CS M146: Introduction to Machine Learning
k-Nearest Neighbors

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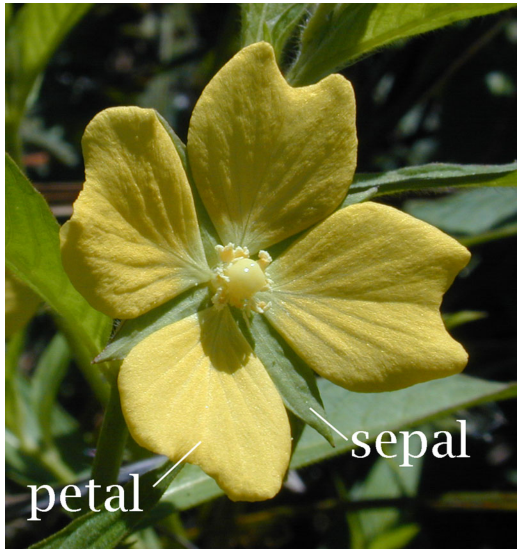
Example: Recognizing flowers

3 types of iris (classes): setosa, veriscolor, virginica

Measuring the properties of flowers

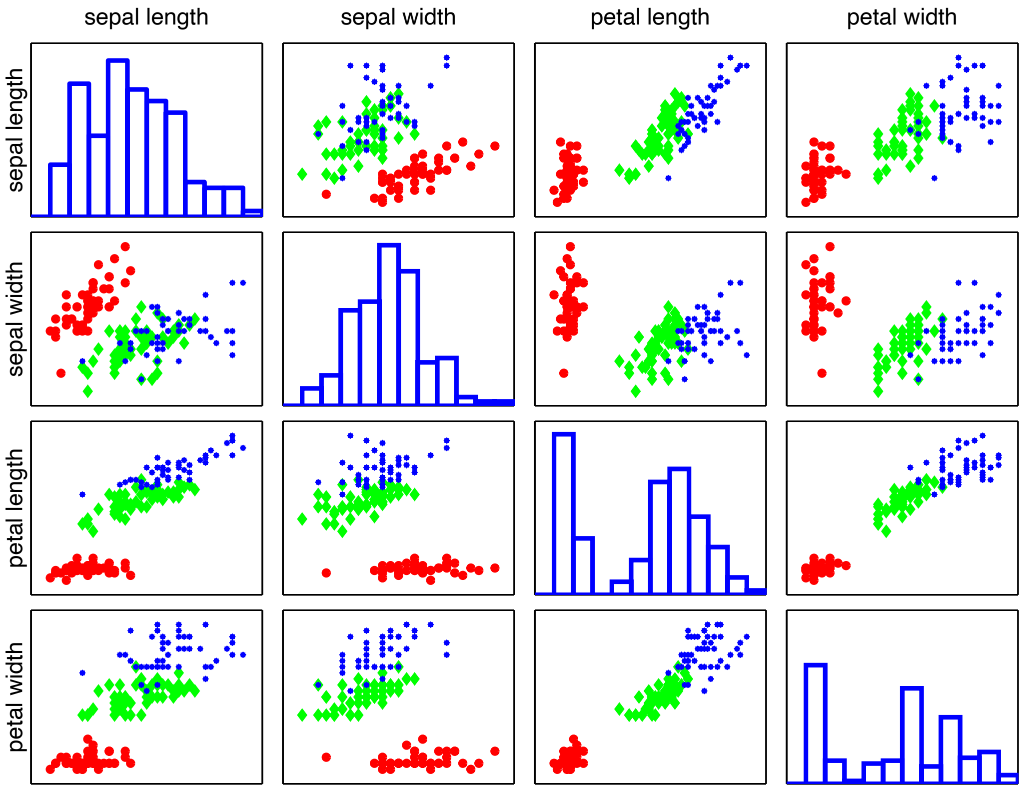
Features: the widths and lengths of sepal and petal

4 features (sepal width, sepal length, petal width, petal length)



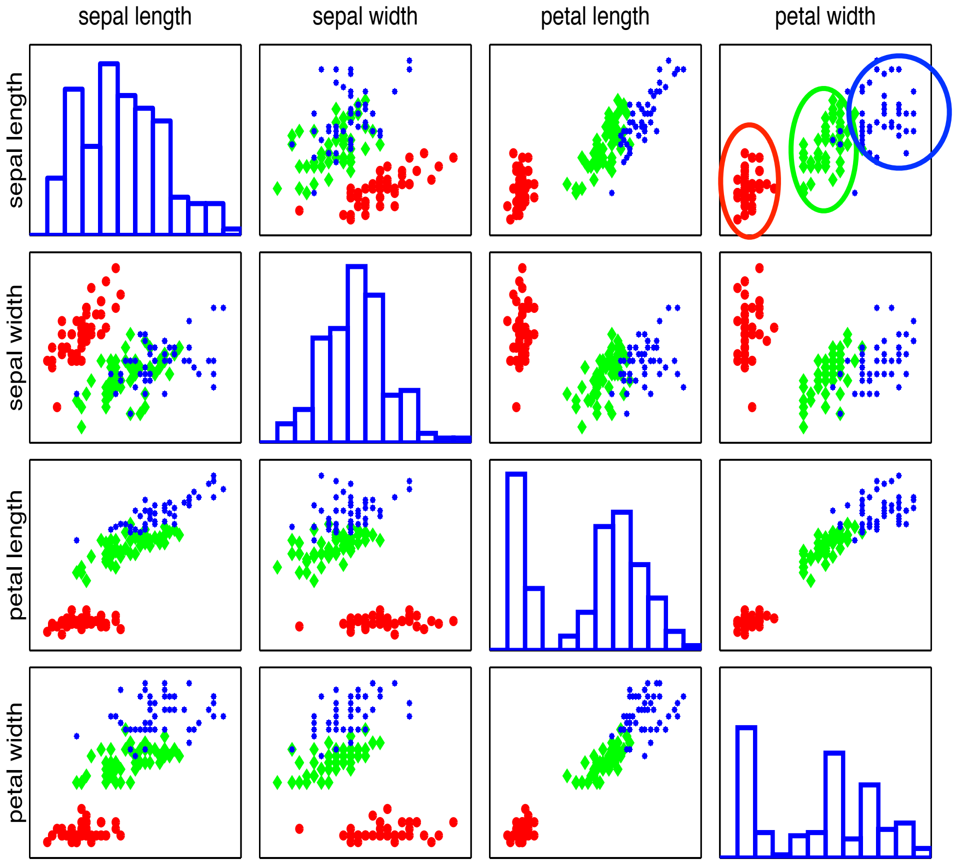
Data Visualization

Each colored point is an instance of a flower: setosa, versicolor, virginica



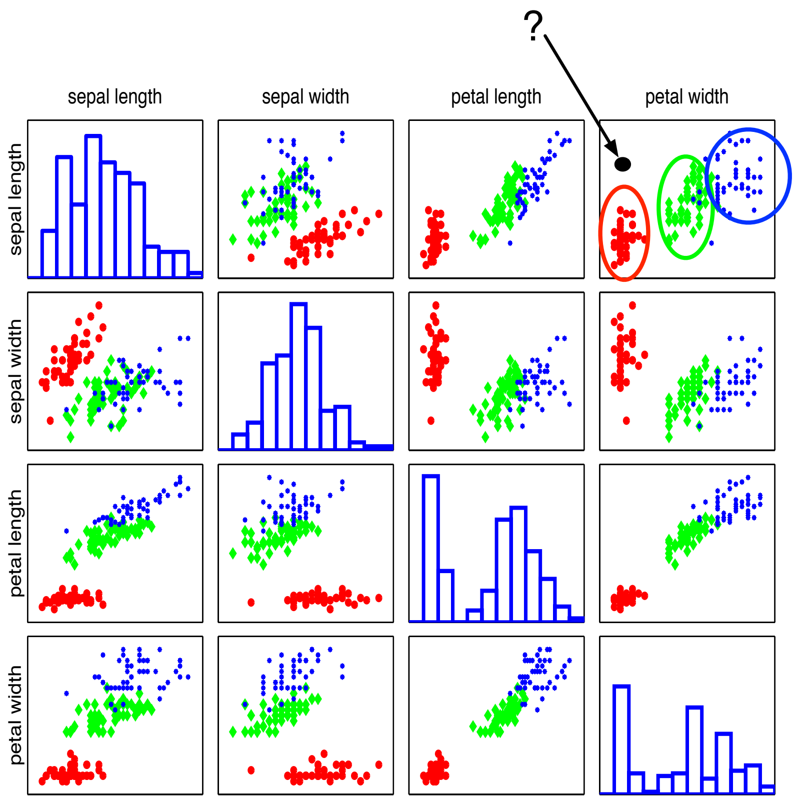
Different types seem well-clustered

Using two features: petal width and sepal length



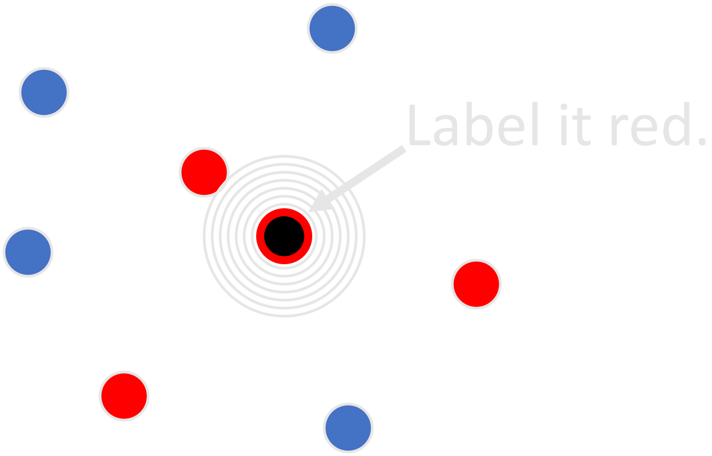
Labeling an unknown flower type

Close to red cluster: so labeling it as setosa



1-Nearest Neighbor

- One of the simplest of all machine learning classifiers
- Idea: label a new point the same as the closest known point



1-Nearest Neighbor

- **Nearest neighbor** is an index to a training instance

$$nn(\boldsymbol{x}) = [i] \text{ where } i \in \{1, 2, \cdots, n\}$$

- To compute nearest neighbor, we need a notion of **distance** between two points, e.g., squared Euclidean (or ℓ_2) distance

$$nn(\boldsymbol{x}) = \underset{i \in [n]}{\operatorname{argmin}} \sum_{j=1}^{d} (x_j - x_j^{(i)})^2$$

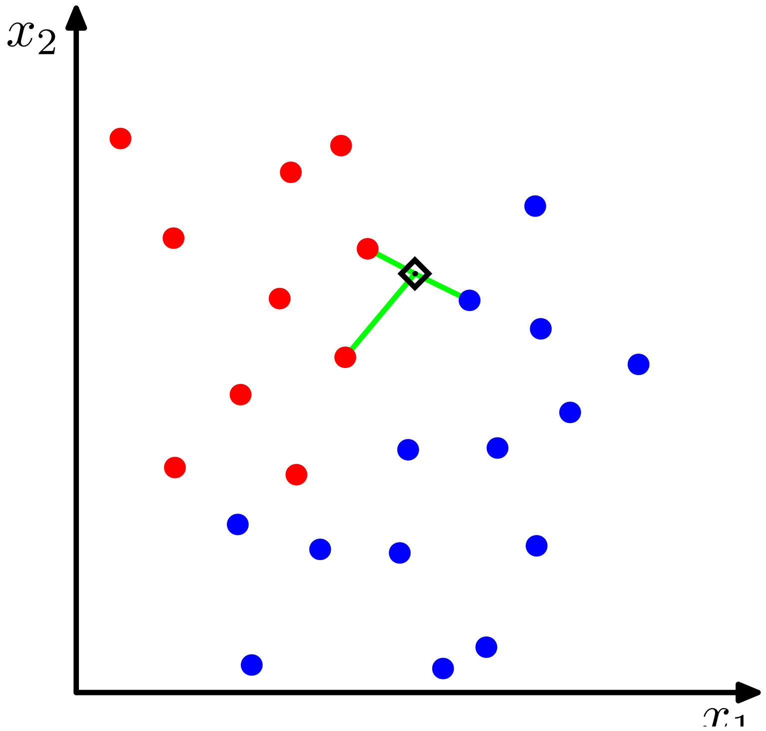
- Classification rule assigns the label of the nearest neighbor

$$h(\boldsymbol{x}) = y_{nn(\boldsymbol{x})}$$

- A type of **non-parametric classifier** (no parameters!)

Visual example

In this 2-dimensional example, the nearest point to $\boldsymbol{x}$ is a red training instance. Thus, $\boldsymbol{x}$ will be labeled red.



Example: classify iris with two features

Training data

ID (n)	petal width (x_1)	sepal length (x_2)	category (y)
1	0.2	5.1	setosa
2	1.4	7.0	versicolor
3	2.5	6.7	virginica

Flower with unknown category

petal width = 1.8, sepal length = 6.4

Calculating distance

ID	distance
1	1.75
2	0.72
3	0.76

Thus, the category is versicolor

How to measure distances?

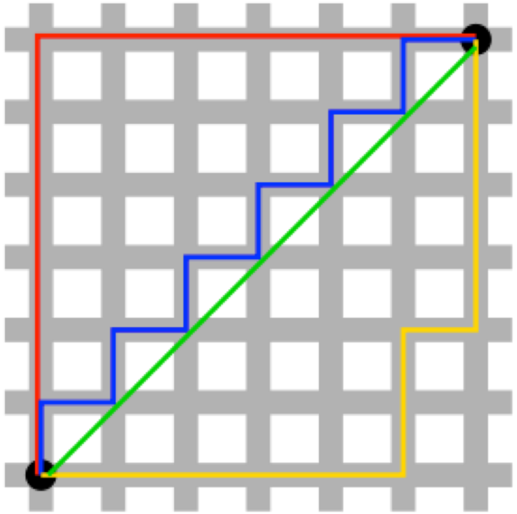
Previously, we used squared Euclidean distance.

$$nn(\boldsymbol{x}) = \underset{i\in[n]}{\operatorname{argmin}} \sum_{j=1}^{d}(x_j - x_j^{(i)})^2$$

Alternative distances

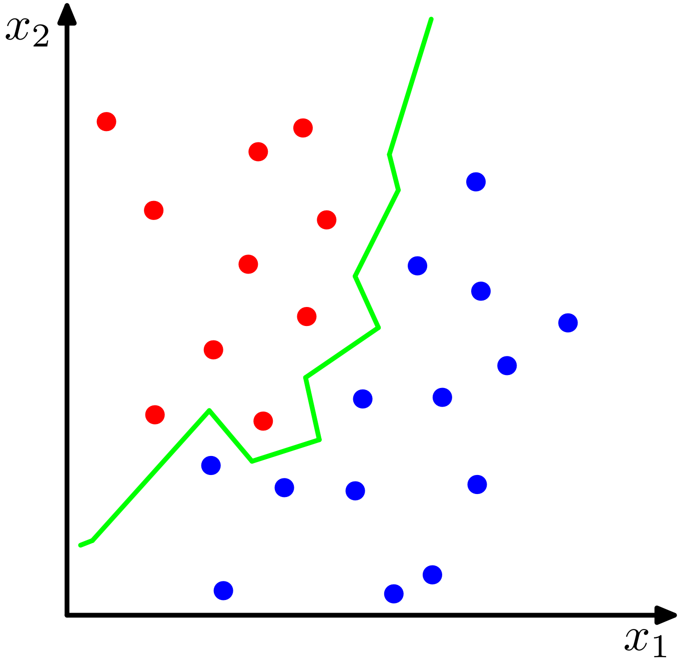
L1 distance

$$nn(\boldsymbol{x}) = \underset{i\in[n]}{\operatorname{argmin}} \sum_{j=1}^{d} | x_j - x_j^{(i)} |$$



Decision boundary

For every point in the space, we can determine its label using the nearest neighbor rule. This gives rise to a decision boundary that partitions the space into different regions.



(b)

k-Nearest Neighbor (kNN) classification

Increase the number of neighbors

1st nearest neighbor

$$nn_1(\boldsymbol{x}) = \underset{i \in [n]}{\operatorname{argmin}} \left\| \boldsymbol{x} - \boldsymbol{x}^{(i)} \right\|_2^2$$

2nd nearest neighbor

$$nn_2(\boldsymbol{x}) = \underset{i \in [n] - nn_1(\boldsymbol{x})}{\operatorname{argmin}} \left\| \boldsymbol{x} - \boldsymbol{x}^{(i)} \right\|_2^2$$

3rd nearest neighbor

$$nn_3(\boldsymbol{x}) = \underset{i \in [n] - nn_1(\boldsymbol{x}) - nn_2(\boldsymbol{x})}{\operatorname{argmin}} \left\| \boldsymbol{x} - \boldsymbol{x}^{(i)} \right\|_2^2$$

The set of k nearest neighbors

$$knn(\boldsymbol{x}) = \{nn_1(\boldsymbol{x}), nn_2(\boldsymbol{x}), \cdots, nn_k(\boldsymbol{x})\}$$

k-Nearest Neighbor (kNN) classification

Classification rule

- Every neighbor votes
- Use majority vote

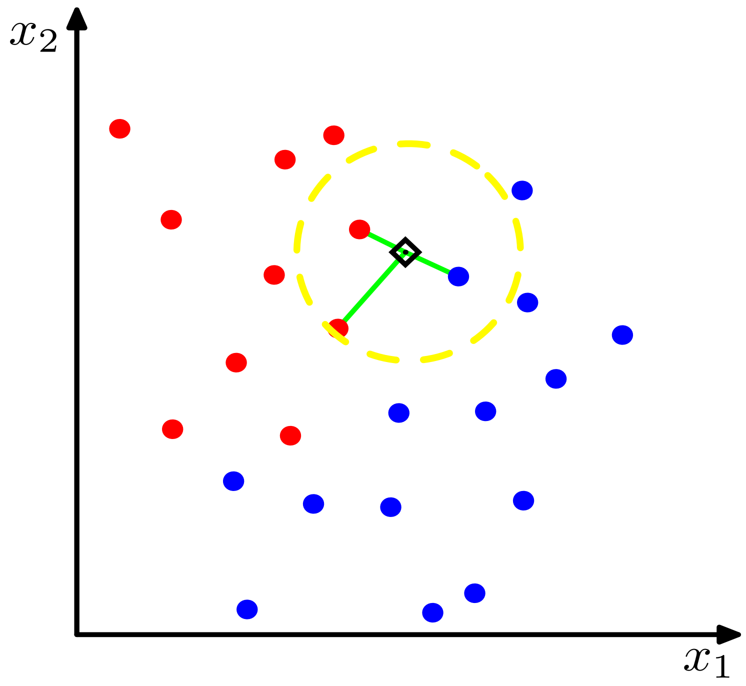
$$h(x) = \text{majority}\{y_{nn_1(\boldsymbol{x})}, y_{nn_2(\boldsymbol{x})}, \cdots, y_{nn_k(\boldsymbol{x})}\}$$

Note:

- kNN assumes all features are equally useful for classification
- Scale of measurement matters
  - Different nearest neighbors if you have {petal width, sepal length} vs {5 petal width, sepal length}

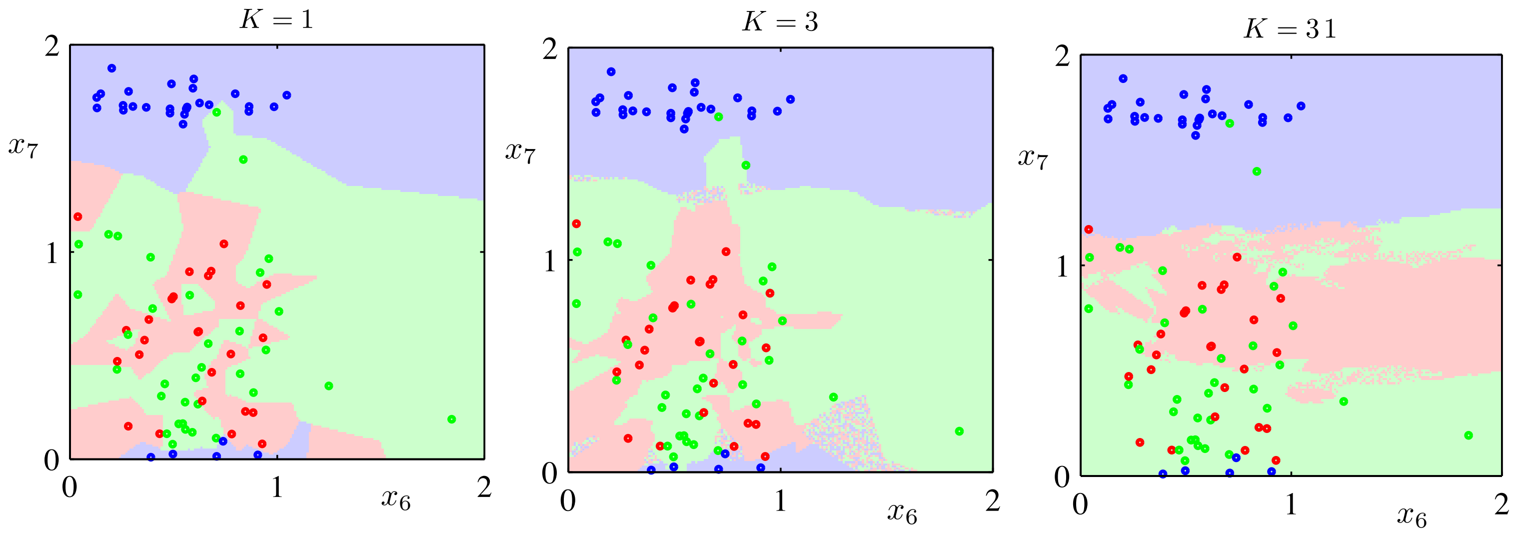
Example

$k = 1$, Label: Red $\quad k = 3$, Label: Red $\quad k = 5$, Label: Blue



How to choose an optimal k? Treat as hyperparameter and validate

Voronoi Diagrams for kNN



- Assign colors to training points based on their class labels
- For every other point, color it with the same color as its k nearest neighbors

Summary

Advantages of kNN

- conceptually simple and easy to implement – just computing the distance
- **non-parameteric** (no parameters, no optimization needed)

Disadvantages

Computationally intensive for large-scale (high dimensionality, high training instances problems

- $O(nd)$ for labeling a data point

Memory intensive

- Need to store the training data even during testing

Needs a suitable notion of distance for computing nearest neighbors

- not always easy for certain data types, e.g., images