ECE 20875

Python for Data Science

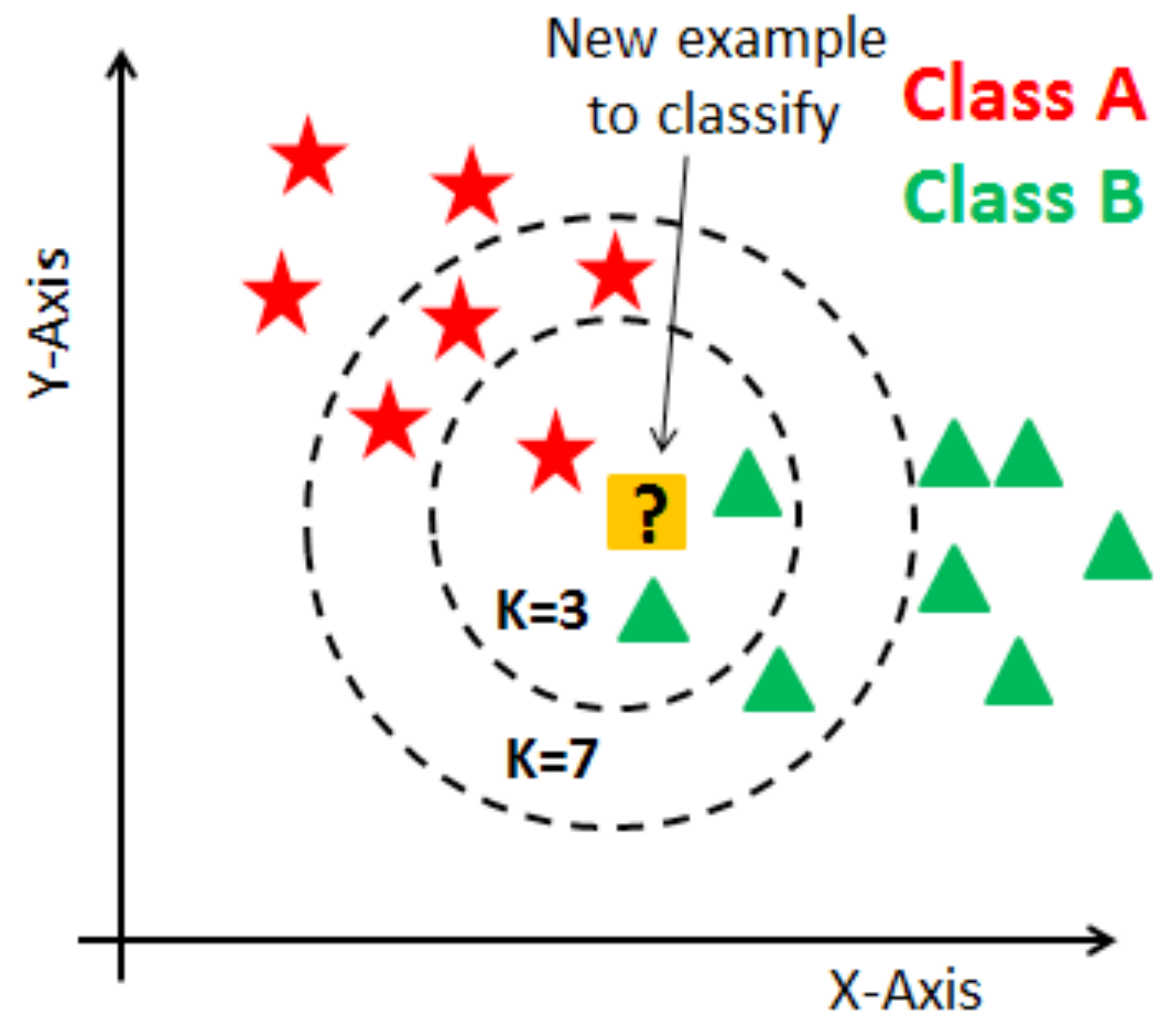
Chris Brinton, Qiang Qiu, and Mahsa Ghasemi

(Adapted from material developed by Profs. Milind Kulkarni, Stanley Chan, Chris Brinton, David Inouye, Qiang Qiu)

classification: k-nearest neighbor

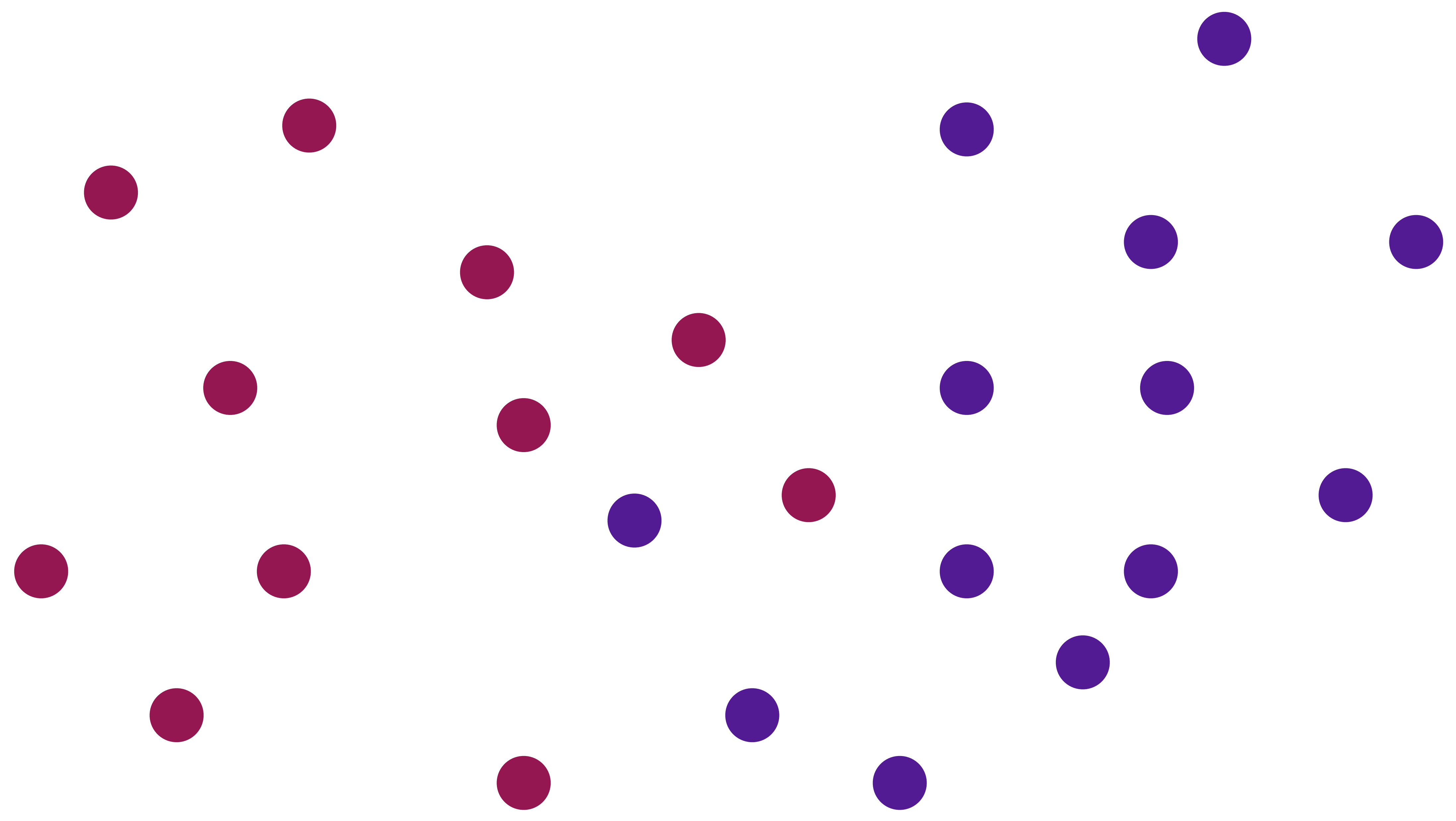
k-nearest neighbor

- Naïve Bayes is a nice classifier, but it is *parametric*
    - We must have a model of the data in mind, and some prior knowledge, to use it effectively.
- What if we don't have any such knowledge? What if all we have is our input data, and it does not seem to fit any existing distribution well?
- **k-nearest neighbor** (**kNN**) is a classifier that requires no assumptions about the data:
    - Look at the classes of the k-nearest points and pick the most frequent one



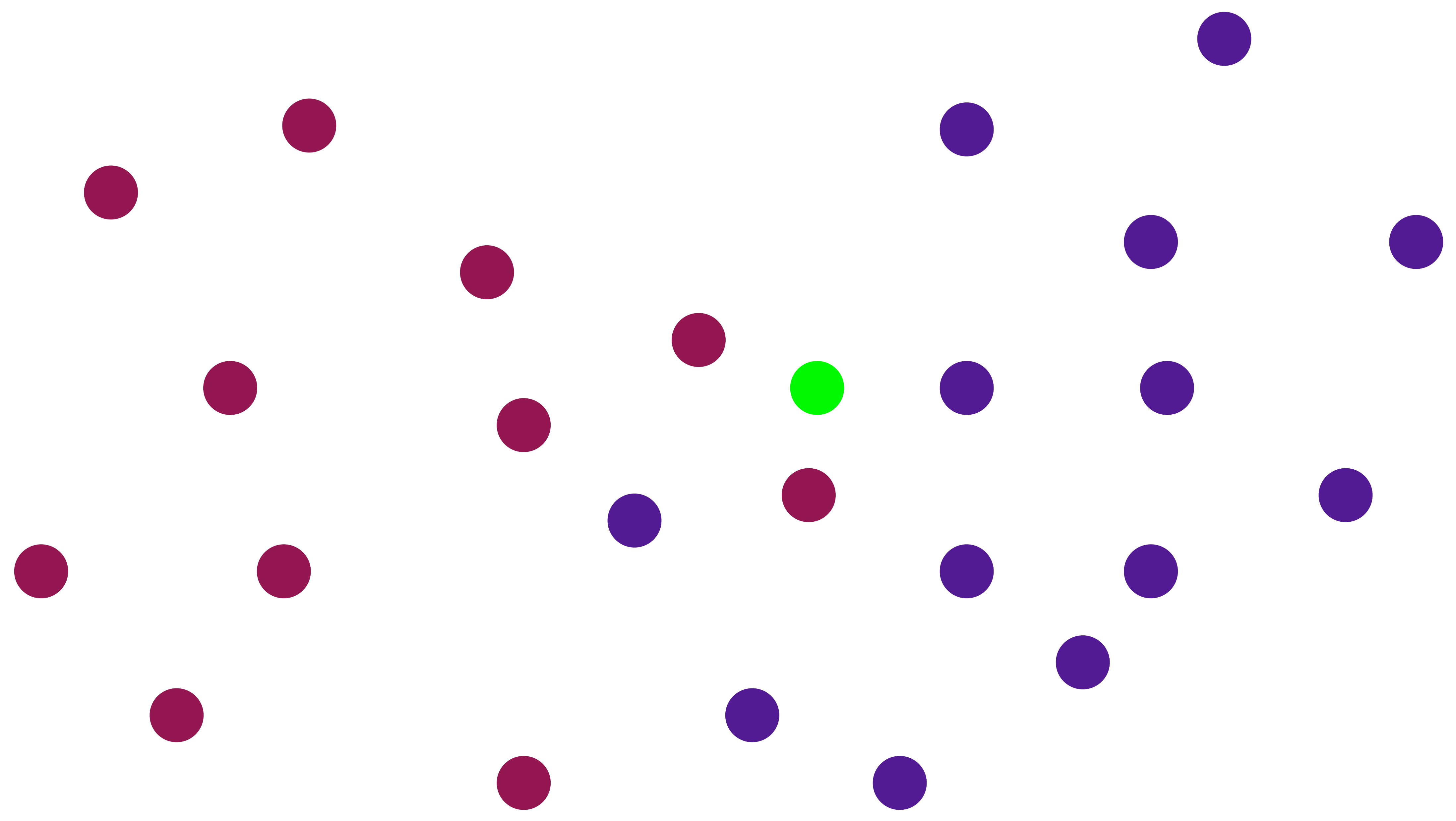
kNN algorithm

- Start with labeled training data, just like naïve Bayes



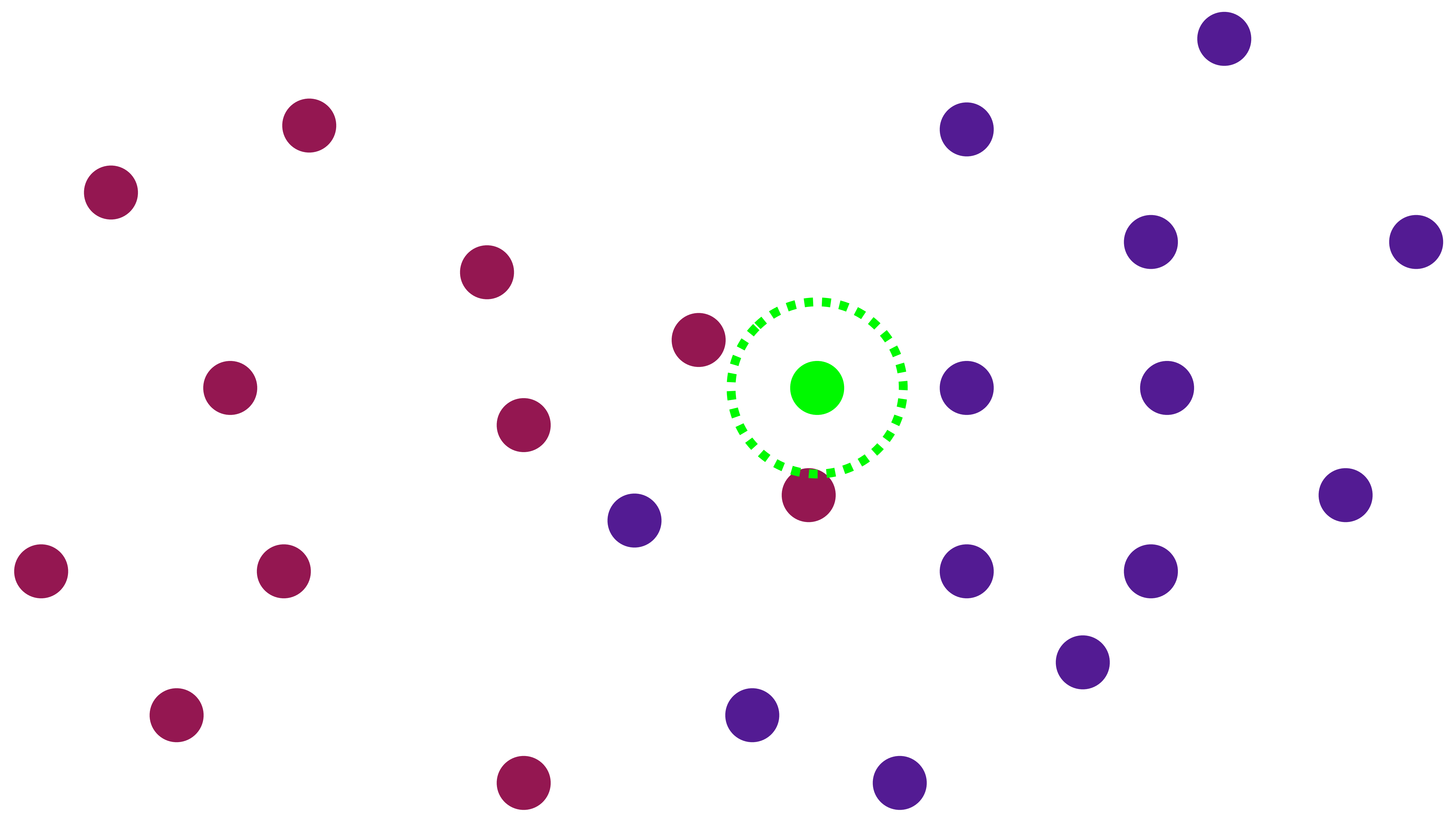
kNN algorithm

- Take new data point



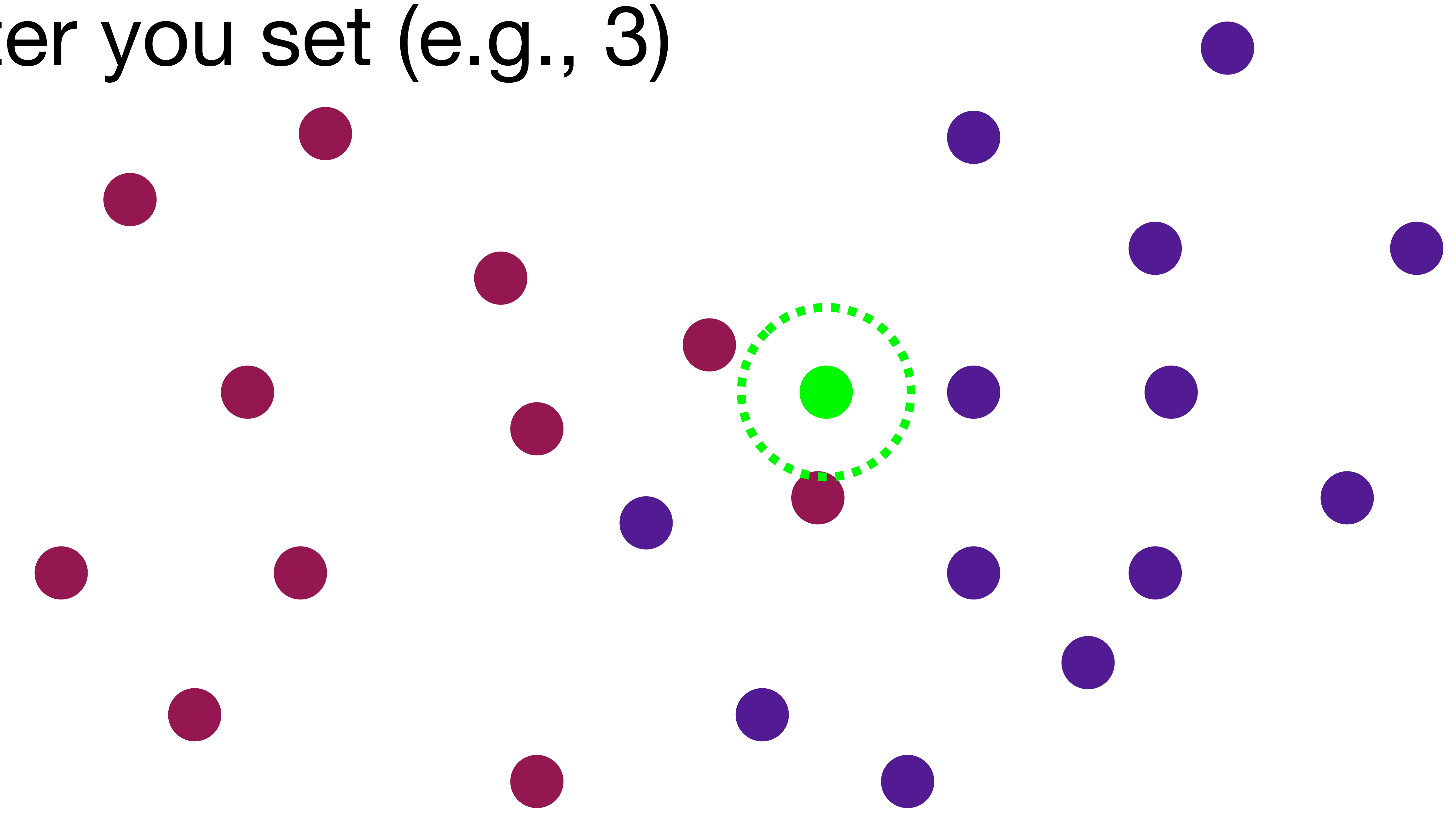
kNN algorithm

- Draw a circle around it



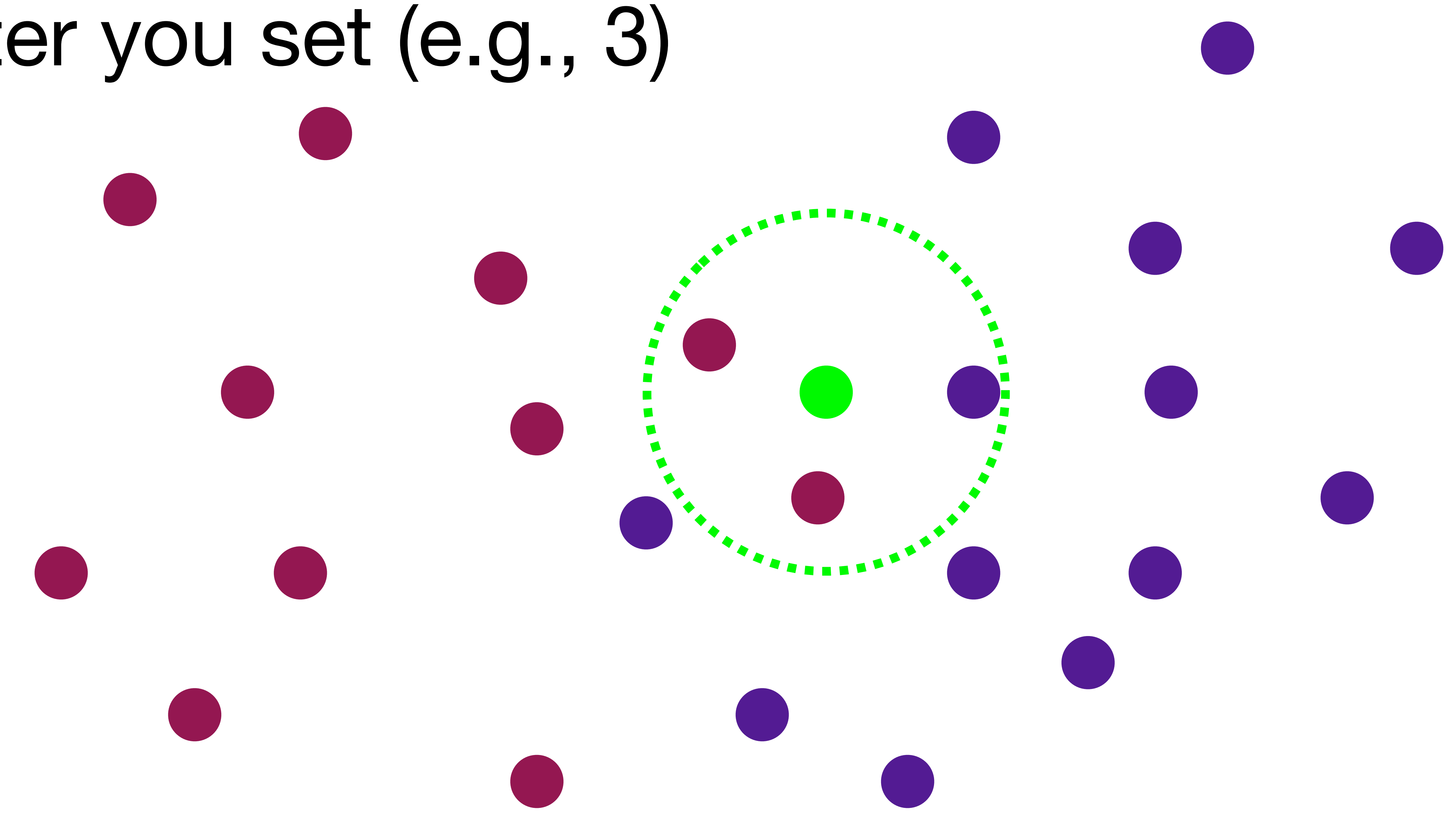
kNN algorithm

- Grow the circle until it has *k* other points in it
    - *k* is a parameter you set (e.g., 3)



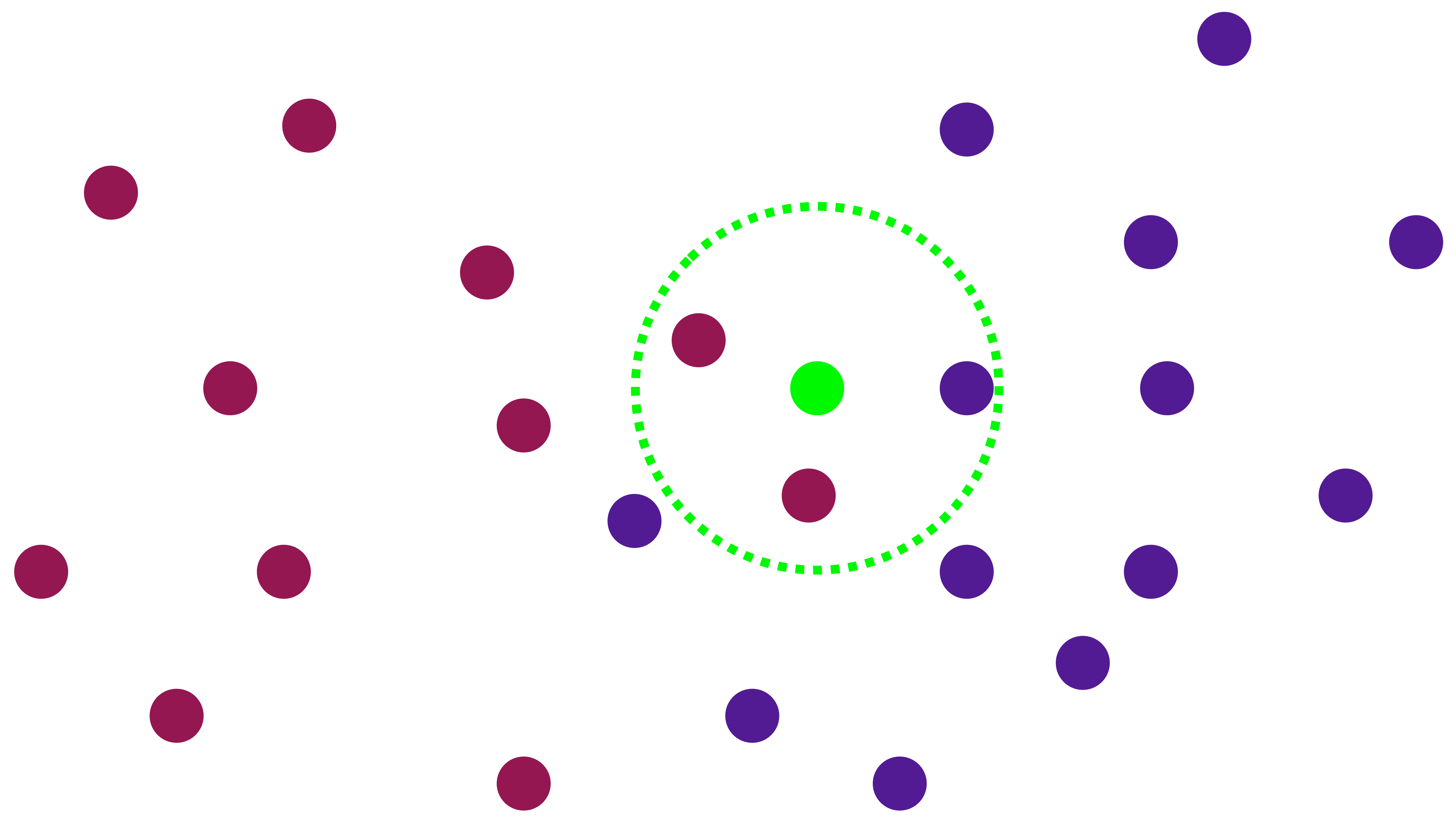
kNN algorithm

- Grow the circle until it has *k* other points in it
  - *k* is a parameter you set (e.g., 3)



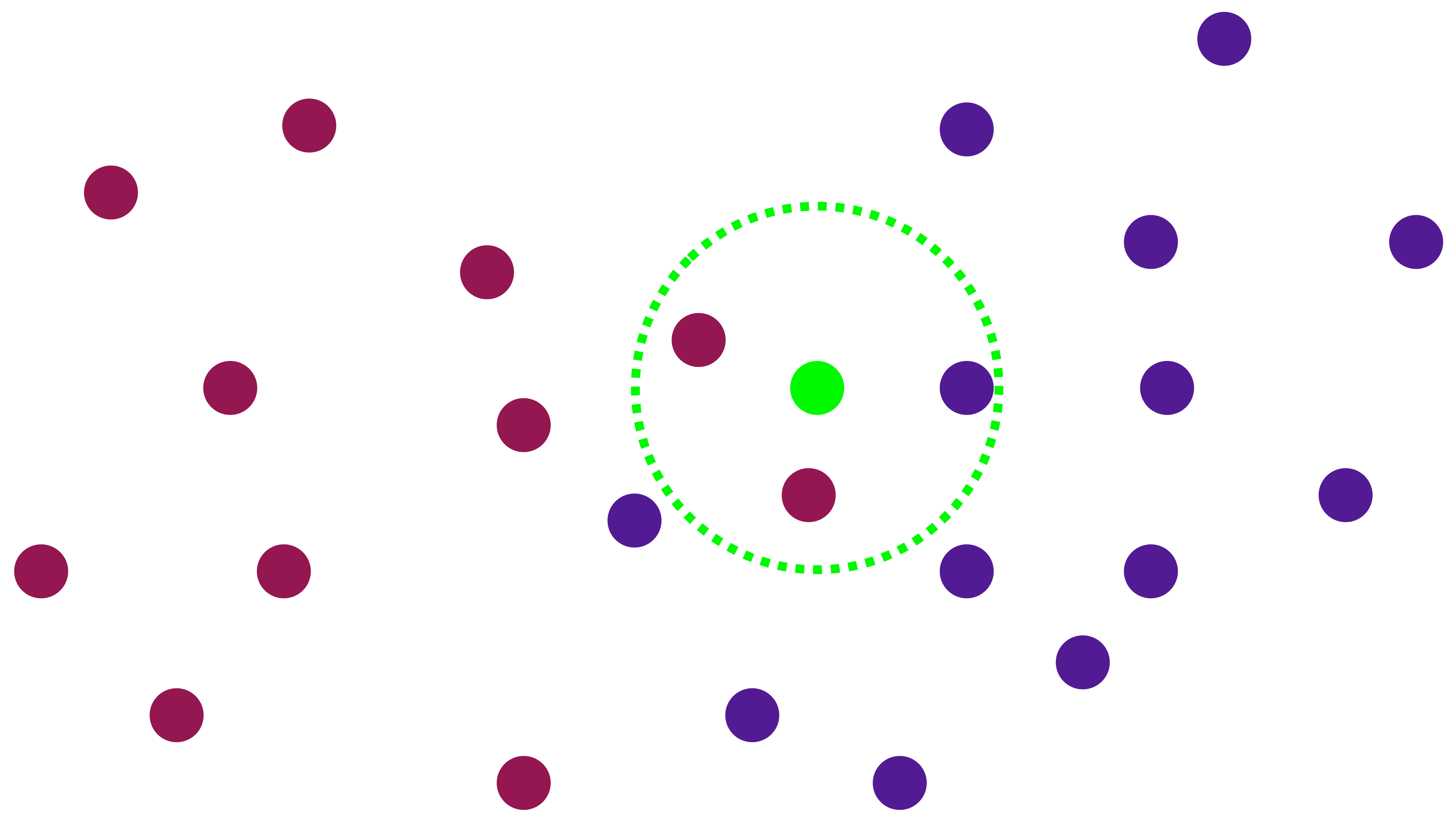
kNN algorithm

- Count how many points from **class 1** are in the circle and how many from **class 2**
  - **Majority wins**



kNN algorithm

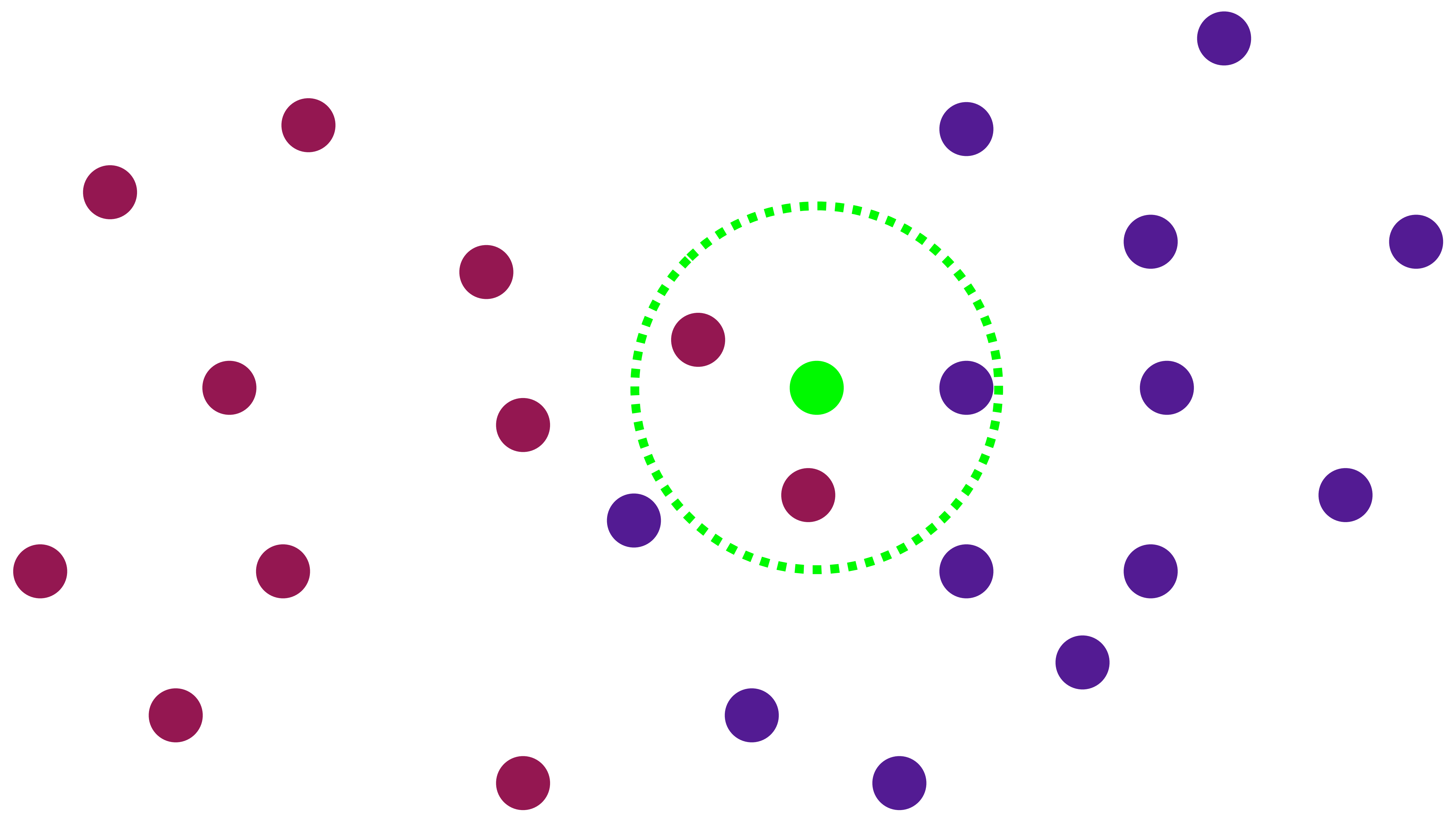
- Count how many points from **class 1** are in the circle and how many from **class 2**
  - **Majority wins**



- How to choose k?
  - Larger k means we are less sensitive to outliers, but also less sensitive to possibly informative (very near) neighbors
  - Cross validation!

formal algorithm and python

- Algorithmic interpretation:
  - Find the distance $||x - x_0||$ from **new point** x_0 to every other point x
  - Sort by distance, pick closest k points
  - Predicted class is the one with the most "votes" from these k
- In Python
  - `from sklearn.neighbors import KNeighborsClassifier`
  - https://scikit-learn.org/stable/modules/classes.html#module-sklearn.neighbors



pros vs cons

+ Simple concept for classifier
+ No models or prior knowledge required
- Expensive to use model (compute distances from all other points)
- Does not help with missing data (classifier is only as good as labeled training data)
- The intuition and usefulness can breakdown in high dimensions (what does it mean to “near” in 1000 dimensions?)

binary evaluation metrics

- With regression, we used MSE (and r^2) as our evaluation metrics

- In classification, these are not valid, because our predictions are either right or wrong

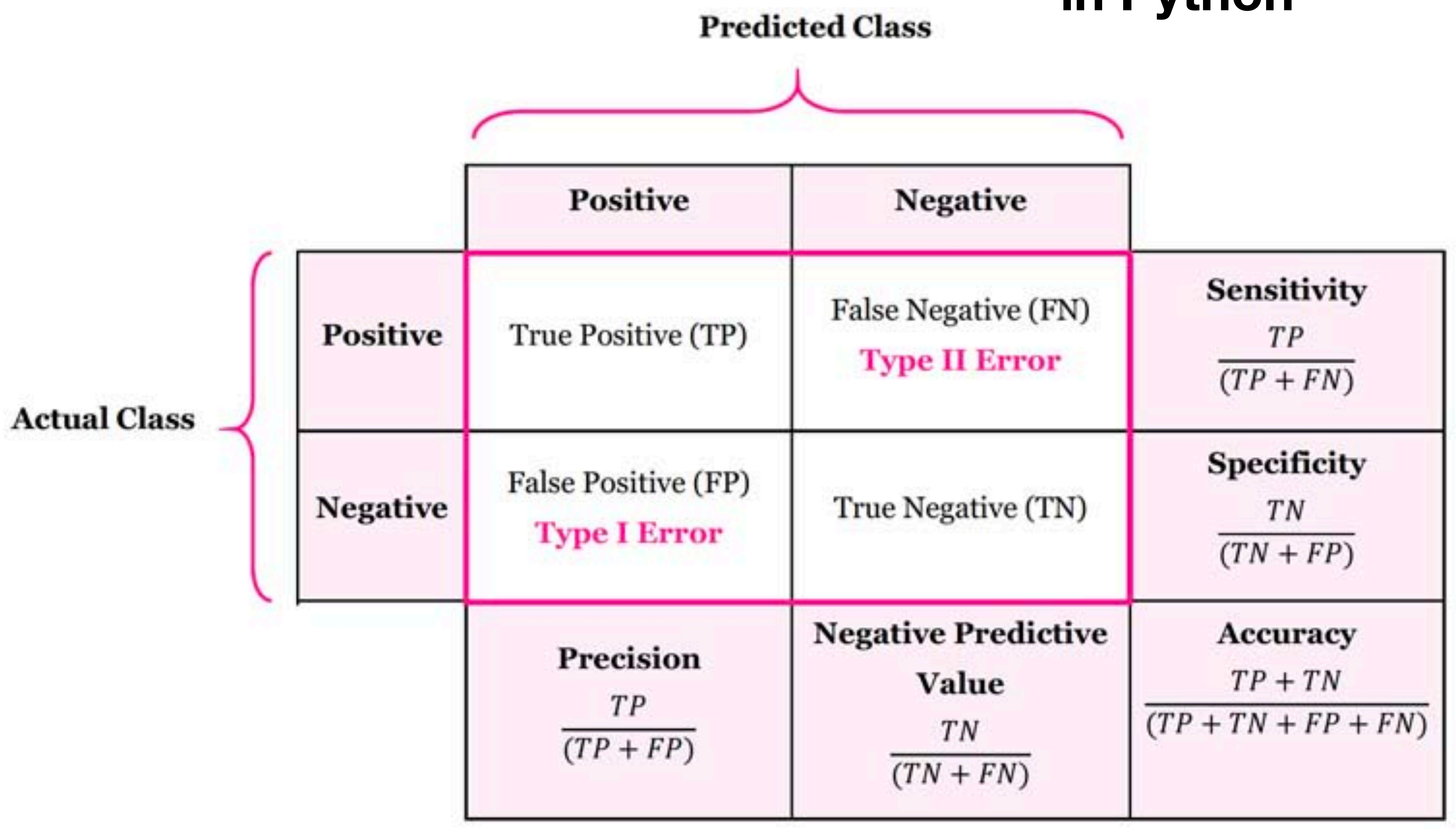
- For binary classification, we typically report several metrics (on a test set), based on a **confusion matrix** (shown to the right). The most common three are:

  - **Accuracy**: Fraction of correct predictions

  - **Precision**: Fraction of correct predictions in the predicted positive class

  - **Recall** (or **sensitivity**): Fraction of correct predictions in the actual positive class

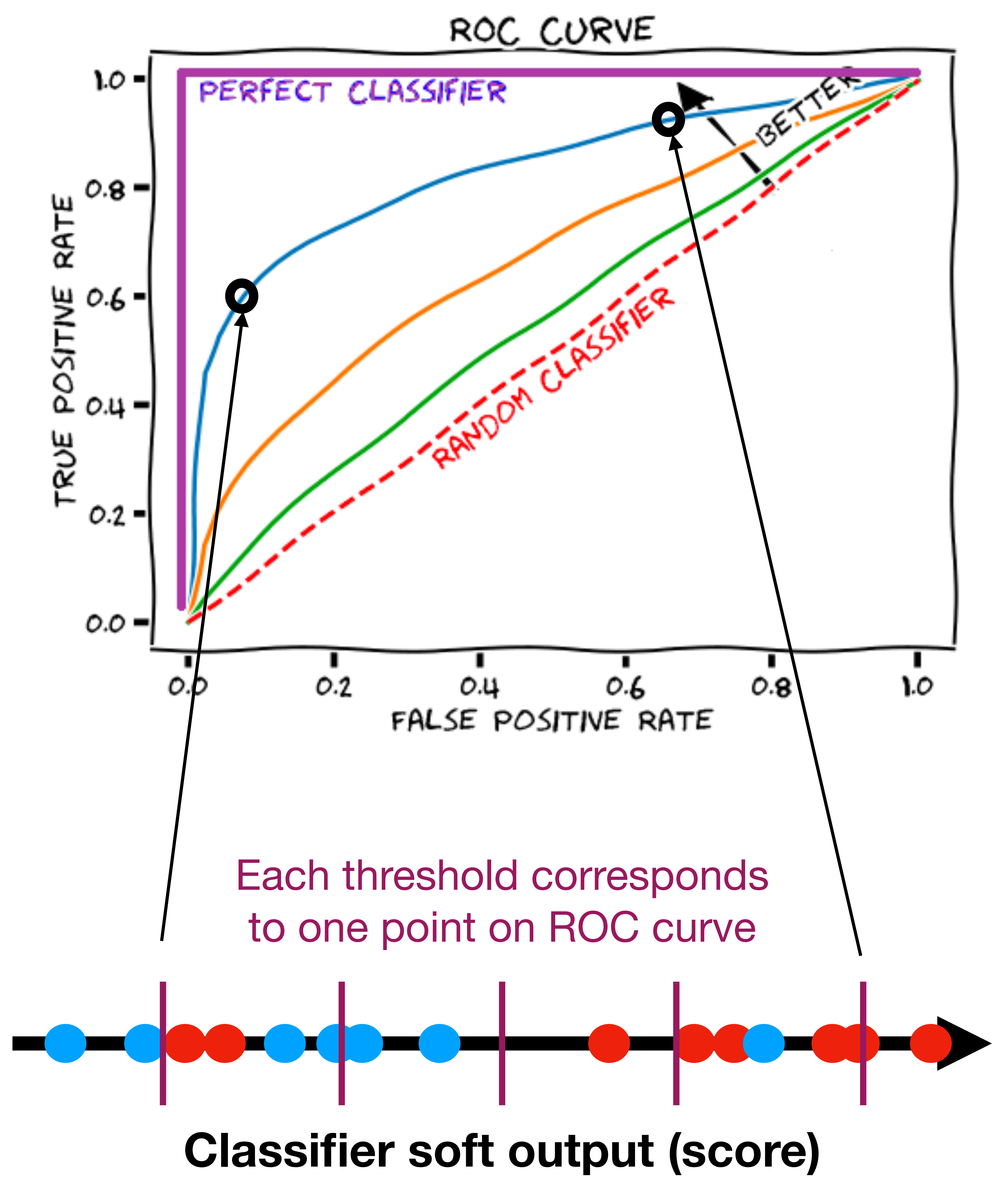
see `sklearn.metrics` in Python



		Predicted Class		
		Positive	**Negative**	
Actual Class	**Positive**	True Positive (TP)	False Negative (FN) **Type II Error**	**Sensitivity** $\frac{TP}{(TP+FN)}$
	Negative	False Positive (FP) **Type I Error**	True Negative (TN)	**Specificity** $\frac{TN}{(TN+FP)}$
		Precision $\frac{TP}{(TP+FP)}$	**Negative Predictive Value** $\frac{TN}{(TN+FN)}$	**Accuracy** $\frac{TP+TN}{(TP+TN+FP+FN)}$

composite binary metrics

- In regression problems, MSE is convenient: Single number that indicates quality
- With classification problems, none of these confusion table metrics tell the whole story:
  - If there is significant **class imbalance**, accuracy can look very good even if the classifier is not
  - For example, suppose 90% of cars are minivans and 10% are sports cars. If we always predict minivan, we will have 90% accuracy!
- There are two composite metrics that can be useful:
  - **F1 score**: Harmonic mean between precision and recall (both need to be high for the F1 score to be high)
  - **AUROC**: Area under true/false positive curve from varying decision threshold from 0 (predict all negatives) and 1 (predict all positives)


ROC CURVE
PERFECT CLASSIFIER
BETTER
RANDOM CLASSIFIER
TRUE POSITIVE RATE
FALSE POSITIVE RATE
0.0
0.2
0.4
0.6
0.8
1.0
Each threshold corresponds to one point on ROC curve
Classifier soft output (score)