11.01.2019

Statistical Methods in AI (CSE/ECE 471)

Lecture-5: K-nearest neighbors classifier

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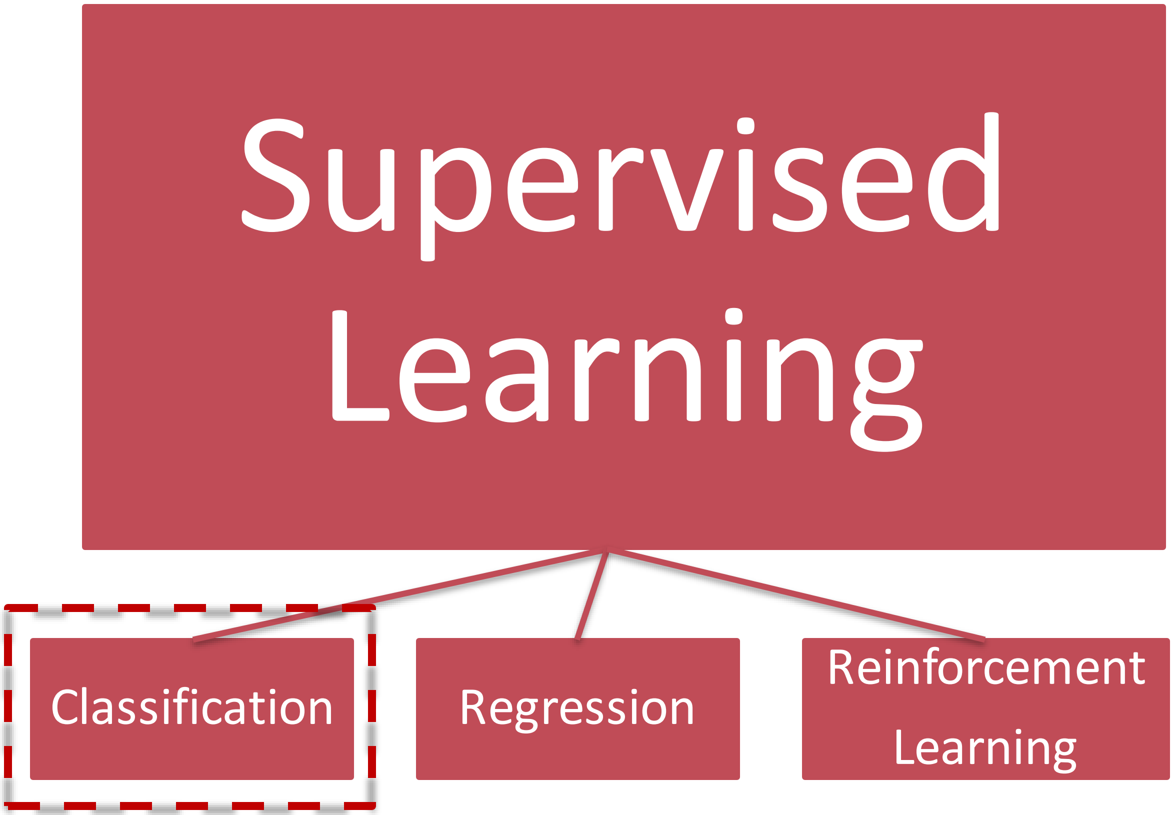
Announcements

- A1 is due **20/1, 11.59 PM**
- No tutorial this Saturday


Felicity
2019
SUPERHERO
FACTS
Wally West (Flash) stated he usually stays awake all night and takes micro sleeps during the day when people are blinking.
Wish we could do that here at IIIT during lectures. :")

third


Supervised Learning
Classification
Regression
Reinforcement Learning

So far

- Decision Tree classifier

Motivation

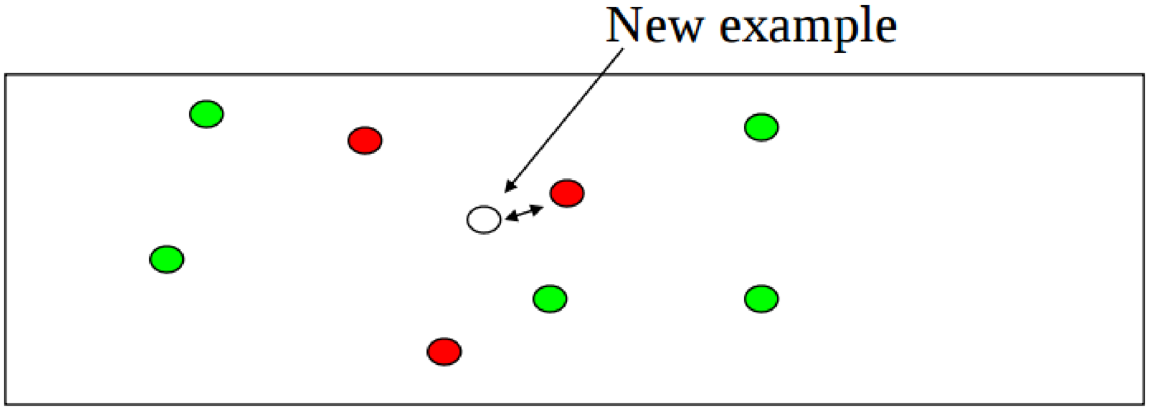
Show me your friends and I will tell you who you are

labeled examples

label

Nearest neighbor classifier

- Given a new example **x**, find the its closest training example <$\mathbf{x}^i$, y^i> and predict y^i



- How to measure distance – Euclidean (squared):

$$\left\| \mathbf{x} - \mathbf{x}^i \right\|^2 = \sum_j (x_j - x_j^i)^2$$

1-NN

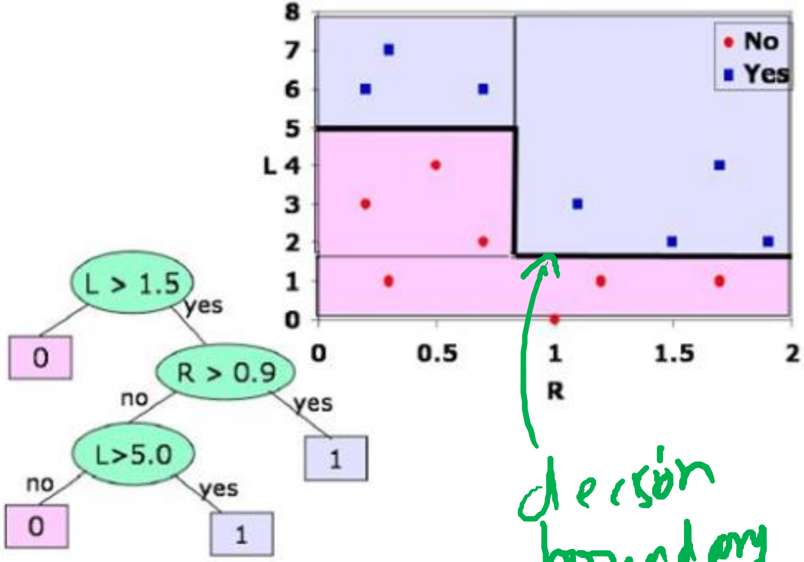
Algorithm:

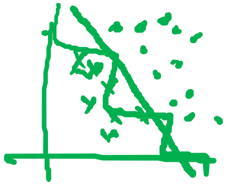
1. Find example $(\mathbf{x}^*, t^*)$ (from the stored training set) closest to the test instance $\mathbf{x}$. That is:

$$\mathbf{x}^* = \underset{\mathbf{x}^{(i)} \in \text{train. set}}{\operatorname{argmin}} \ \text{distance}(\mathbf{x}^{(i)}, \mathbf{x})$$

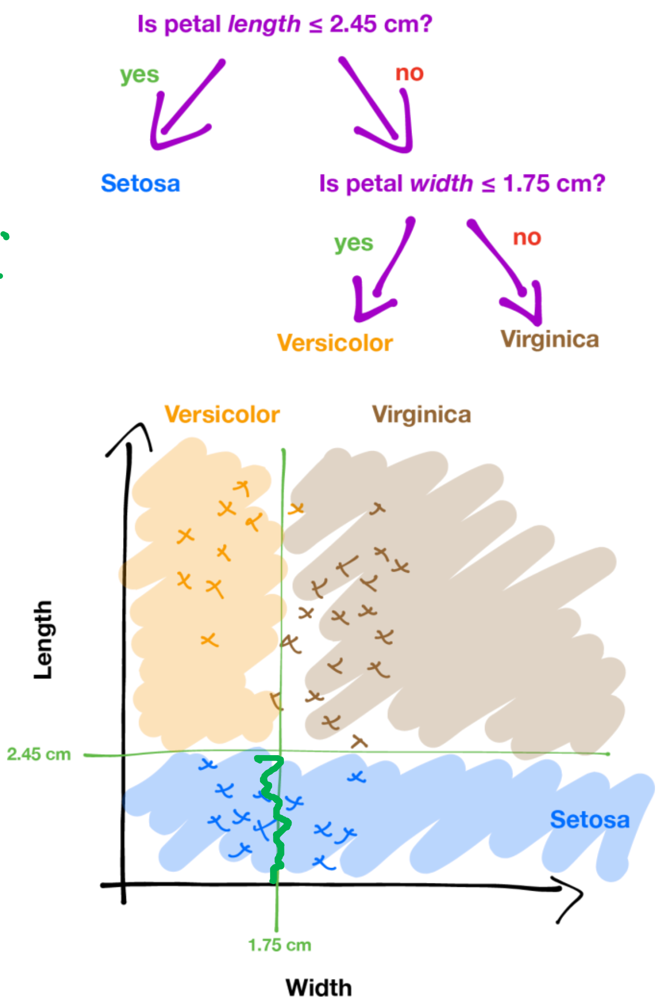
2. Output $y = t^*$

Recap: Decision Boundaries



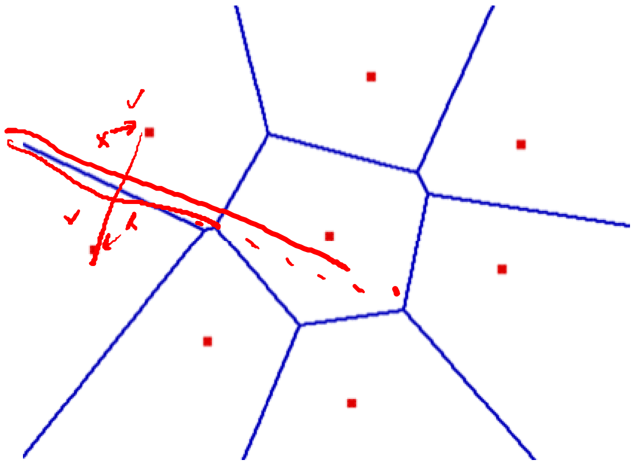


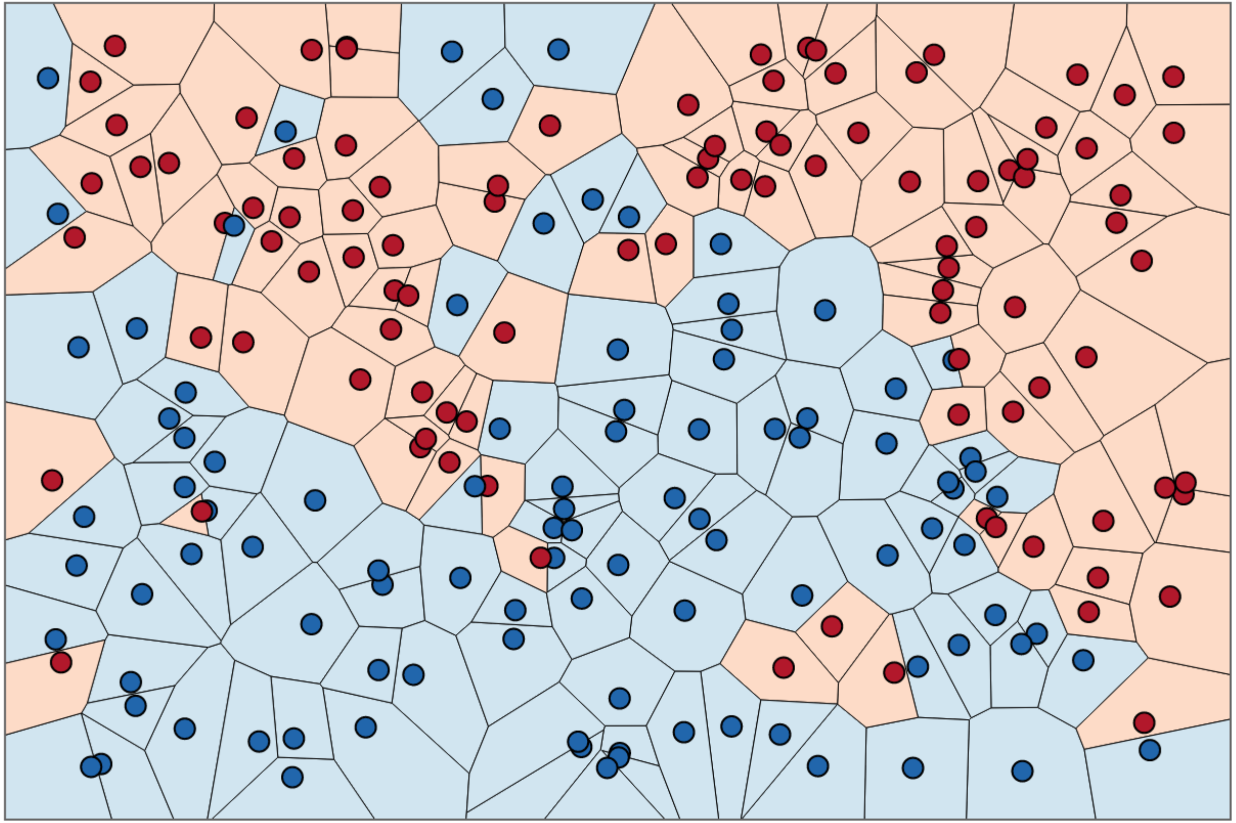
decision boundary

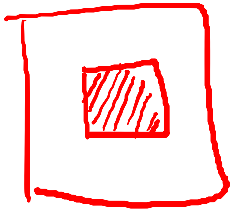


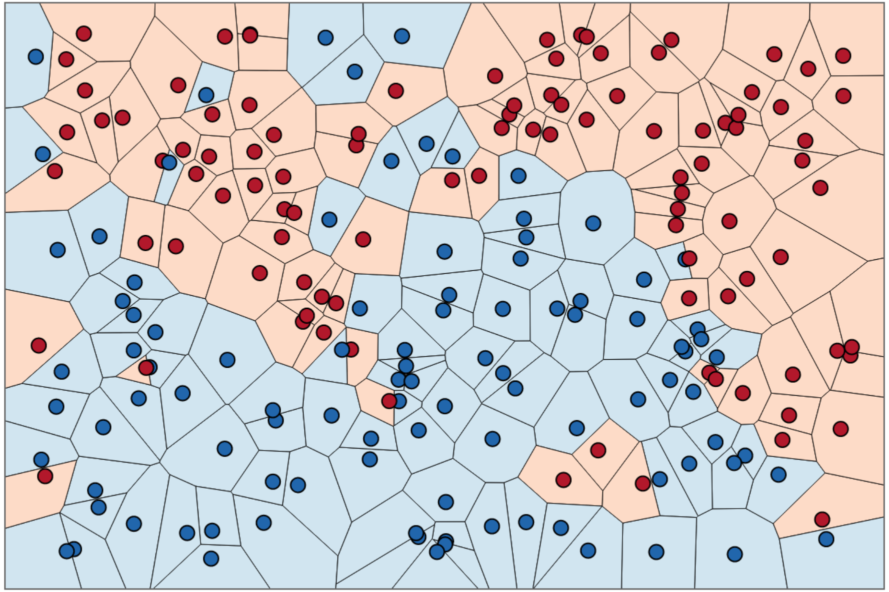
Decision Boundaries: The Voronoi Diagram

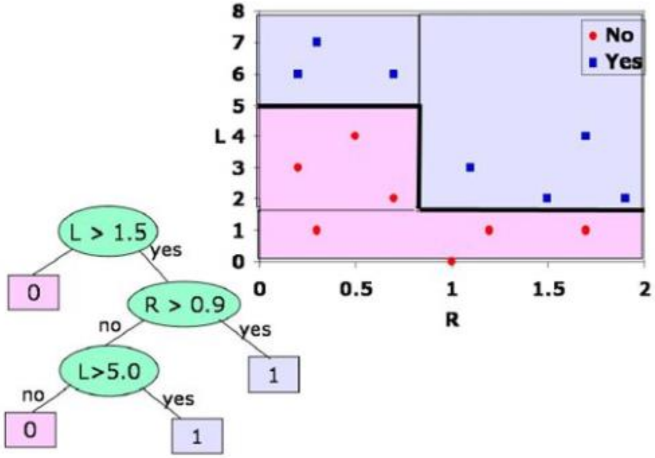
- Given a set of points, a **Voronoi diagram** describes the areas that are nearest to any given point.
- These areas can be viewed as zones of control.





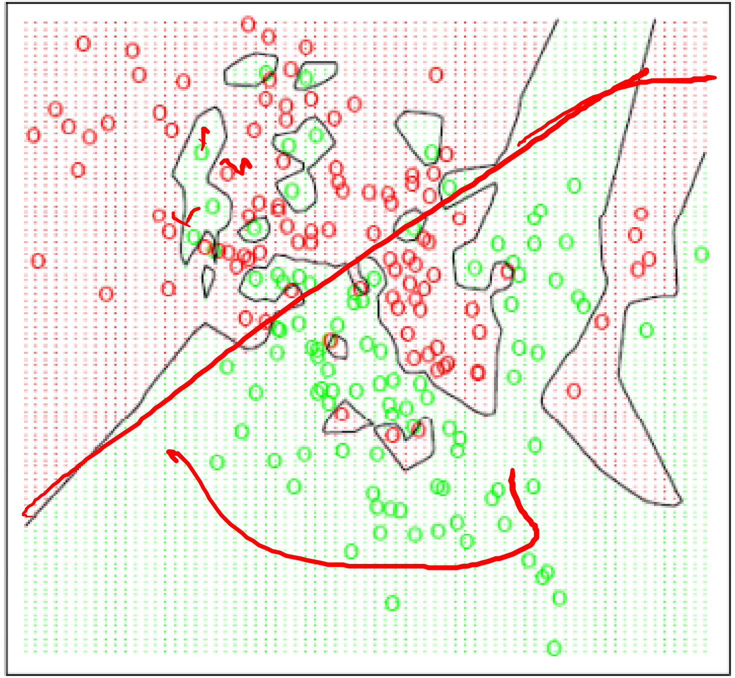






L > 1.5
yes
0
R > 0.9
no
yes
L>5.0
no
yes
1
0
1
8
7
6
5
L 4
3
2
1
0
0
0.5
1
1.5
2
R
No
Yes

Decision Boundaries

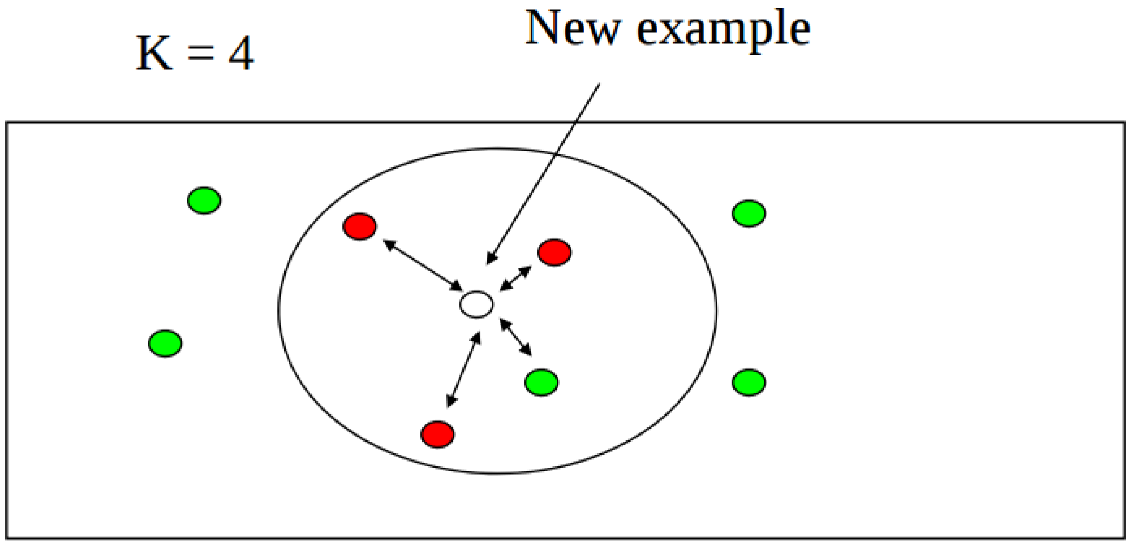


With large number of examples and possible noise in the labels, the decision boundary can become nasty!

We end up overfitting the data

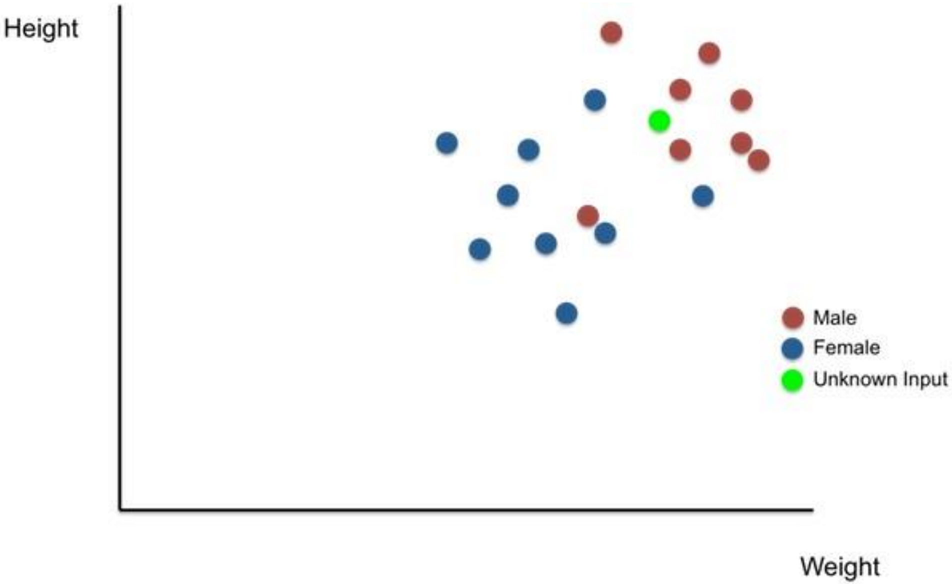
K-Nearest Neighbor

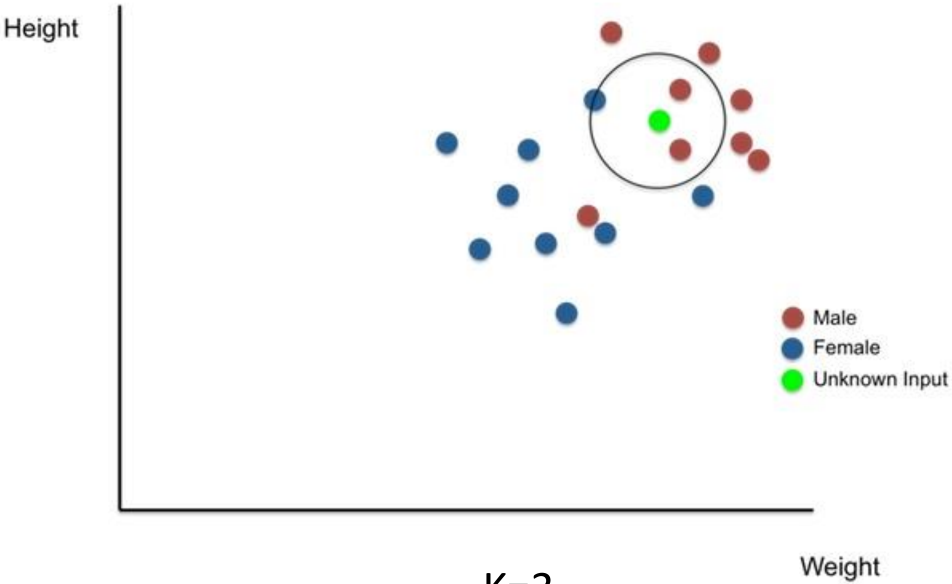
Example:



Find the ***k*** nearest neighbors and have them vote. Has a smoothing effect. This is especially good when there is noise in the class labels.

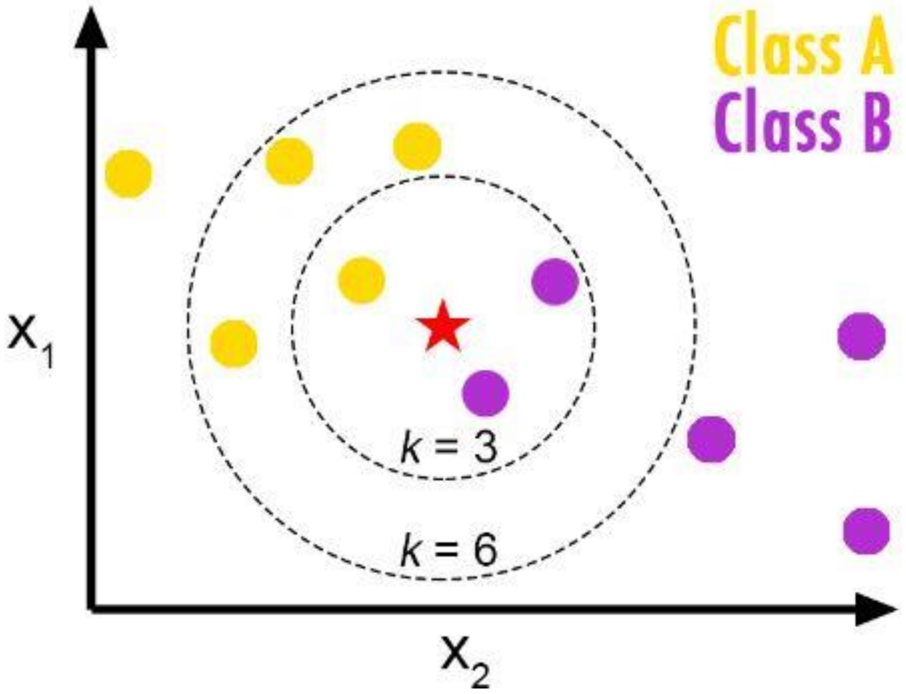
k-nearest neighbor classifier





K=3

k-nearest neighbor classifier



K is usually an odd number

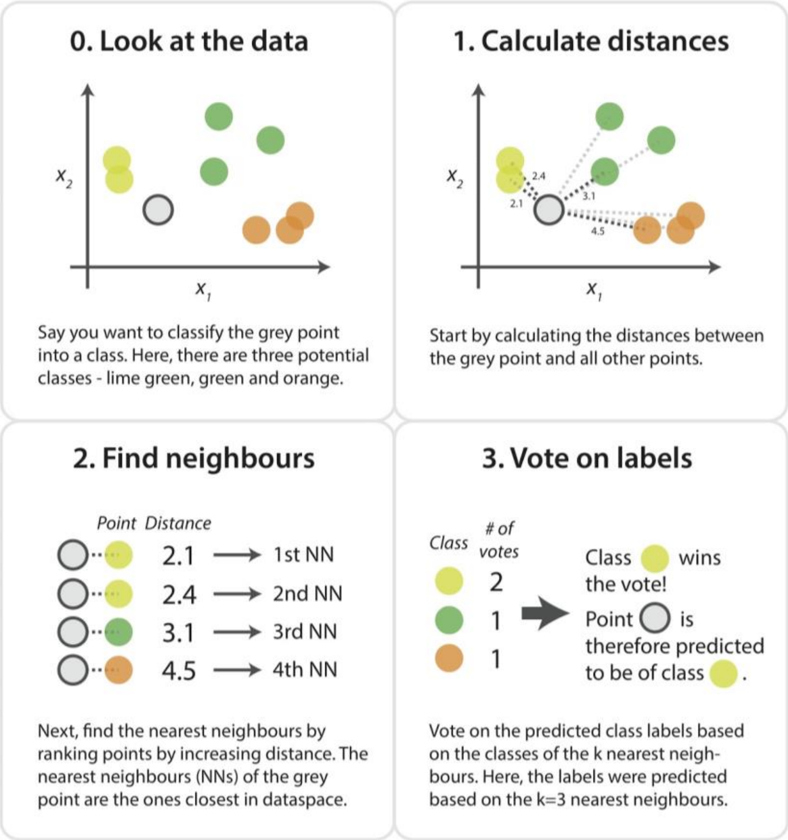
k-NN

Algorithm (kNN):

1. Find k examples $\{\mathbf{x}^{(i)}, t^{(i)}\}$ closest to the test instance $\mathbf{x}$
2. Classification output is majority class

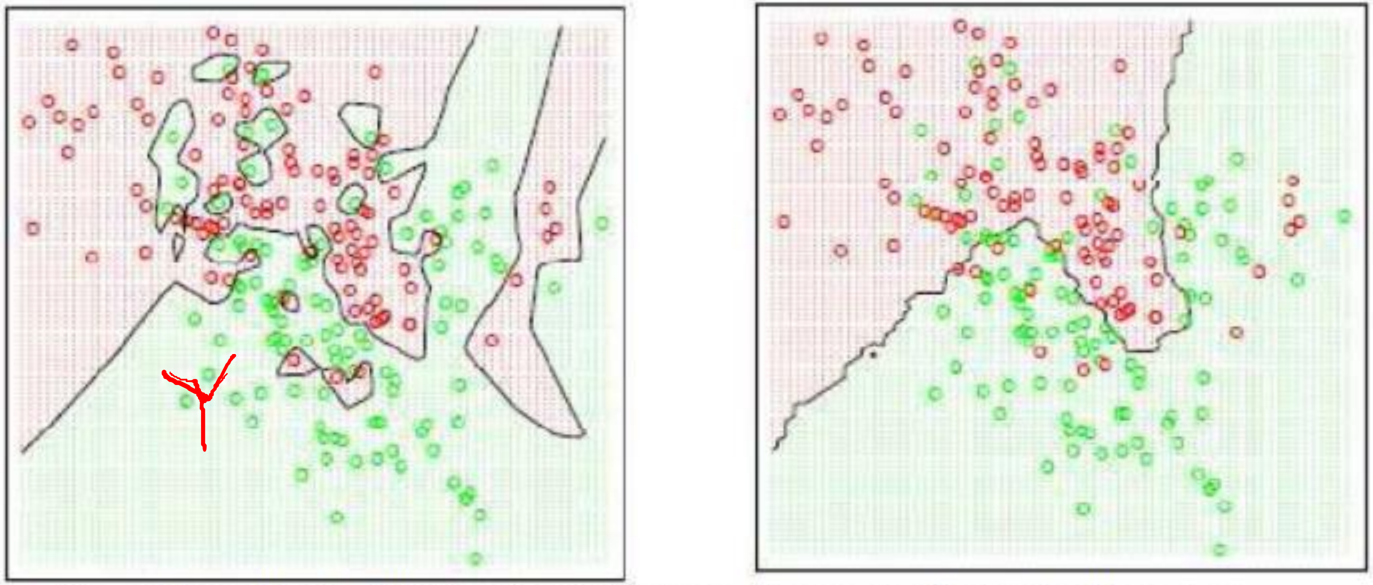
$$y = arg \max_{t^{(z)}} \sum_{r=1}^{k} \delta(t^{(z)}, t^{(r)})$$

k-NN algorithm in pictures



Effect of K

K=1 K=15



Figures from Hastie, Tibshirani and Friedman (Elements of Statistical Learning)

Larger k produces smoother boundary effect and can reduce the impact of class label noise.

Complexity of k-NN

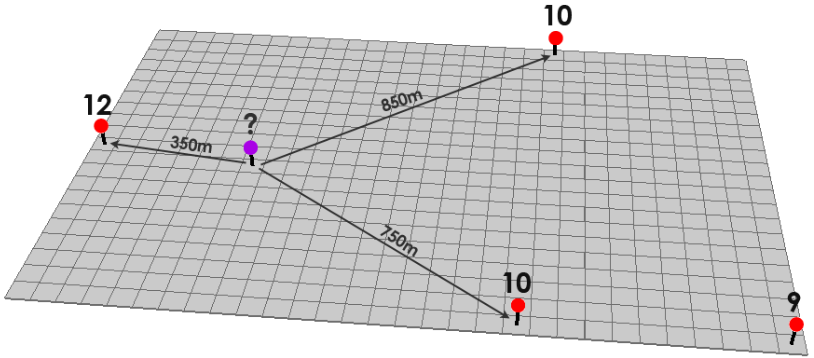
$[\leftarrow d \rightarrow]$

N

$\mathbb{R}^d$

	1-NN	k-NN
Training		
– Time:	$O(1)$	$O(1)$
– Space:	$O(Nd)$	$O(Nd)$
Testing		
– Time:	$O(Nd)$	$O(Nd + Nk\log k)$
– Space:	$O(d)$	$O(kd)$?

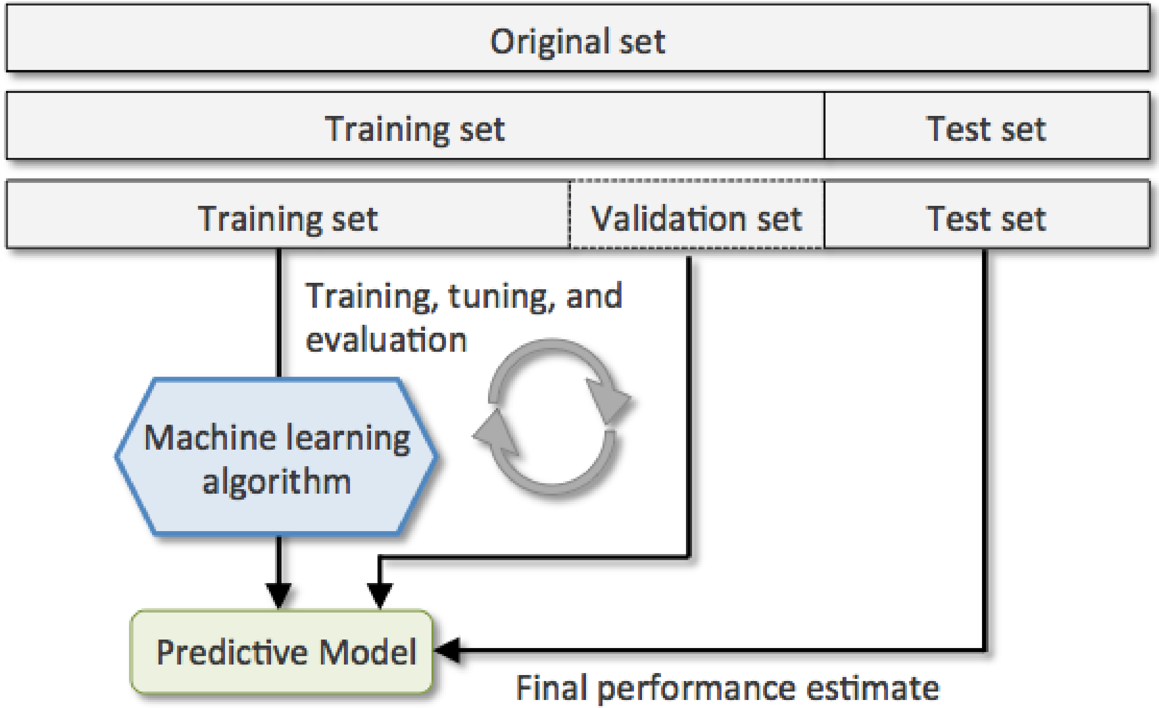
Weighted k-NN



- Helps in case of class skew

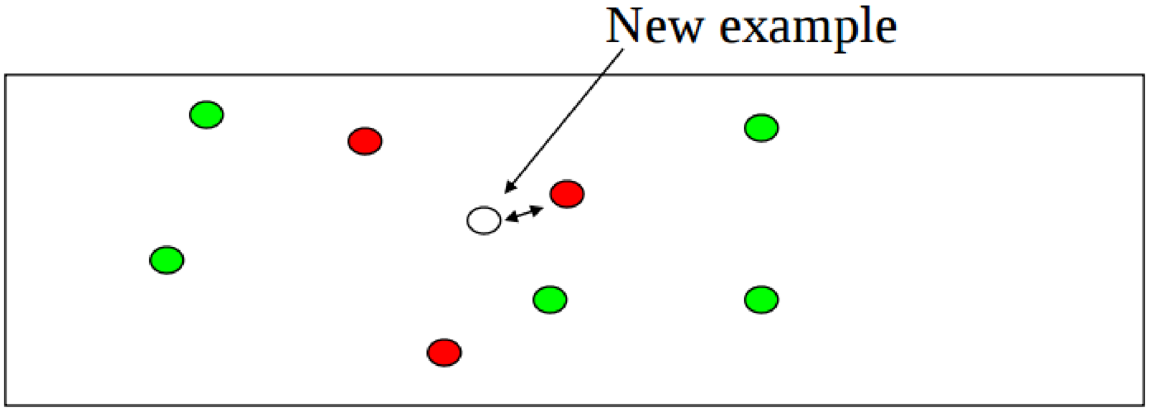
How to choose k ?

👉 Rule of thumb: $k < \sqrt{n}$, where n is the number of training examples



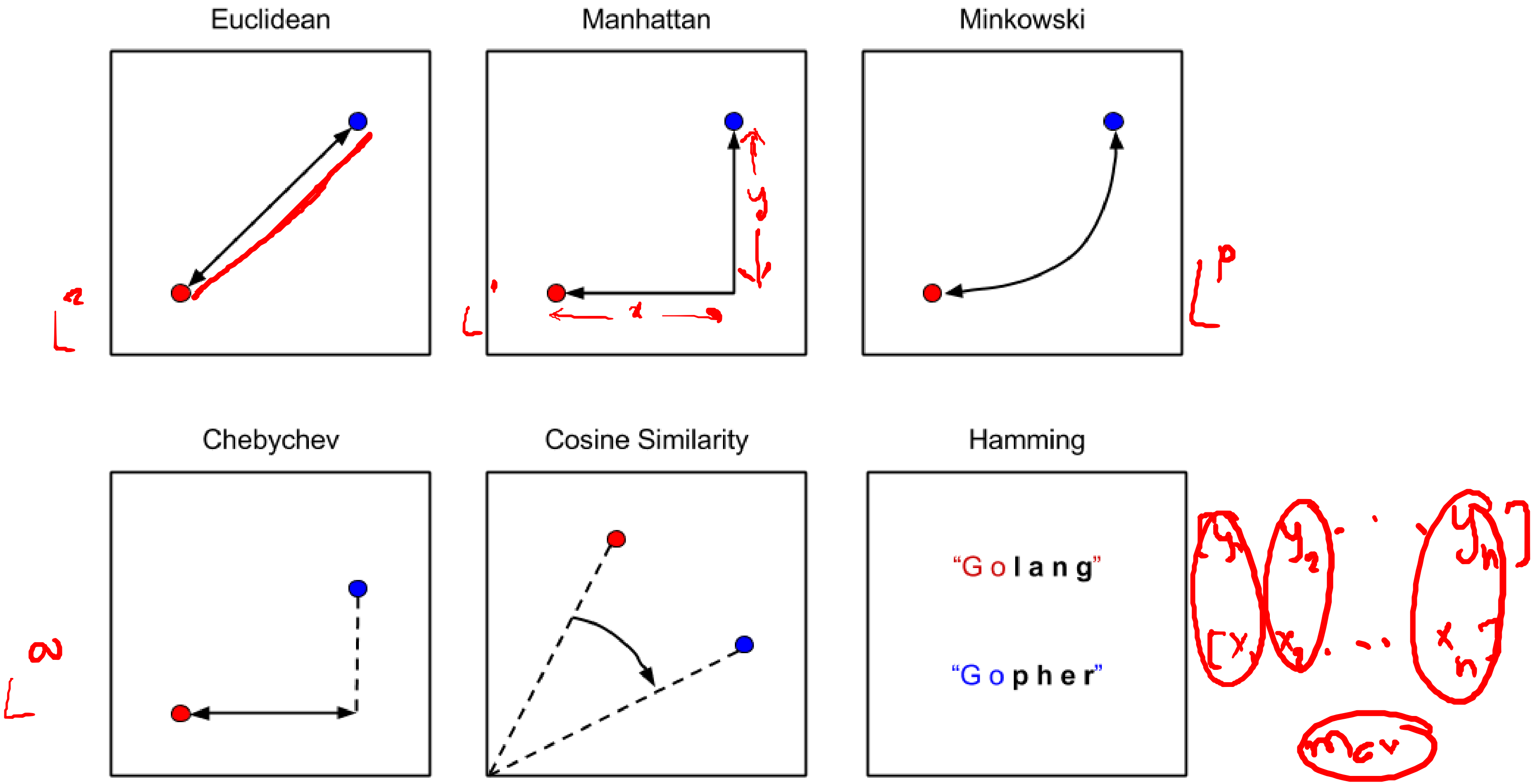
Nearest neighbor classifier

- Given a new example **x,** find the its closest training example $<\mathbf{x}^i, y^i>$ and predict y^i



"Closest" →

Distance measures



Distance measures

Minkowski distance:

$$d_p = \|x_i - y_i\|_p = \sqrt[p]{\sum_{i=1}^{n} |x_i - y_i|^p}$$

Chebyshev distance:

$$d_\infty = \|x_i - y_i\|_\infty = \max_{i=1..n} |x_i - y_i|$$

Cosine distance:

$$d_{cos} = 1 - \frac{\sum_{i=1}^{n} x_i * y_i}{\sqrt{\sum_{i=1}^{n} (x_i)^2} * \sqrt{\sum_{i=1}^{n} (y_i)^2}}$$

Mahalanobis distance:

$$d_M = \sqrt{\sum_{i=1}^{n} |x_i - y_i|^2 / s_i^2}$$

Euclidean distance:

$$d_2 = \|x_i - y_i\|_2 = \sqrt{\sum_{i=1}^{n} |x_i - y_i|^2}$$

Manhattan:

$$d_1 = \|x_i - y_i\|_1 = \sum_{i=1}^{n} |x_i - y_i|$$

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Hellinger distance:

$$d_H = \frac{1}{\sqrt{2}} \sqrt{\sum_{i=1}^{n} |\sqrt{x_i} - \sqrt{y_i}|^2}$$

Manhattan:

$$d_1 = \|x_i - y_i\|_1 = \sum_{i=1}^{n} |x_i - y_i|$$

Bray-Curtis distance:

$$d_{BC} = \sum_{i=1}^{n} |x_i - y_i| \Big/ \sum_{i=1}^{n} |x_i + y_i|$$

Canberra:

$$d_C = \sum_{i=1}^{n} |x_i - y_i| / (|x_i| + |y_i|)$$

Cosine distance:

$$d_{cos} = 1 - \frac{\sum_{i=1}^{n} x_i * y_i}{\sqrt{\sum_{i=1}^{n} (x_i)^2} * \sqrt{\sum_{i=1}^{n} (y_i)^2}}$$

Distance based on Pearson correlation:

$$d_{corr} = 1 - \frac{\sum_{i=1}^{n} (x_i - \acute{x}) * (y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n} (x_i - \acute{x})^2} * \sqrt{\sum_{i=1}^{n} (y_i - \bar{y})^2}}$$

Properties and Issues with k-NN

- Non-parametric
- ‘Lazy’ learner (c.f. ‘eager’ learner in decision trees)
- Simple baseline (after 0-effort baselines)
- GOOD
  - No training
  - Learns highly non-linear decision boundaries
- BAD
  - Need to keep all training points around
  - Curse of dimensionality ! (suggested #dims < 20)

Properties and Issues with k-NN

- If some attributes (coordinates of $\mathbf{x}$) have larger ranges, they are treated as more important

[0-1 2M-3M]

Properties and Issues with k-NN

- If some attributes (coordinates of $\mathbf{x}$) have larger ranges, they are treated as more important
    - normalize scale
        - Simple option: Linearly scale the range of each feature to be, e.g., in range [0,1]
        - Linearly scale each dimension to have 0 mean and variance 1 (compute mean μ and variance σ^2 for an attribute x_j and scale: $(x_j - m)/\sigma$)

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- Irrelevant, correlated attributes add noise to distance measure
  - eliminate some attributes
  - or vary and possibly adapt weight of attributes
- Non-metric attributes (symbols)
  - Hamming distance

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Some use cases for k-NN

- Decent performance when lots of data

- Yann LeCunn – MNIST Digit Recognition
  - Handwritten digits
  - 28x28 pixel images: d = 784
  - 60,000 training samples
  - 10,000 test samples
- Nearest neighbour is competitive

	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

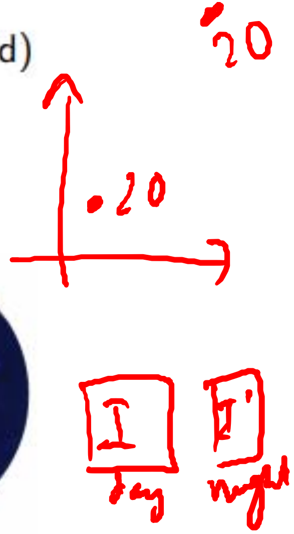
Some use cases for k-NN

- Problem: Where (e.g., which country or GPS location) was this picture taken?

[Paper: James Hays, Alexei A. Efros. im2gps: estimating geographic information from a single image. CVPR'08. Project page: http://graphics.cs.cmu.edu/projects/im2gps/]

Some use cases for k-NN

- Problem: Where (eg, which country or GPS location) was this picture taken?
  - Get 6M images from Flickr with gps info (dense sampling across world)
  - Represent each image with meaningful features
  - Do kNN (large k better, they use $k = 120$)!



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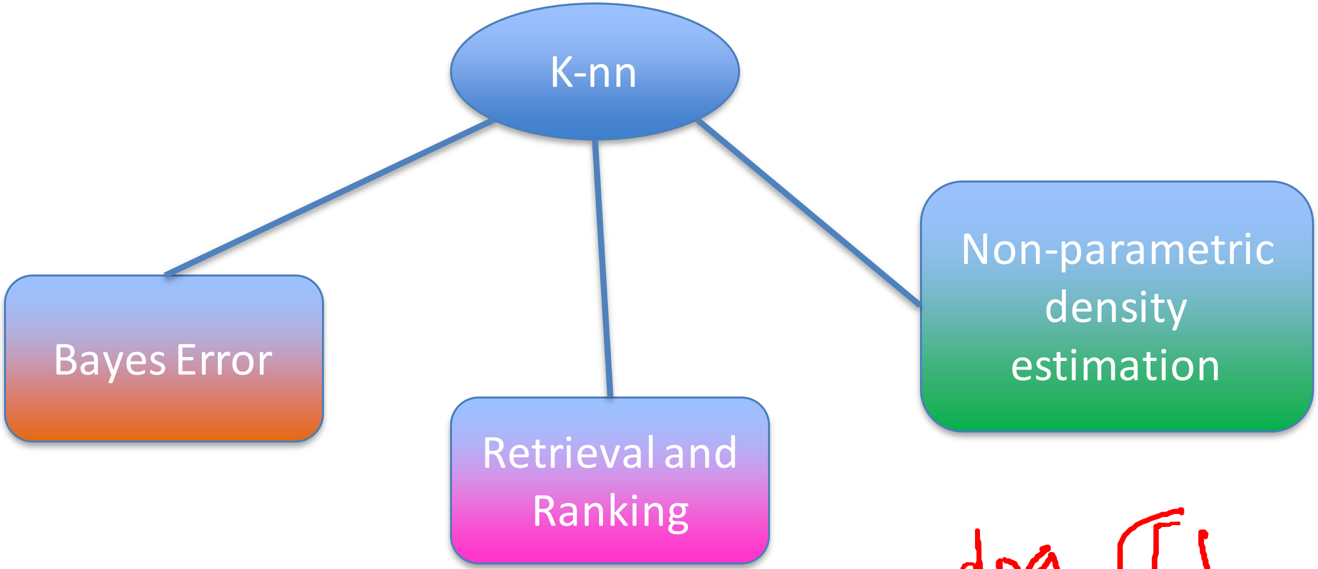
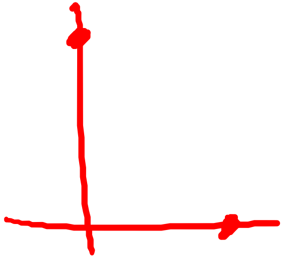
Related topics



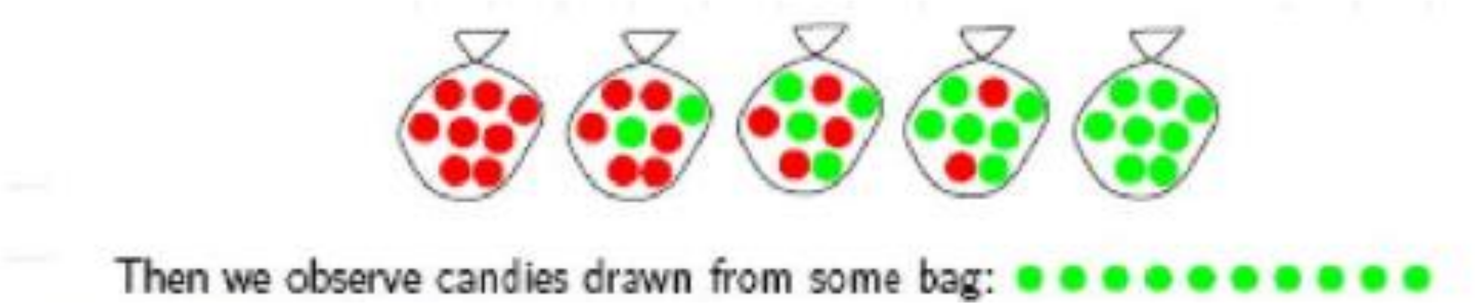


$$\begin{array}{l} \text{dog} \\ \text{cat} \\ \text{wolf} \end{array} \begin{pmatrix} [1 & 0] & 0 \\ [0 & 1] & 0 \\ 0 & 0 & 1 \end{pmatrix}$$


PROBABILITY = EVENT / OUTCOMES
wikiHow to Calculate Probability

Data – a probability-based perspective

- The basis for Statistical Learning Theory

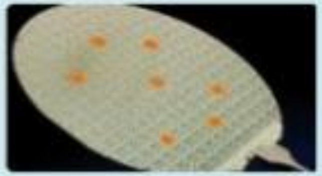


  - Domain described by random variables (r.v.)
    - X = {apple, grape}
    - $b_i \in [1,5]$
  - **Data = Instantiation of some or all r.v.'s in the domain**

Uncertainty arises from many sources

Process Uncertainty
Processes contain "randomness"

Uncertain travel times



Semiconductor yield

Data Uncertainty
Data input is uncertain

Intended Spelling — Text Entry — Actual Spelling

GPS Uncertainty

Testimony

{Paris Airport}

Ambiguity

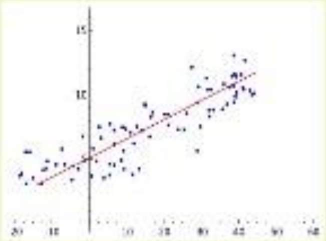
Contaminated?

Rumors

{John Smith, Dallas}
{John Smith, Kansas}

Conflicting Data

Model Uncertainty
All modeling is approximate



Fitting a curve to data

Forecasting a hurricane (www.noaa.gov)

Data: a probabilistic perspective

	DBAName	AKAName	Address	City	State	Zip
t1	John Veliotis Sr.	Johnnyo's	3465 S Morgan ST	***Chicago***	IL	***60608***
t2	John Veliotis Sr.	Johnnyo's	3465 S Morgan ST	Chicago	IL	***60609***
t3	John Veliotis Sr.	Johnnyo's	3465 S Morgan ST	Chicago	IL	***60609***
t4	***Johnnyo's***	Johnnyo's	3465 S Morgan ST	***Cicago***	IL	60608

Conflicts

Does not obey data distribution

Conflict

Output

Proposed Cleaned Dataset

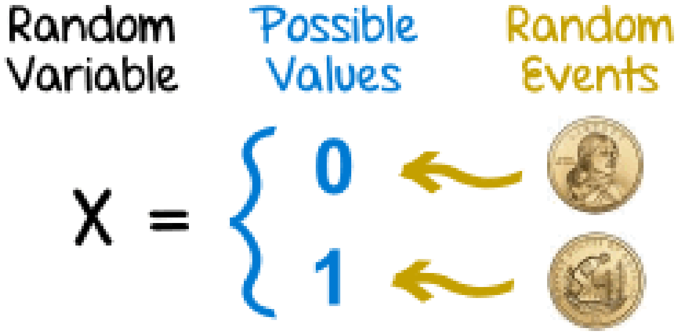
	DBAName	Address	City	State	Zip
t1	John Veliotis Sr.	3465 S Morgan ST	Chicago	IL	60608
t2	John Veliotis Sr.	3465 S Morgan ST	Chicago	IL	**60608**
t3	John Veliotis Sr.	3465 S Morgan ST	Chicago	IL	**60608**
t4	**John Veliotis Sr.**	3465 S Morgan ST	**Chicago**	IL	60608

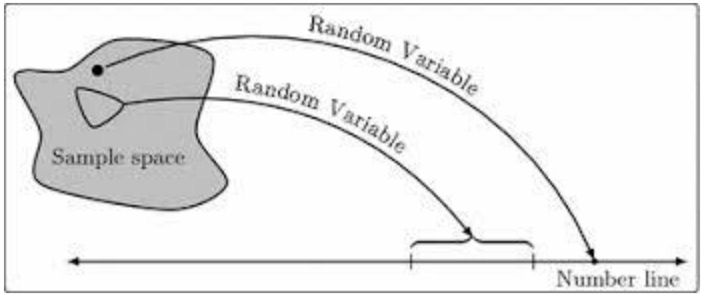
Marginal Distribution of Cell Assignments

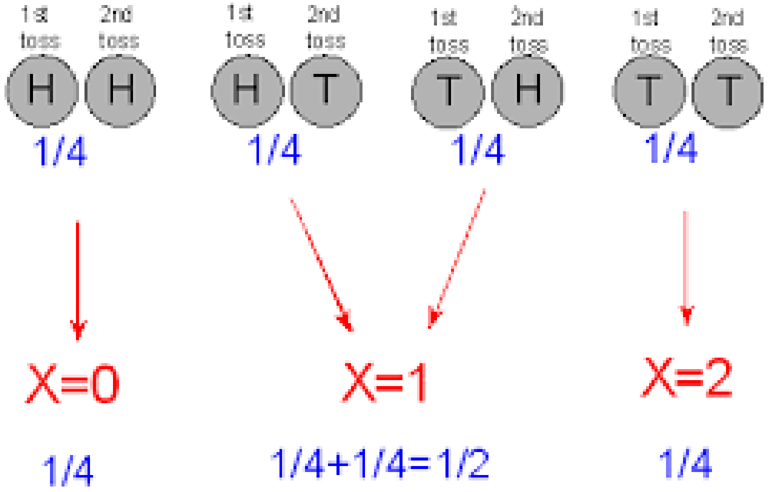
Cell	Possible Values	Probability
t2.Zip	60608	0.84
	60609	0.16
t4.City	Chicago	0.95
	Cicago	0.05
t4.DBAName	John Veliotis Sr.	0.99
	Johnnyo's	0.01

Random Variables

R.V. = A numerical value from a random experiment







Random variables

- A **discrete random variable** can assume a countable number of values.
  - Number of steps to the top of the Eiffel Tower*

Random variables

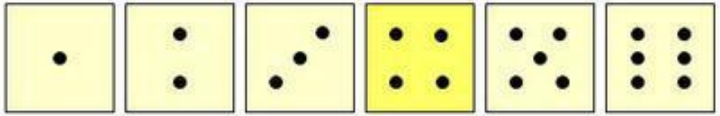
- A **discrete random variable** can assume a countable number of values.
  - Number of steps to the top of the Eiffel Tower*
- A **continuous random variable** can assume any value along a given interval of a number line.
  - The time a tourist stays at the top once s/he gets there

*Believe it or not, the answer ranges from 1,652 to 1,789. See Great Buildings

Discrete Random Variables

- Can only take on a countable number of values

Examples:

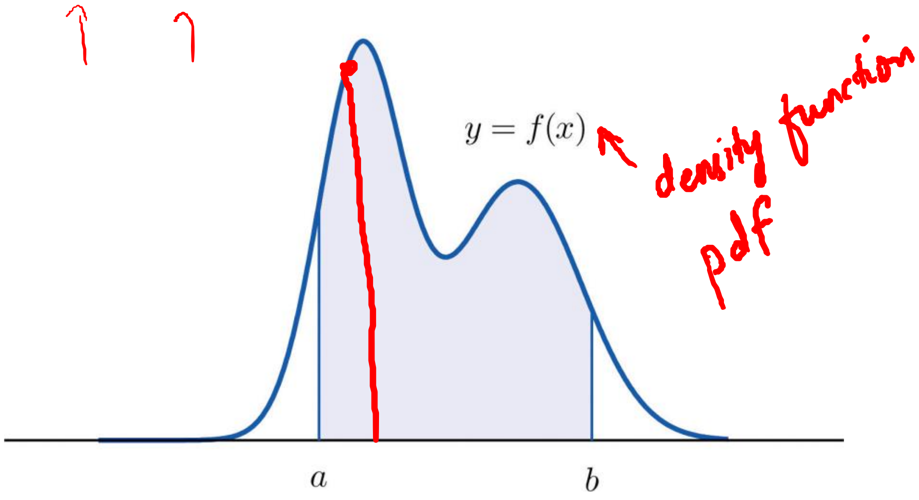


- **Roll a die twice**
  Let X be the number of times 4 comes up
  (then X could be 0, 1, or 2 times)

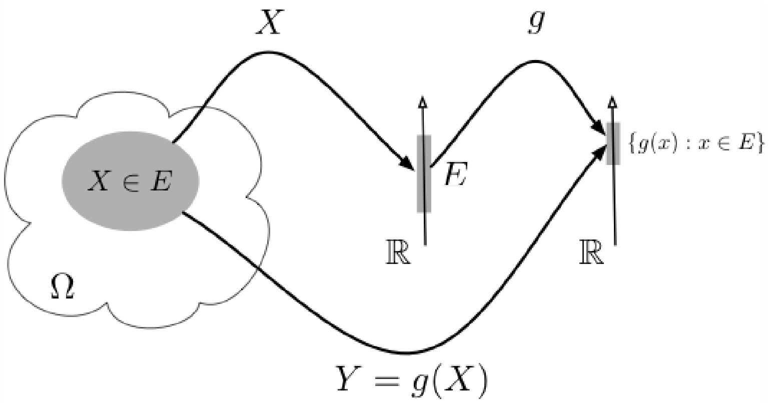
- **Toss a coin 5 times.**
  Let X be the number of heads
  (then X = 0, 1, 2, 3, 4, or 5)

Continuous random variable

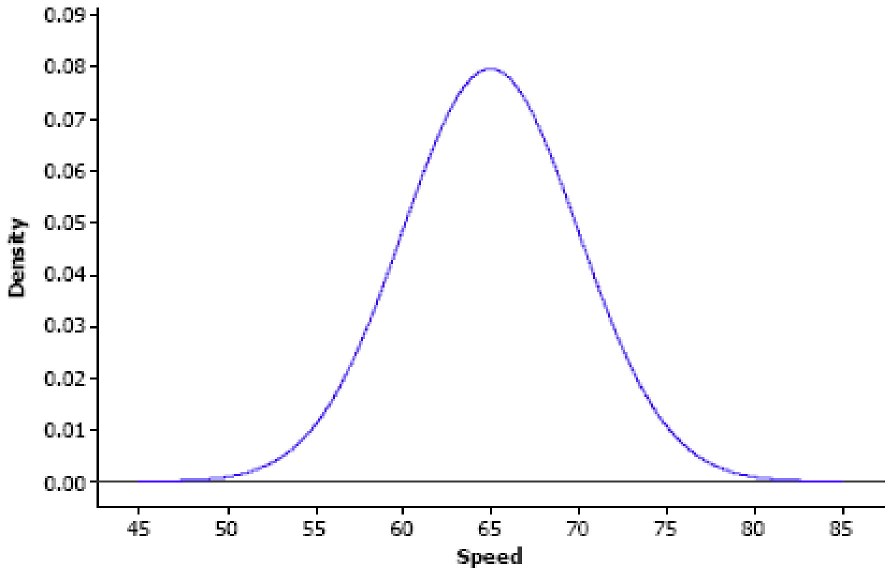
$P(a < X < b) =$ area of shaded region

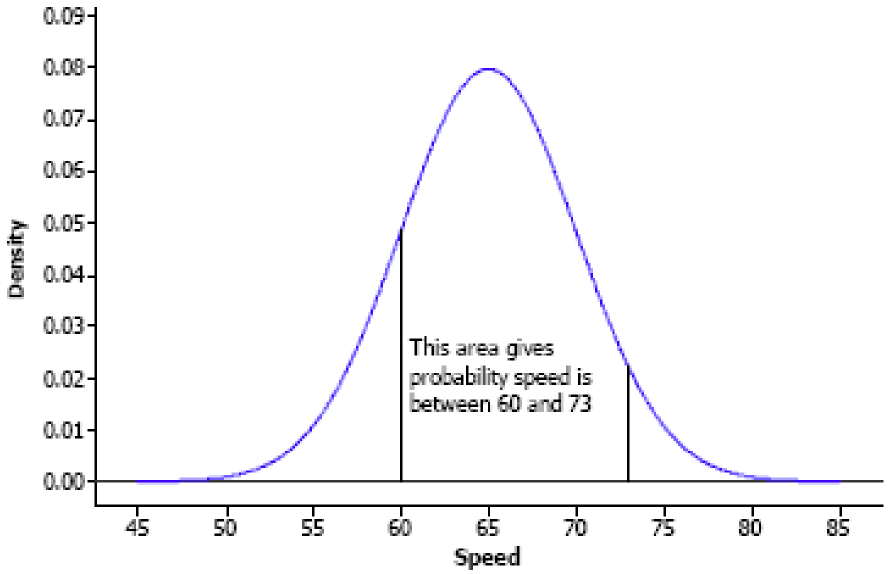


$P(Y = 0.2) = 0$

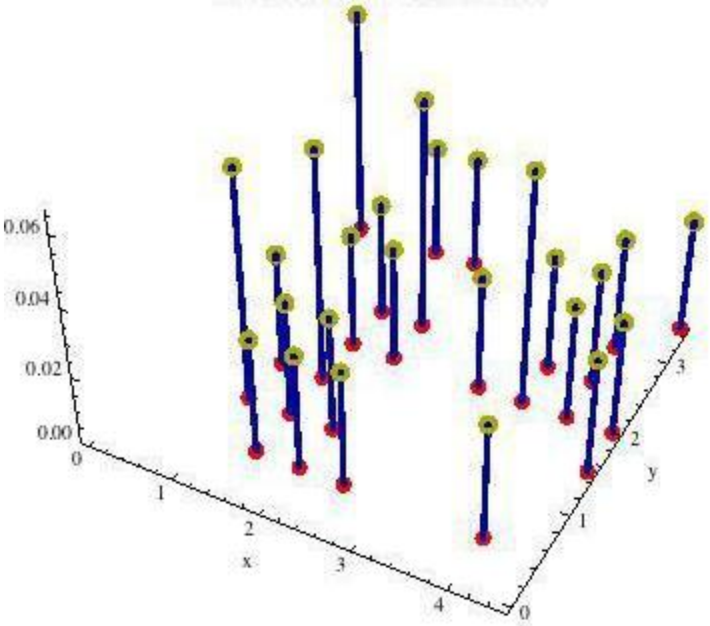


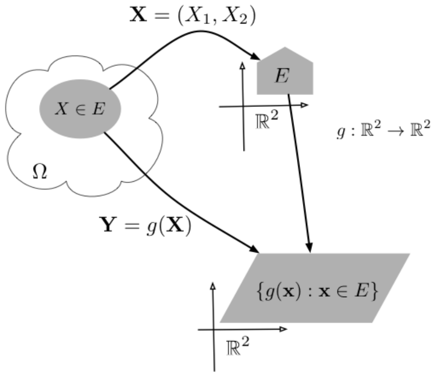
Continuous random variable

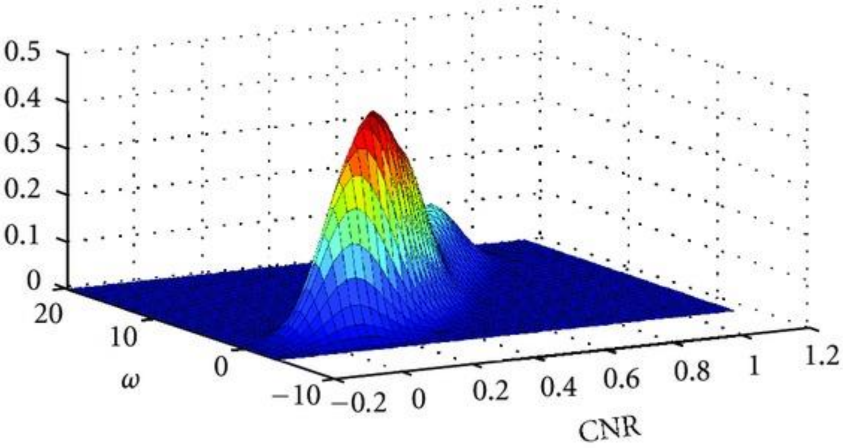




Random vectors







References and Reading

- https://en.wikipedia.org/wiki/K-nearest_neighbors_algorithm

- Euclidean v/s Cosine distance
  - Code example: https://cmry.github.io/notes/euclidean-v-cosine
  - https://stackoverflow.com/a/53175061
  - https://www.quora.com/Why-cosine-is-better-than-Euclidean-in-high-dimensional-data-as-in-text-documents