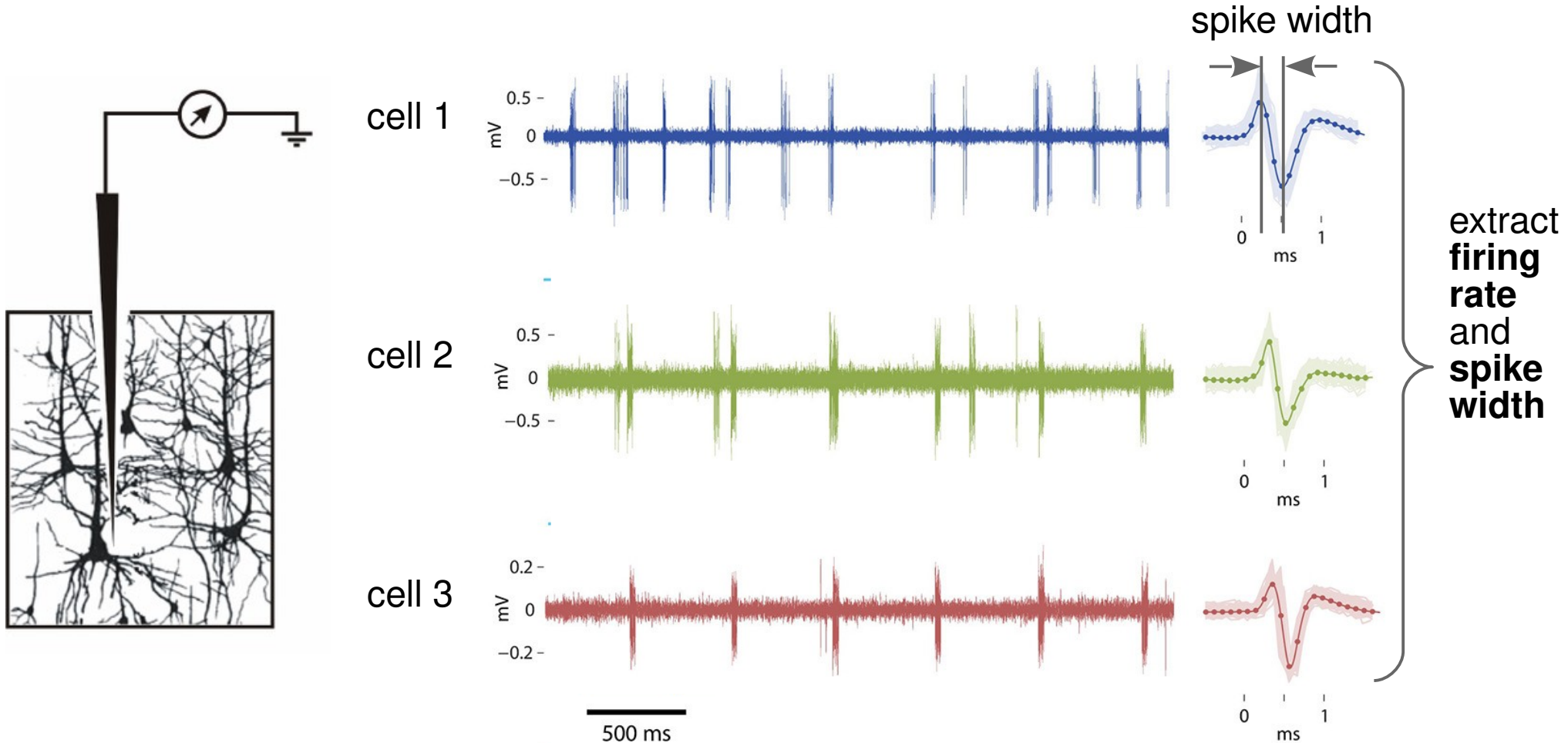
2) Resolve typical programming errors (bugs) in form of a quiz

3) Re-work on programming concept/analysis concept suggested by YOU.

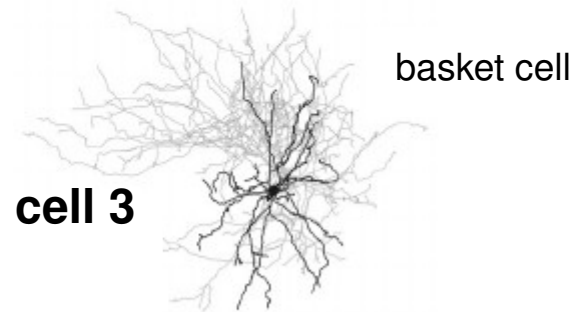
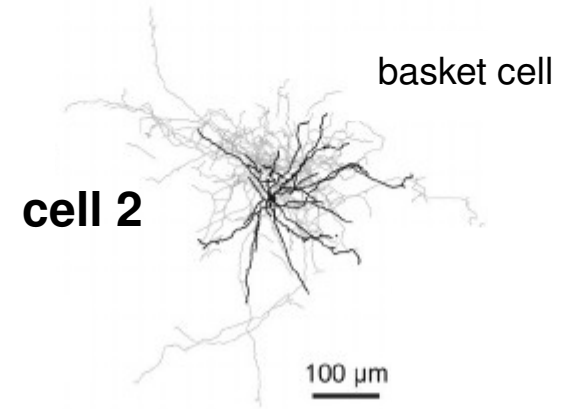
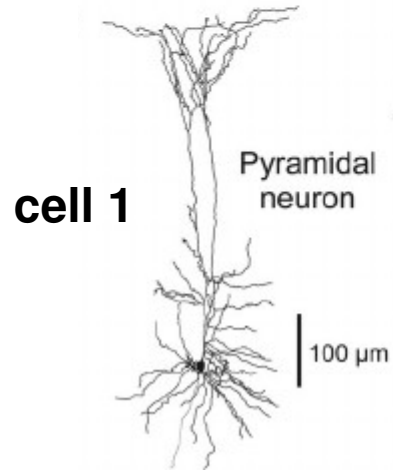
4) Start to work on a “fictive” end-of-course project : discuss approach, tips, tricks, typical problems

Slido Link : <https://app.sli.do/event/pZ7KRRPsGkfTD8KioD56Y8/embed/polls/73a60122-8717-4539-8ba8-d25cd314451f>

# Example : extracellular single unit recording

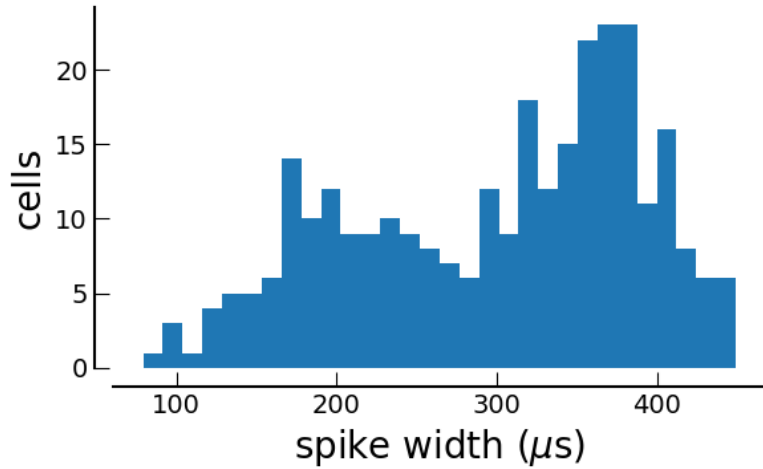


# Example : single unit recording + reconstruction

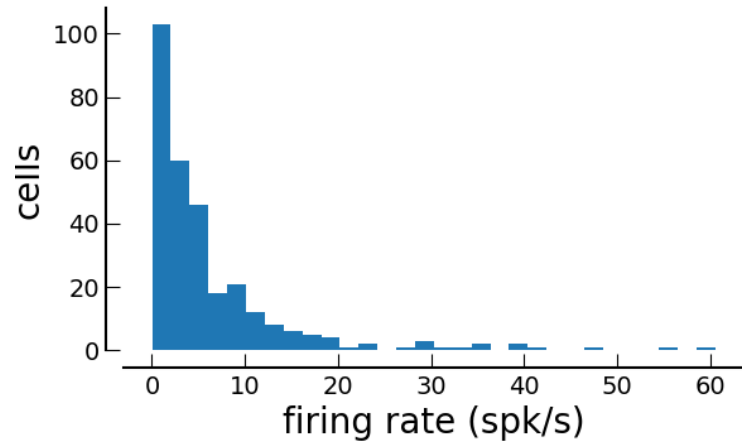


# Example: ephys summary of recordings from all cells

histogram of spike widths

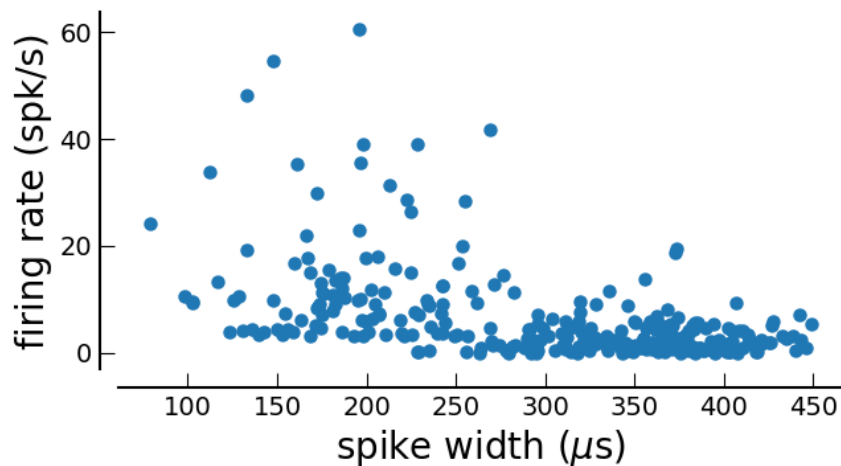


histogram of firing rates

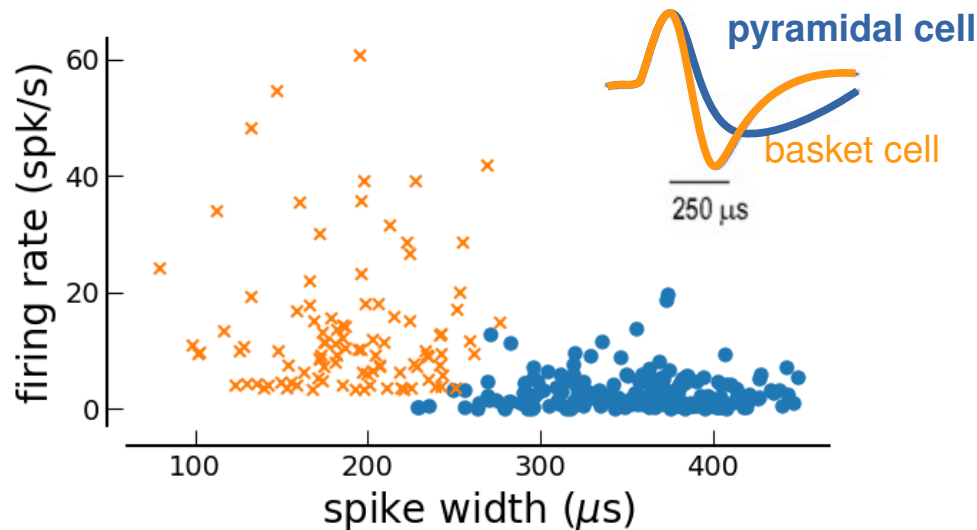


# Example: summary of recordings from all cells

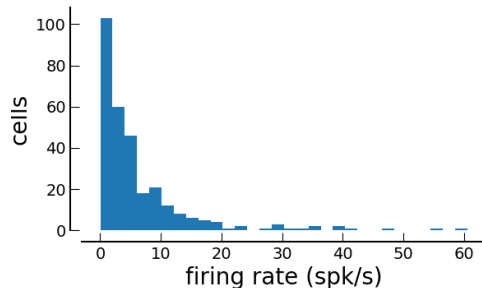
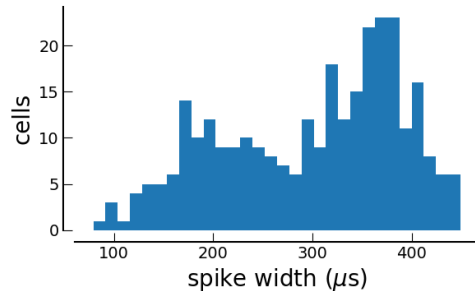
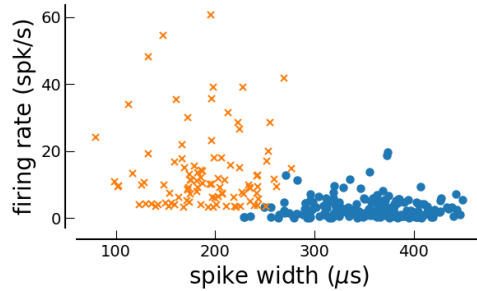
spike widths over firing rates  
(all cells)



spike widths over firing rates :  
using additional information of cell  
identity from reconstruction



# Example: summary of recordings from all cells



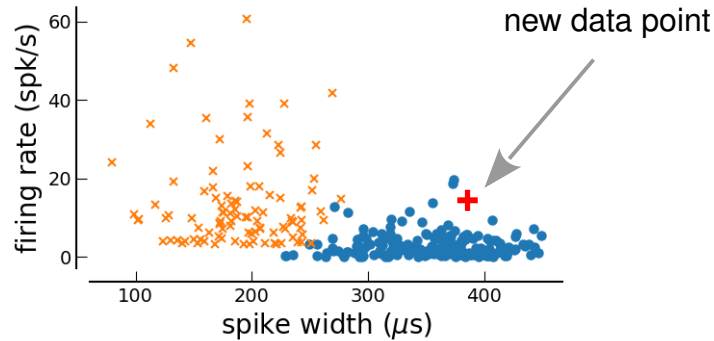
Averaging throws away specific information:

- ok if one averages over members of the same group
- problematic if not, looking for groups before averaging

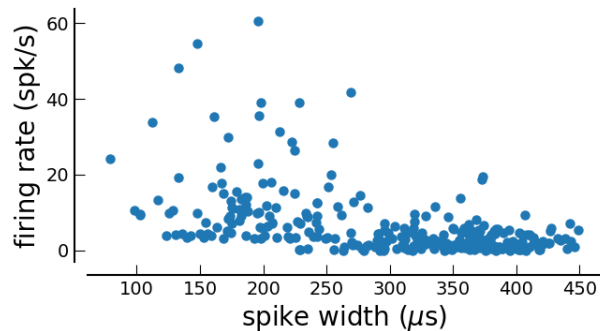


need to identify sub-groups in order to refine analysis and obtain deeper insights

# Aim : classification and clustering



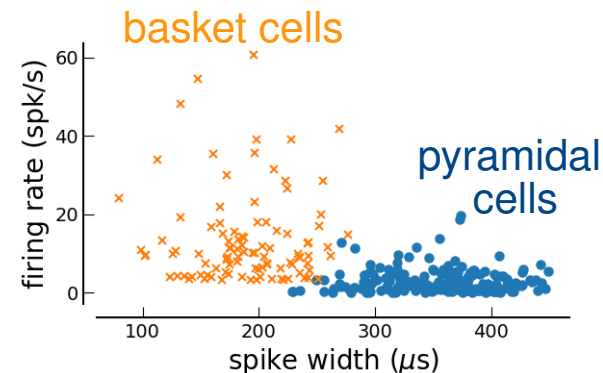
**Classification** is the task of predicting the group of new data points based on past observations.



**Clustering** is the task of dividing the data into a number of groups such that data points in the same groups are more similar to other data points in the same group than those in other groups. In simple words, the aim is to segregate groups with similar traits and assign them into clusters.



# Classification vs. Clustering



**Example :** 2 classes with labels “pyramidal cells” and “basket cells”

| Classification                                   | Clustering   |
|--|--|
| supervised learning technique (labels are known) | unsupervised learning technique (labels are not known) |
| known number of classes                          | unknown number of classes                              |
| used to classify future observations             | used to understand (explore) data structure            |

# Classification: supervised learning

classes (output variables)

input variables

$$Y = f(X)$$




mapping function

Classification is where you have input variables (X) and output category/class (Y) and you use an algorithm to learn the mapping function (f) from the input to the output.

| input variables: X |                     | mapping function | classes: Y       |
|--------------------|---------------------|------------------|------------------|
| spike width (μs)   | firing rate (spk/s) | classifier       | neuron type      |
| 335                | 5                   | →                | Pyramidal neuron |
| 167                | 34                  | →                | Basket cell      |
| 212                | 43                  | →                | Basket cell      |

⋮

# Classification: supervised learning

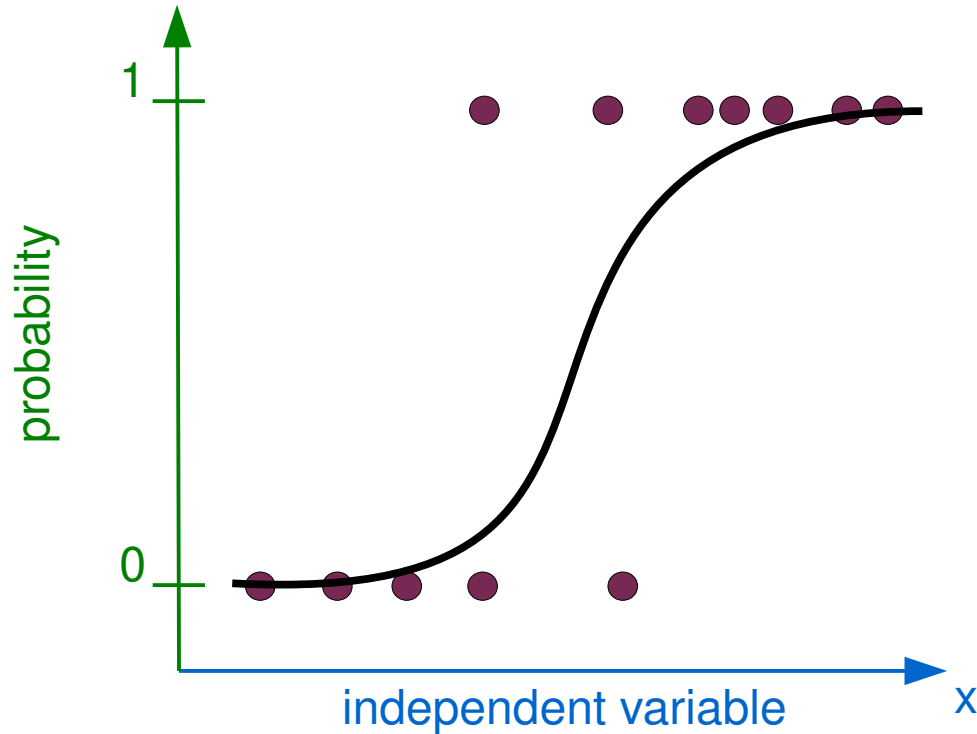
| input variables: X     |                     | mapping function  | classes: Y       |
|------------------------|---------------------|---|------------------|
| spike width ( $\mu$ s) | firing rate (spk/s) | classifier  | neuron type      |
| 335                    | 5                   |  | Pyramidal neuron |
| 167                    | 34                  |  | Basket cell      |
| 212                    | 43                  |  | Basket cell      |

⋮

**Classification aim :** Learn mapping to predict neuron type of new recordings.

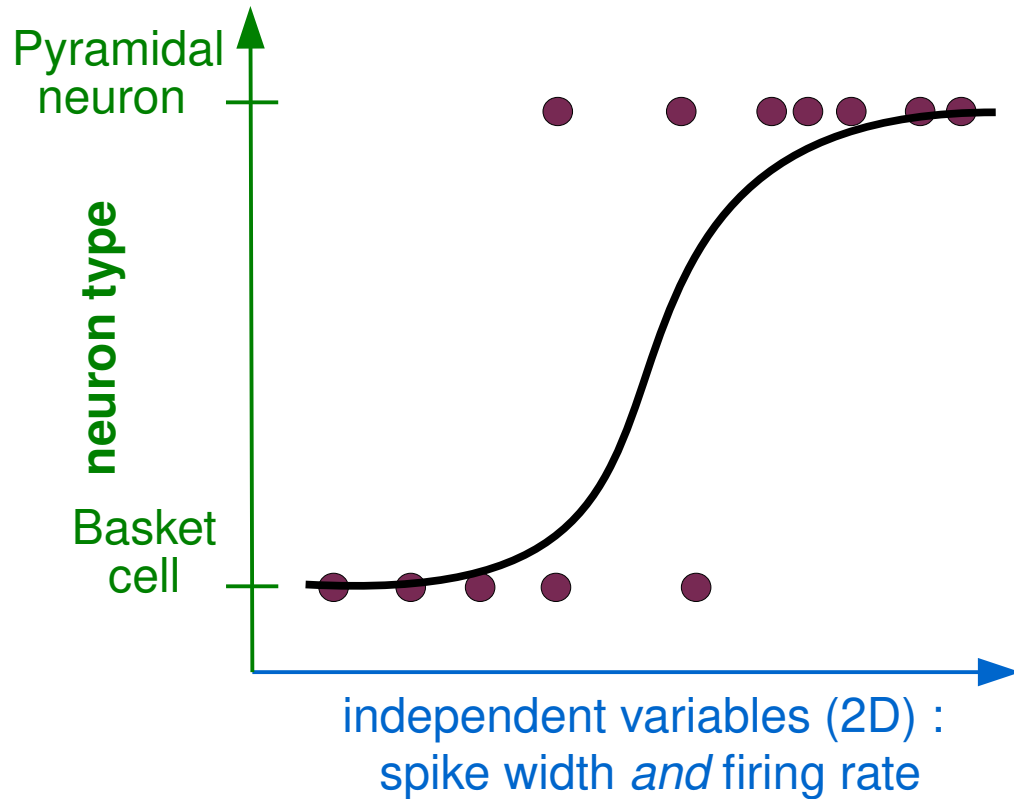
|     |    |   |      |
|-----|----|---|------|
| 412 | 12 |  | ???? |
|-----|----|---|------|

# Classification method 1: Logistic regression



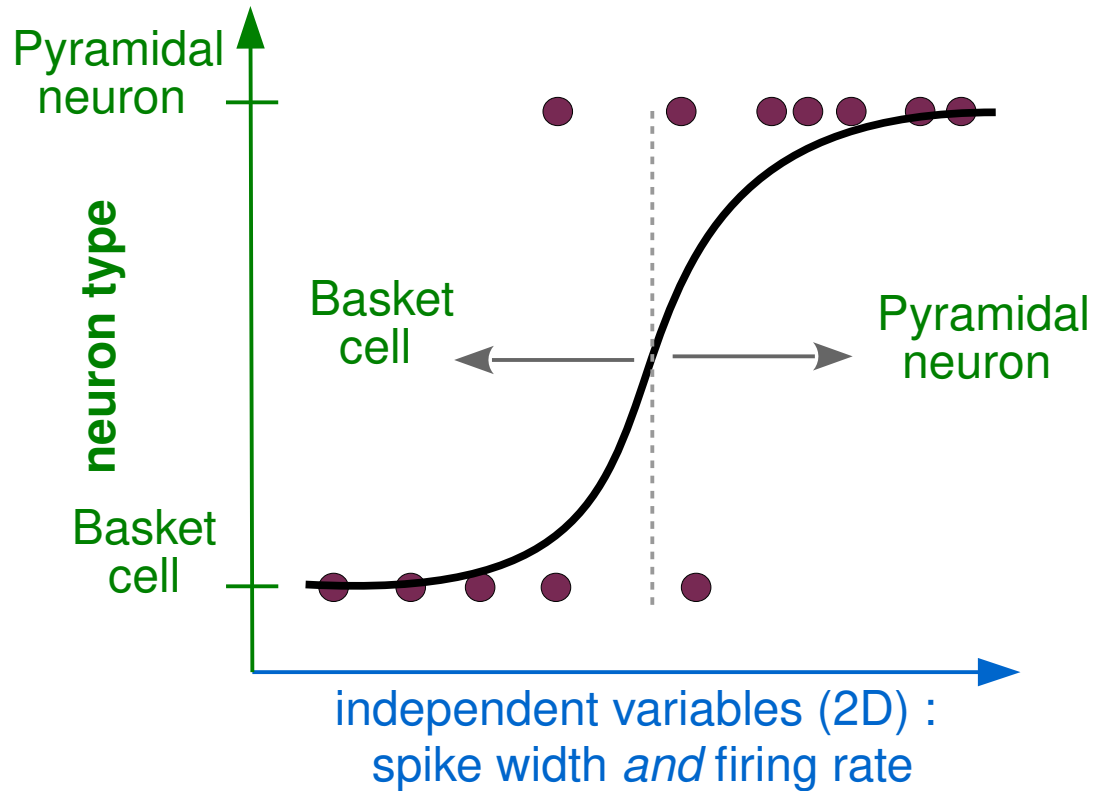
Logistic regression is a nonlinear model to link predictors and outcomes through a *sigmoidal* function. It gives the *odds* that an outcome happens – vs. it not happening for a given value of the independent variable (predictor value).

# Logistic regression and our example



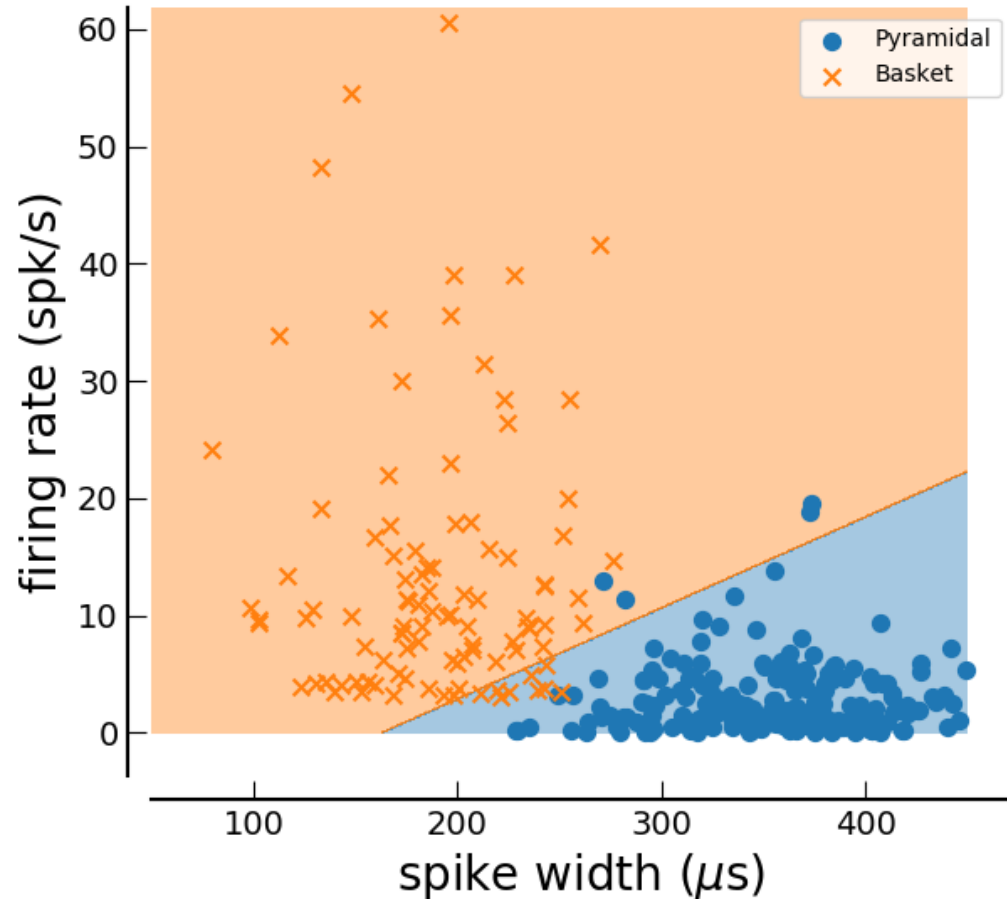
**Task :** fit the sigmoidal function to predict likelihood of neuron type.

# Logistic regression and our example



**Task :** fit the sigmoidal function to predict likelihood of neuron type.

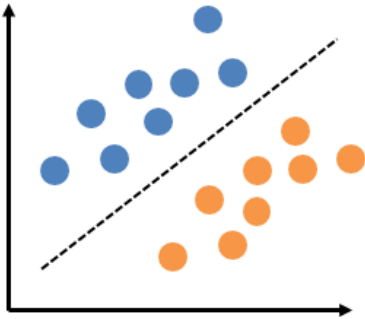
# Logistic regression on recording example



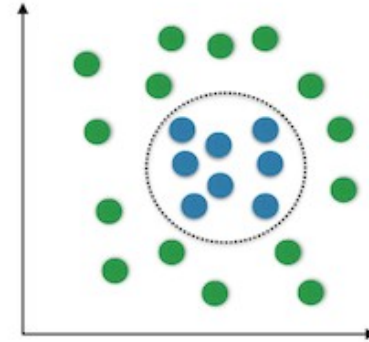
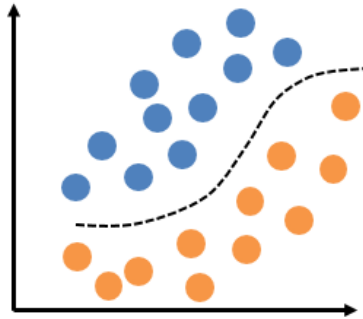
- does a pretty good job of separating the two neuron groups based on spike width and firing rate
- logistic regression give probability of being in either group (here we plot which of the groups the points are more likely to belong to)
- one-dimensional *linear* classifier

# Linear vs. nonlinear separation of groups

Linear

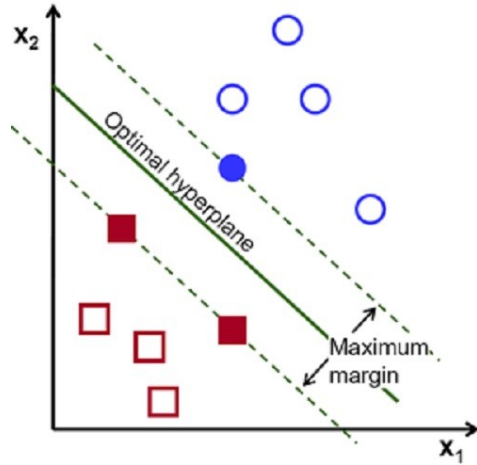


Nonlinear

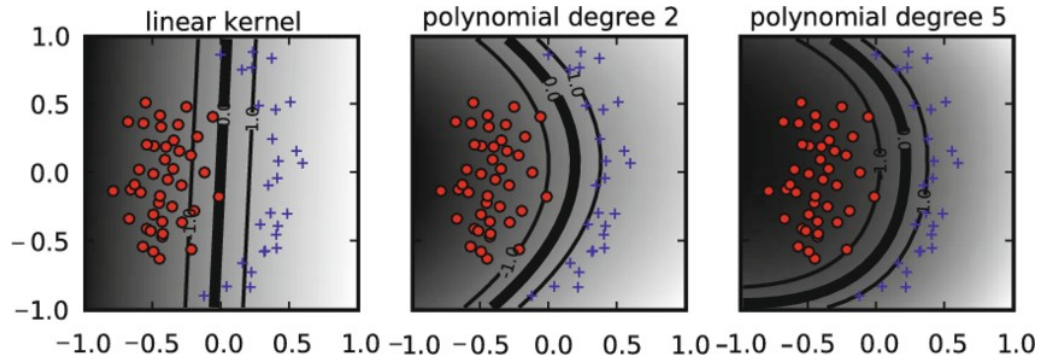




# Classification method 2: support-vector machine

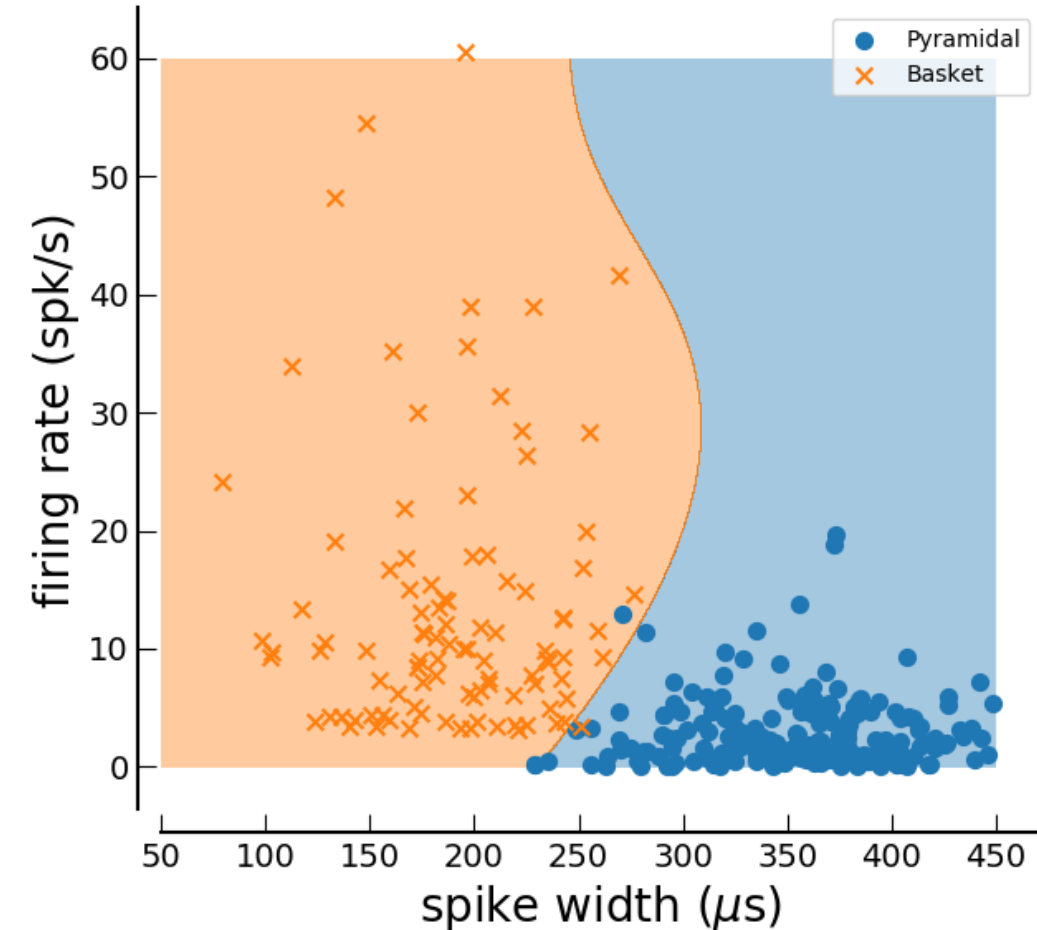


**Support vector machine (SVM)** : find the separating line (in higher dimensional space : hyperplane) that is equidistant to the two classes of datapoints, such that it maximizes the distance btw. the hyperplane and the nearest datapoint on each side.



The SVM classifier can be linear (finding a hyperplane) or non-linear using different kernels (e.g. polynomials).

# Classification method 2: support-vector machine



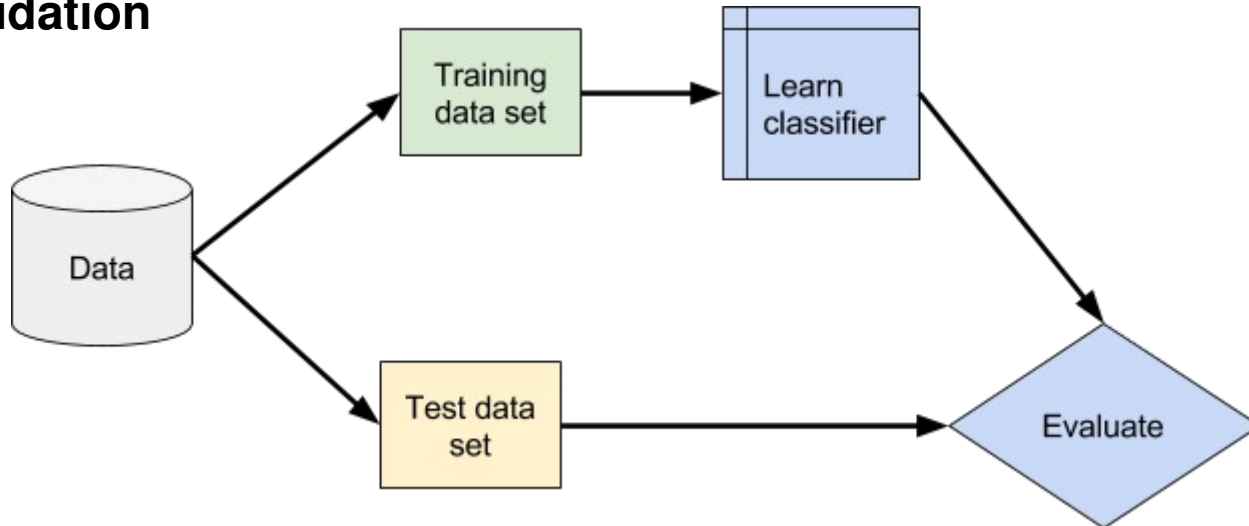
**SVM classification :** we use *polynomial kernel* which finds a higher-order polynomial that separates the classes of points.

**Note :** SVM classification can be linear in which case the algorithm finds a line to separate the classes.

# Predictions, validation and cross-validation

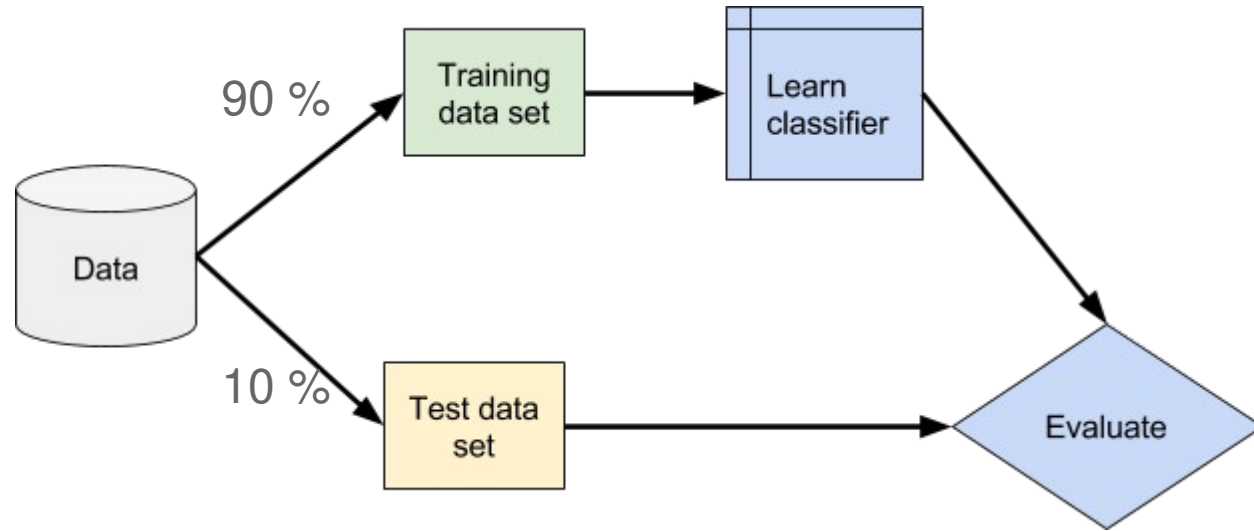
- How good is the classification ?
- How do we know that the separation is true ?
- How do we know that the classifier didn't just over-fit the data ?  
(over-fitting : the production of an analysis that corresponds too closely or exactly to a particular set of data, and may therefore fail to classify additional data reliably)

## → Cross-validation



# Predictions, validation and cross-validation

- data is split in training (90 %) and test (10 %) set
- training set is used to build classifier
- test set (never seen by classifier) is used to check whether prediction is correct
- this process is typically repeated multiple times with different splits between training and test data



# Clustering

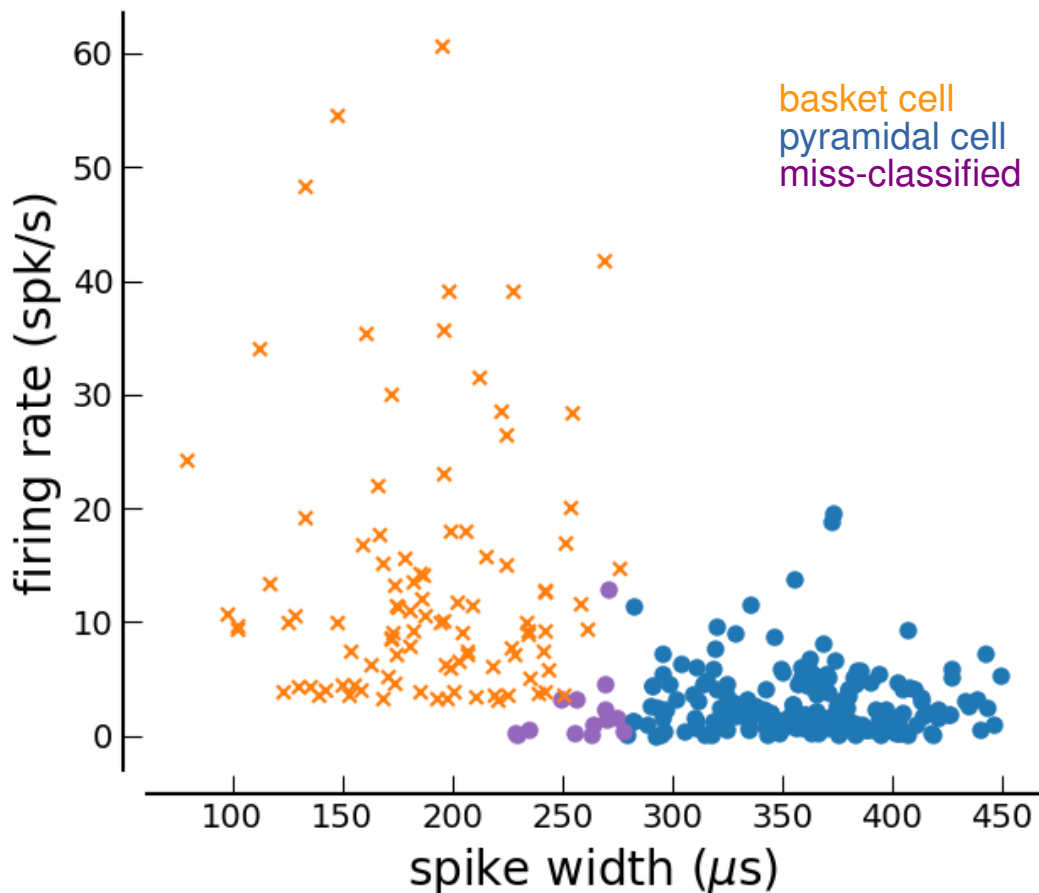
| Classification                                      | Clustering   |
|---|--|
| supervised learning technique<br>(labels are known) | unsupervised learning<br>technique (labels are not<br>known) |
| known number of classes                             | unknown number of classes                                    |
| used to classify future<br>observations             | used to understand (explore)<br>data                         |

We know the classes.

Have to figure out classification.

# Clustering method: k-means clustering

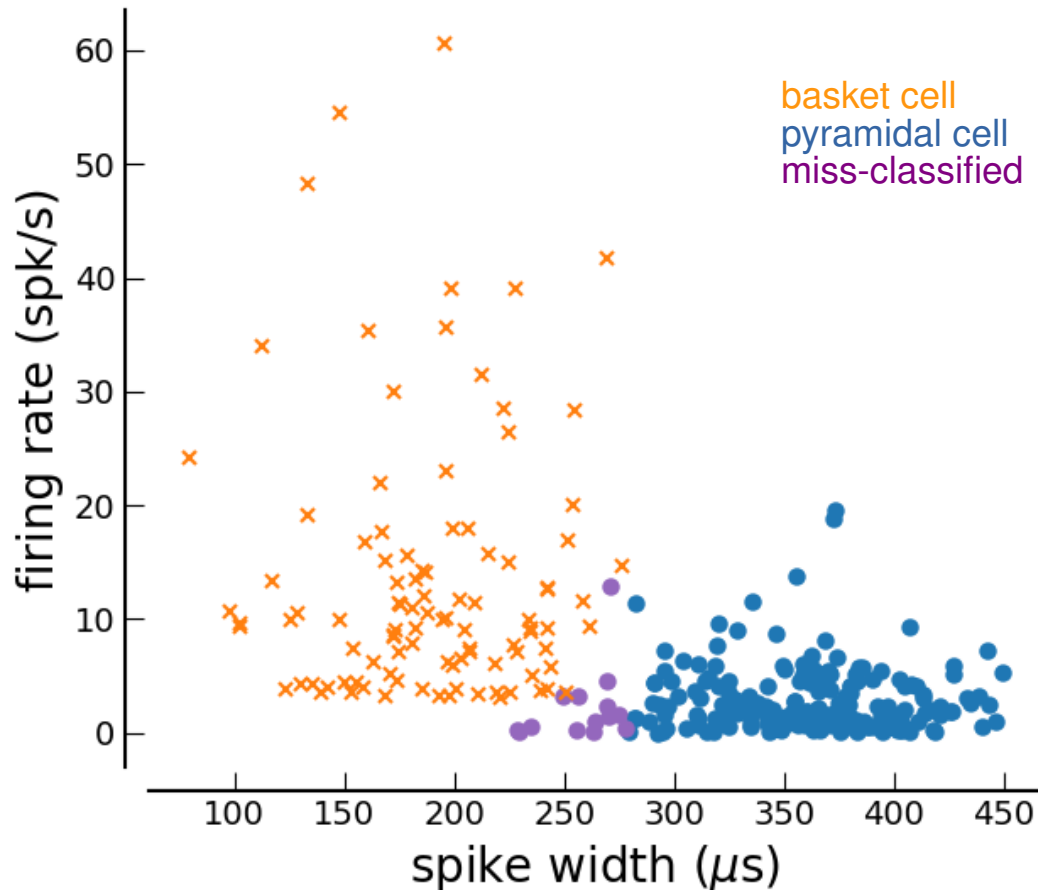
*k-means* on our example ( $k=2$ )



- **k-means** : algorithm is an iterative algorithm that tries to partition the dataset into  $K$  *pre-defined* distinct non-overlapping clusters
- each data point belongs to only one cluster
- It assigns data points to a cluster such that the sum of the squared distance between the data points and the cluster's centroid (arithmetic mean of all the data points that belong to that cluster) is at the minimum

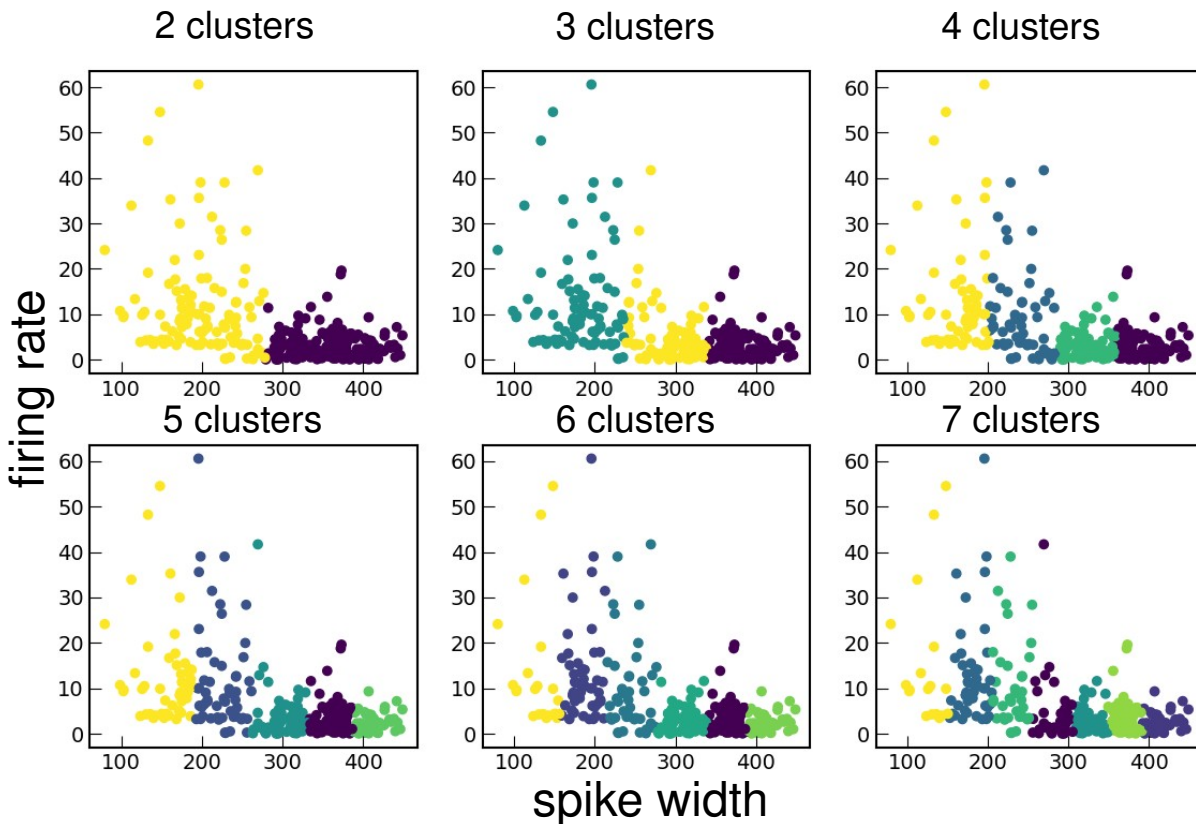
# k-means clustering: how many clusters to use ?

*k-means* on our example ( $k=2$ )



- **k-means** : tells you where the cluster centers (centroids) are but NOT how many there are
- **problem** : in actual data, you don't know the number of clusters
- **solution** : *silhouette analysis* to determine how many clusters are likely to be valid

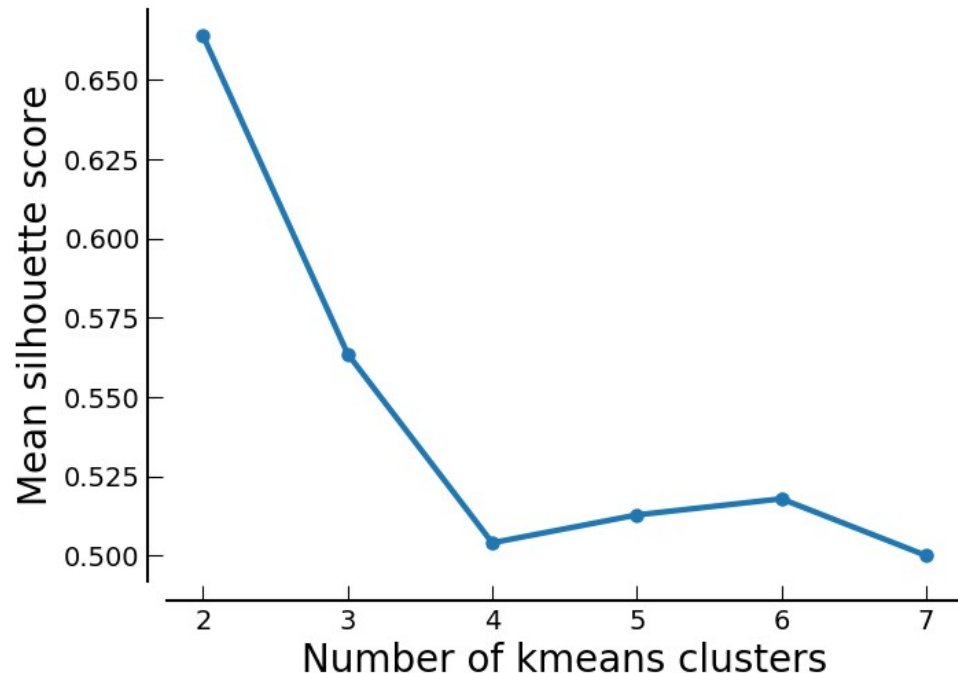
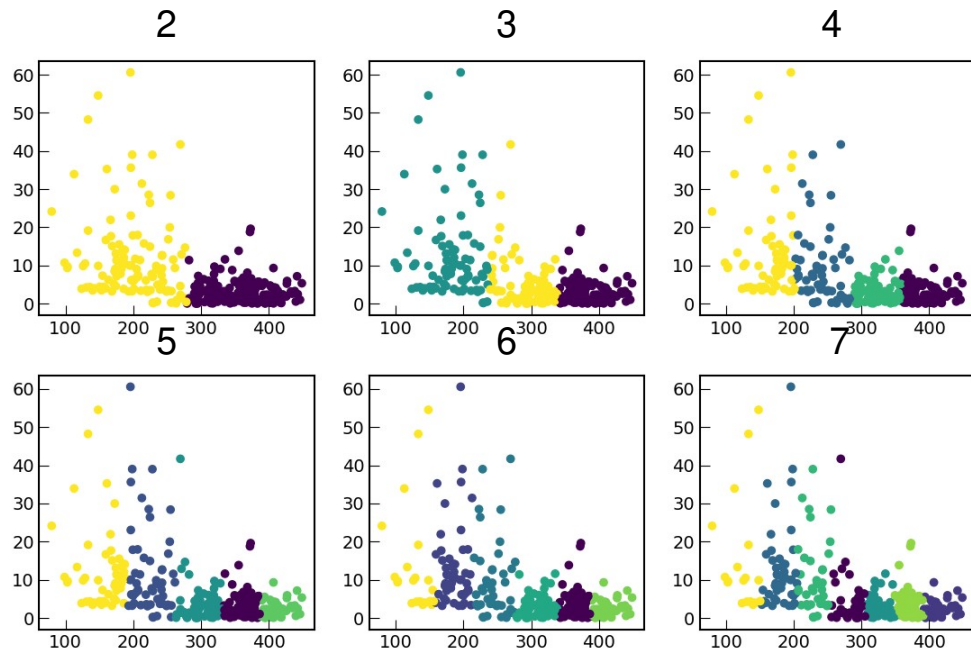
# k-means clustering : silhouette analysis



- Silhouette analysis gives a perspective into the density and separation of the formed clusters
- measures of how close each point in one cluster is to points in the same cluster compared to the neighboring clusters
- values range between  $[-1, 1]$  :
  - '1' good separation between clusters
  - '0' classification is almost arbitrary
  - '-1' indicates missclassification



# k-means clustering : silhouette analysis



- for our example : 2 clusters yield the highest, average silhouette score  
→ best separation with 2 clusters