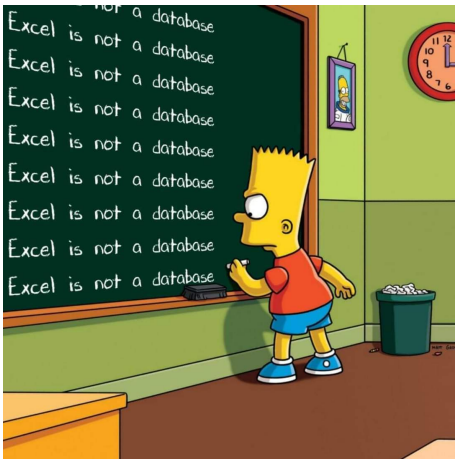
Topics in data management

Mark van der Loo



Version: November 2021

Version: November 2021
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To the author's best knowledge, the cover picture was published first by Stuart McMillan in the context of the UK government misreporting the number of SARS-COVID-19 cases becase of faulty data management using Excel. https://twitter.com/mcmillanstu/status/1313520477919498246
Typeset with LaTeX, December 21, 2021.

Preface

These notes are based on several versions of a twelve-hour course that was taught as part of the European Master's of Official Statistics track (EMOS). The course was given by the author for students of the University of Utrecht (since 2016) and Leiden University (since 2019). The Master's track is followed by a broad class of studens, but most of them have a bachelor's degree in one of the social sciences with an emphasis on quantitative research in that area.

The topics have changed a few times during the four years this course was given. They now cover a broad range of areas including data validation, the statistical value chain, data structures, relational data management and more. Although each topic could only be touched upon given the short time available for the course, it was always attempted to treat both theoretical and practical aspects.

Reading guide

Important terminology are presented in a frame for easy lookup.

Terminology
Important terms are presented here like this.

Every Chapter has exercises. When there are answers, there is a link to the page number where you can find the answers below the exercises. You can click on the link in the section heading of the answers to jump back to the exercises.

Acknowledgments

Part of this work was written during a visiting professorship at Universidade Federal de Pelotas (Br) in 2019, where I taught a four day course on data management for scientists. I like to thank professors Maximiliano (Max) Cenci, Tatiana Pereira Cenci and Marcos Britto Correa for their kind hospitality and pleasant collaboration. The visit was funded by CAPES Grant Agreement No 88887.368241/2019-00.

I am greatly indebted to Ronald Ossendrijver for carefully reviewing the manuscript. Any errors are of course on account of the author.

Mark van der Loo, October 2020

Contents

Chapter 1

The faces of data

The main purpose of this chapter is to raise awareness of the different ways data are used, and how and why data should be structured for a specific purpose. The reader is also acquainted with a few common terms related to data management.

1.1 Introduction

Data are created and used for many different purposes, and it should therefore not be surprising that the same data occurs in different guises that are geared for a specific type of use. One of the most common mistakes made in data analyses or data management is to take data that is structured for one purpose, say presentation, and try and use it in that form for another purpose like statistical analyses. The purpose of this chapter is to give an overview of the main types of uses of data, the way data is typically structured for each purpose, and to compare their relative advantages and disadvantages.

The main uses of data distinguished here are storage, transport, analyses, and presentation. Each use comes with its own conventions of how to structure and manipulate data that stem from the different demands that the different uses imply. For example, for reliable storage, retrieval and updating of information it is beneficial to store each piece of information exactly once, while it may be beneficial for interactive data analyses to have multiple copies of the same data available. Similarly, when transporting data from one computer system to another, it is important that data can be 'packed' and 'unpacked' quickly with a variety of tools. When presenting data, it is important that the relevant information can be grasped quickly by users.

Working with data is more comfortable when data is structured especially for

a specific purpose. As a trade-off the other purposes suffer: data formatted for communicating between web services is hardly fit for human interpretation. One important aspect of data management is therefore the ability to recognize the task at hand and transform data into a suitable format.

As an example, consider a table of (fictional) CO_2 emission figures by fuel source. Pay special attention to how the data are formatted.

CO_2 emission (kiloton per annum)

fuel	**emission**
Petrol	215
– of which bio	75
Diesel	456
– of which bio	89

(1.1)

This type of format is very common. One frequently encounters it for example in official statistics publications or in financial reports of businesses. Table (1.1) is optimized so people can quickly eyeball the contribution of biofuels as a fraction of total emissions for each fuel type. As a trade-off this table is not very suited for analysis. For example, to derive the contribution of regular fuels, one needs to subtract the emission value in the second line from the value in the first line, and do this again for line three and four. Performing such calculations is much easier, and less error-prone when the analyst does not have to worry about in what line which data item is stored exactly.

This situation can be improved by realizing that the first column actually hides a two-level classification: fuels are split into Petrol and Diesel while each of those is split into the bio and regular type. Knowing this, the same information can be represented as follows.

fuel	**type**	**emission**
Petrol	regular	140
Petrol	bio	75
Diesel	regular	367
Diesel	bio	89

(1.2)

The totals represented in the first table are no longer explicitly represented in Table (1.2). This is because the totals in Table (1.1) present the result of an analyses while Table (1.2) represents the basis of an analyses, that is: the raw underlying data. The benefit of the second representation over the first is that it allows for more general analyses like computing the total contributions of regular and biofuels.

A good way to think of the difference is that Table (1.1) is a presentation of results, while Table (1.2) represents a data set for analyses. The advantage of the second for over the first is that it allows general analyses, like computing the

total emission contribution of regular fuels. Thus, although both tables communicate the same information they differ in area of application. Unfortunately, the presentation form is very often used in analyses, especially in spreadsheet software.

Next, have a look at the following format, where the data has been transformed to a machine-readable string of characters.

```
[{"fuel":"petrol","type":"regular","emission":140},
↪  {"fuel":"petrol","type":"bio","emission":75},
↪  {"fuel":"diesel","type":"regular","emission":367},
↪  {"fuel":"diesel","type":"bio","emission":89}]
```
(1.3)

Here the little ↪ indicates that a line break was inserted only to fit the code on the page. The actual string has no spaces and no line endings or newlines. The format presented here is called javascript object notation (JSON). The main purpose of this format is to provide a general way to represent all sorts of data in a standardized way so it can be sent from one piece of software to another. Now there are many of such formats, but this particular one is very commonly used for communication between web services and clients. Clearly, this format is not meant for presentation to people or for statistical analyses. One advantage of JSON is that it is very generic: data need not fit in a table to be stored in a JSON string, and in principle any kind of data can be packed as JSON. Another advantage is that all wide-spread programming languages have libraries that allow programmers to read, write, and manipulate JSON data. It is thus a good format to interchange data between different systems.

Finally, consider the same information but now organized as it would be, when stored in a database.

Fuel

id	**name**
11	petrol
12	diesel

,

Type

id	**name**
1	regular
2	bio

,

Emission

id	**fuel**	**type**	**amount**
120	11	1	140
121	11	2	75
123	12	1	367
124	12	2	89

(1.4)

Now each classification and each concept is given it's own table. There is a 'Fuel' table where each fuel is given a meaningless identifying number, and a name. The same happened for the subclass 'Type'. The table on emission sources now has a unique id for each emission, and the fuel and type are identified by the id's in their respective table. The reason data is stored in such a format in database systems is that they are optimized for consistency. For example, if one needs to replace the fuel name 'petrol' with 'gasoline', then the formats presented in (1.1), (1.2), and (1.3) require multiple changes in multiple places, which is both inefficient and error-prone. The database format ensures that in

case of an update, only a single item needs to be touched and everything else is updated immediately. This benefit of easy and consistent updates comes with a cost: the data in the Emission table is not understandable unless one knows the other tables as well. We shall go into more detail when we discuss relational data in Chapter 4.

The above examples give some intuition to why it is important to structure data in a way that is suited for purpose. Below the main types of uses, specific demands that come with it and typical tools are summarized.

Storage. When data is formatted for storage, this is typically done with the four basic operations in mind that are often referred as the CRUD operations.

CRUD.
Creating, Retrieving, Updating, and Deleting data.

To facilitate this, data storage systems must have a way of uniquely identifying each data item entrusted to them, regardless, for example of the order in which the data is stored. The database example (1.4) satisfies extra demands such as a form of consistency, but there are other storage solutions that do not satisfy this consistency but that do support CRUD operations. Software for data storage is often characterised as either relational or non-relational. The table set in (1.4) is an example of how data is structured in a relational database. Examples of non-relational databases include key-value stores, document databases or graph (network) databases.

Transport. When transporting data from one machine to another, it is important that every value can be packed, send, unpacked and recognized correctly. Over time many standards have been developed. Important formats include the JSON format that was mentioned earlier and XML (eXtensible Markup Language). Both formats are supported by many programming languages and they can therefore be used by developers to exchange information between systems. The formats still leave a lot of choice for how to store data precisely. For example, in (1.3), the order of variables in each record is fuel–type–emission. Changing this order would still yield a valid JSON format. For this reason, developers usually fix the way a JSON or XML document must look like in something called a schema.

Schema.
A schema describes the structure of a data format for a specific type of data, within a chosen standard (e.g. XML, JSON).

Both JSON[1] and XML[2] have their own ways of denoting a schema. Some schemas are fairly simple, such as the JSON schema defined by the European Statistical System for exchanging information about data validation results[3]. Other schemas are large and elaborate, such as the SDMX standard[4], for standardized exchange of statistical information between institutions.

Analysis. To analyze data interactively, it is important that it is formatted so that typical operations such as filtering, plotting, and modeling are made as easy as possible. The most important demands are that a data set represents a single type of entity and that each data item represents the properties of one unique entity. Furthermore, there should be no duplicate entries and all properties should be stored in the correct type (integer, numeric, nominal, ordinal, text).

Entity type, population, entity, population unit, attribute, variable.
In computer science and specifically in the area of databases, the term *entity type* refers to a collection of real-world objects or events such as persons, clicks on a web page, buildings in some city, and so on. In statistics this concept is usually referred to as a *population*, or target population.

Similarly, in computer science an *entity* is an instance of an entity type, while in statistics one often refers to a population element as a *population unit*.

All elements of a population (entities of an entity type) share a set of properties. Computer scientists often refer to a property as *attributes* while statisticians call them *variables* or *stochastic variables* when probabilistic properties of the data are important.

In many, but not all cases (See Section 1.2) this means that data is represented in a tabular format such as (1.2) where each row represents one entity, each column represents one attribute and each entity appears only once. A good rule of thumb to decide whether a tabular data set is fit for analyses is to answer the

[1] `https://json-schema.org/`
[2] `https://www.w3schools.com/xml/schema_intro.asp`
[3] `https://ec.europa.eu/eurostat/cros/content/validation-report-structure_en`
[4] `https://sdmx.org`

question: are summary statistics of the attribute columns meaningful? Compare for instance Tables (1.1) and (1.2): is it meaningful to compute the sum of the numeric column?

Presentation. The main purpose of data in a presentable format is to convey a message as clearly and objectively as possible. This means that presentation is adapted to the expected audience and one may even choose different presentations for different audiences. Typical tools for data presentation include spreadsheet software, or business intelligence software like Tableau. Almost all statistical software packages also offer some kind of support for data presentation.

In practice, the lines between various uses of data are often blurred by software tools. Spreadsheet software is optimized for presentation of data but also offer limited analytical and data management features. Many commercial databases offer some form of in-database analytical capabilities mixing storage and analyses while users of spreadsheet software often confuse a spreadsheet file with a data storage format. Although this blurring can seem convenient it is almost always better to separate concerns and choose a specialized tool and data format for the task at hand. The main reason for this is that reproducibility, maintainability and understandability suffer when a tool is used for purposes for which it is not designed. Notorious examples include complex interlinked sets of spreadsheets where it is very difficult to track how the results are derived. The lack of systematic testability as well as their opaqueness renders spreadsheets all but useless for reliable and reproducible research. They do shine when it comes to presentation, with features like conditional formatting or interactive pivoting. A second example of such misuse of a tool is when programming a data analyses in Structured Query Language (SQL). SQL is optimized for CRUD operations on data bases, but expressing analytical operations such as computing a summary statistics or model parameters cumbersome when expressed in pure SQL. This then tends to lead to code that is hard to read and difficult to maintain. So as a general rule, it is a good idea to choose the data structure and associated tools that are designed for a specific type of use.

1.2 Data types and data manipulation

We have seen that data can be formatted in different ways for different purposes. The structure we use —a database schema, a JSON string, in principle says nothing about the *intrinsic* structure of data, which is the discussion of the following paragraphs.

Relational data. The running example of the previous section is a data set where there is no intrinsic relation between the different data points: the order of columns and rows in Table 1.2 have no meaning. And any analyses performed on this dataset will be insensitive to permutations of rows or columns as long as we refer to the columns by their name rather than position. Data satisfying this requirement is called 'relational data': each relation (row in a table) represents values of attributes of a single population unit. Typical operations that one performs on relational data include filtering or sorting rows, or adding or deleting columns. These operations consume relational data and produce relational data. The result of certain analyses can also be meaningfully stored in a relational data set. For example grouped aggregation.

There are many cases where data points represented in a data set do possess intrinsic interrelations, and this always requires specialized theoretical and computational tools to analyze. Let us look at some important practical examples.

Time series. A time series is a sequence of values (or value-tuples) that correspond to a sequence of equidistant times or periods. Examples include monthly GDP estimates, daily closing levels of the stock market or quarterly estimates of immigration. Many outputs in official statistics are as time series, and much effort is spent on constructing them. Important operations performed on economic time series include inflation correction, taking account of calendar effects, decomposition into trend and seasonal effects, decomposition into long-term trend and business cycle effects, increasing or decreasing the frequency by disaggregation or aggregation, and more. All these operations have in common that they they both accept and produce time series. They make explicit use of the fact that data is organized as a time series and are therefore not invariant under permutation of the elements of a time series.

Geospatial data. This data type is used to visualise and analyse phenomena where geographical location or geospatial patterns are important. Some examples from official statistics where geospatial analyses plays a role include land use, population density, biodiversity, and environmental accounting. In geospatial data, each value is related to a point, line, or region (a polygon) that is represented in a certain co-ordinate system. Typical operations include co-ordinate transformations, geospatial smoothing, and merging or splitting of regions. Again, permuting the values with respect to their geospatial features (point, line, region) would make such operations useless. Also observe that again, the 'typical operations' mentioned here both consume and produce geospatial data.

Network data. A network consists of nodes, connected by links. Nodes represent entities while links represent connections between them. For example a client–server relationship between companies, a family link between persons, or a shared employer between persons. At the time of writing, official statisticians are just beginning to explore the uses of network data, but it is likely that a more 'systemic' approach to describing the economy and society based on network science will play a role in the future of official statistics. For networks, the structure *is* the data. In network analyses one is interested in summarizing or using network structure as a means to gain insight in the phenomenon described by it. Typical operations on networks include subnetwork selection or CRUD operations like adding or deleting nodes or links. Again (and notice this is becoming a theme now), these operations consume and produce networks.

Other. There are many more data types that are useful but not naturally represented in relational format. Examples include images, videos, or event logs. All these data types come with their own 'natural' transformations.

By now, attentive readers have probably detected a recurring theme across these examples. Each data type comes with a set of 'natural' operations that leave the data type intact. This phenomenon is so important that mathematicians and computer scientist have a name for it.

Algebraic closure.
Given a data type T, and an operation that manipulates data of that type. We say that T is *algebraicly closed* under this operation when the result of the operation is again of the same type T.

In practice, things are easier when you work in an algebraically closed system of operations. For example. Given a relational data set, we can develop a script where we first filter, then sort, and then merge the data set with another data set. These operations are easy to perform in sequence because the output of one operation can serve as input to the next. If we discover a bug and find out we need to merge before filtering, the only thing we need to do is swap the two operations. Indeed, working within an algebraically closed system feels so natural that one can focus on *what* of the data manipulation, rather than at the *how*.

There are other advantages that are facilitated by algebraic closure. For example, most modern database systems are capable of re-ordering instructions to increase speed of execution. For example it is faster to first filter records and then sort them then the other way around (because there is less to sort that way). Algebraic systems generally come with a set of re-ordering rules that can

be taken advantage of by software that executes it. Important examples of algebraic systems are the various query languages that implement CRUD operations for different data types. Examples include Structured Query Language (SQL) for relational data, Cypher for network data and Spatial SQL for geographic data.

The main takeaway of this section is that it is useful to distinguish between *data transformations* where data is manipulated but the type does not change, and *type transformations* where data manipulation yields data of a new type. Third, we saw in §1.1 there are format transformations that change the technical layout of data.

A typical step in a statistical production system starts with reading data from a file or database. This is a format transformation, possibly followed by a type transformation. For example when a JSON string is read into a relational format. Next, depending on the task several type-conserving transformations and/or type-transforming data manipulations are carried out after which the data is again formatted for output.

Where are we?

We have seen that data is a representation of information, and that data may be formatted in several ways depending on its intended use. We have also seen that data types can be distinguished by looking at their intrinsic structure. Depending on intrinsic structure, a number of 'natural' operations are associated with data that leave its characteristic structure intact. It is useful to distinguish between formatting, type-conserving, and type-changing data transformations.

1.3 Exercises

1. Explain why Table (1.1) is unsuited for storage or transport of data.
2. Acquaint yourself with storage solutions by reading through the Wikipedia entries for Database[5] and NoSQL[6].
3. Find out what OLTP and OLAP means.
4. Explain why or not the following data structures are suitable for analyses.

(a)

	Alice	Bob	Carol
Shoe size	38	43	41
Income	3300	2800	4000

(b)

Income	0k – 20k	20k – 40k	40k – 80k	80K+
Amsterdam	20%	40%	35%	5%
Rotterdam	30%	30%	38%	2%
Den Haag	25%	35%	30%	10%

(c)

Name	Age	has job
Dave	36	No
Eve	5	Yes

(d)

Sector	costs	profit
Retailers	50	10
Wholesalers	20	5
Total	70	15

5. Name three operations on image data that leave the data type intact.
6. Explain why each of the following statements is true or false.
   (a) The natural numbers $\mathbb{N} = \{1, 2, \ldots\}$ are closed under multiplication.
   (b) The rational number s $\mathbb{Q}$ are closed under addition.
   (c) The real numbers $\mathbb{R}$ are closed under division.
   (d) We denote with Σ^* the set of all finite strings that can be created with an alphabet Σ. For example if $\Sigma = \{a, b, \ldots, z\}$ then Σ^* is the set of all finite concatenations of letters from the Latin alphabet, plus the empty string (the string without characters). Statement: Σ^* is closed under concatenation of strings (pasting one string behind the other).
   (e) The function zero returns 0 for each value it is given. For Example $\mathrm{zero}(\pi) = 0$. Statement: the integers $\mathbb{Z} = \{\ldots, -2, -1, 0, 1, 2, \ldots\}$ are closed under zero.

[5] https://en.wikipedia.org/wiki/Database
[6] https://en.wikipedia.org/wiki/NoSQL

(f) The natural numbers are closed under zero.

(g) (Bonus question) The function a_n adds the number 1, n times to its input. For example $a_3(2) = 2 + 1 + 1 + 1 = 5$. Statement: the natural numbers are closed under a_∞.

Check your answers on page 79.

Chapter 2

The statistical value chain

In this Chapter we look at some general principles that help to organize data processing, going from raw data to statistical output[1].

2.1 Statistical value chain

A national statistical institute (NSI) can in many ways be seen as a data factory. Indeed, both nationally and internationally official statisticians refer to their work as 'production', to their data as 'raw data' and to their statistics as 'output'. All terms that are borrowed from phyiscal production processes. In this sense it is no surprise that the idea of a Statistical Value Chain has become the preferred way of organizing statistical production in many statistical offices.

Value chain.
The idea of the value chain is based on the process view of organizations, the idea of seeing a manufacturing (or service) organization as a system, made up of subsystems each with inputs, transformation processes and outputs [IfM, 2013].

A value chain, roughly, consists of a sequence of activities that step by step increase the value of a product. The idea of a statistical value chain has become a common term in the official statistics community over the last two decades or so, although a single common definition seems to be lacking[2]. Roughly then, a statistical value chain is constructed by defining a number of meaningful

[1] Partly based on Van der Loo and De Jonge [2018, Chapter 1]
[2] One of the earliest references seems to be by Willeboordse [2000]

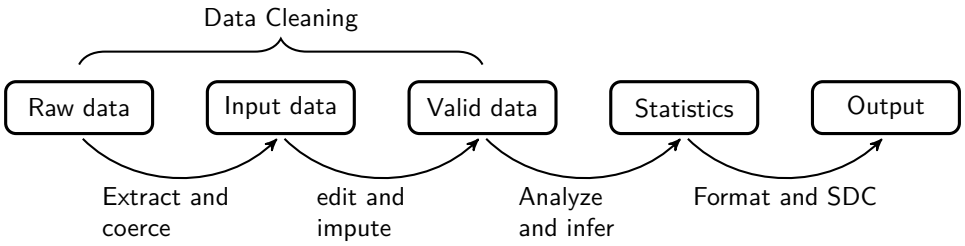


Figure 2.1: Part of a statistical value chain, showing five different levels of statistical value going from raw data to statistical product.

intermediate data products, for which a chosen set of quality attributes are well-described [Renssen and Van Delden, 2008]. There are many ways to go about this, but the picture shown in Figure 2.1 has proven to be a fairly generic and useful picture to organize thoughts around a statistical production process. A nice trait of the schema in Figure 2.1 is that it naturally introduces activities that are typically categorized as 'data cleaning' into the statistical production process. From the left we start with raw data. This must be worked up to satisfy (enough) technical standards so it can serve as input for consistency checks, data correction and imputation procedures. Once this has been achieved, the data may be considered valid (enough) for the production of statistical parameters. These must then still be formatted to be ready for deployment as output.

More generally, a statistical production process is designed by viewing input, output and a number of intermediate states as statisitical products.

Statistical product.
A state of data that is guaranteed to satisfy a predifined set of quality demands.

Thus each state, represented by a rectangle in Figure 2.1 is fixed by specifying precisely when a data set is allowed to be called 'raw', or 'valid' and so on. Physically, each state may be represented by a table in a data base, a set of files, or any other way data can be represented. A description should be accurate enough to understand the contents of a data set as well as the limits of its usability. To describe usability, the five quality aspects defined in the Eurpean Quality Assurance Framework (QAF): relevance, accuracy, timeliness, accessibility and comparability serve as a guide of things to describe. For example, a good description of the file format falls under accessibility while an accurate description of logical restrictions that the data satisfy (like 'Age is nonnegative') falls under 'accuracy and reliability'.

The five quality aspects of data.
In the European Quality Assurance Framework, the following five quality dimensions are defined.

- **Relevance.** The degree to which the statistical product meets user needs in both coverage and content.
- **Accuracy & Reliability.** Accuracy is the proximity between an estimate and the unknown true value. Reliability is the closeness of early estimates to subsequent estimated values.
- **Timeliness and Punctuality.** Timeliness refers to the time gap between publication and the reference period. Punctuality refers to the gap between planned and actual publication dates.
- **Accessibility and Clarity.** Accessibility is the ease with which users are able to access the data, also reflecting the format in which the data are available and the availability of supporting information. Clarity refers to the quality and sufficiency of the metadata, illustrations and accompanying advice.
- **Comparability and Coherence.** Comparability is the degree to which data can be compared over time and domain. Coherence is the degree to which data that are derived from different sources or methods, but refer to the same topic, are similar.

Having solid descriptions of each state are an important step of making data usable for other production processes or incidental analyses. It makes different statistical production chains composable by using the output of one chain as input for another. The definition of statistical products allows one to systematically disentangle a complex set of activities going from input to output into manageable chunks of well-defined tasks with clear beginnings and clear ends. This allows one to design the process going from say 'input data' to 'valid data' independent from the other steps in the chain. If two statistical production processes have similar intermediate states, there is a chance that tooling and methodology might be shared between them, thus enhancing standardisation, which in turn should improve comparability between statistics and overall efficiency.

One generally distinguishes two approaches in designing statistical production chains. The first and traditional way is called *output-driven* design. Here, one first investigates the need of end-users and based on that, describes the output state with all quality aspects. For example, the output may be an interactive

dashboard that gives a coherent view on the state of a certain economic sector. Given this description, one can then describe what statistics should be available, and with what quality. Knowing this, one can describe the necessary microdata and it's quality necessary to produce the statistics. This process continues until the necessary raw data is defined.

The second and more recent approach to Statistical Value Chain design is called the *data-driven* approach. The motivation is usually the availability of a new type of data source that is potentially interesting for the production of official statistics. Either by creating an opportunity for new output or for replacing or augmenting an existing data source. In this case, the 'design' process is more informal and proceeds iteratively, starting with investigating the usability of the data. Once usability is established, more iterations are necessary to actually bring the new process into production.

We conclude this section by describing the five data states of Figure 2.1 in some more detail.

Raw data

With raw data we mean the data as it arrives at the place where it is to be processed. The state of such data may of vary enormously depending on the data source. Raw data is often characterized by limited amount of control over how the data was collected, as is the case with administrative data. However, it is possible to describe the state of the data as it arrives and perhaps to create agreements with data suppliers about data form and quality. In any case, a version of the raw data is to be stored as-is to ensure reproducibility.

Raw data.
Raw data is 'data as it arrives'. We only demand that it is adequately described so further processing can take place.

The first production step, consist of making the data readily accessible and understandable. After the first processing step, we demand that each value in the data can be identified with the real-world object they represent (person, company, something else), for each value it is known what variable it represents (age, income, ...), and the value is stored in the appropriate technical format (number, string).

Depending on the technical raw data format, the activities necessary to achieve the desired technical format typically include file conversion, string normalization, and standardization and conversion of numerical values. Joining the data

against a backbone population register of known statistical objects, possibly using procedures that can handle inexact matches of keys is also considered a part of such a procedure.

Input data

Input data are data where each value is stored in the correct type and identified with the variable it represents and the statistical entity it pertains to. In many cases such a dataset can be represented in tabular format, rows representing entities, columns representing variables. In the R community this has come to be known as 'tidy' data [Wickham et al., 2014]. Here, do not force a particular data format. Many data can be usefully represented in the form of a tree or graph (e.g. web pages, XML structures). As long as all the elements are readily identified and of the correct format, it can serve as Input data.

Input data.
Input data satisfies the following demands.

- Each unit in the data is identified with a unit in the population register.
- Each unit occurs only once in the data.
- Each value is stored in the correct type (a data type defines the values that a variable can assume).
- Each value is identified with a single population unit and a single attribute of that unit.

A rule of thumb for input data is that it can be easily imported into an appropriate tool. For example by reading it from a data base, or a well-described textual format, in a single line of script.

Once a dataset is at the level of input data, the treatment of missing values, implausible values, and implausible value combinations must take place. This process is commonly referred to as data editing and imputation. It differs from the previous steps in that it focuses on the consistency of data with respect to domain knowledge. Such domain knowledge domain knowledge can often be expressed as a set of rules, such as `age >= 0`, or `mean(profit) > 0`, or `if ( age < 15 ) has_job = FALSE`. We will have a further look into such rules in Chapter 3.

Valid data

Data are valid once they are trusted to faithfully represent the variables and objects they represent. Making sure that data satisfies the domain knowledge expressed in the form of a set of validation rules is one reproducible way of doing so. Often this is complemented by some form of expert review, for example based on various visualizations, or reviewing of aggregate values by domain experts.

Valid data.
Data is 'valid' when it contains no invalid values, is free of internal contradictions, and does not conflict common domain knowledge.

Once data is deemed valid, the statistics can be produced by known modeling and inference techniques. Depending on the preceding data cleaning process, these techniques may need those procedures into account. For example when estimating variance after certain imputation procedures.

Statistics

Statistics are simply estimates of the output variables of interest. Often these are simple aggregates (totals, means) but in principle they can consist of more complex parameters such as regression model coefficients, or a trained machine learning model.

Statistics.
A statistic is an estimate of a population property based on valid data.

Once statistics are computed, they need to be formatted to be transferred to other organizations or for presentation.

Output

Creating output begins where the analysis stops. Output is created by taking the statistics and preparing them for dissemination. This may involve technical formatting, for example to make numbers available through a (web) API or layout formatting, for example by preparing a report or visualization. In the case of technical formatting, a technical validation step may again be necessary,

for example by checking the output format against some (json or XML) schema. In general, the output of one institute or department is raw data for another.

Output.
Data formatted for dissemination.

2.2 Exercises

1. Explain where in the value chain of Figure 2.1 the following activities take place. Sometimes multiple options are possible. Explain why.
   (a) Formatting a date-time variable to ISO8601 format.
   (b) Estimate the covariance between unemployment rate and age.
   (c) Join survey data with a survey reference frame, using unique identifiers (such as social security number) so all elements in the survey data can be identified.
   (d) Join administrative data with a reference frame, using approximate record linkage, based on approximate matches in name-addres data.
   (e) Clean up a text variable that contains values such as `"M"`, `"Man"`, `"Fem"`, and `"woman"` and replace them with valid codes from a code list, like `"male"` `"female"`, `"other/non-binary"`.
2. Discuss advantages and disadvantages of the data-driven versus the output-driven approach to designing statistical production systems.

Check your answers on page 80.

Chapter 3

Data validation

In this Chapter we look at formal ways of testing whether data is good enough for its intended use[1].

3.1 Introduction

Informally, data validation is the activity where one decides whether or not a particular data set is fit for a given purpose. The decision is based on testing observed data against prior expectations that a plausible dataset is assumed to satisfy. Examples of prior expectations range widely. They include natural limits on variables (weight cannot be negative), restrictions on combinations of multiple variables (a man cannot be pregnant), combinations of multiple entities (a mother cannot be younger than her child) and combinations of multiple data sources (import value of country A from country B must equal the export value of country B to country A). Besides the strict logical constraints mentioned in the examples, there are often 'softer' constraints based on human experience. For example, one may not expect a certain economic sector to grow more than 5% in a quarter. Here, the 5% limit does not represent a physical impossibility but rather a limit based on past experience. Since one must decide in the end whether a data set is usable for its intended purpose, we treat such assessments on equal footing.

Data validation (definition of the ESS).
Data validation is an activity in which one verifies whether or not a combination of values is a member of a set of acceptable combinations.

[1] Based on van der Loo and de Jonge [2020].

The purpose of this Chapter is to formalize the definition of data validation and to demonstrate some of the properties that can be derived from this definition. In particular, it is shown how a formal view of the concept permits a classification of data validation rules (assertions), allowing them to be ordered in increasing levels of 'complexity'. Here, the term 'complexity' refers to the amount of different types of information necessary to evaluate a validation rule. A formal definition also permits development of tools for automated validation and automated reasoning about data validation [Zio et al., 2015, Van der Loo and De Jonge, 2018, 2019]. Finally, some subtleties arising from combining validation rules are pointed out.

3.2 Formal definition of data validation

Intuitively, a validation activity classifies a dataset as acceptable or not acceptable. A straightforward formalization is to define it as a function from the collection of data sets that could have been observed, to $\{\text{True}, \text{False}\}$. One only needs to be careful in defining the 'collection of data sets', to avoid a 'set of all sets' which recursively holds itself. To avoid such paradoxes, a data set is defined as a set of key-value pairs, where the keys come from a finite set, and the values from some domain.

Definition 1 *A* data point *is a pair* $(k, x) \in K \times D$*, where* k *is a* key*, selected from a finite set* K *and* x *is a* value *from a* domain D*.*

In applications the identifier k makes the value interpretable as the property of a real-world entity or event. The domain D is the set of all possible values that x can take, and it therefore depends on the circumstances in which the data is obtained.

As an example, consider an administrative system holding age and job status of persons. It is assumed that 'job' takes values in $\{\texttt{"employed"}, \texttt{"unemployed"}\}$ and that 'age' is an integer. However, if the data entry system performs no validation on entered data, numbers may end up in the job field, and job values may end up in the age field. In an example where the database contains data on two persons identified as 1 and 2, this gives

$$\begin{aligned} K &= \{1, 2\} \times \{\texttt{"age"}, \texttt{"job"}\} \\ D &= \mathbb{N} \cup \{\texttt{"employed"}, \texttt{"unemployed"}\}. \end{aligned} \tag{3.1}$$

This definition allows for the occurrence of missing values by defining a special value for them, say 'NA' (not available) and adding it to the domain.

Once K and D are fixed it is possible to define the set of all observable datasets.

Definition 2 *A* dataset *is a subset of $K \times D$ where every key in K occurs exactly once.*

Another way to interpret this is to say that a data set is a total function $K \to D$. The set of all observable data sets is denoted D^K. In the example, one possible dataset is

$$\{((1, \texttt{"age"}), 25), ((1, \texttt{"job"}), \texttt{"unemployed"}),$$
$$((2, \texttt{"age"}), \texttt{"employed"}), ((2, \texttt{"job"}), 42)\}$$

Observe that the key consists of a person identifier and a variable identifier. Since type checking is a common part of data validation these definitions deliberately leave open the possibility that variables assume a value of the wrong type.

Data validation can now be formally defined as follows.

Definition 3 *A* data validation function *is a surjective function*

$$v : D^K \twoheadrightarrow \{\textit{False}, \textit{True}\}.$$

A data set $d \in D^K$ for which $v(d) =$ True is said to *satisfy* v. A data set for which $v(d) =$ False is said to *fail* v.

Recall that surjective means that there is at least one $d \in D^K$ for which $v(d) =$ False and at least one $d \in D^K$ for which $v(d) =$ True. A validation function has to be surjective to have any meaning as a data validation activity. Suppose $v' : D^K \to \{\text{False}, \text{True}\}$ non-surjective function. If there is no data set d for which $v'(d) =$ False, then v' is always true and it does not validate anything. If, on the other hand, there is no d for which $v'(d) =$ True then no data set can satisfy v'. In short, a function that is not surjective on $\{\text{False}, \text{True}\}$ does not separate valid from invalid data.

A data validation function is reminiscent of a predicate as defined in first-order logic. Informally, a predicate is a statement about variables that can be True or False. The variables can take values in a predefined set (referred to as the *domain* of the predicate). Since validation functions map elements of D^K to $\{\text{False}, \text{True}\}$, it is tempting to equate a validation function as a predicate over D^K. However, the elements of D^K are instances of possible data sets, and validation is based on statements involving variables of a single observed data set. It is therefore more convenient to adopt the following definition.

Definition 4 *A* validation rule *is a predicate over an instance $d \in D^K$ that is neither a tautology nor a contradiction.*

The elements of D^K are sufficiently similar so that any validation rule over a particular data set $d \in D^K$ is also a validation rule over another data set in $d' \in D^K$, where the truth value of a validation rule depends on the chosen data set. This also allows us to interpret a tautology as a predicate that is True for every element of D^K and a contradiction as a predicate that is False for every element of D^K.

The equivalence between an assertion about a data set and a function classifying possible data sets as valid or invalid instances is a rather obvious conclusion. The actual value of the above exercise is the strict definition of a data point as a key-value pair. As will be shown below, inclusion of the key permits a useful classification of data validation rules.

To demonstrate that many types of validation rules can be expressed in this framework a few examples based on the example of Equation (3.1) will be considered. The following rule states that all ages must be integer.

$$\forall((u, \texttt{"age"}), x) \in d : x \in \mathbb{N}.$$

Here, $((u, \texttt{"age"}), x)$ runs over the person-value pairs where the value is supposed to represent an age. Similarly, it is possible express a nonnegativity check on the age variable.

$$\forall((u, \texttt{"age"}), x) \in d : x \geq 0.$$

In these examples a data set fails a validation rule when not all elements satisfy a predicate. Such rules are not very informative when it comes to pinpointing what elements of the data set cause the violation. It is customary to perform data validation on a finer level, for example by checking nonnegativity element by element. Based on the definitions introduced here this is done by fixing the key completely.

$$\begin{aligned}\forall((1, \texttt{"age"}), x) \in d : x \geq 0 \\ \forall((2, \texttt{"age"}), x) \in d : x \geq 0.\end{aligned}$$

Now consider the cross-variable check that states that employed persons must be 15 or older.

$$\forall((u, \texttt{"age"}), x), (u, \texttt{"job"}), y) \in d : y = \texttt{"employed"} \Rightarrow x \geq 15,$$

where $\Rightarrow$ denotes logical implication (if $y = \texttt{"employed"}$ then $x \geq 15$). Finally, consider the cross-person check that states that we expect the average age in the data set to be larger then or equal to 5.

$$\frac{\sum_{(u,\texttt{"age"},x)\in d} x}{\sum_{(u,X,x)\in d} \delta(X, \texttt{"age"})} \geq 5,$$

where $\delta(X, Y) = 1$ when $X = Y$ and otherwise 0.

In practical applications validation rules are often expressed more directly in terms of variable names, such as $age \geq 0$. Such expressions are specializations where one silently assumes extra properties such as that the rule will be evaluated for the entry for age in every record.

Remark 1. In Definition 3, (and also 4) a validation function is defined as a surjection $D^K \twoheadrightarrow \{\text{False}, \text{True}\}$. In practical applications it is often useful to also allow the value `NA` (not available) for cases where one or more of the data points necessary for evaluating the validation rule are missing. In that case the domain D in the Equation (3.1) must be extended to $D \cup \{\texttt{NA}\}$. See Van der Loo and De Jonge [2019] for an implementation.

Remark 2. The current formalization of data validation excludes checking for completeness of the key set: it is assumed by definition that each data set in D^K is a complete set of key-value pairs where the keys cover all of K. The above definitions therefore create a clean distinction between what is metadata (the keys and their interpretation) and data (key-value pairs). It is possible to check for uniqueness of variables.

Remark 3. The formal definition of data validation rules also allows a formalization of data validation software tools or domain specific languages, such as in Bantilan [2020], Van der Loo and De Jonge [2019].

Remark 4. In official (government) statistics, validation rules are referred to as *edit rules* rather than data validation rules. See De Waal et al. [2011] and references therein.

3.3 Classification of validation rules

Validation rules defined by domain experts may be easy for humans to interpret, but can be complex to implement. Take as an example the assertion 'the average price of a certain type of goods this year, should not differ more then ten percent from last year's average'. To evaluate this assertion one needs to combine prices of multiple goods collected over two time periods. A practical question is therefore if the 'complexity of evaluation', in terms of the amount of information necessary, can somehow be measured. In this section a classification of data validation rules is derived that naturally leads to an ordering of validation rules in terms of the variety of information that is necessary for their evaluation.

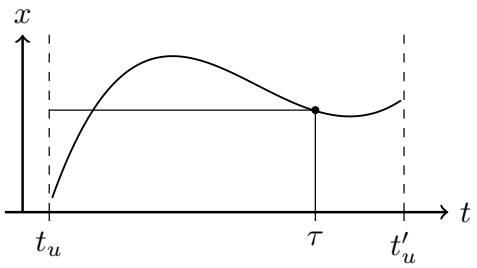


Figure 3.1: A unit u of type U exists from t_u to t'_u. From t_u onward it has an attribute X with its value x possibly changing over time. At some time τ this value is observed. The observed value is thus fully characterized by the quartet (U, τ, u, X).

One way to measure the amount of information is to look at the predicate defining a data validation rule and to determine how many different (k, x) pairs are needed to evaluate it. This is not very useful for comparing complexity across different data sets that are not from the same D^K since the numbers will depend on the size of the key set K. One measure that does generalize to different D^K is the measure 'does a rule need one, or several (k, x) to be evaluated?'.

This measure is not very precise, but it can be refined when a key consists of multiple meaningful parts such as in the running example where the key consists of the id of a person and the name of a variable. One can then classify a rule according to two questions: 'are multiple person id's necessary for evaluation?', and: 'are multiple variables necessary for evaluation?'. This gives a four-way classification: one where both questions are answered with 'no', two where one of the questions is answered with 'yes' and one where both questions are answered with 'yes'. Although this refinement improves the accuracy of the classification, it only allows for comparing validation rules over data sets with the exact same key structure. It would therefore be useful to have a generic key structure that can be reused in many situations. One such structure can be found by considering in great generality how a data point is obtained in practice.

A data point usually represents the value of an attribute of an object or event in the real world: a person, a web site, an e-mail, a radio broadcast, a country, a sensor, a company, or anything else that has observable attributes. In what follows, an object or event is referred to as a 'unit' for brevity. A data point is created by observing an attribute X from a unit u of a certain type U at time τ, as in Figure 3.1. Using the same reasoning as above, this yields a $2^4 = 16$-way classification of validation rules: for each element U, τ, u, X a validation rule requires a single or multiple instances to be evaluated. However, there are some restrictions. Any unit u can only be of one type. So evaluating a validation

rule will never require multiple types and a single unit. Second, the type of a unit fixes its properties. So a validation rule will never need a single variable for multiple types. With these restrictions considered, the number of possible classes of validation rules reduces from sixteen to ten.

To distinguish the classes the following notation is introduced. For each element U, τ, u, X assign an s when a validation rule pertains to a single value of that element and assign an m when a validation rule pertains to multiple values of that element. For example, a validation rule of class $sssm$ needs a single type, a single measurement, a single object and multiple variables to be evaluated.

The ten possible classes can themselves be grouped into *validation levels*, according to whether a class is labeled with no, one, two, three, or four m's. A higher validation level indicates that we need a larger variety of information in order to evaluate the rule. The classification, and their grouping into validation levels is summarized in Table 3.1.

Table 3.1: The ten possible classes of validation rules, grouped into 'validation levels'. A higher level indicates that a wider variety of information is necessary to evaluate a validation rule.

Validation level				
0	1	2	3	4
ssss	sssm	ssmm	smmm	mmmm
	ssms	smsm	msmm	
	smss	smms		

Going from level 0 to 4 corresponds to a workflow that is common in practice. One starts with simple tests such as range checks. These are of level zero since a range check can be performed on a single data point. That is, one only needs a value that corresponds to a single type, measurement, unit, and variable. Next, more involved checks are performed, for instance, involving multiple variables ($sssm$, e.g. the ratio between two properties of the same unit must be in a given range), multiple units ($ssms$, e.g. the mean of a variable over multiple units must be within a specified range), or multiple measurements ($smss$, e.g. the current value of the property of a unit cannot differ too much from a past value of the same property of the same unit). Going up in level, even more complex rules are found until rule evaluation involves multiple variables of multiple units of multiple types measured at multiple instances ($mmmm$).

This classification also has an immediate interpretation for data stored in a data base that is normalized in the sense of Codd [1970]. In such a data base, records represent units, columns represent variables, and tables represent types. The 'time of measurement' is represented as a variable as well. The classification indicates whether a rule implementation needs to access multiple

records, columns or tables.

3.4 Properties of validation rule sets

Definition 4 implies that a validation rule is a predicate over a data set that is not a tautology nor a contradiction. This means that combining two validation rules with $\wedge$ or $\vee$ does not automatically yield a new validation rule. Consider for example the rules $x \geq 0$ and $x \leq 1$ (using shorter notation for brevity). The rule $x \geq 0 \vee x \leq 1$ is a tautology. The rule $x \geq 0 \wedge x \leq -1$ is a contradiction. In fact, the only operation that is guaranteed to transform a validation rule into another validation rule is negation.

The fact that validation rules are not closed under conjugation ($\wedge$) or disjunction ($\vee$) has practical consequences. After all, defining a set of validation rules amounts to conjugating them together into a single rule since a data set is valid only when all validation rules are satisfied. A set of rules may be such that their conjugation is a contradiction. Such a rule set is called *infeasible*. More subtle problems involve unintended consequences, including *partial infeasibility* [Bruni and Bianchi, 2012], and introduction on fixed values or range restrictions. Other problems involve the introduction of several types of redundancies [Dillig et al., 2010, Paulraj and Sumathi, 2010], which make rule sets both harder to maintain and hamper solving problems such as error localization [Bruni, 2005, De Jonge and Van der Loo, 2019a]. In the following, some examples of unintended effects and redundancies are discussed. The examples shown here are selected from a more extensive discussion in Van der Loo and De Jonge [2018, Chapter 8]. For simplicity of presentation the rules are expressed as simple clauses, neglecting the key-value pair representation.

Partial inconsistency is (often) an unintended consequence implied by a pair of rules. For example the rule set

$$\begin{aligned} gender = \texttt{"male"} &\Rightarrow income > 2000 \\ gender = \texttt{"male"} &\Rightarrow income < 1000, \end{aligned}$$

is feasible, but it can only be satisfied when $gender \neq$ `"male"`. Thus, the combination of rules (unintentionally) excludes an otherwise valid gender category.

A simple redundancy is introduced when one rule defines a subset of valid values with respect to another rule. For example if $x \geq 0$ and $x \geq 1$, then $x \geq 0$ is redundant with respect to $x \geq 1$. More complex cases arise in sets with multiple rules. A more subtle redundancy, called 'nonrelaxing clause' occurs in

the following situation.

$$\begin{aligned} x \geq 0 \Rightarrow y \geq 0 \\ x \geq 0. \end{aligned}$$

Here, the second rule implies that the condition in the first rule must always be true. Hence the rule set can be simplified to

$$\begin{aligned} y \geq 0 \\ x \geq 0. \end{aligned}$$

Another subtle redundancy, called a 'nonconstraining clause' occurs in the following situation.

$$\begin{aligned} x > 0 \Rightarrow y > 0 \\ x < 1 \Rightarrow y > 1 \end{aligned}$$

Now, letting x vary from $-\infty$ to ∞, the rule set first implies that $y > 1$. As x becomes positive, the rule set implies that $y > 0$ until x reaches ∞. In other words, the rule set implies that y must be positive regardless of x and can therefore be replaced with

$$\begin{aligned} y > 0 \\ x < 1 \Rightarrow y > 1 \end{aligned}$$

Methods for algorithmically removing such issues and simplifying rule sets have recently been discussed by Daalmans [2018], and have been implemented by De Jonge and Van der Loo [2019b]. In short, the methods are based on formulating Mixed Integer Programming (MIP) problems and detecting their (non)-convergence after certain manipulations of the rule sets. General theory and methods for rule manipulation have also been discussed by Chandru and Hooker [1999] and Hooker [2000] in the context of optimization.

Where are we?

We have seen that data validation (checking data) can be formally defined in terms of logical statements (predicates) over a data set. Equivalently, we can define it as a function that accepts a data set and takes values in $\{\text{False}, \text{True}\}$. It is possible to define a very general classification of validation rules, based on a generic decomposition of the metadata. Combining validation rules into a set can lead to subtle and unintended consequences that can be solved in some cases with algorithmic methods.

3.5 Exercises

1. In September 2018 we ask the two Dutch citizens Alice and Bob the following questions.

   X: Do you have a job? (`yes`, `no`)

   Y: What is your age? (`under-aged`, `adult`, `retired`)

   (a) Describe the domain D

   (b) Give all values of k (this constitutes K)

   (c) What is the size of D^K? That is, how many data sets are possible?

2. Using the same case as in the previous exercise, we now restrict the possible data sets by approving only data points that satisfy the following restrictions.

   $job \in \{\texttt{yes}, \texttt{no}\}$

   $age \in \{\texttt{under-aged}, \texttt{adult}, \texttt{retired}\}$

   $job = \texttt{yes} \Rightarrow age = \texttt{adult}$

   How many data sets are now possible?

3. Decide and explain for the following cases whether it describes a validation function or not.

   (a)
   $$v(x) = \begin{cases} \texttt{TRUE} \text{ if } x \geq 3 \text{ and } x \geq 5 \\ \texttt{FALSE} \text{ otherwise} \end{cases}$$

   (b)
   $$v(x, y) = \begin{cases} \texttt{TRUE} \text{ if } x + y = 3 \text{ and } x - y = 0 \text{ and } x \leq 1 \\ \texttt{FALSE} \text{ otherwise} \end{cases}$$

   (c)
   $$v(x) = \begin{cases} \texttt{TRUE} \text{ if } x \leq 10 \text{ or } x \geq 3 \\ \texttt{FALSE} \text{ otherwise} \end{cases}$$

4. Classify the following rules according to their complexity (Table 3.1).

   (a)
   $$\frac{\text{mean}(price_{2018})}{\text{mean}(price_{2017})} \leq 1.1$$

   (b)
   $$\text{mean}(price) \geq 1$$

(c)
$$\max\left(\frac{x}{\text{median}(X)}, \frac{\text{median}(X)}{x}\right) < 10$$

(d) The following rule is the fundamental equation for National Accounts

$$\underbrace{COE + GOS + GMI + T_{P\&M} - S_{P\&M}}_{\text{GDP, Income approach}} = \underbrace{C + G + I + (X - M)}_{\text{GDP, expenditure approach}}$$

where

COE: Compensation of employees
GOS: Gross operating surplus
GMI: Gross mixed income
$T_{P\&M} - S_{P\&M}$: Taxes minus subsidies on production and import
C: Consumption by households
G: Government consumption and investment
I: Gross private domestic investment
$X - M$: Export minus Imports of goods and services

5. This is a lab assignment using R. Load the `validate` package and load the `SBS2000` dataset.

```
library(validate)
data(SBS2000)
```

This dataset represents a number of records from the Structural Business Survey (SBS). If you do not have `validate` installed, you can install it once using

```
install.packages("validate")
```

(a) Read the help file of the dataset: `?SBS2000`.
(b) Work through the introductory example of the 'data validation cookbook' `vignette("cookbook", package="validate")`
(c) Create a new textfile
(d) Define at least 10 rules for the `SBS2000` dataset
(e) Provide rationales in comments
(f) Read, and `confront()` rules with data
(g) Summarize and plot the results.
(h) Use `as.data.frame` and `View` to convert and display the results.

(i) Make a `plot` of the `validator` object.

(j) (Bonus) If you are familiar with `rmarkdown`: create a data quality report.

6. Find an implied rule for the following rule set.

```
turnover >= 0
other.rev >= 0
turnover + other.rev == total.rev
```

7. What are the allowed ranges for *age* and *income* implied by the following rule set?

```
age >= 18
if (job == TRUE) age <= 70
if (income > 0) job == TRUE
income >= 0
```

Try doing it first by hand. Verify your answer using the `validatetools` R package with the function `detect_boundary_num()`.

8. Simplify the following rule set.

```
if ( income > 0 ) age >= 16
age < 12
```

Try doing it first by hand. Verify your answer using the `validatetools` R package with the function `simplify_conditional()`.

9. Which of these rules can be left out?

```
age >= 18
age >= 12
```

Try doing it first by hand. Verify your answer using the `validatetools` R package with the function `remove_redundancy()`.

Check your answers on page 80.

Chapter 4

Relational data

Much of the well-structured data used in statistical organizations is stored in the form of *records*, more formally called *relations*. This Chapter gives a brief introduction to classical relational database theory.

4.1 Relations

The basic concept underlying classical databases is the idea of a combination of values, called a *tuple* that are related to one another. The relation between the values consists of the fact that they are pertain to the same entity. As an example consider the following tuple.

$$(Id = 1, Name = \text{"}Alice\text{"}, Age = 7, Owns = \{puzzle, bicycle\}). \quad (4.1)$$

This tuple describes several attributes of a real-world person. In this case, the tuple holds the name of a 7 year old person called Alice, who owns a bicycle and a puzzle.

Tuple.
A *tuple* is a combination of values $(x_1, x_2, \ldots, x_p)$ that take values in predefined domains.

We have introduced a bit of terminology here that needs to be made more precise for the coming discussion. First of all, we introduced the term *entity*. An entity is a particular object or event in the real world. An example of a real-world entity is *Willem-Alexander Claus George Ferdinand, King of the Netherlands, Prince of Oranje-Nassau, Squire of Amsberg*. Each entity is of a certain *entity type*.

The entity type describes all entities that that belong to a certain group. What constitutes an entity type is in practice largely a matter of choice. For example we could think of the entity type 'people living in the Netherlands', and define it as 'any person who is registered to live in a Dutch municipality'. Under this condition *Willem-Alexander Claus George Ferdinand, King of the Netherlands, Prince of Oranje-Nassau, Squire of Amsberg* is indeed of entity type 'people living in the Netherlands'. Sometimes this is also expressed by saying that *Willem-Alexander Claus George Ferdinand, King of the Netherlands, Prince of Oranje-Nassau, Squire of Amsberg* is an *instance* of the type 'people living in the Netherlands'.

Entity and Entity Type.
An *entity type* defines a population of entities. An entity is a real-world object or event. If an entity belongs to a certain entity type, we say that it is an *instance* of this type.

Entities are characterised by their properties. In database-language these are called *attributes* while statisticians call them *variables*. It is important to realize that entities of the same type share an attribute set. For example, every 'person living in the Netherlands' has a 'municipality of residence', namely the municipality where they are registered. Some persons living in the Netherlands may also own a house on a Greek peninsula. But since this is not true for all persons living in the Netherlands, the attribute 'size of house on Greek peninsula' is not an attribute for this entity type.

Attribute.
An attribute is a property associated with an entity. If two entities are of the same type, they have the same set of attributes, possibly with different attribute values.

This example highlights another common principle: entity types are usually defined by starting with a broad type and then fixing one or more attributes. For example, we can start with the entity type 'person' and fix the attribute 'municipality' to municipality in the Netherlands. There is one other way of defining an entity type, and that is by simply listing the entities that belong to the type. For example, one may define the entity type of 'All People with Dutch Nationality in 2017' by giving a list of all Dutch Social Security numbers that existed in 2017.

4.2 Normalization

A relational database stores collections of similar tuples. Normal people call such a collection a Table, but database theorists call this a *Relation*.

Relation.
A *relation* is a set of tuples, where all tuples have attributes in the same domains, in the same order.

For two tuples (normal people call them records) to be in the same relation, they must have the same number of attributes and those attributes must be of the same data type. There are generally several ways of distributing the same information over relations and tuples in a database. For example, the information about Alice in Equation (4.1) can also be represented as a set of tuples, like so.

$$\begin{aligned} &(Id = 1, Name = \text{“}Alice\text{”}) \\ &(Id = 1, Age = 7) \\ &(Id = 1, Owns = \{puzzle, bicycle\}). \end{aligned} \tag{4.2}$$

The choice of representation depends on the intended purpose, as also discussed in Section 1. Historically, focus has been on properties that were important for business administration systems. Exemplary applications that drove the development of early database theory are financial and logistic databases where possibly many users can simultaneously add, remove, or update data. An example to keep in mind is a company that buys, sells, and stores goods at multiple locations. There are tables of product availability and location, tables of sales and purchases (transactions) and so on. At any given time, an employee of the sales department must be able to see whether there is enough in stock for their next order. A widely applied approach to normalizing databases was presented in a seminal paper by Codd [1970]. In this approach, three levels of database normalization are defined which are still very much in use today.

4.2.1 First normal form

The idea of the first normal form is to make tuples as simple as possible. Remember that a tuple is a combination of values, coming from predefined domains. Another way of expressing this, is to say that the data types of the values in a tuple must be fixed beforehand. In principle, data types can be very complex. For example a calendar date is specified by a year, month, and day (and a time

zone which we ignore here) .

$$(Name = \texttt{"Alice"}, Birthday = (Year = 1991, Month = 05, Day = 13"))$$

So here, the value of $Birthday$ is also a tuple. The domain of $Birthday$ consists of all triples in $\mathbb{N} \times \mathbb{N} \times \mathbb{N}$ that represent a valid calendar date when their elements are interpreted respectively as year, month and day. The first normal form is all about making tuples as simple as possible, by not allowing data types that are composed of simpler types.

First normal form (1NF).
A relation is said to be in first normal form (1NF) when:

- All tuples have values from the same domains, in the same order.
- There are no duplicate tuples in a relation.

It is worth noting that there is no intrinsic ordering of tuples (records) in a relation. This means that in general you can not assume records to be sorted in any particular way in a database except if you explicitly sort them.

Continuing with the example, we can store Alice's birthday as

$$(Name = \texttt{"Alice"}, Birthday = \texttt{"19910513"})$$

The main advantage of 1NF is that operations on the level of relations, like searching, filtering and sorting are easier to reason about compared to the situation where tuples might contain complex data values.

The definition of 1NF does raise the question of when something is *atomic*. In practice this usually means either a string, a predefined categorical variable, a Boolean, or a number type such as integer or double precision, or a date/datetime type.

From a mathematical point of view the idea of atomicity is more subtle. A data type is atomic only under the set of operations that leave it intact (see also the definition of algebraic closure in Chapter 1). To clarify this let us discuss an physical example. In chemistry, atoms and molecules (and some of their ions) form the 'data type' under chemical reactions. Which ever chemical reaction you perform, you can never produce a particle that is not either an atom (ion) or a molecule. So the set of atoms, molecules and their ions are closed under chemical reactions. If we allow other, non-chemical operations, like nuclear fission, we can create particles that are not in the periodic system,

like neutrons, or neutrinos. This shows that the meaning of 'atomic' depends on the operations that you allow.

Similar to the atoms and molecules in chemistry, we could allow operations on an `Integer` type in a database, other than the familiar arithmetic operations. For example by pulling them apart into separate bytes, or bits even. The moral of the story is that there is no absolute definition of atomicity when it comes to *atomic domains*. In practice, the atomic types are the simplest data types offered by a programming language or database system.

4.2.2 Second normal form

The intuition behind second normal form, or 2NF in short, is to reduce the amount of redundancy in storing information and to guarantee a certain simplicity for each relation. The explicit definition sounds a bit more formal and requires some explanation.

Second normal form (2NF).
A relation is said to be in second normal form (2NF) when

- it is in 1NF
- it has no partial dependencies.

To understand this definition, we need to understand what *partial dependencies* are. To do so, suppose we have a database with the following relations.

Ownership

PersonId	ProductId	Nr	Shop
1	107	2	Toy store
1	101	1	Bicycle store
2	104	1	Toy store

Products

Id	Product
101	bicycle
104	ball
107	puzzle

Persons

Id	Name	Age
1	Alice	7
2	Bob	6

In the first relation, the key 'PersonId' identifies a person whose properties are stored in the third relation, while the key 'ProductId' identifies an object in the

second relation. Together, these two keys completely identify how many objects of a given type each person owns. For example, we can ask: 'how many puzzles does Alice own?' and look up that information by finding the key combination $(\mathrm{Id} = 1, \mathrm{Object} = 107)$ in the relation 'Ownership'. Compare this with the situation for the 'Shop' attribute. The value of 'Shop' does not depend on 'PersonId' and 'ProductId', but only on 'ProductId'. One could say that it is over-identified, or in data-base terminology it only *partially depends* on the keys available in the relation. We can improve this situation by moving the 'Shop' variable to the 'Products' relation.

Ownership

PersonId	ProductId	Nr
1	107	20
1	101	5
2	104	3

Products

Id	Product	Shop
101	bicycle	Bicycle store
104	ball	Toy store
107	puzzle	Toy store

Persons

Id	Name	Age
1	Alice	7
2	Bob	6

Now none of the relations have attributes with partial dependencies, which brings them in second normal form. Of course, we do see that there is some redundancy in data storage since we have some duplicates for the 'Shop' variable. This will be remedied in the third normal form. But before we get to that, we need to discuss something about keys.

As you may have noticed, we silently introduced the term 'key' into the discussion. In real-world databases, each and every tuple (record) is uniquely identified by an explicitly defined key or combination of keys. Such a key is usually an otherwise meaningless number that carries no information except the identity of the entity that is described by the tuple. Examples include social security and passport document number. When a single key identifies each tuple, this is called the *primary key*. If no such key is provided by the database designer, database software will typically create one in the background, possibly invisible to the user. In formal database theory however, there is no concept of key as a special kind of attribute. In formal theory one works with sub-tuples, called *candidate keys* that uniquely identify the other values in the tuple. For a given relation, there may be multiple candidate keys, with different numbers of attributes in them. This level of abstraction makes database theory more general but also more cumbersome to discuss, which is why they we do not discuss it here.

4.2.3 Third normal form

The intuition behind the third normal form is again fairly easy to state. To avoid duplication of information, store tuples that represent different entity types in different relations. Continuing with the example of the previous paragraph, we see that in the second relation, values of the attribute 'Shop' are duplicated in the second relation. Now suppose we want to change 'Toy store' into 'Department store'. For data in this form we need to update two fields in the second relation. We can solve this by creating a fourth relation with different 'Shops'. The result is a set of relations that are interlinked by shared keys, without data duplication.

Ownership

PersonId	ProductId	Nr
1	107	20
1	101	5
2	104	3

Products

Id	ProductId	ShopId
101	bicycle	S2
104	ball	S1
107	puzzle	S1

Persons

Id	Name	Age
1	Alice	7
2	Bob	6

Shops

Id	Shop
S1	Toy Store
S2	Bicycle Store

Now, if we update the label 'Toy store' to 'Department store' it only needs to be done in a single attribute of a single tuple in a single relation, and all queries on this set of relations done afterwards must return the new label.

We are now ready to move on to the formal definition of the third normal form.

Third normal form (3NF).
A relation is said to be in third normal form when

- it is in 2NF
- there are no non-prime attributes that are transitively dependent on a key.

A non-prime attribute is an attribute that is not a key or part of a set of attributes that together form a key (that is, a set of attributes that uniquely identify each record). This non-primality condition is really just theoretical fine-print. It is necessary to define 3NF without explicitly assuming that one of the attributes

in a relation is an identifying variable. In databases we always do have such a variable, so we'll use that in the example. The key concept in the definition is *transitive dependency*. We have seen what a dependency is: the value of variable X determines what the value of variable Y must be. We can denote this with $X \to Y$. For example in the the following table we have $\mathrm{Id} \to \mathrm{Object}$.

Products

Id	Product	Price	Shop
101	bicycle	250,00	Bicycle store
104	ball	3,50	Toy store
107	puzzle	5,00	Toy store

Such a dependency is called a *functional dependency*. To be precise, the notation $X \to Y$ means that 'whenever two tuples have the same value for X, they have the same value for Y. It follows that if we have $X \to Y$ and we have $Y \to Z$ then this must imply $X \to Z$. This is called the *transitive property* of functional dependencies.

Now let's take a look at the above table. We have $\mathrm{Id} \to \mathrm{Product}$, but we also have $\mathrm{Product} \to \mathrm{Shop}$. Namely, for any two Objects that are the same, we have the same Shop (observe that the converse is not true). This is trivial here, since every 'Product' occurs only once, but nevertheless we see that

$$\mathrm{Id} \to \mathrm{Product} \text{ and } \mathrm{Object} \to \mathrm{Shop}$$

and therefore we must have the transitive dependency

$$\mathrm{Id} \to \mathrm{Shop}.$$

In other words, the shop type depends indirectly on the identifying key for 'Product'.

Bringing a relation into third normal form amounts to bringing it first into second normal form, and then identify the attribute or attributes that show transitive dependence on other (sets of) attributes. The transitively dependent attributes are then moved to a separate table.

Any database can in principle be automatically put into 3NF, although in general there may be more than one solution and some steering based on domain knowledge is likely to be necessary. For example, we see in the example that 'Price' also transitively depends on 'Id' even though in reality it is an attribute of a 'Product'. In practice, databases are designed by information analysts and database administrators to be in third normal form in the first place. And this brings us to the topic of the next section.

4.3 Entity-Relationship diagrams

The basic recipe for designing a particular database structure sounds deceivingly simple:

1. Identify all the entity types and their properties.
2. Create relations with tuples of the form
$$(Id, Property_1, Property_2, \ldots, Property_n),$$
where Id is a *primary key*.
3. A connection between two entities of different entity types is represented as a relation that contains the primary keys of both entities.

In practical situations, the number of entity types can grow quickly. Consider again as an example the situation of Alice and Bob, who own a few objects, that were bought in a few stores. We've seen that in 3NF there are three obvious entity types involved, namely 'Person' (Alice and Bob), 'Object' (bicycle, ball, puzzle), and 'Shop'. Moreover there is an entity type that expresses an 'Ownership' relation between 'Person' and 'Object'. This is an entity type because it has unique properties that can not be attributed to a person or object alone. Here it is only the Size of the ownership ('Nr'), but we can also think of a starting and ending time of ownership as relevant attributes of this relation.

Because relations and their interconnections tend to quickly gain complexity, their design is usually represented graphically in something called an *entity-relationship diagram* (ERD). As an example, consider the ERD of the Alice and Bob example in Figure 6.1. In this diagram, each entity type and its properties are represented in a box. In this case we also added the type of each property, and labeled the unique identifier with an asterisk. Whenever the unique identifier (*primary key*) of one entity occurs in the table of another entity, this is called a *foreign key*. This is indicated with a line between boxes that connects the primary key of one relation with the foreign key in another relation. The lines are labeled with the type of relationship. For example, the 'Id' of a Person can occur multiple (n) times as a foreign key in the 'Ownership' relation. Whether a connection between two relations is one-to-one, one-to-many, or many-to-many is called the *arity* of the connection.

Primary key, foreign key.
A primary key is a code that uniquely identifies an entity in the relation representing that entity type. A foreign key is an identifier of one entity type that occurs in the relation representing another entity type.

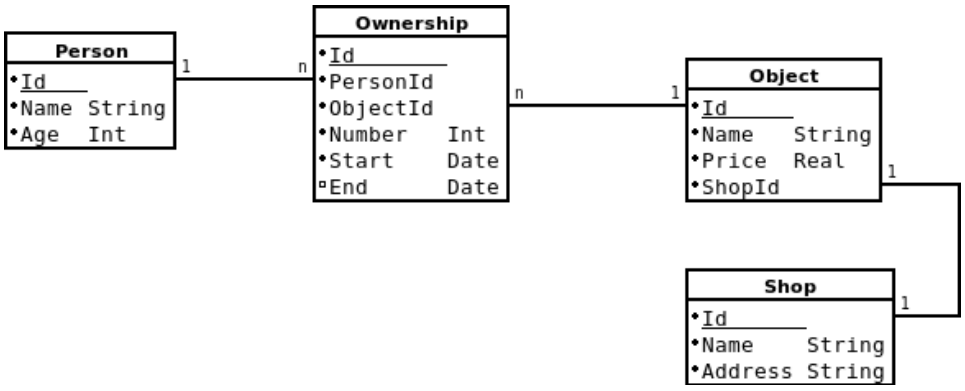


Figure 4.1: Entity-Relationship diagram of people owning objects bought in shops for a certain price.

The entity-relationship diagram shown in Figure 6.1 graphically represents a simple *database schema*. A database schema is a formal representation of the structure of a database, this includes choices such as which relations are there, what data is allowed to enter those relations (and what not) and what are the interconnections between the relations. There are many tools available that allow one to specify a schema graphically, as in Figure 6.1. The software then creates a formal specification for a particular database management system (DBMS).

Database schema.
A database schema denotes, in a formal (programming) language the structure of a database.

Over time, many variations of entity-relationship diagrams have been developed. They differ for example in the way the *arity* of connections are represented. In some styles an entity type must always be a noun, while a relation must always be a verb. In this paragraph we only highlight the most important bits, as we will return to more formal information modeling in Chapter 6. The elements we have discussed here are enough to give a rough sketch for databases

4.4 Introduction to relational algebra

Relational algebra consists of a set of basic operations that combine or alter relations (sets of similar tuples). The basic operations are very general, and do not depend on type of database, programming language used, or other implementation details. In fact there are many implementations of these basic ideas,

an we will discuss two of them at the end of this Section.

But before continuing it is worth spending a few words on why having an 'algebra' is important. Recall that the important property of being algebraic is to have operations that turn things into other things of the same type. Let us illustrate this with a little algebra we all know. Consider the following exercise.

$$\frac{3 \cdot 2 + 3 \cdot 5}{7}$$

There are several ways to compute the result. The most straightforward way is the following.

1. Compute $3 \cdot 2 = 6$, and store the result as x.
2. Compute $3 \cdot 5 = 15$, and store the result as y.
3. Compute $x + y = 6 + 15 = 21$, and store the result as z.
4. Compute $z/7 = 21/7 = 3$.

In total we have done three additions and one division. However, since we know the rules of arithmetic we can do things more efficiently as follows.

1. Rewrite the exercise as $3 \cdot (2 + 5)/7$
2. Compute $2 + 5$ and rewrite by substituting the answer. We are left with $3 \cdot 7/7$
3. cross out the 7 in the denominator against the 7 in the numerator, and we are done.

Here, we only needed to evaluate a single calculation (adding 2 and 5) explicitly. Thus, by using algebraic properties of addition, multiplication and division we were able to save on the number of calculations, at the cost of some rewriting.

Having an algebra of operations, together with strict rules about their like execution order, allows one to simplify calculations significantly. For a simple calculation as just shown, rewriting may actually take more time than a straightforward calculation. But when the objects of calculation are possibly large relations with data rather than a few numbers, this balance is likely to tilt the other way. Indeed, database systems will typically optimize user-defined operations on data by shuffling their order to minimize execution time, memory usage, or a combination of both.

4.4.1 Basic operations

The basic operations on relations are usually divided into set operations (remember that a relation is a set of tuples) unary operations, and binary operations (joins). The fact that tables are sets is important insofar that it implies that the relations can not be expected to be ordered in any way. So as far as relational algebra is concerned, the tables

$Name$	$Height$
$Mary$	167
$Eddy$	180
$John$	178

and

$Name$	$Height$
$John$	178
$Eddy$	180
$Mary$	167

are exactly the same. In fact, the tabular representations above should be considered just as a convenience. In principle we are working with a set of ordered tuples, for which the standard mathematical notation is

$$\{(John, 178), (Eddy, 180), (Mary, 167)\}.$$

There are three binary set operations that work on relations with the same attributes: set Union $A \cup B$, set Difference $A - B$, and set Intersection $A \cap B$. Below are examples of each operation.

Union (only works for relations with the same attributes).

$Name$	$Height$
$Eddy$	180

$\cup$

$Name$	$Height$
$Mary$	167
$John$	178

$=$

$Name$	$Height$
$Eddy$	180
$Mary$	167
$John$	178

Difference (only works for relations with the same attributes).

$Name$	$Height$
$Eddy$	180
$Mary$	167
$John$	178

$-$

$Name$	$Height$
$Eddy$	180
$John$	178

$=$

$Name$	$Height$
$Mary$	167

Intersection (only works for relations with the same attributes).

$Name$	$Height$
$Eddy$	180
$Mary$	167
$John$	178

$\cap$

$Name$	$Height$
$Eddy$	180
$John$	178
$Alice$	192

$=$

$Name$	$Height$
$Eddy$	180
$John$	178

In principle one of these 'basic relations' is redundant since we can write intersection as a combination of union and difference (see Exercise 5). Having these

three basic operations is thus more a matter of convenience than of theoretical minimalism.

Unary operations are operations that act on a single relation. There are three unary operations: Projection, Selection, and Rename. The Projection operation selects zero or more columns from a relation, returning a possibly smaller relation. It is denoted as $\Pi_{a_1,\ldots,a_p}$ where the subscripts denote what columns to select. Here's an example.

$$\Pi_{Name}\begin{array}{|ll|}\hline Name & Height \\ \hline Mary & 167 \\ Eddy & 180 \\ John & 178 \\ \hline\end{array} = \begin{array}{|l|}\hline Name \\ \hline Mary \\ Eddy \\ John \\ \hline\end{array}.$$

The second unary operation is called Selection. It is denoted σ_ϕ, where ϕ is a Boolean proposition (a selection rule) stating a condition on attributes in the relation.

$$\sigma_{Height \leq 170}\begin{array}{|ll|}\hline Name & Height \\ \hline Mary & 167 \\ Eddy & 180 \\ John & 178 \\ \hline\end{array} = \begin{array}{|ll|}\hline Name & Height \\ \hline Mary & 167 \\ \hline\end{array}$$

The last unary operation is called Rename. It is denoted $\rho_{a/b}$ where a is the name of the attribute to be renamed, and b is the new name.

$$\rho_{Name/FirstName}\begin{array}{|ll|}\hline Name & Height \\ \hline Mary & 167 \\ Eddy & 180 \\ John & 178 \\ \hline\end{array} = \begin{array}{|ll|}\hline FirstName & Height \\ \hline Mary & 167 \\ Eddy & 180 \\ John & 178 \\ \hline\end{array}$$

Finally, there are several types of *join* operations that merge two relations into a single new relation, based on common values in shared attributes. The most important one is the *natural join*, denoted with a 'bowtie' symbol: $\bowtie$. This merges two datasets and only keep the records that can be merged. This is often referred to as an *inner join*.

$$\begin{array}{|ll|}\hline Name & Age \\ \hline John & 25 \\ Mary & 34 \\ \hline\end{array} \bowtie \begin{array}{|ll|}\hline Name & Height \\ \hline Mary & 167 \\ Eddy & 180 \\ John & 178 \\ \hline\end{array} = \begin{array}{|lll|}\hline Name & Age & Height \\ \hline John & 25 & 178 \\ Mary & 34 & 167 \\ \hline\end{array}$$

In formal relational algebra, it is assumed that there are no duplicate keys to merge on. So for example *Mary* will occurs maximally once in each table on the left-hand-side (recall the definition of 1NF). In practice duplication can occur, and we will see in the next section how this is dealt with in implementations.

The *outer join*, merges two tables on shared attributes with common values, but also keeps the records that can not be matched. Attributes of one table that have no match with the other one are left empty.

$Name$	Age
$John$	25
$Mary$	34
$Alice$	57

$\times$

$Name$	$Height$
$Mary$	167
$Eddy$	180
$John$	178

$=$

$Name$	Age	$Height$
$John$	25	178
$Mary$	34	167
$Alice$	57	
$Eddy$		180

Both the natural join and the outer join are symmetric, that is $A \bowtie B = B \times A$ and $A \times B = B \times A$ for any two relations A and B. There are also variants that are *not* symmetric. The *left join*, denoted $\ltimes$, keeps all records from the left hand side and adds records at the right hand side where possible. Attributes for records with no match are left empty.

$Name$	Age
$John$	25
$Mary$	34
$Alice$	57

$\ltimes$

$Name$	$Height$
$Mary$	167
$Eddy$	180
$John$	178

$=$

$Name$	Age	$Height$
$John$	25	178
$Mary$	34	167
$Alice$	57	

Similarly, there is a *right join* denoted $\rtimes$, that keeps all records of the right hand side. Finally, there is the *antijoin* operation, denoted $\triangleright$. The antijoin is not really a join operation. It selects records from the relation on the left-hand side that can not be matched with the relation on the right hand side.

$Name$	Age
$John$	25
$Mary$	34
$Alice$	57

$\triangleright$

$Name$	$Height$
$Mary$	167
$Eddy$	180
$John$	178

$=$

$Name$	Age
$John$	25
$Mary$	34

Observe that the difference between the antijoin and set intersection is that for set intersection, we demand that the relation on the left hand side has the exact same attributes as the relation on the right hand side while this is not the case for antijoin.

To complete our discussion of relational algebra, we need to define the operator precedence. That is, just like we agreed that in normal arithmetic, multiplication comes before addition, we need to define the order of execution when combining multiple relational operations. The order is defined as follows.

1. σ, Π, ρ (highest precedence —execute this first when possible)
2. $\bowtie$, $\times$, $\ltimes$,$\rtimes$, $\triangleright$

3. $\cap$
4. $\cup$, $-$.

In this booklet we shall always use brackets to make order of execution absolutely clear.

4.4.2 Implementations

Relational algebra has been implemented, fully or partially in many tools. Here we shall briefly discuss two of them: SQL and R package 'dplyr'. The latter tool will be used in the workshop exercise. The goal of this chapter is not to learn how to work with SQL, but to raise awareness that the formal concepts introduced so far have real and practical implementations that are used every day.

The most important implementation of relational algebra is SQL, which stands for Structured Query Language. SQL is in itself not a tool, but the definition of a programming language that treats tables as a basic type. This programming language is implemented in many (commercial) database systems where different vendors typically create their own dialect of SQL, for example by extending it with certain capabilities for data analyses. However the basic operations treated here are usually all present.

Here is an example. Suppose we have a table called 'A' and we wish to select the attribute called 'Height'. In SQL this would look something like this.

```
SELECT Height FROM A
```

So here, `SELECT HEIGHT` is a direct translation of Π_{Height} and the whole expression means $\Pi_{Height}A$. If we want to do a left join on the Name attribute between A and B, and subsequently select 'Age' and 'Height', we get the following.

```
SELECT Height, Age FROM
  A LEFT JOIN B ON Name
```

Observe that the operator precedence discussed in the previous section ensures that $A \ltimes B$ is computed first and next 'Height' and 'Age' are selected. Readers interested in learning SQL could have a look at the online tutorial of the W3Schools organization[1].

[1] https://www.w3schools.com/sql/default.asp

A second –sort of– implementation comes with R package 'dplyr'. In R, a relation is represented by something called a *data.frame*. There are no ways to force the absence of duplicates, or even atomicity of its contents, so this data type is more flexible than the type of relations where relational algebra was designed for. Although R [R Core Team, 2020] comes with implementations of all relational operators that work on data frames, many people find the syntax implemented in the `dplyr` package easier to work with, so this is what we will discuss here.

To select a column called 'Height' from a data frame called 'A', in `dplyr` one calls a function called `select`.

```
select(A, Height)
```

Since 'dplyr' does not offer a programming language, but a set of functions, some syntax is needed to take the output of one function and pass it to the next function. Here we use the so-called pipe operator and work out the second example.

```
A %>%
  left_join(B, Name) %>%
  select(Height, Age)
```

Here, the %>% operator takes the output on the left hand side and feeds it as the first argument of the functions on the right hand side. This is equivalent to storing intermediate results and reusing that in the calculations.

```
X <- left_join(A, B, Name)
select(X, Height, Age)
```

Which syntax is preferred is to an extend a matter of taste. The former syntax with %>% is quicker to develop, the latter syntax is easier to debug since intermediate results are available.

Where are we?

We have see that the concepts of tables and records can be treated formally in database theory, where they are called respectively relations and tuples. The formal treatment yields normalized forms that can be described and designed graphically using entity-relationship diagrams (database diagrams). Moreover, there is a small number of basic operations that can be used to manipulate of sets of relations. Many commonly used tools implement these operations or variants thereof so they are ubiquitous in data management.

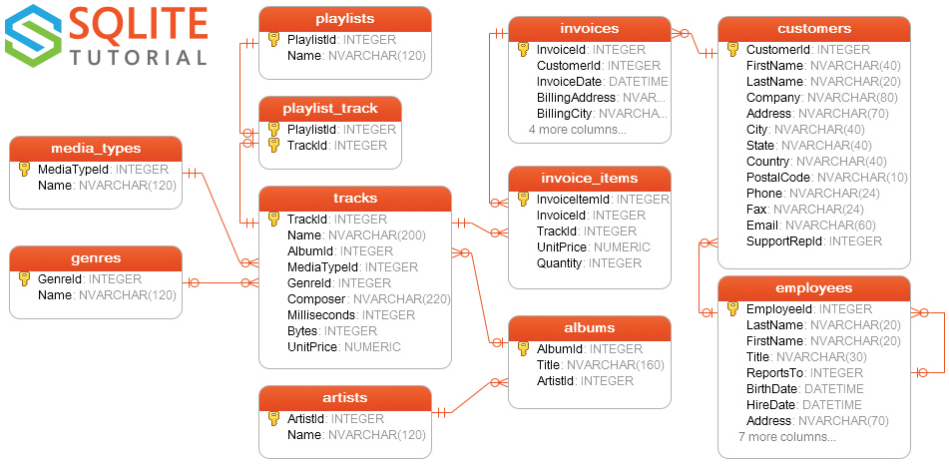


Figure 4.2: A database scheme for record sales, taken from from the SQLite tutorial (https://www.sqlitetutorial.net/sqlite-sample-database/).

4.5 Exercises

1. Put the following table in 1NF

Id	Name	Age	Owns
1	Alice	7	{puzzle, bicycle}
2	Bob	6	{ball}

2. In official statistics, there are several ways to count businesses. There are 'legal units' which are defined by their registration at the Chamber of Commerce. There are 'Tax' units which are defined as one or more legal units that together file a tax report. And then there are 'Economic units'. These are constructed by Official Statisticians by combining one or more legal units into an establishment that coherently conducts its business. Exemplary cases are large (multinational) companies that separate activities into different legal units. It is also possible for multiple legal units to form a new Tax unit, but those legal units do not necessarily come from the same economic unit. How would you store such data? Create a database schema to reflect that.

3. Consider the database schema in Figure 4.2 and answer the following questions.

   (a) How many attributes are there in the employees table?

   (b) What are the foreign keys in the 'tracks' table?

   (c) What is the type of the primary key in 'customers'?

4. Create a database schema for the case in Section 4.A.

5. Consider the sets $V = \{a, b, c, d, e\}$ and $W = \{b, d, f\}$. Show that in this case $V \cap W$ gives the same result as $V \cup W - (V - W) - (W - V)$. Bonus question: can you prove this is true for any two sets V and W?

6. Consider the following two tables.

$$A = \begin{array}{|ll|}\hline Name & Age \\ \hline John & 25 \\ Mary & 34 \\ Alice & 57 \\ \hline \end{array} \qquad B = \begin{array}{|ll|}\hline Name & Height \\ \hline Mary & 167 \\ Eddy & 180 \\ John & 178 \\ \hline \end{array}$$

   Compute the following relations, try to simplify the calculations before filling in the actual relations.

   (a) $\Pi_{a \in A}(A \ltimes B)$, where $a \in A$ means all attributes occurring in A.

   (b) $\sigma_{Age>40}(A \bowtie B)$.

   (c) $\sigma_{Age \leq 40 \wedge Height \leq 170}(A \times B)$. (The symbol $\wedge$ means 'AND').

   (d) $\Pi_{Height} A \bowtie B$.

7. Take a look again at the schema in Figure 4.2. How would you create the following relations? Use notation from relational algebra to express this.

   (a) A relation with one tuple for each track, holding Album Title and Track Name.

   (b) A relation with Artist, Track, and customerId, so we can identify in what artists each customer is interested.

   (c) A relation with TrackId and EmployeeId so we can analyze which employee sells most tracks.

Check your answers on page 81.

4.A Case: car rentals

Your job is to design a database schema for the case below. You can do it on pen and paper (great to get started!), use a drawing programme, or one of the many (online) free database schema creators. An example is dbdesigner[2]. You can use the guest login or create a free trial account. (Note: you will not be able to save your schema, but you can export an image or SQL code)[3].

[2] `https://www.dbdesigner.net`

[3] This assignment was taken from the Master's Thesis of Zhang [2012].

Part 1

Our company does car rental business and has several locations with different address (address consist of street with the number, city, and postal code). In large cities there can be multiple locations. The cars are classified as subcompacts, compacts, sedans, or luxury. Each car has a particular model, year made, and color. Each car has a unique identification number and a unique license plate.

Part 2

Cars rented in a particular location may be returned to a different location (pickup and drop-off). For every car we keep the odometer (km traveled) reading before it is rented and after it is returned. The car is rented out with full tank and we record the volume of gas in the tank when the car is returned, but we only indicate if the tank is empty, quarter full, half full, three quarters full, or full.

Part 3

We keep track of which day a car was rented, but not of the time, similarly for car returning. If a customer requests a specific class (say sedan), we may rent the customer a higher-class car if we do not have the requested class in the stock, but we will price it at the level the customer requested (so-called upgrade). Each car class has its own pricing, but all cars in the same class are priced the same.

Part 4

We have rental policies for 1 day, 1 week, 2 weeks, and 1 month. Thus, if a customer rents a car for 8 days, it will be priced as 1 week + 1 day. The drop-off charge only depends on the class of the rented car, the location it was rented from and the location it is returned to. About our customers, we keep their names, addresses, possibly all phone numbers, and the number of the driver's license (we assume a unique license per person).

Part 5

About our employees we keep the same basic information as our customers (we require that all our employees have a driver's license). We have several categories of workers, drivers, cleaners, clerks, and managers. Any of our employees can rent a car from our company for a 50less than 2 weeks. However, for any longer rental they must pay 90regular price. Every employee works in one location only.

Chapter 5

Data in organizations

In this Chapter we discuss some high-level ideas on how databases can be implemented in an organization. We also discuss one theoretical result that helps to guide the choice of database implementation.

5.1 Data architecture

Understanding relational database theory and implementations thereof is one thing. It is another thing entirely to actually use these ideas in production environments. In practice one needs to make trade-offs between availability, consistency, flexibility, and database performance. It has to be decided which users have access to what data, what actions each user is allowed to perform. For example, a data analyst may only temporarily need read-only access while data base administrators have the ability to create or delete whole tables. Especially in larger organisations, one needs to have procedures in place to decide who is granted what rights, for how long, and on what grounds.

Since there are many choices to be made, it is advantageous to have a global overview of all things related to data in an organisation. Such an overview is called a 'data architecture'. To be precise, The Open Group on Architecture Frameworks (TOGAF[1]) defines a data architecture as follows.

Data Architecture.
A description of the structure and interaction of the enterprise's major types and sources of data, logical data assets, physical data assets, and data

[1] `https://pubs.opengroup.org/architecture/togaf9-doc/arch/index.html`

management resources.

Architecture documents can describe the state of an organisation as it currently works, but they can also serve as the design of how an organisation should work in the future. The idea is that this helps decision makers across the organisation to make consistent choices. Nowadays, many large organizations employ enterprise and data architects. For official statistics, a Common Statistical Data Architecture was developed under the auspices of the United Nations initiative on the modernisation of official statistics (CSDA[2]).

Architectures include a broad range of aspects, ranging from organizational issues to technical (software) and physical (hardware) choices.

In this section we will focus on a few well-known methods for organizing databases.

As long as databases have been used in the industry, people have discussed how to organize them. Over time, several general ideas on how to structure databases in an organization have evolved. Many of these ideas have been developed over time in industry, and the terminology used is not always consistent. Most of these ideas have first been published in white papers, or blog posts or other publications that have not been peer reviewed. However some of these ideas have become commonplace in industry and it is well worth taking note of them as they do demonstrate how the theoretical ideas discussed in Chapter 4 end up being used in practice. In the following subsections we give an overview of some of the most well-known database architectures, and discuss some of their advantages and disadvantages.

5.1.1 Data Warehouse and Data Mart

The data warehouse is the classical data base architecture. It is designed to be a *single source of truth* for the whole organization. This means that the traditional data warehouse typically consists of a single database system where all data is stored. Data that is sent to the data warehouse has to pass strict checks before being allowed to enter. Data warehouses are governed and centrally within an organization. Technically, they are often implemented as relational databases.

Data warehouses typically harbour data that is absolutely necessary to run a business (mission-critical), and that must be consistent across the organization. In NSIs, sampling frames that are used by various departments fall under that category. When two sample surveys are to be used to make inferences about the same population, the samples should be drawn from the same population

[2] `https://statswiki.unece.org/display/DA`

register. In businesses, customer administration and human resources typically also fall under that category.

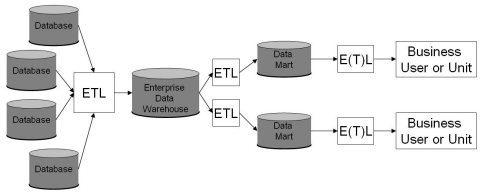


Figure 5.1: A data warehouse, feeding data marts. ETL stands for Extraction, Transformation and Loading. Picture from Wikimedia commons.

Thus, the advantage of a data warehouse architecture is that data is reliable and strictly maintained. An immediate disadvantage is lack of flexibility. With centrally controlled systems it may be cumbersome to create custom tables for ad hoc analyses, or to add variables or otherwise manipulate the database schema in ways that are interesting for analyses, since such changes potentially have consequences in many places in the organization.

An early answer to this disadvantage is the 'data mart' architecture. In this design, there is a central data warehouse but different users are allowed to create their own local data bases that combine data from the warehouse with locally created data. For example, in the case of an NSI a department that conducts a certain business survey may join that data to a centrally stored register of tax data and data from the Chamber of Commerce. This way, analysts have freedom to set up local systems while the 'single source of truth' stays intact. Typical disadvantages of the data mart structure include proliferation of data base systems and duplication of work.

5.1.2 Data Lake

The idea of a data lake was invented as an answer to the disadvantages caused by the rigidity of centralized data warehouses. Recall that in a data warehouse, the data base schemas are strictly controlled and therefore it may take a lot of effort to condition data for it to be accepted into the database. Also, as the types of data that are interesting for an organization to harvest become more diverse and larger, keeping everything in a central data warehouse becomes more or less impossible to organize.

The term data lake was invented by James Dixon, who wrote a blog post about it in 2010[3]. It was further elaborated upon in a white paper of Stein and Morrison [2014]. Dixon summarizes the idea as follows.

[3] `https://jamesdixon.wordpress.com/2010/10/14/pentaho-hadoop-and-data-lakes/`

> If you think of a datamart as a store of bottled water —cleansed and packaged and structured for easy consumption— the data lake is a large body of water in a more natural state. The contents of the data lake stream in from a source to fill the lake, and various users of the lake can come to examine, dive in, or take samples.

The idea is to remove the barrier for storing data completely. In a data lake, all data is stored in a key-value store. Data can in principle be anything, including documents, images, videos, audio or other formats. There is little organization in storing the data, except for a unique identifier attached to each item. The main task of a data lake is to store data so it can in principle be analyzed later. The technical solution proposed by Dixon is to use a Hadoop-like key value store.

The main disadvantage of a data lake is that data needs to be gathered and cleaned for every separate task. Having little structure in the data means that it is hard to automate over and generally it requires more advanced skills to work with data from a data lake than data from a data warehouse.

5.1.3 Data Virtualisation

In both the data warehouse and data lakes, data is moved from the data source into a central or distributed database system. This may become cumbersome, especially for very large and very diverse datasets. In data virtualisation, data stays at the source, and instead there is a database that stores where data can be found. Since users may access that database more or less as if it were a regular database, this is called 'data virtualisation'. The data is retrieved by the 'virtualisation' software as needed.

An advantage of data virtualisation is that the technical introduction into an organization is relatively easy. Hardly any changes are necessary in existing systems. The main challenges are organisational. For example in the situation of a data mart, it needs to be decided which local databases must be connected to the virtualisation software, and how.

5.2 The CAP theorem

For large datasets, data that needs to be accessed by many users, or data that needs to be available at many places simultaneously, it is common to use some form of distributed database.

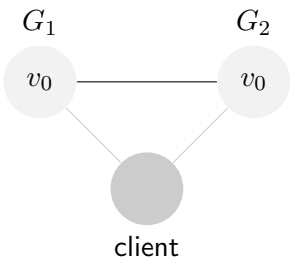
Distributed database.
A distributed database is a database system that is spread over two or more nodes.

The term 'node' is just a fancy word for a computer in a network, or an application that runs as if it was on a separate computer in a network. When a database is running on multiple nodes, there has to be some communication between the nodes to synchronize information between them. The CAP theorem demonstrates that there are fundamental limits on what one can expect from such a system.

CAP Theorem.
A distributed database can not simultaneously be Consistent, Available, and Partition-tolerant.

The CAP theorem was conjectured in 2002 by Eric Brewer [2002] and proven quickly thereafter by Gilbert and Lynch [2002]. The original proof is a bit technical and requires a fair amount of technical definitions. In the current discussion we use the visual proof as discussed by Whittaker[4], which is easier to follow and captures the main arguments.

First consider a network composed of two nodes, called G_1 and G_2. The network hosts a database, and both nodes have access to a stored variable with value v_0.



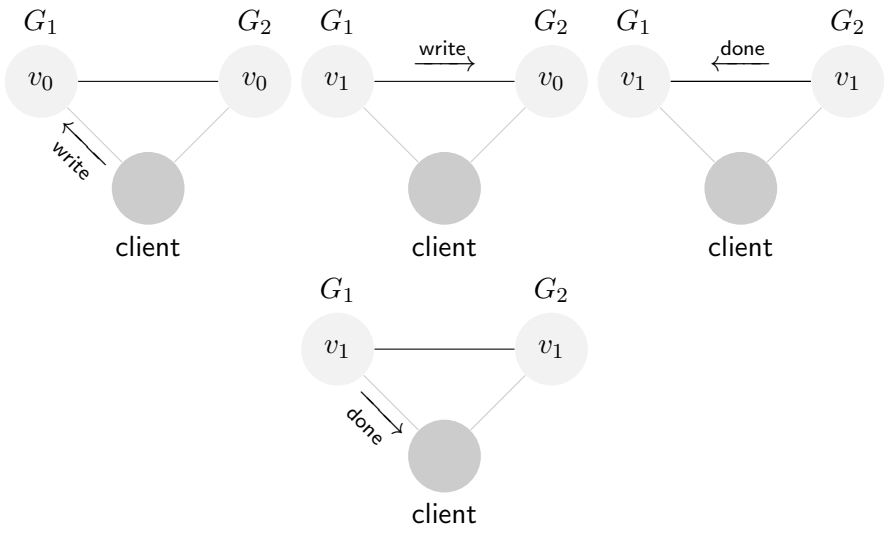
The two nodes can be accessed by a client, that can request each node to return the current value (a 'read' operation) or to overwrite the current value with another value, say v_1.

Now, for the database to be *consistent*, means that

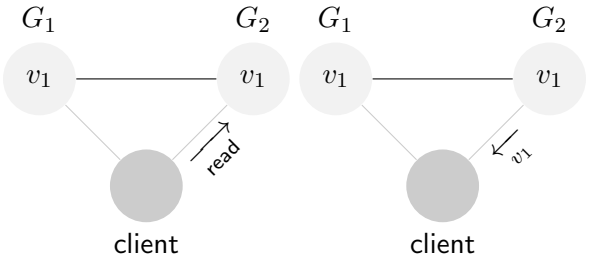
[4] https://mwhittaker.github.io/blog/an_illustrated_proof_of_the_cap_theorem/

> any read operation that begins immediately after a write operation is completed must return that value.

The important thing is that this must hold regardless of which nodes are receiving the read or write request. Here is how the two-node database can be consistent: it needs to synchronizes before it is done with a 'write' operation.



Now the client can read from either node and receive the same answer.



The *availability* demands entails the following.

> every request received by a non-failing node must result in a response.

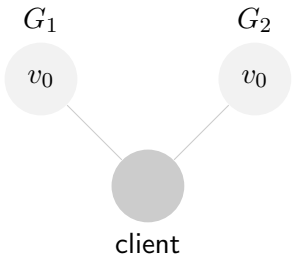
This means that in an available system, if the client sends a request to a node that is 'up' (i.e. not crashed), the node must eventually return a result: nodes are not allowed to ignore requests.

Finally, *partition-tolerance* means that

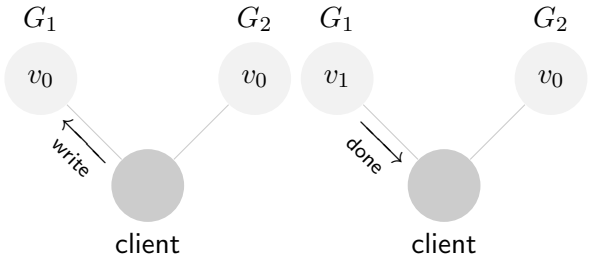
the network will be allowed to loose arbitrary many messages sent from one node to another.

In particular, partition-tolerance means that the system keeps working even when one or more nodes are completely separated from the others.

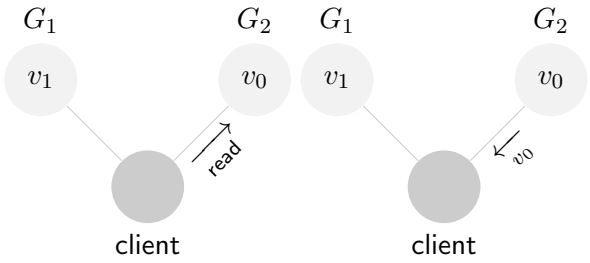
By now, it is probably clear that the CAP theorem must hold: after all, how can a set of nodes stay synchronized when they can not communicate write requests? Explicitly, assume that the CAP theorem does hold and consider the situation where G_2 is separated from G_1, so no messages can be send in either direction.



The client sends a write request. Because Availability is assumed, G_1 must answer.



The consistency demand is now violated, since reading from G_2 does not return the value written by the last completed write operation.



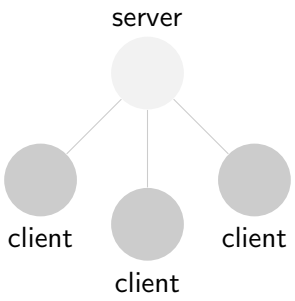


Figure 5.2: Consistent and available: all data on a single node.

In conclusion, assuming consistency, availability and partition-tolerance leads to a contradiction. The above example demonstrates that a partitioned network can not host a database that is both available and consistent.

5.3 Practical consequences of the CAP theorem

Since the CAP theorem tells us that we can't have partition tolerance while being consistent and available, this means we need to choose what is most important for a certain application. Let us discuss a few ways in which different types of database systems (CA, CP, or AP) can be implemented.

5.3.1 Consistent, Available

A partition-tolerant system can be created by using a single storage facility. The architecture looks like in Figure 5.2. There are one or more clients that send requests to a single data storage node. Requests are handled in order of arrival by the server and a new request is not handled until the previous one has been completed. We have consistency since no synchronisation needs to take place, and since every request to a non-failing node (a single server node here) will indeed yield a response. The idea of partition-tolerance becomes irrelevant in this architecture since there are no data storage nodes to partition by breaking links between them.

The point is that if you want a system that is 100% Consistent and Available, you are forced to create a centralized system. Many traditional transactional database solutions are built this way.

5.3.2 Consistent, Partition-tolerant

Here, we drop availability. The simplest solution for creating a database that is both consistent and partition tolerant is by building a system where every node ignores every request. This means that every read operation receives the same answer: none. It is also partition-tolerant since all nodes always behave the same and no synchronisation is necessary.

More realistically, a master node can be appointed to distribute data across nodes, and to queue requests from clients. A read operation cannot take place before the last write operation is fully complete across all nodes. This means that when one client issues a request, the others have to wait. An example of such architecture is shown in Figure 5.3. Now, if the connection between the

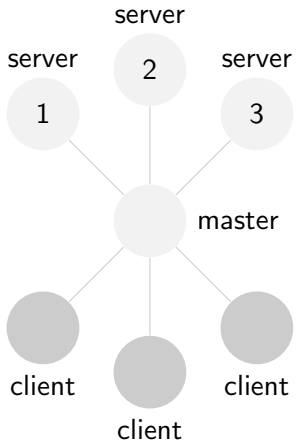


Figure 5.3: Consistent and partition-tolerant: a single node handles all requests.

master node and server 1 is severed, then any request that would involve reading from or writing to server 1 will be dropped (loss of availability). The data that is still reachable on servers 2 and 3 is still consistent across read/write requests. Such problems can be avoided by partially duplicating data across servers. An example of this is Hadoop/HBase. Here, a central node distributes data across multiple nodes. All data is written to say, three out of n nodes. This means that availability is only compromised when all three servers that hold a certain value become unreachable. In practice the probability of such an event may be low but in terms of the CAP theorem it does mean dropping the Availability property.

5.3.3 Available and Partition-tolerant

Here we drop the demand that a read request always returns the latest write result. In Figure 5.4, a client may write something to one node and request a value from another node before the write operation has spread across the network. Or, client 1 may write something to server 1, and client 2 reads the same information from server 3 before the nodes have synchronized. An example

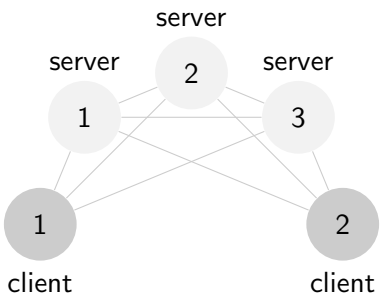


Figure 5.4: Available and partition-tolerant: there's always a node that answers, but the servers may not have synchronized information.

of such behavior is in social media or online search engines (Google) where users from different locations may not always get the same search result at the same time (of course such differences are also obscured by personalisation).

Where are we?

We have seen that there are a few main architectural paradigms on organizing data in large organizations. These paradigms are based on, and evolve with practical experience and increasing technological capabilities. The CAP theorem is a theoretical result that forces one to decide between consistency, availability or partition-tolerance of a distributed database.

5.4 Exercises

1. Go to the TOGAF website, and read the Executive Overview[5]. Pay attention to how the term 'enterprise' is defined.
2. Look up the entries of Data Warehouse, Data Mart, Data Lake, and Data Virtualisation on Wikipedia. Create a table with pro's and cons in the columns and an architecture on each row.

[5] `https://pubs.opengroup.org/architecture/togaf9-doc/arch/chap01.html#tag_01_03`

3. Using the same system as in Section 5.2, demonstrate that a distributed database that does not satisfy the availability condition can be consistent and partition-tolerant. Tips: consider nodes that can send a 'fail' message when they find out that a 'write' message is lost.

4. Below are three fictional cases. In this assignment, students are grouped in teams of 3-5 students.

   Discuss, in about 20-30 minutes, which of the four architectural patterns: Data Warehouse (DW), Data Mart (DM), Data Lake (DL) or Data Virtualization (DV) would be preferred. Consider things like the CAP requirements, and realize that it may be possible to combine strategies. If you have questions about details in the example just make a reasonable assumption. Feel free to read online blogs/opinions by data architects for inspiration, or dig up the definitions on e.g. Wikipedia.

   Each team will give a presentation of about 5 minutes, covering the following aspects.

   (a) Type of organization as defined in the above description.

   (b) The choice you made: DW, DM, DL, DV? and

   (c) most importantly: why you made this choice.

5.A Cases

5.A.1 The startup

You work for a fast-growing online startup called 'Borkly'. Their product is a *Next-Generation Search Engine for Old People* with a freemium business model: customers either use the service for free with adds or choose to take an add-free subscription with monthly payments. The company works remote-first, so almost everybody works from home. There are currently 40 people in the company (not all of them full-time): 3 owner/managers, 22 developers, 5 data analysts and 10 customer support employees.

For their growing customer support department they are looking to replace their current ad hoc customer administration (CRM) database backend. The current system is slow, buggy, and even some simple administrative activities sometimes take a lot of 'manual' work. There are really only two people who understand how it works. At the moment Borkly only stores the bare necessities to keep administration going. In the future they want to be able to store everything they can get from every customer, including site visits/audit trails, e-mails, and so on, to be able to serve their data analysts with information.

5.A.2 The statistical office

You work for the *Center of Statistical Information for the Country*. This bureau is responsible for collecting, producing, and publishing, all national statistics. It is an organization with about 1000 employees, who all work in the same building. Although there is one organization, historically each statistical domain collected and processed its own data, leading to a broad and varying landscape of data storage solutions, varying from text-files (csv) to professional data bases. Although such solutions are locally optimal (i.e. they can be maintained by the departments using them, with some help from the IT department), management feels that some form of unification would benefit the Center as a whole.

In the future, the organization would like to cut costs by removing overlapping information from the organization. They would also like to develop new, frequently published, statistical products based on the combination of various data streams in the Center. They would also like data analysts to be able to quickly create one-off on-demand analysis for external customers. Finally, they would like to leverage the large quantities of information coming from the internet of things (IoT) such as mobile phone data for their statistical products.

5.A.3 The government

You work at the National Office of Employment. This office is responsible for registering the unemployed, and for payment of unemployment benefits. Historically, the office was created by merging several regional offices with a similar task. Although there have been some attempts to unify the legacy data warehouses into a single data warehouse, the differences between storage solutions and (meta)data are so large that the office in some respects works more like a cluster of local offices than as a single unified entity.

The NOE's board recently decided that fraud detection is a spear point within the organization. To do this it is necessary to integrate both existing data sources, and new external sources, for example tax records and sometimes social media records from suspects. The data analyses department is given extra budget to hire data scientists and they are now talking to the IT department on how to shape the data landscape.

Chapter 6

Information modeling

In this Chapter we introduce some ideas and methods that have been designed formally model the entities and relationships that are important for an organisation. In particular, we will give a brief introduction into Unified Modeling Language.

6.1 Information models

An information model is an attempt to capture the essence of the real-life thing or process in simpler, abstract terms. We have seen an example of an information model in Chapter 4.3, when we talked about Entity-Relationship Diagrams, see also Figure 6.1.

Information models are often separated into three layers, that differ in their level of detail and precision. The first type is *conceptual*. Conceptual models are often presented as text or schematic visualisations and their main purpose is to communicate the bare essentials, for example to high-level management. There is no formal language for conceptual models, although UML can be used for this purpose. The second layer is the *logical* information model (LIM). A LIM describes all information elements in a structured way and serves as a blueprint for development of for example, a database. A LIM is typically platform-independent. That is to say, it does not depend on any particular programming language, database system, or other implementation details. Again, UML can be used in this manner but the Entity-Relationship Diagram of Figure 6.1 is also a good example. The last layer is the *physical* layer, which describes all technical choices including database type and configuration input file format, connections to other databases and so on.

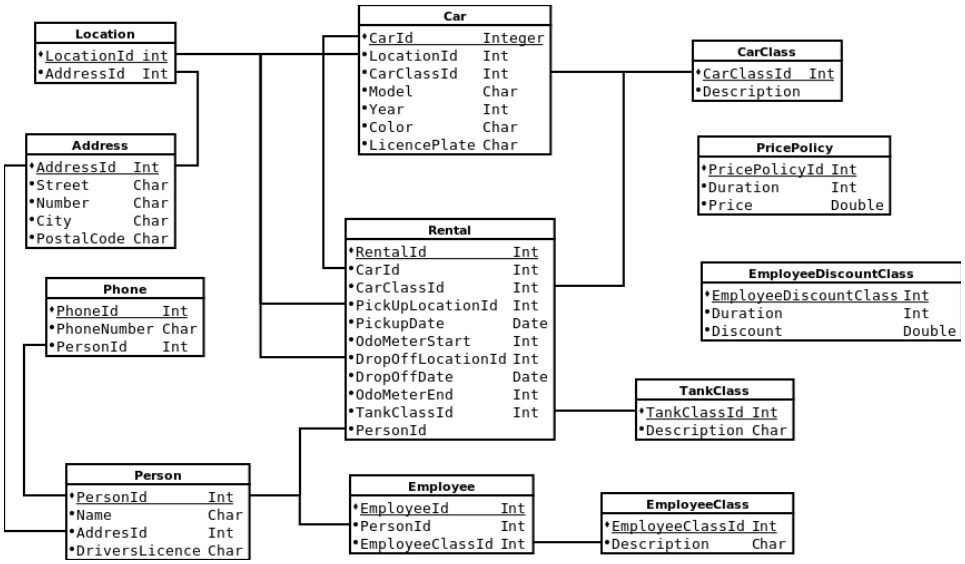


Figure 6.1: An Enterprise-Relationship Diagram

6.2 Introduction to Unified Modeling Language

UML is a formal graphical language that was developed in the 1990's to cope with increasing complexity of large software projects. The idea is to systematically capture all components and the typed relationships between them in a formal graphical representation that would both be easy to create and easy to understand. The idea was that ideally, a program can be defined in UML and the software code can be generated automatically based on the UML specification. The UML specification itself, is platform-independent and can be transformed between for example database systems or operating systems.

Like information models in general, UML can be used in roughly three different ways. It can be used as a sketch tool to outline the most important part of a process or application. Sketches can be made on a whiteboard or a piece of paper. Second, it can be used as a blueprinting tool that documents all components of (for example) a database and the relations between it. In this case, it is common to use an UML drawing tool. The resulting document is then part of the formal specification of a database (or other software system). Finally, UML can be used as a programming language. Theoretically, if a system is modeled in enough detail, the UML description can be translated to executable code on any system where an UML translator is available. In practice this is cumbersome and not many applications are developed in that way.

Here we will focus on UML as a sketching tool and treat only a few of the most important aspects of it. Nevertheless, these aspects can be useful to focus one's

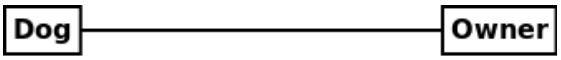
thinking about complex systems or to communicate ideas and designs. Readers interested in learning more about UML can refer to textbooks, such as that by Miles and Hamilton [2006].

The main advantages of UML include its generality, understandability and wide applicability. It can be used to model software, databases, but also the structure of organisations or physical installations. A disadvantage is that UML drawings quickly become too large and cluttered to interpret in full. A more formal disadvantage is that UML is static, in the sense that there is no algebra of manipulations that allow one to simplify or otherwise manipulate an UML diagram automatically.

6.2.1 Classes and Relations

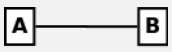
UML is used to describe *classes* and their relations. Term class is an UML term, and would in the language we've developed in Chapter 4 called an 'entity type'. Information objects are represented as blocks, and relations are represented as possibly decorated lines between them. The relationships are decorated depending on their type.

The simplest type of relation is an *association*. For example, the following diagram displays an association between a pet and an owner.



Although the box labels are suggestive, in UML this diagram does actually not say anything about who owns who, or any other property the association might have. It merely states that a pet is associated with an owner.

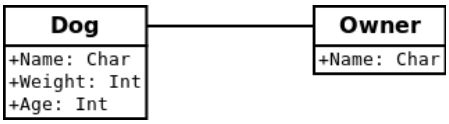
Association.
An association between two classes is a relation that has no direction. It is represented as a solid line between two information elements.



Associations are allowed to have an *arity*, to be labeled, and to have a direction (See Equation 6.1).

Classes may be endowed with *attributes* of a certain type. These properties

that may take different values for different elements of the class.



So far, we have done nothing that we have not seen when we discussed entity-relationship diagrams (Chapter 4.3). This changes when we add the *arity* of an association. For example, we can annotate the association between 'Dog' and 'Owner' to indicate that a single Owner is associate with zero or more dogs.

Here the asterisk stands for 'zero or more' and the 1 stands for, well, one.

Arity.
The *arity* describes the multiplicity on both ends of a relationship. It expresses how many instances of one class can be associated with how many instances of another. The arity is notated at the beginning and end of a relation. The notations used are as follows.

- $*$ means 0 or more
- n, with n a number means 'exactly n' (for example $n = 1$)
- $n \ldots m$ means $n, n+1, \ldots, m$.
- $n \ldots *$ means n or more.

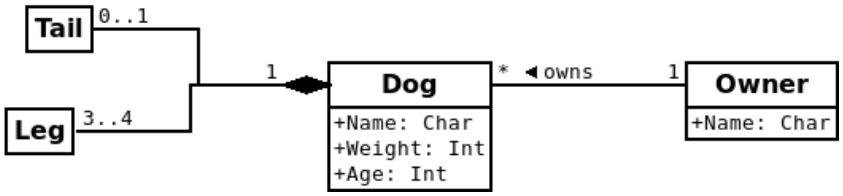
Relations can be labeled, in which case they possibly also gain a direction.

(6.1)

Here, the owner 'owns' a dog. The fact that it is the owner who owns is signified by the arrow on the label.

Thus far we have discussed associations between classes. A second, more specific type of relation is the *composition* relation. This occurs when every entity

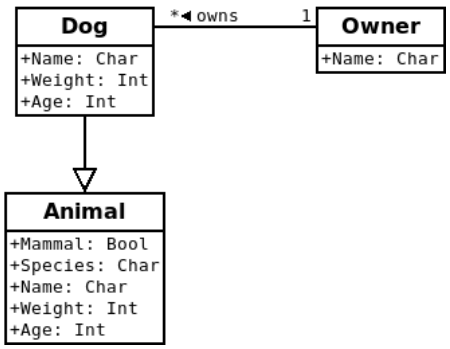
of a certain class is composed of elements of other classes. Composition is graphically represented with a solid diamond on the side of the composed class.



Here, a single 'Dog' entity is contains 0 or 1 'Tail' entities and 3 to 4 'Leg' entities. The fact that the lines coming from 'Tail' and 'Leg' combine before entering the diamond has no significance; it is just a consequence of the graphical representation.

Composition.
Composition is an association that describes a part-whole relationship. The line connecting the two classes is decorated with a solid diamond on the side of the whole class.

The last and slightly more complicated type of association we discuss here is *inheritance*. For any class with a nonempty set of attributes, we can define a subclass by fixing one or more attributes. For example, we can define the class 'Animal'. If we fix the Boolean attribute 'Mammal' to True and fix the Species to Dog, we get an inherited class called 'Dog'.



An equivalent way to think of inheritance is to say that any entity of class 'Dog' is also an 'Animal' but not vice versa.

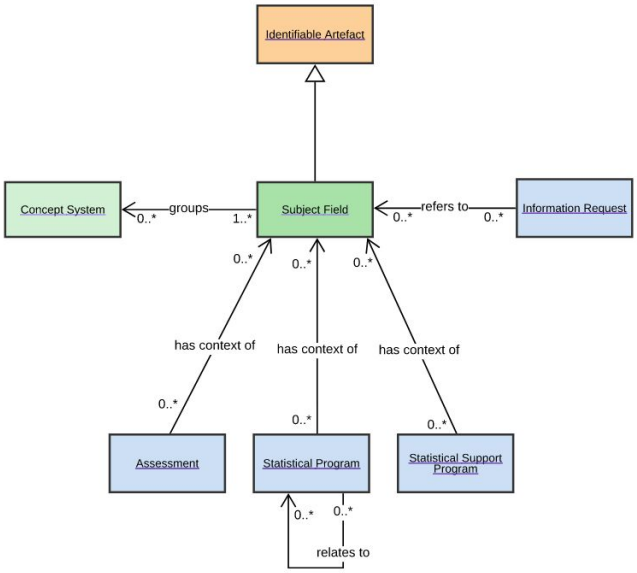
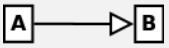


Figure 6.2: The UML diagram surrounding 'Subject Field' in the Concept Group of the General Statistical Information Model. The open arrows indicate the direction of the label in each association.

Inheritance.
Inheritance is an association that defines a class-subclass relationship. It is represented by an arrow, where the arrow points from the subclass to the superclass.



Here 'A' is a subclass of 'B'. An entity of class 'A' has all attributes that an entity of 'B' has, but not the other way around.

6.2.2 An application in Official Statistics

The High-Level Group on Modernisation of Official Statistics (HLG-MOS) is an initiative of the United Nations Economic Committee for Europe's (UNECE) Statistical Commission. This initiative is an ongoing effort to both standardize and modernize how official statistics are produced. HLG-MOS is steered by a coalition of high level managers (typically director general or deputy director general) who initiate several modernisation projects each year.

In one of these projects, called Generic Statistical Information Model (GSIM)[1] an attempt was made to model all information objects in a statistical organisation. The resulting UML diagrams can be found at

`https://statswiki.unece.org/display/gsim/`.

The aim of this effort is not to create databases or software but to have a reference document that describes the most important things and their interrelations that are encountered by Official Statistical offices in a standardized way. You can think of it as a fancy glossary that can be reused by statistical organizations. For example by using the same terms for the same things in their documents and (international) communications. The idea is that having a common understanding about all these concepts will facilitate common a understanding of them; having a common understanding again, makes working together in international context easier.

There are four main UML diagrams covering Business (design and planning of statistical programs), Concepts (to define the meaning of what data are measuring), Exchange (to catalogue information entering and exiting an organization), and Structure (to structure information throughout the statistical process). Figure 6.2 shows a piece of the UML diagram from the 'Concepts' group, surrounding the term 'Subject Field'. Each such diagram als comes with a description of the main concept. For example, concept 'Subject Field' comes with the following description.

Definition	**Explanatory text**
One or more *Concept Systems* used for the grouping of *Concepts and Categories* for the production of statistics.	A *Subject Field* is a field of special knowledge under which a set of *Concepts* and their *Designations* is used. For example, labour market, environmental expenditure, tourism, etc.

Where are we?

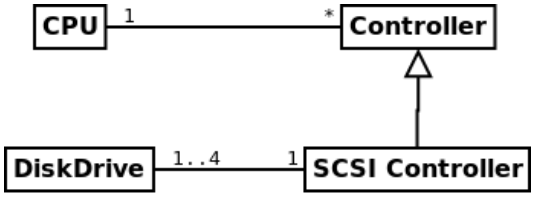
The term 'information modeling' refers to a set of techniques that allow one to systematically describe complex systems. This can be done in ways that vary from sketchy and high-level to formal and detailed approaches. The Unified Modeling Language supports all these approaches and lets the user decide what level of detail is sufficient for their purpose.

[1] `https://statswiki.unece.org/display/gsim/`

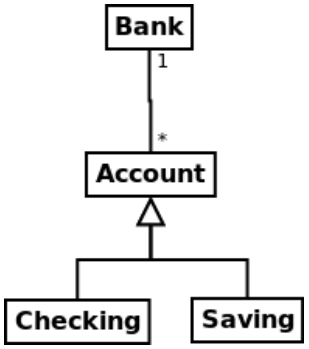
6.3 Exercises

1. Describe the classes and relationships between them for each of the following UML diagrams.

   (a)



   (b)



2. Complete the UML diagram of Figure 6.1, see also Case 4.A for a full description. You can draw your own diagram or use the diagram on page 73.

Check your answers on page 82.

CarClass
•Description
PricePolicy
•Duration Int
•Price Double
EmployeeDiscountClass
•Duration Int
•Discount Double
TankClass
•Description Char
Car
•Model Char
•Year Int
•Color Char
•LicencePlate Char
EmployeeClass
•Description Char
Rental
•PickupDate Date
•OdoMeterStart Int
•DropOffDate Date
•OdoMeterEnd Int
Location
Employee
Address
•Street Char
•Number Char
•City Char
•PostalCode Char
Phone
•PhoneNumber Char
•PersonId Int
Person
•Name Char
•AddresId Int
•DriversLicence Char

Bibliography

Niels Bantilan. pandera: Statistical data validation of pandas dataframes. In *SciPy2020*, 2020.

Eric A. Brewer. Towards robust distributed systems, 2002. Principles of Distributed Computing.

Renato Bruni. Error correction for massive datasets. *Optimization Methods and Software*, 20(2-3):297–316, 2005.

Renato Bruni and Gianpiero Bianchi. A formal procedure for finding contradictions into a set of rules. *Applied Mathematical Sciences*, 6(126):6253–6271, 2012.

V. Chandru and J. Hooker. *Optimization methods for logical inference*, volume 34 of *Wiley Series in Discrete Mathematics and Optimization)*. John Wiley & Sons, 1999.

Edgar F Codd. A relational model of data for large shared data banks. *Communications of the ACM*, 13(6):377–387, 1970.

Jacco Daalmans. Constraint simplification for data editing of numerical variables. *Journal of Official Statistics*, 34(1):27–39, 2018.

E. De Jonge and M. Van der Loo. *Error Localization*. John Wiley & Sons, Inc, 2019a. to be published.

Edwin De Jonge and Mark Van der Loo. *validatetools: Checking and Simplifying Validation Rule Sets*, 2019b. URL `https://CRAN.R-project.org/package=validatetools`. R package version 0.4.6.

T. De Waal, J. Pannekoek, and S. Scholtus. *Handbook of statistical data editing and imputation*. Wiley handbooks in survey methodology. John Wiley & Sons, 2011. ISBN 978-470-54280-4.

Isil Dillig, Thomas Dillig, and Alex Aiken. Small formulas for large programs: On-line constraint simplification in scalable static analysis. In *International Static Analysis Symposium*, pages 236–252. Springer, 2010.

Seth Gilbert and Nancy Lynch. Brewer's conjecture and the feasibility of consistent, available, partition-tolerant web services. *Acm Sigact News*, 33(2): 51–59, 2002.

John Hooker. *Logic-based methods for optimization: combining optimization and constraint satisfaction*, volume 2 of *Wiley Series in Discrete Mathematics and Optimization*. John Wiley & Sons, 2000.

IfM. Porter's value chain, 2013. link via web.archive.org.

Russ Miles and Kim Hamilton. *Learning UML 2.0*. " O'Reilly Media, Inc.", 2006.

S Paulraj and P Sumathi. A comparative study of redundant constraints identification methods in linear programming problems. *Mathematical Problems in Engineering*, 2010, 2010.

R Core Team. *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria, 2020. URL `https://www.R-project.org/`.

RH Renssen and Arnout Van Delden. Standardisation of design and production of statistics; a service oriented approach at statistics netherlands. In *IAOS conference, Shanghai*, 2008.

Brian Stein and Alan Morrison. The enterprise data lake: Better integration and deeper analytics. *PwC Technology Forecast: Rethinking integration*, 1 (1-9):18, 2014.

M.P.J. Van der Loo and E. De Jonge. *Statistical data cleaning with applications in R*. John Wiley & Sons, Inc, New York, 2018. ISBN 1118897153.

M.P.J. Van der Loo and E. De Jonge. Data validation infrastructure for R. *Journal of Statistical Software*, 2019. Accepted for publication.

MPJ van der Loo and E de Jonge. *Data Validation*, pages 1–7. American Cancer Society, 2020. ISBN 9781118445112. doi: 10.1002/9781118445112.stat08255. URL `https://onlinelibrary.wiley.com/doi/abs/10.1002/9781118445112.stat08255`.

Hadley Wickham et al. Tidy data. *Journal of Statistical Software*, 59(10):1–23, 2014.

A. Willeboordse. Towards a new Statistics Netherlands; blueprint for a process-oriented organisation structure. *Netherlands Official Statistics*, 15:46–50, 2000. The journal has been discontinued, but the paper is still available online.

Weiguang Zhang. A suite of case studies in relational database design. Master's thesis, McMaster University, Hamilton, Ontario, 2012.

M Di Zio, N Fursova, T Gelsema, S Giessing, U Guarnera, J Ptrauskiene, L Quensel von Kalben, M Scanu, K ten Bosch, M van der Loo, and K Walsdorfe. Methodology for data validation. Technical Report deliverable of Work Package 2, ESSNet on validation, 2015. URL `https://ec.europa.eu/eurostat/cros/content/methodology-data-validation-handbook-final_en`.

Appendix A

Answers to selected exercises

Answers for section 1.3

1. For data that is stored (in a database) and data that is transported we want each value to be described unambiguously. Here, we have two values where 'fuel' is described as '– of which bio'. This makes interpretation dependent on the order of records.

4. (a) Not suited.
   (b) Not suited.
   (c) Suited for analyses (but note that a 5-year old has a job in this data, so the data is invalid).
   (d) Not suited.

5. Basically anything that you can do with image-processing software, e.g.: format conversion from png to jpg, zoom, blur, rotate, flip, and so on. A counter example is Optical Character Recognition, where image data is converted to character strings.

6. True.

7. True.

8. False.

9. True.

10. False.

11. False.

Answers for section 2.2

1. (a) Between raw and input, or between statistics and output.
   (b) Between valid and statistics, or perhaps between input and valid as auxiliary information.
   (c) Between raw and input.
   (d) Between raw and input.
   (e) Between raw and input.

Answers for section 3.5

1. (a) $D = \{\texttt{yes}, \texttt{no}, \texttt{under-aged}, \texttt{adult}, \texttt{retired}\}$.
   (b) $K = \{(Alice, Job), (Alice, Age), (Bob, Job), (Bob, Age)\}$.
   (c) Four keys, and for each we have 5 options, so the size of D^K equals $5^4 = 625$.

2. There are 4 valid job-age combinations, and 2 persons, so $4^2 = 16$ possibilities.

3. (a) validation rule.
   (b) not a validation rule.
   (c) not a validation rule.

4. (a) $smms$, validation level 2.
   (b) $ssms$, validation level 1.
   (c) $ssms$, validation level 1.
   (d) $mmmm$, validation level 4.

6. `total_rev >= 0`

7. $age \geq 0$, $income \geq 0$

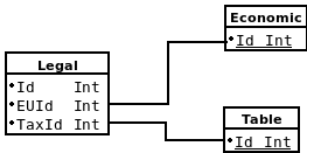
8. `income <= 0`

9. `age >= 12` can be left out.

Answers for section 4.5

1.

Id	Name	Age	Owns
1	Alice	7	{puzzle}
1	Alice	7	{bicycle}
2	Bob	6	{ball}

2. 

3. (a) 15 (including the primary and foreign keys).
   (b) AlbumId, MediatypeId, GenreId.
   (c) Integer

4. See figure A.1 on page 83.

5. $\{a, b, c, d, e\} \cap \{b, d, f\} = \{b, d\}$. Furthermore $V \cup W = \{a, b, c, d, e, f\}$, $V - W = \{a, c, e\}$, and $W - V = \{f\}$. So $\{a, b, c, d, e, f\} - \{a, c, e\} - \{f\} = \{b, d\}$.

6. (a) $\Pi_{a \in A}(A \ltimes B) = A$ (note: this is true for any A).
   (b) $\sigma_{Age>40}(A \times B) = \sigma_{Age>40}(A) \times B =$

$Name$	Age	$Height$

   (table with zero rows and three columns).
   (c)

$$\sigma_{Age \leq 40 \wedge Height \leq 170}(A \times B) = \sigma_{Age \leq 40}(A) \times \sigma_{height \leq 170}(B)$$

$Name$	Age	$Height$
$Mary$	34	167

   (d)

$$\Pi_{Height} A \bowtie B =$$

$Height$
178
167

7. (a) $\Pi_{Title,Name}(\texttt{tracks} \ltimes_{AlbumId} \texttt{albums})$

(b) For readability we define two intermediate results: X and Y.

$$X = \texttt{tracks} \ltimes_{AlbumId} (\texttt{albums} \ltimes_{ArtistId} (\rho_{Name/Artist}\texttt{artists}))$$
$$Y = (\texttt{invoice\_items} \ltimes_{TrackId} X) \bowtie \texttt{invoices} \bowtie_{CustomerId} \texttt{customers}$$
$$\Pi_{Artist,Name,CustomerId}(Y)$$

(c) $\Pi_{TrackId,EmployeeId}(Y \bowtie \texttt{employees})$.

Answers for section 6.3

1. (a) One CPU is associated with 0 or more controllers. An SCSI Controller is a type of controller. One SCSI controller is associated with 1 to 4 DiskDrives.

   (b) One Bank is associated with 0 or more Accounts. Checking and Saving are types of Accounts.

2. See Figure A.2 on page 83.

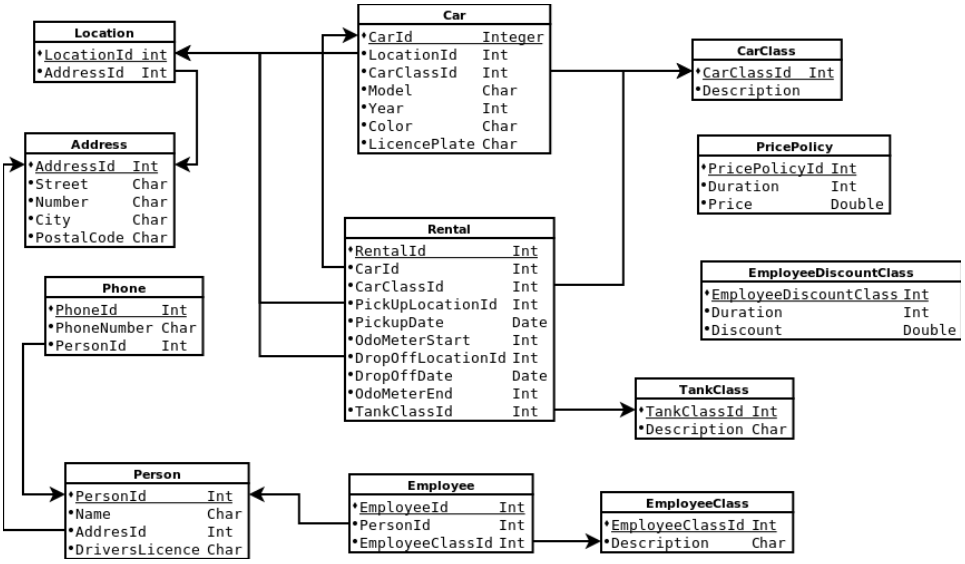


Figure A.1: Car rental ERD.

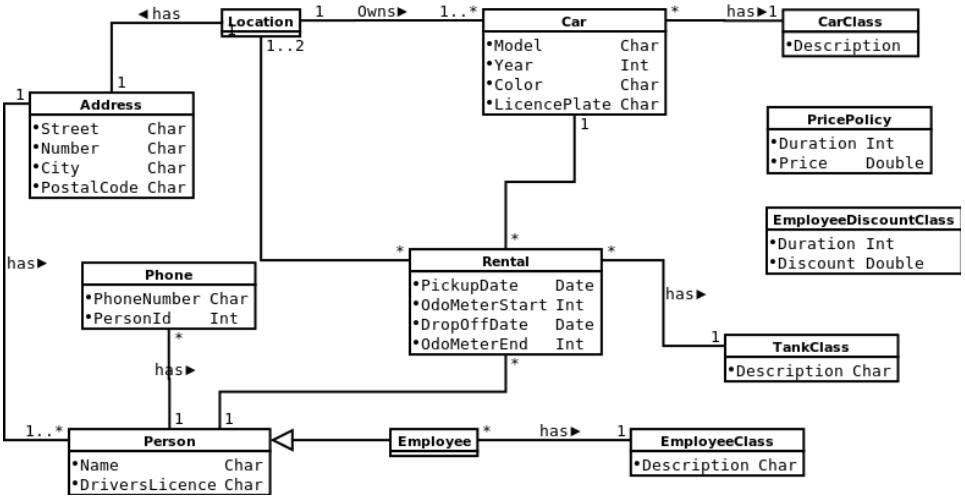


Figure A.2: Car rental UML diagram.

Index