University of Udine

Big Data Management, Analysis, and Presentation

A whirlwind introduction to Data Mining

Andrea Brunello
andrea.brunello@uniud.it

Outline

1. What is data mining
2. Model evaluation
3. Data exploration and preparation

What is data mining

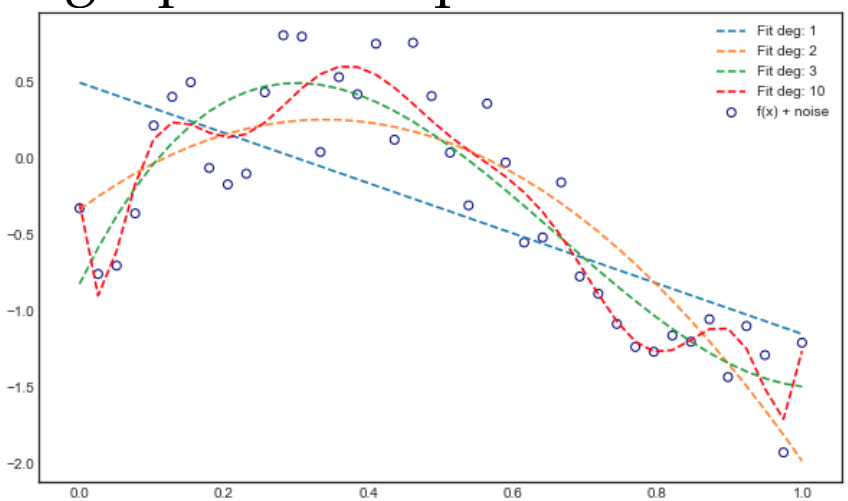
What is Data Mining

- **Data** $\approx$ **facts** recorded, stored
- **Information** consists of the set of **concepts**, regularities, patterns that are "hidden" within the data
- **Data Mining** deals with the **extraction** and presentation of useful, previously unknown **information**, implicitly contained in a (large) amount of data
  - It is a process of abstraction, which leads to the generation of a *model*
- Such models, in our case, are built by **machine learning** algorithms

Models and reality

"A model is a selective abstraction of reality"
(A. Einstein)

- In our case, the "reality" is represented by the data we have at our disposal
- We want to build a **simplified description** of this reality
- The model is therefore a (simplified) conceptual representation of the real world or a part of it, capable of approximating a particular phenomenon



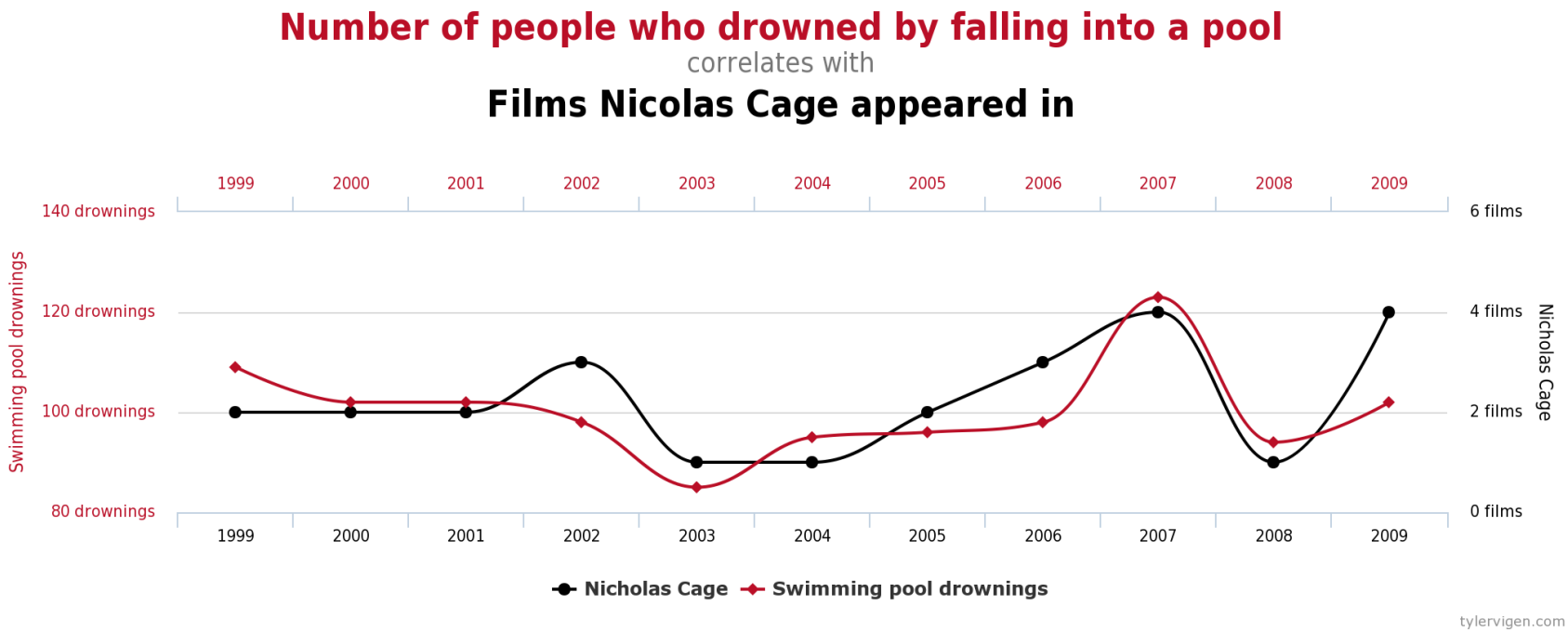
Using models

- Models can be used to:
  - **Understand**: identify how certain features of a house are more important than others in determining its value
  - **Predict**: determine the final value of a house based on a set of its features
- These uses can overlap

$$\begin{aligned} value = & -34.8 * surface \\ & + 57740.3 * rooms \\ & + 39347.8 * marble \\ & + 49276.1 * restored \\ & - 7843.3 \end{aligned}$$

Correlation does not imply causation!

Often, discovered patterns may be trivial, the result of random correlations, or not entirely accurate



Types of data

- Data Mining can be applied to various types of data:
  - **Structured**: tabular data
  - **Unstructured**: text, images, audio, video
- Traditional machine learning techniques require converting unstructured data into structured forms
- *Deep learning* approaches (neural networks) allow for direct handling of unstructured data
- In this course, we will focus on structured data

Structured data

A tabular dataset used by traditional machine learning algorithms has the following structure:

Temperature	Outlook	Humidity	Windy	Played?
Mild	Sunny	80	No	Yes
Hot	Sunny	75	Yes	No
Hot	Overcast	77	No	Yes
Cool	Rain	70	No	Yes
Cool	Overcast	72	Yes	Yes
Mild	Sunny	77	No	No

- Each row represents **an instance**, i.e., an example of the concept to be learned
- The rows are independent of each other
- Each instance describes the values of a given set of attributes (columns), which can be numerical or categorical

The Data Mining process

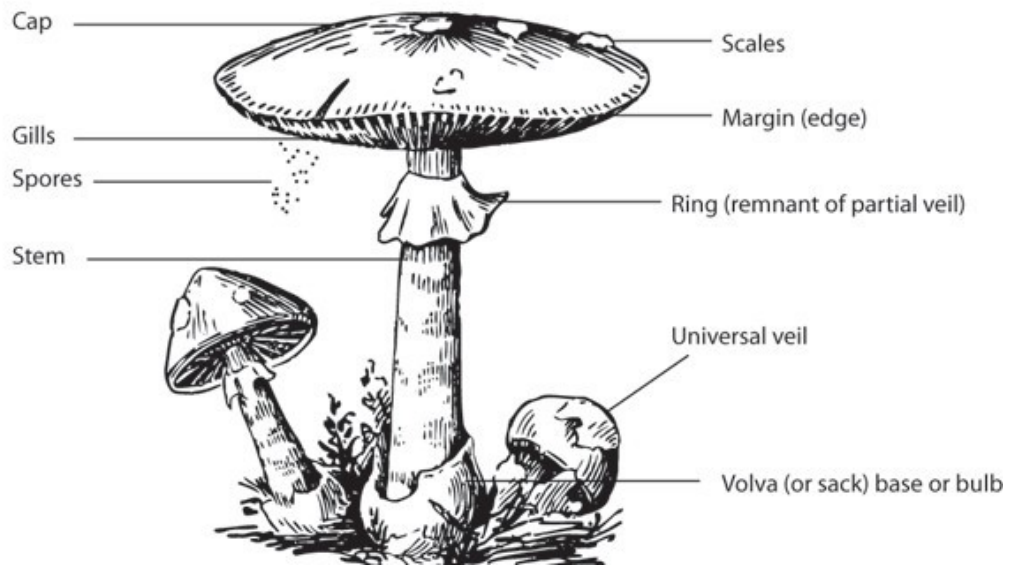
Generally, the Data Mining process unfolds as follows:

- It all starts with posing a specific **question**
- Next, relevant **data** is gathered to use as input to the analysis
- Through an *exploration* phase, the data is examined (e.g., missing values, outliers), and pre-processing is carried out
- A set of attributes considered important for the data and the goal is selected
- A machine learning **algorithm** is applied to the dataset to "train" a model
- Finally, the model produced by the algorithm is **evaluated**

An example: Mushroom dataset

Let's walk through the Data Mining process with an example focused on prediction

- **Question**: is it possible to automatically distinguish between poisonous and edible mushrooms?
- **Data**: 8124 instances of already classified mushrooms, each described by 22 attributes, plus the class label
  - `https://archive.ics.uci.edu/ml/datasets/mushroom`



An example: Mushroom dataset (2)

Content of the first 11 rows of the *dataset*

cap_shape	cap_surface	cap_color	bruises_or_not	odor	gill_attachment	gill_spacing	gill_size	gill_color	stalk_shape	stalk_root	stalk_surface_above_ring
convex	smooth	brown	bruises	pungent	free	close	narrow	black	enlarging	equal	smooth
convex	smooth	yellow	bruises	almond	free	close	broad	black	enlarging	club	smooth
bell	smooth	white	bruises	anise	free	close	broad	brown	enlarging	club	smooth
convex	scaly	white	bruises	pungent	free	close	narrow	brown	enlarging	equal	smooth
convex	smooth	gray	no	none	free	crowded	broad	black	tapering	equal	smooth
convex	scaly	yellow	bruises	almond	free	close	broad	brown	enlarging	club	smooth
bell	smooth	white	bruises	almond	free	close	broad	gray	enlarging	club	smooth
bell	scaly	white	bruises	anise	free	close	broad	brown	enlarging	club	smooth
convex	scaly	white	bruises	pungent	free	close	narrow	pink	enlarging	equal	smooth
bell	smooth	yellow	bruises	almond	free	close	broad	gray	enlarging	club	smooth
convex	scaly	yellow	bruises	anise	free	close	broad	gray	enlarging	club	smooth

stalk_surface_below_ring	stalk_color_above_ring	stalk_color_below_ring	veil_type	veil_color	ring_number	ring_type	spore_print_color	population	habitat	class
smooth	white	white	partial	white	1	pendant	black	scattered	urban	poisonous
smooth	white	white	partial	white	1	pendant	brown	numerous	grasses	edible
smooth	white	white	partial	white	1	pendant	brown	numerous	meadows	edible
smooth	white	white	partial	white	1	pendant	black	scattered	urban	poisonous
smooth	white	white	partial	white	1	evanescent	brown	abundant	grasses	edible
smooth	white	white	partial	white	1	pendant	black	numerous	grasses	edible
smooth	white	white	partial	white	1	pendant	black	numerous	meadows	edible
smooth	white	white	partial	white	1	pendant	brown	scattered	meadows	edible
smooth	white	white	partial	white	1	pendant	black	several	grasses	poisonous
smooth	white	white	partial	white	1	pendant	black	scattered	meadows	edible
smooth	white	white	partial	white	1	pendant	brown	numerous	grasses	edible

52% of the instances are classified as *edible*, 48% as *poisonous*

An Example: Mushroom Dataset (3)

Idea:

1. Partition the instances based on the value of the attribute *bruises_or_not*
2. Determine that an instance is classified as *edible* if and only if *bruises_or_not* = *bruises*

$\rightsquigarrow$ Based on this simple rule (= the model approximating the reality described by our data), we achieve a classification accuracy of 74%

Note: The model is not error-free, meaning it doesn't perfectly describe the data we observe; this is generally expected

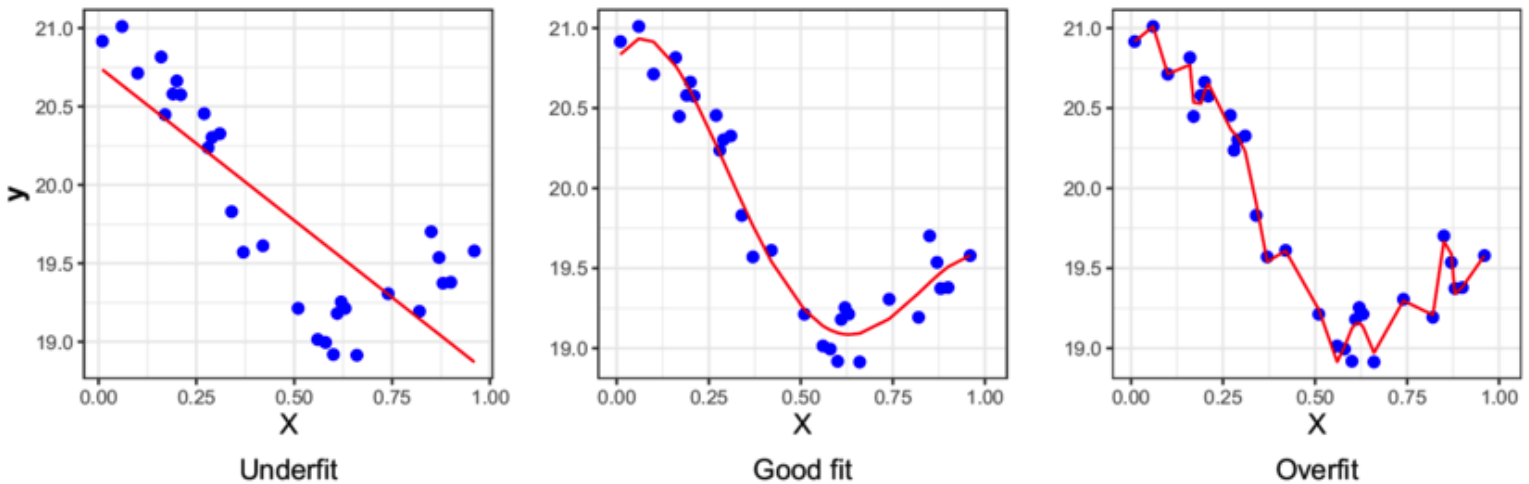
Model evaluation

Models and generalization

- It is close to impossible for the instances in a dataset to cover all possible cases within a given domain
- *Example:* a housing dataset, where each instance describes a house (e.g., size, number of rooms, presence of a garden) and its value
- Therefore, the machine learning algorithm must generate a **model that can generalize well, and work even for instances it hasn't seen during training**
- *Example:* a model that can predict the value of a new house based on certain patterns learnt from previously sold ones

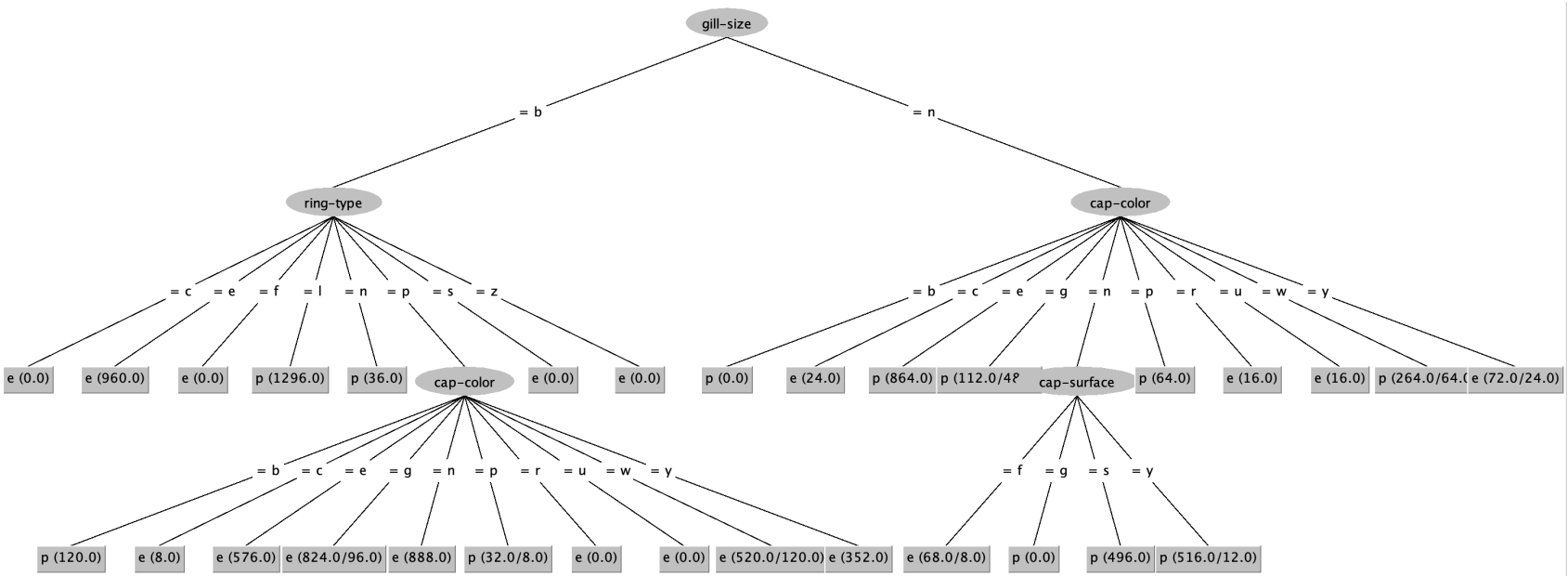
Models and generalization (2)

- The ability of models to generalize is a fundamental aspect of the data mining process, when making predictions
- It is not guaranteed that a prediction model that achieves excellent results on the data provided for training will also perform well on new data
- Intuitively, this happens because the model might have learned spurious patterns due to "noise" (*overfitting*)



Models and generalization (3)

- Let's see what happens on our Mushroom dataset if we train a more powerful and complex model
- We use a *decision tree*

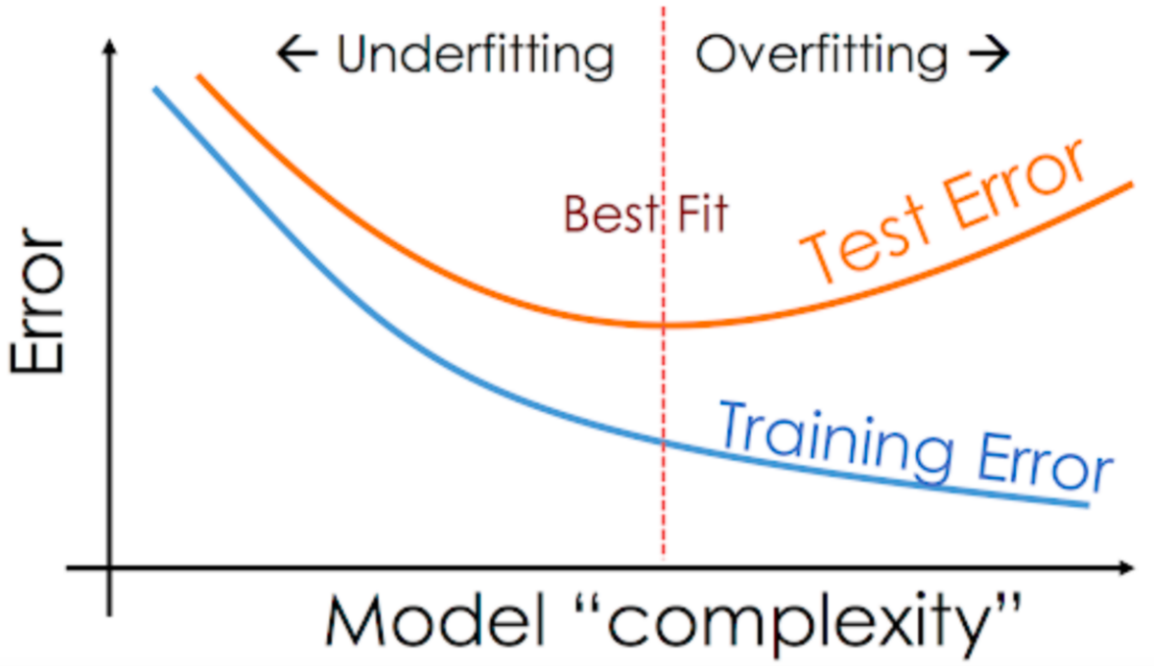


Training and test data

- The decision tree has an accuracy of over 95%
- Still, this doesn't mean that, given a new, never seen before mushroom, we have over 95% probability of classifying it correctly!
- We must determine the generalization capability of the model and, to do that:
  1. We randomly split (50-50) the dataset instances into a training and a test subsets
  2. We build the decision tree just by looking at the training set instances
  3. We evaluate how the tree performs over the test instances
- We obtain a lower accuracy of 92%

Model complexity and generalization

Complex models (e.g., large decision trees) tend to perform well on training data but may generalize less effectively on new data compared to simpler models



Confusion matrixes

- Classification errors are not born equal
- E.g., we would prefer the model to incorrectly classify an edible mushroom as poisonous (False Negative) rather than misclassify a poisonous one as edible (False Positive)
- A confusion matrix allows us to take a closer look at the classification performance of a model

		Predicted	
		Negative (**N**) -	Positive (**P**) +
Actual	Negative -	True Negatives (**TN**)	False Positives (**FP**) **Type I error**
	Positive +	False Negatives (**FN**) **Type II error**	True Positives (**TP**)

Classification matrix, mushroom dataset

How does our decision tree perform in this scenario?

```
=== Confusion Matrix ===

   p     e   <-- classified as
1796   179   |    p
 122  1965   |    e
```

Notice that:

- $(1796 + 1965)/(1796 + 179 + 122 + 1965) \approx 0.92$
- $179/(1796 + 179 + 122 + 1965) \approx 0.04$
- $122/(1796 + 179 + 122 + 1965) \approx 0.03$

Supervised vs Unsupervised learning

- In our mushroom example, we built a model with a clear objective in mind, and guided by the value of an attribute we wanted to predict "edible or not"
- This is called **supervised learning**: the learning algorithm is provided with a known label for each instance in the dataset (the target attribute), and the goal is to obtain a model capable of determining the label for new instances based on a set of attributes called predictors
- Another class of **unsupervised learning** methods aims to discover general patterns and structures in the data without the information from any pre-defined labels
  - E.g., *clustering*; we are not going to cover it here

Data exploration and preparation

Introduction

- Very rarely a dataset can be used as it is for analysis tasks
- The most time-consuming phase of the entire data mining process is data exploration and preparation
- **It is a crucial step**, as all subsequent analyses depend on it
- Some typical tasks:
  - choices regarding the encoding of attributes
  - detection and handling of missing values
  - removal of columns with low variance
  - identification of outliers
  - dependencies between columns
  - feature selection, removal of irrelevant columns

Attribute encoding

- Example: attribute related to *pH*: should we keep the numerical values or use "coarser" categorical values (acidic, neutral, basic)?
- What precision should be considered for numerical attributes? (e.g., integers, decimals, how many decimal places, . . .)
  - for example, if a temperature sensor is capable of providing an accurate measurement to the second decimal place, it is unnecessary to keep a number like 37.234664367

Missing values

What to do when some instances have unknown (null) values?

Temperature	Outlook	Humidity	Windy	Played?
Mild	Sunny	?	No	Yes
Hot	?	75	?	No
Hot	Overcast	77	No	Yes

Several solutions, for example:

- remove those instances
- remove columns with too many null values
- replace null values with a default value
- replace null values with the mean/mode of the column
- other more sophisticated imputation techniques

Additionally, the "type" of missing value plays an important role (why is it missing?)

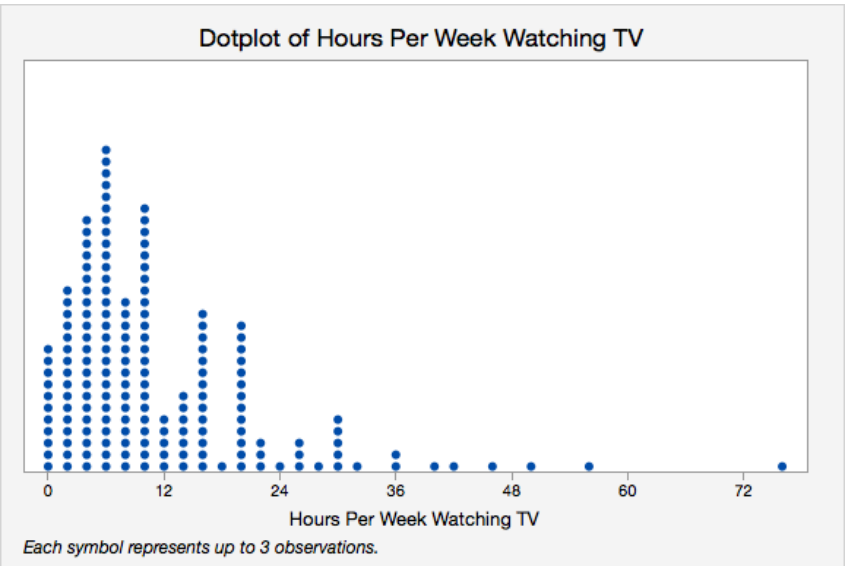
Low variance columns

- In the dataset, there may be columns that have only one value or a very imbalanced distribution of values
- *Typically*, such columns provide little information
- A machine learning algorithm may detect this and disregard them when generating models
- However, removing them beforehand leads to a more efficient learning process

ID	season	holiday	workingday	weather	f5	temp	atemp	humidity	windspeed	count
AB101	1	0	0	1	7	9.84	14.395	81	0.0000	16
AB102	1	0	0	1	7	9.02	13.635	80	0.0000	40
AB103	1	0	0	1	7	9.02	13.635	80	0.0000	32
AB104	1	0	0	1	7	9.84	14.395	75	0.0000	13
AB105	1	0	0	1	7	9.84	14.395	75	0.0000	1
AB106	1	0	0	2	7	9.84	12.880	75	6.0032	1
AB107	1	0	0	1	7	9.02	13.635	80	0.0000	2
AB108	1	0	0	1	7	8.20	12.880	86	0.0000	3
AB109	1	0	0	1	7	9.84	14.395	75	0.0000	8
AB110	1	0	0	1	7	13.12	17.425	76	0.0000	14

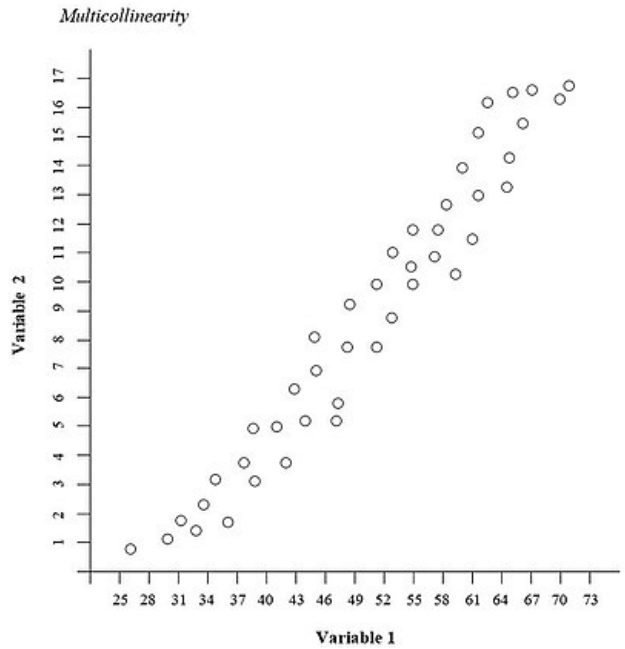
Outliers

- In statistics, an outlier is a term used to define, in a set of observations, an anomalous value, that is, a value clearly distant from the other observations
- An outlier may be due to errors in data collection or measurement
- There is no unique mathematical definition of an outlier
- Be cautious when removing or correcting them



Dependencies between columns

- It may happen that the values of some columns are strongly related (correlated) to each other
- In such cases, it is sufficient to keep only one column
- This not only makes the analysis phase more efficient but also allows the trained models to correctly determine the "contribution/role" of each predictor



Note. The plot depicts the predictor variables, Variable 1 and Variable 2, as highly linearly related.

Feature selection

- The process of determining which attributes to keep and which to discard is called *feature selection*
- In the previous slides, we saw some examples of column removal
- There are many techniques in the literature for performing feature selection, as it plays a crucial role before the actual analysis:
  - creation of simpler models
  - creation of more accurate models
  - creation of more interpretable models
  - creation of models that can better generalize to new data

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