APL 405: Machine Learning for Mechanics

Lecture 3: k-Nearest Neighbour

by

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Supervised Learning: Recap

Supervised Learning

Learning (training, estimating) a function (or model) f so that it best fits the relationship between

- the input $\mathbf{x}$, and
- the output y

from observed training data (the individual data points are assumed to be (probabilistically) ***independent***)

$$D_{\text{train}} = \left\{\left(\mathbf{x}^{(1)}, y^{(1)}\right), \left(\mathbf{x}^{(2)}, y^{(2)}\right), \cdots, \left(\mathbf{x}^{(N)}, y^{(N)}\right)\right\}$$

End goal will be to construct an output prediction $\hat{y}(\mathbf{x}^*)$ for unseen input $\mathbf{x}^*$ so that it is close to y^*

Types of Supervised learning: **Classification** and **Regression**

- Output variable y? → **categorical** → **Classification**
- Output variable y?→ **numerical** → **Regression**
- Input variable can be categorical or numerical or mix of both

Supervised Learning: Recap

- **Parametric vs Non-parametric models**

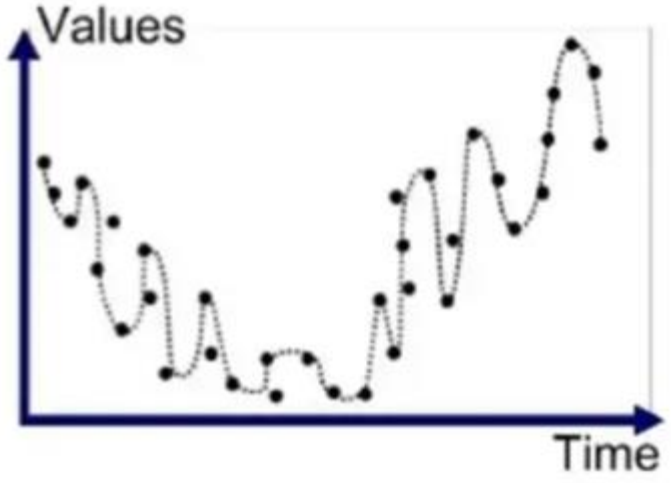
- Prediction errors caused due to **bias**, **variance** and **irreducible** errors

- Bias make algorithms easier to understand but are generally less flexible
  - Low bias: Suggests less assumptions about the function f
  - High bias: Suggests more assumptions about the function f

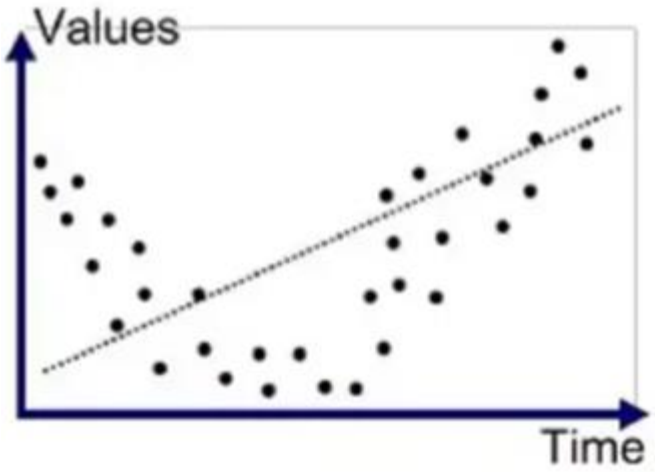
- Machine learning algorithms that have a high variance are strongly influenced by the specifics of the training data
  - Low variance: Suggests small changes to the estimated function f with changes to the training dataset
  - High variance: Suggests large changes to the estimated function f with changes to the training dataset

Overfit vs Underfit

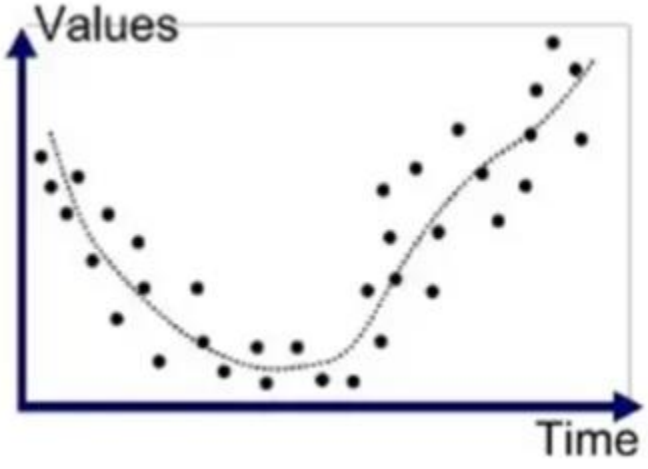
- **Overfitting** refers to the phenomenon when a model fits the training data "too well"
  - It happens when a model learns the detail and noise in the training data. This means that the noise or random fluctuations in the training data is picked up and learned as concepts by the model.
  - Models that have high variance and low bias leads to overfitting
  - Does not generalize to new unseen data well



Overfitting



Underfitting



Balanced fit

- **Underfitting** refers to the phenomenon when a model is unable to fit to the training data
  - It happens when a model is "too rigid"
  - Models that have high bias and low variance leads to underfitting
  - Does not generalize to new unseen data well

Introduction to k-Nearest Neighbours (k-NN)

- We will start with the relatively simple k-nearest neighbours (k-NN) method.

  Can be used for *both* regression and classification

- Most ML algorithms are based on the intuition that *if the unseen data point* $\mathbf{x}^*$ *is close to training data point* $\mathbf{x}^{(i)}$*, then the prediction* $\hat{y}(\mathbf{x}^*)$ *should be close to* $\mathrm{y}^{(i)}$.

- A simple way to implement this idea is to find the "nearest" training data point
  - Compute the Euclidean† distance between the unseen input and all training inputs.

$$\text{The } i\text{th Euclidean distance: } \left\|\mathbf{x}^{(i)} - \mathbf{x}^*\right\|_2 = \sqrt{\left(x_1^{(i)} - x_1^*\right)^2 + \left(x_2^{(i)} - x_2^*\right)^2 + \cdots + \left(x_p^{(i)} - x_p^*\right)^2}$$

  - Find the data point $\mathbf{x}^{(j)}$ with the *shortest distance* to $\mathbf{x}^*$, and use its output as the prediction, $\hat{y}(\mathbf{x}^*) = y^{(j)}$

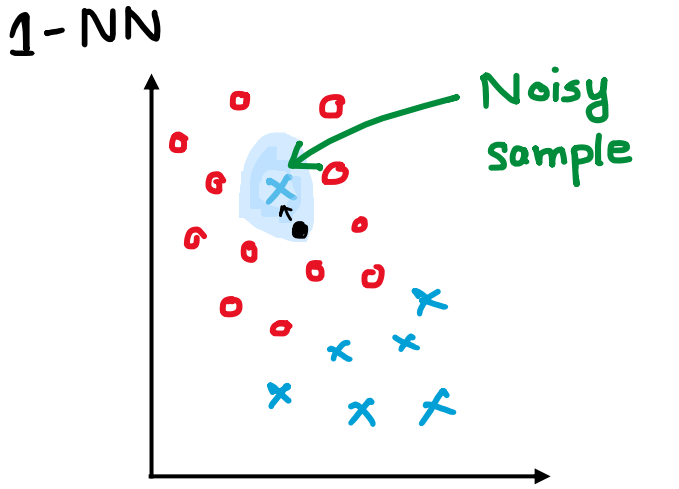
- This is the 1-nearest neighbour algorithm

† There are many other distances: Manhattan, Mahalanobis, cosine similarity, etc. Use Manhattan if inputs variables are not similar in type (such as age, gender, height, etc.)

Introduction to k-Nearest Neighbours (k-NN)

- In practice we can rarely say *for certain* what the output value y will be!
- Mathematically, we handle this by describing y as a random variable. That is, we consider the data as *noisy*, meaning that it is affected by random errors referred to as noise.

- **Shortcoming**: 1-nearest neighbour algorithm is sensitive to **noise** in data and **mis-labelled** data



Every test example in the blue shaded area will be mis-classified as the blue class

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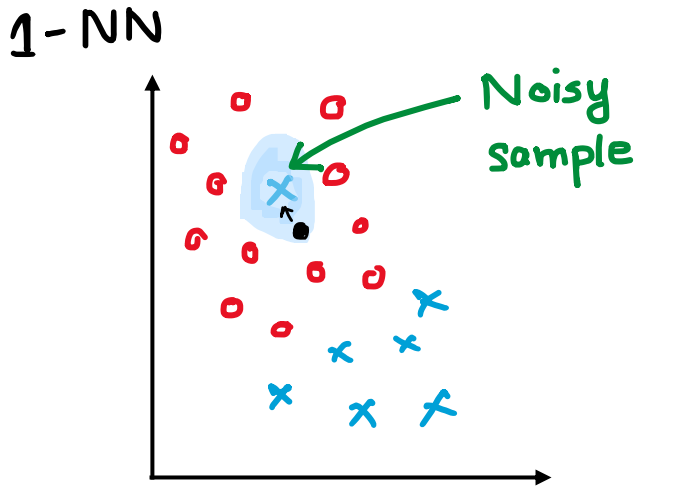
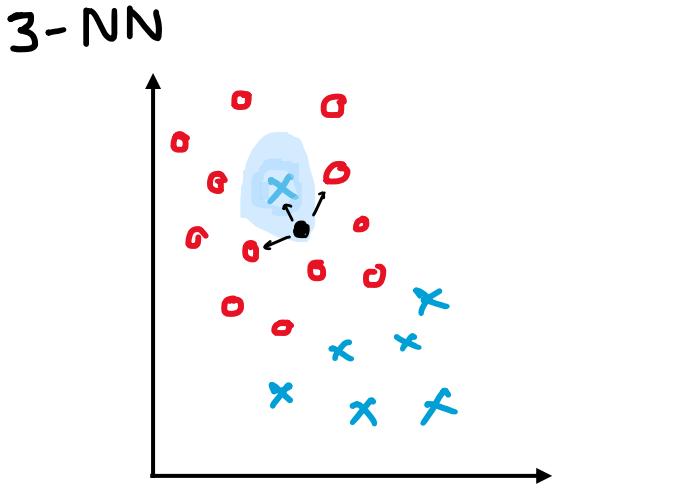


Every test example in the blue shaded area will be mis-classified as the **blue** class



Every test example in the blue shaded area will be classified as the **red** class

- **How to improve**: Use k-nearest neighbours to obtain a majority vote (or take an average)

Introduction to k-Nearest Neighbours (k-NN)

k-NN algorithm

Data: Training data $\left(\mathbf{x}^{(i)}, y^{(i)}\right)_{i=1}^{N}$ and unseen (test) input $\mathbf{x}^*$

Result: Predicted test output $\hat{y}(\mathbf{x}^*)$

1. Compute the distances $\left\|\mathbf{x}^{(i)} - \mathbf{x}^*\right\|_2$ for all training data points $i = 1,2,\cdots,N$
2. Find k examples $\left(\mathbf{x}^{(i)}, y^{(i)}\right)$ closest to the test instance $\mathbf{x}^*$
3. Compute the prediction $\hat{y}(\mathbf{x}^*)$

$$\hat{y}(\mathbf{x}^*) = \begin{cases} \text{Mean (or median) of } k \text{ closest examples} & (\textbf{Regression}) \\ \text{Majority vote (mode) of } k \text{ closest examples} & (\textbf{Classification}) \end{cases}$$

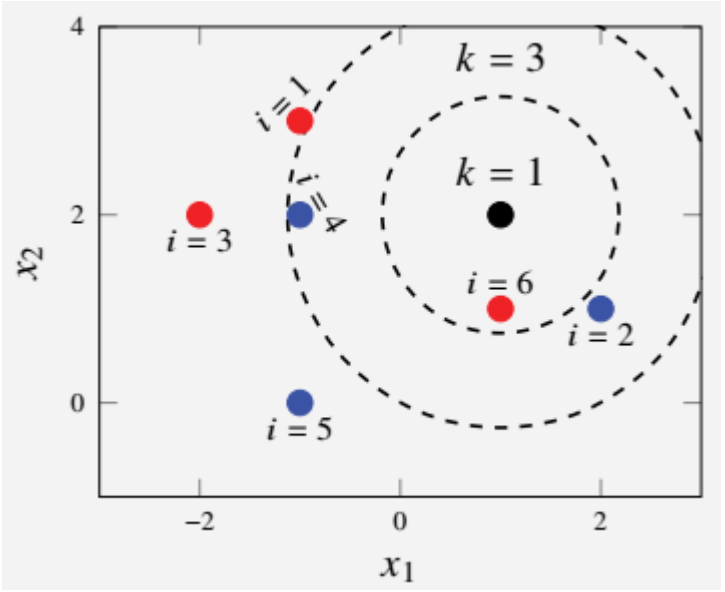
- k-NN is a non-parametric algorithm; makes no assumptions about the functional form and has no fixed set of parameters. Uses the entire training data when making predictions

Example of kNN for binary classification

i	x_1	x_2	y
1	-1	3	Red
2	2	1	Blue
3	-2	2	Red
4	-1	2	Blue
5	-1	0	Blue
6	1	1	Red

- Predict the output for $\mathbf{x}^* = [1 \quad 2]^T$
- Consider two different kNN classifiers
  - one using $k = 1$, and (result is red)
  - another using $k = 3$ (result is blue)

i	$\left\|\mathbf{x}^{(i)} - \mathbf{x}^*\right\|_2$	y_i
6	$\sqrt{1}$	Red
2	$\sqrt{2}$	Blue
4	$\sqrt{4}$	Blue
1	$\sqrt{5}$	Red
5	$\sqrt{8}$	Blue
3	$\sqrt{9}$	Red

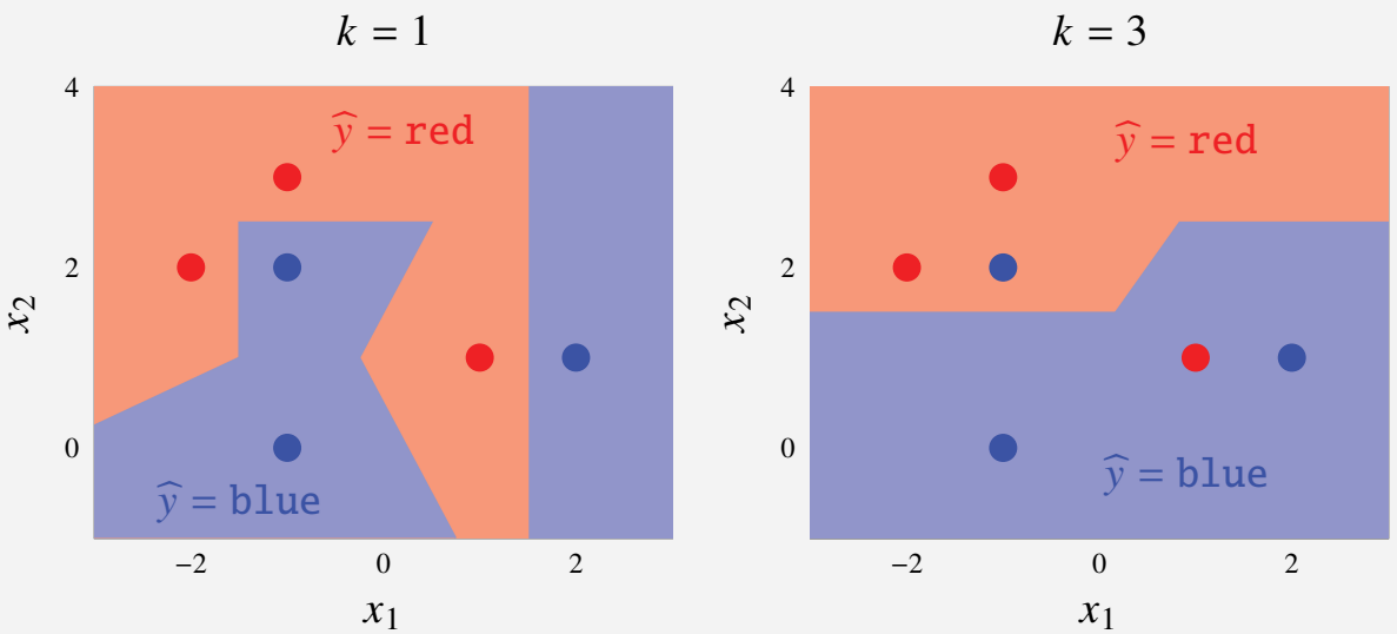


Decision boundary of a classifier

i	x_1	x_2	y
1	-1	3	Red
2	2	1	Blue
3	-2	2	Red
4	-1	2	Blue
5	-1	0	Blue
6	1	1	Red

- Predict the output for $\mathbf{x}^* = [1 \quad 2]^T$
- Consider two different kNN classifiers
  - one using $k = 1$, and
  - another using $k = 3$

- **Decision boundaries** are the points in input space where the class prediction changes, that is, the borders between different classes
- They can help to understand a classifier and given a concise summary of a classifier



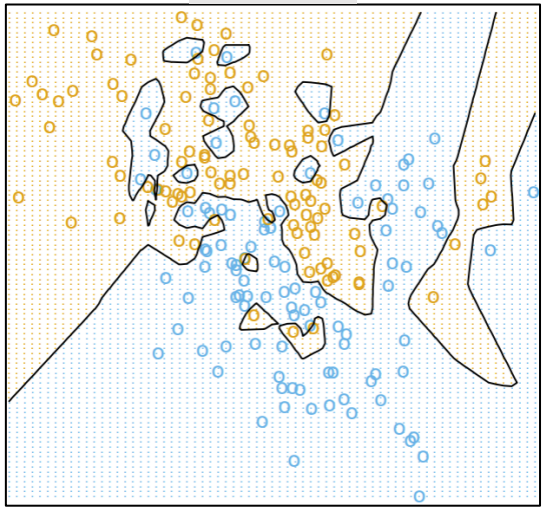
How to choose k?

- The number of neighbours k is chosen by the user

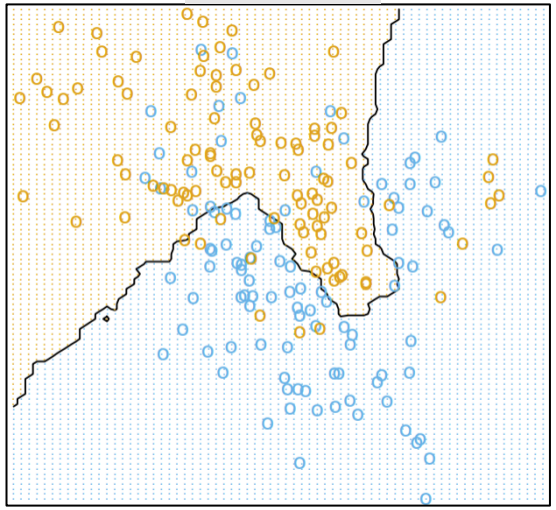
- Since it is not learned, it is not a parameter, and we refer to it as the **hyperparameter**

- The choice of hyperparameter k has a big impact on the predictions made by k-NN
  - Small k
    - Good at capturing fine-grained patterns
    - May **overfit**, i.e. be sensitive to random errors in the training data
  - Large k
    - Makes stable predictions by averaging over lots of samples
    - May **underfit**, i.e. fail to capture important patterns
  - Balancing k (trade-off between flexibility and rigidity)
    - Optimal choice of k depends on the number of data points N
    - Rule of thumb: choose $k < \sqrt{N}$
    - We can choose k using **cross-validation**

$k = 1$

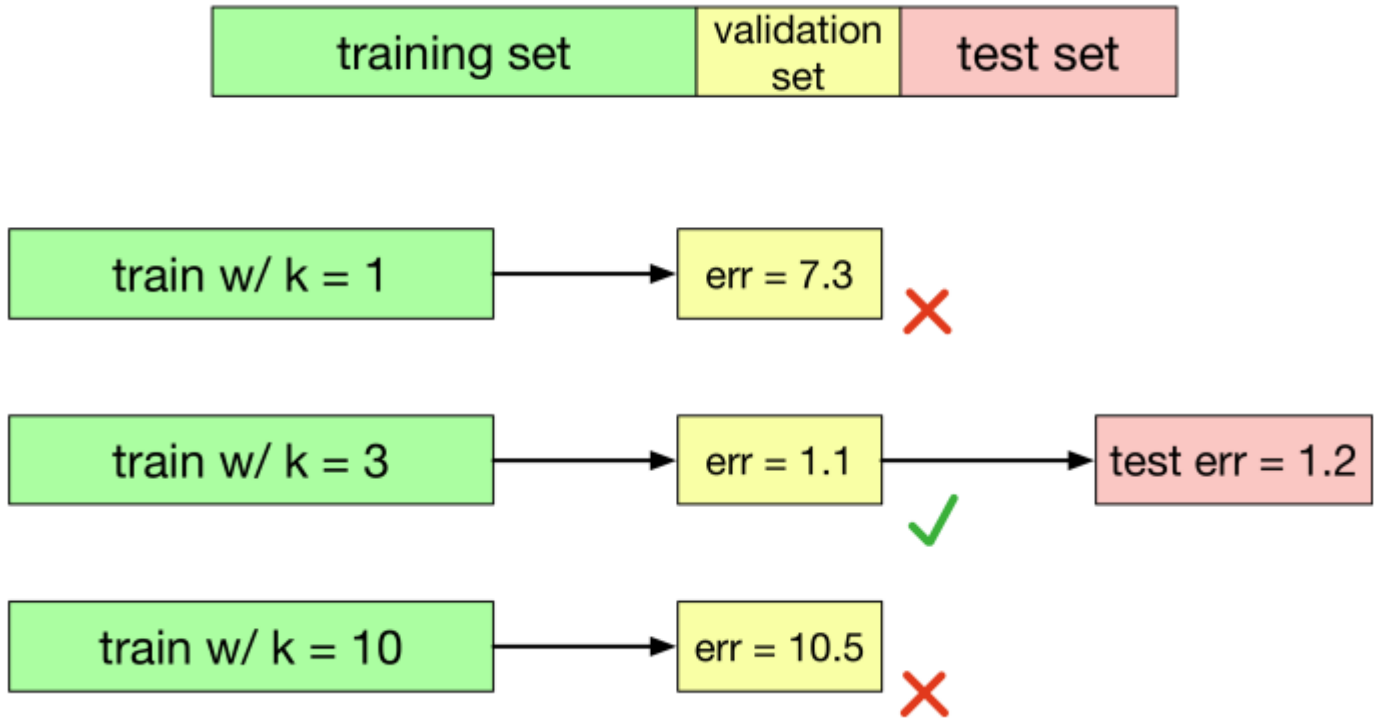


$k = 15$



Validation and Test sets

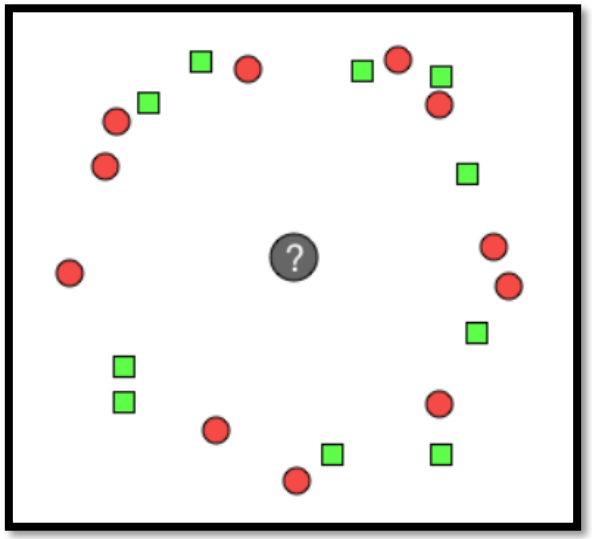
- We can tune the hyperparameters using a **validation set**:



- The **test set** is used only at the very end, to measure the generalization performance of the algorithm.

Pitfalls of kNN: Curse of dimensionality

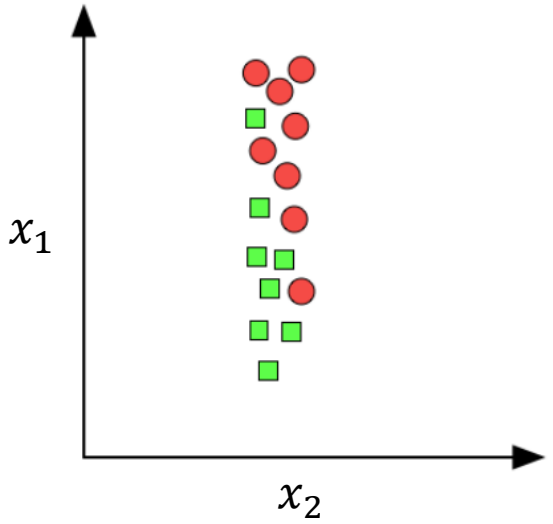
- kNN works well with a small dimension of inputs (e.g. 2-3), but struggles when the input dimension is high
- In high dimensions, “most” points are far apart and are approximately at the same distance
  - Hence, our intuition that works for distances in 2- and 3- dimensional spaces breaks down in higher dimensions



- We can show this by applying the rules of expectation and covariance of random variables (HW maybe)

Pitfalls of kNN: Normalization

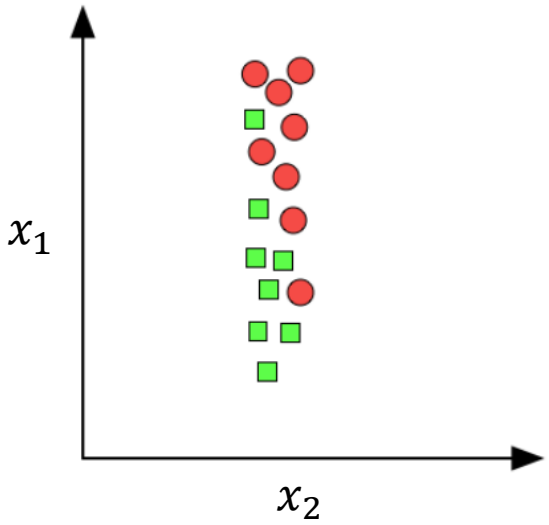
- kNN can be quite sensitive to the range of the input features
- Example, $\mathbf{x} = [x_1 \quad x_2]^T$, where x_1 is in the range [100, 1000] and the values of x_2 is in the range [0, 1] (or vice-versa)



- The Euclidean distance between a test point $\mathbf{x}^*$ and a training data point $\mathbf{x}^{(i)}$ is $\sqrt{\left(x_1^{(i)} - x_1^*\right)^2 + \left(x_2^{(i)} - x_2^*\right)^2}$
- The Euclidean distance is dominated by the first term $\left(x_1^{(i)} - x_1^*\right)^2$ simply due to the larger magnitude of x_1
- Thus, the variable x_1 gets considered much more important than x_2 by kNN

Pitfalls of kNN: Normalization

- kNN can be sensitive to the ranges of the input features



- **Simple fix**: Normalize each dimension to be in the range [0, 1]
  - $\bar{x}_j^{(i)} = \frac{x_j^{(i)} - \min_i\left(x_j^{(i)}\right)}{\max_i\left(x_j^{(i)}\right) - \min_i\left(x_j^{(i)}\right)}$ for all $i = 1,2,\cdots,N$ and $j = 1,2,\cdots,p$

- **Simple fix**: Standardize each dimension using mean and standard deviation of data
  - $\bar{x}_j^{(i)} = \frac{x_j^{(i)} - \mu_j}{\sigma_j}$ for all $i = 1,2,\cdots,N$ and $j = 1,2,\cdots,p$

Pitfalls of kNN: Computationally costly

- Computational cost for training time: 0
- Computational cost at test time, per test data point
  - Calculate p-dimensional Euclidean distances with N data points: $\mathcal{O}(Np)$
  - Sort the distances: $\mathcal{O}(N \log N)$
- This must be done for each test data point, which is very expensive by the standards of a learning algorithm!
- Need to store the entire dataset in memory!
- Gives decent accuracy when there is lots of data

MNIST digit classification
- Handwritten digits
- 28x28 pixel images: $p = 784$
- 60,000 training samples
- 10,000 test samples

	Test Error Rate (%)
Linear classifier (1-layer NN)	12.0
K-nearest-neighbors, Euclidean	5.0
K-nearest-neighbors, Euclidean, deskewed	2.4
K-NN, Tangent Distance, 16x16	1.1
K-NN, shape context matching	0.67
1000 RBF + linear classifier	3.6
SVM deg 4 polynomial	1.1
2-layer NN, 300 hidden units	4.7
2-layer NN, 300 HU, [deskewing]	1.6
LeNet-5, [distortions]	0.8
Boosted LeNet-4, [distortions]	0.7

Summary

- k-Nearest Neighbors algorithm can be used for both classification and regression

- kNN stores the entire training dataset in memory which it uses as its representation
  - kNN does not learn any model

- kNN makes predictions just-in-time by calculating the similarity between a test input and each training sample
  - There are many distance measures to choose from to match the structure of your input data

- It is a good idea to rescale your data, such as using normalization, when using kNN