

# Data Engineering for Data Analytics: A Classification of the Issues, and Case Studies

Alfredo Nazabal

The Alan Turing Institute, London, UK

Christopher K.I. Williams

Giovanni Colavizza

Camila Rangel Smith  
The Alan Turing Institute, London, UK

Angus Williams

## Abstract

Consider the situation where a data analyst wishes to carry out an analysis on a given dataset. It is widely recognized that most of the analyst's time will be taken up with *data engineering* tasks such as acquiring, understanding, cleaning and preparing the data. In this paper we provide a description and classification of such tasks into high-levels groups, namely data organization, data quality and feature engineering. We also make available four datasets and example analyses that exhibit a wide variety of these problems, to help encourage the development of tools and techniques to help reduce this burden and push forward research towards the automation or semi-automation of the data engineering process.

## 1 Introduction

A large portion of the life of a data scientist is spent acquiring, understanding, interpreting, and preparing data for analysis, which we collectively term *data engineering*<sup>1</sup>

<sup>1</sup>Another term often used is data wrangling.

. This can be time-consuming and laborious, for example [1] estimate that these tasks constitute up to 80% of the effort in a data mining project. Every data scientist faces data engi-

neering challenges when carrying out an analysis on a new dataset, but this work is often not fully detailed in the final write-up of their analysis.

Our focus is on a task-driven analysis scenario, where a data scientist wants to perform an analysis on a given dataset, and they want to obtain a representation of the data in a format that can be used as input to their preferred machine learning (ML) method. Interestingly, there is no unique or correct way of wrangling a messy dataset. For example, features and observations with missing values can be deleted or imputed using different approaches; observations can be considered anomalous according to different criteria; or features can be transformed in different ways.

Furthermore, most publicly available datasets have already undergone some form of pre-processing. While providing a clean version of the data is extremely helpful from a modeling perspective, data engineering researchers suffer from a limited availability to public messy datasets. This leads to researchers addressing some of the problems by synthetically corrupting clean datasets according to the data wrangling problem to be solved. However, such synthetic corruption is often not sufficient to capture the wide variety of corruption processes existing in real-world datasets. All of this variability in terms of data engineering issues and possible solutions, and the lack of public messy datasets and their final cleaned version makes attempting to automate this problem extremely challenging.

In this paper we first provide a classification of data engineering problems appearing in messy datasets when a data scientist faces an analytical task, and give practical examples of each of them. We have identified three high-level groups of problems: **Data Organization** issues (DO), related to obtaining the best data representation for the task to be solved, **Data Quality** issues (DQ), related to cleaning corrupted entries in the data, and **Feature Engineering** (FE) issues, related to the creation of derived features for the analytical task at hand. Additionally, we have further divided the DO and DQ groups according to the nature of data wrangling problem they face. Under Data Organization we include data parsing (DP), data dictionary (DD), data integration (DI) and data transformation (DT). Under Data Quality we include canonicalization (CA), missing data (MD), anomalies (AN) and non-stationarity (NS). Providing a classification of wrangling challenges not only pushes research in these individual fields, but also helps to advance the automation or semi-automation of the whole data engineering process.

A second contribution of the paper is to make available four example messy datasets, each with an associated analytical task. The analyses were carried out by data scientists at the Alan Turing Institute (in some cases replicating steps that were taken for published analyses). In the appendices we describe the cleaning operations they needed to perform in order to obtain a version of the data that could be used for the analysis task at hand. These provide practical examples of the issues identified in our classification, and give an insight of what constitutes a practical pipeline during a data wrangling problem.

The structure of the paper is as follows: Section 2 introduces the four cases studies that will provide examples throughout the paper. Section 3 describes our classification of data engineering challenges, broken down under the headings of Data Organization, Data Quality and Feature Engineering. Section 4 discusses related work. Section 5 provide details of the data engineering and modelling steps carried out for each of the four datasets, and our conclusions appear in section 6.

## 2 Overview of Case Studies

We have identified four case studies, drawing data from a variety of domains and having a variety of formats: plant measurements, household electricity consumption, health records, and government survey data. We refer to Section 5 for detailed descriptions of the data engineering challenges and modelling approaches of each dataset. We also provide a GitHub repository with the datasets and the wrangling processes.<sup>2</sup>

<sup>2</sup><https://github.com/alan-turing-institute/aida-data-engineering-issues>

Table 1 shows an overview of the wrangling challenges present in each of our use cases. Note that the actual challenges that an analyst encounters depend on the particular analysis that is undertaken, which in turn will depend on the particular analytical task being addressed. **justifyTundra Traits dataset:** The Tundra Traits data consists of measurements of the physical characteristics of shrubs in the Arctic tundra, as well as the data wrangling scripts that were used to produce a “clean” version of the dataset [2]. The analytical challenge entails building a model to gauge the effect of temperature and precipitation on specific shrub traits related to plant growth (see Section 5.1). **justifyHousehold Electricity Survey (HES) dataset:** The Household Electricity Survey (HES) data contains time-series measurements of the electricity use of domestic appliances, as well as a report on data cleaning by Cambridge Architectural Research [3]. Our chosen analytical challenge is to predict the energy consumption of a household given its appliance profile (see Section 5.2). **justifyCritical Care Health Informatics Collaborative (CleanEHR) dataset:** The CleanEHR data contains a sample of anonymized medical records from a number of London hospitals, including demographic data, drug dosage data, and physiological time-series measurements [4], together with publicly available data cleaning scripts. Our chosen analytical challenge is to predict which patients die in the first 100 hours from admission to the hospital. See Section 5.3. **justifyOfcom Consumer Broadband Performance dataset:** The Consumer Broadband Performance dataset contains annual surveys of consumer broadband speeds and other data, commissioned and published by Ofcom<sup>3</sup>

<sup>3</sup>The UK Office of Communications.

, and available as a spreadsheet for each year [5]. The data engineering challenge here is primarily one of matching common features between the data for any two years, as the names, positions, and encodings change every year. There was no given analytical chal-

lenge with the data as published, so we have chosen to build a model to predict the characteristics of a region according to the properties of the broadband connections (see Section 5.4).

Table 1: List of wrangling issues encountered in the datasets.

	Data Organization				Data Quality				Feature Engineering
Dataset	DP	DD	DI	DT	CA	MD	AN	NS	FE
Tundra		•	•	•	•	•	•		•
HES		•	•	•	•	•			•
CleanEHR		•	•	•	•	•		•	•
Broadband	•	•	•			•		•	•

### 3 Classification of Wrangling Challenges

When data analysts want to employ their preferred machine learning models, they generally need the data to be formatted in a single table. Although data engineering issues extend to other forms of data such as images, text, time series or graph data, in this work we take the view that the data analyst wishes to obtain a clean regular table that contains the information needed to perform the desired analytical task. To define notation, a table is assumed to consist of  $n$  rows and  $D$  columns. Each row is an *example* or *instance*, while each column is a *feature* or *attribute*, and attributes can take on a set of different *values*.

We mainly focus on two large groups of data wrangling issues: those related with *organizing* the data and those related with improving the *quality* of the data. We also include a third group on *feature engineering*, where the separation between wrangling issues and modelling choices starts to become blurred. In Table 3 at the end of this section we provide a summary of all the data wrangling problems addressed in this work. Notice that this classification should not be considered as a sequential process. Depending on the dataset and the analytical task some challenges are necessary while others are not, and the order of solving these problems can be variable.

#### 3.1 Data Organization

When data scientists start to work on a specific problem with real data, the first problem they face is obtaining a representation or view of their data that is best suited for the task to be solved. Data scientists usually perform several operations while organizing their data: the structure of the raw data is identified so that it can be read properly (data parsing); a basic exploration of the data is performed, where basic metadata is inferred for all the elements in the data (data dictionary); data from multiple sources is grouped into a

single extended table (data integration); and data is transformed from the raw original format into the desired data structure (data transformations).

3.1.1 Data Parsing

Data parsing refers to the process of identifying the structure of the raw data source so that it can be read properly. Raw data sources come in many different formats, from CSV files to flat files, XML, relational databases, etc. Some file formats can be read using open source programs while others are only readable using proprietary software.

Even when data comes in a well-structured file format, it can present a wide variety of encodings. For example, the well-known CSV format allows a wide variety of delimiter, quote and escape characters, and these have to be determined before the file can be loaded into an analysis program. Additionally, multiple tables may appear together in a single file, making it necessary to identify them and extract them properly. Even though many CSV files can be easily read by standard libraries, it is not uncommon to find files where this process fails, and the analyst needs to manually select the parameters to properly parse the data; see [6] for state-of-the-art performance on this task.

Table 2: An example of an ambiguous CSV file from [6].

Mango; 365,14; 1692,64
Apple; 2568,62; 1183,78
Lemon; 51,65; 685,67
Orange; 1760,75; 128,14
Maple; 880,86; 323,43

*Practical Example:* Table 2 shows an example of ambiguous CSV files appearing in real-world scenarios. A wrong detection of the CSV parameters can lead to a completely different table output (e.g. notice how choosing either semicolon, space or comma as the field separator results in different structured tables with three columns).

3.1.2 Data Dictionary

The term *Data Dictionary* refers to *understanding* the contents of the data and translating that knowledge into additional metadata. Ideally a dataset should be described by a data dictionary or metadata repository which gives information such as the meaning and type of each attribute in a table, see e.g. [7]. This information is normally provided by the data collectors and may come in many different formats, e.g. text documents with a profile of the data, extra headers in the data with information about its features in the data, or addi-

tional CSV files with descriptions for all the features. When data scientists are working with the data it is common that they need to go back and forth from the data to the metadata to understand the meaning of the tables and features and to detect possible inconsistencies that are not obvious from a simple exploration of the data. Even more importantly, it is not uncommon that this metadata is missing or out-of-date, making it necessary to infer it from the data itself. This process of data dictionary creation takes place at the level of tables, features and feature values: **justifyTable understanding:** The first problem data scientists face is to understand what is the global information contained in the tables, or *what is this table about?*. Often the owners of the data provide this information directly to the data scientists, or in some cases the name of the files reflect broadly the information contained in the data, but this is not always so. Data scientists then proceed to *explore* the data and try to understand their contents, by answering questions such as: How many tables are contained in the data? How many features? How many instances? Is there metadata with information about the features in the data? Additionally, understanding whether the data is a relational table, a time series or another format is a key process to decide how to work with this data. Unfortunately, data scientists might not be able to fully understand the contents of the data simply by exploration (e.g. headers might be missing, file names might be non-informative, etc.). In such cases, table understanding involves an interaction with a domain expert or the data collectors.

*Practical example:* In the Broadband dataset all basic information about the tables is summarized in the names of the different directories that contained the dataset. Each folder name contained the year and month of each annual survey. Most of the time, each folder only contained a CSV file with the different measurements for that year (panellist data). However, some of these folders also contained an additional CSV file (chart data) with a collection of tables and captions for those tables, with some basic summaries about the complete dataset. **justifyFeature understanding:** Normally, some basic information on the features contained in the table is provided, either by a header giving the name of each feature, or by an additional file with detailed information of each feature. When this information is not provided, either a domain expert should be involved to help complete the missing information, or this information must be inferred directly from the data. Feature understanding can take place at a semantic level (e.g. a feature with strings representing countries, see e.g. [8]), or at a syntactic level (e.g. a feature is an integer, or a date [9]). Feature understanding is a crucial process that must be addressed when working with a new dataset. Depending on the predictive task, the data scientist might need to remove features that leak information on the target feature, remove unnecessary features for the task at hand, transform some of these features, or create new features based on existing ones. This process relates heavily with *Feature Engineering* (see Section 3.3).

*Practical example 1:* From the latitude and longitude features in the Tundra dataset, we can get a sense of the locations around the world where plant traits were measured. From the experimental protocol (metadata), for each observational site there were a number of individual plots (subsites), and all plants within each plot were recorded. Unfortunately,



there was no indication in the data whether the latitude and longitude for each plant was recorded at the site or plot level. Further exploration of the data was needed to discover that the coordinates apply at site level.

*Practical example 2:* In the CleanEHR demographics dataset, the names of the features in the header were not informative for a non domain expert, with names like DOB, WKG, HDIS or DOD. A systematic matching process of each feature name in the dataset with a website containing the descriptions and information of the different features was necessary to understand the data. **Value understanding:** Exploring the values contained in the different features give data scientists a better sense of what is contained in the data, and it is the first step towards fixing possible errors in the data. Some common questions data scientists normally try to answer during this process are: if a feature is categorical, how many unique elements does it have? Do some features contain anomalous values? Do values outside the expected range of values of a given feature exist? Value understanding is especially important during the feature understanding process when insufficient information about the features was provided.

*Practical example:* the “HouseholdOccupancy” feature in the HES dataset, which was inferred to mean “number of people living in the house” from its name, was not numeric. A value “6 + ” was used to encode that a household had six or more tenants. Since the data scientist wanted this feature to be numerical, these “6 + ” entries were transformed into “6”.

### 3.1.3 Data Integration

Data integration involves any process that *combines* conceptually related information from multiple sources. Data analysts usually try to aggregate all the information they need for their task into a single data structure (e.g. a table, or time series, etc.), so they can use their desired machine learning model for the predictive task. However, data is often received in installments, (e.g. monthly or annual updates), or separated into different tables with different information and links between them (e.g. demographic information about patients, and medical tests performed on each patient.). Additionally, it is not uncommon that the structure of the data may change between installments (e.g. an attribute is added if new information is available). Commonly, data integration consists of either *joining* several tables together, i.e., adding new features to an existing table (usually referred as record linkage), or *unioning* several tables, i.e., adding new rows to an existing table. Further issues arise when the original data sources contain different data structures (e.g. relational tables and time series). **Record linkage and table joining:** This process involves identifying records across multiple tables that correspond to the same entity, and integrating the information into a single extended table. (Record linkage is also called entity disambiguation, or record matching *inter alia* [10], [11].) If *primary keys* exist in the data, the process is relatively straightforward. In such cases, joining two or more tables is usually performed by identifying the common keys across tables and creating an extended table with the information of the multiple tables. However, more involved link-

age processes are common during data integration: the name of primary keys can change across tables, a subset of features in the data might be needed to perform the record linkage (e.g. one feature identifies a specific table and another the entity (row) in that table), or even more specialized mappings between features might be needed (e.g. in Tundra Traits as per Practical example 2 below). The record linkage process is even harder when explicit keys are not available in the data. In such cases, a *probabilistic* record linkage problem arises. A broad subset of potential features are assigned with some weights that are used to compute the probability that two entities are the same. The probability of a pair of entities exceeding a given threshold is used to determine whether they are a match or not. Early work on a theoretical framework for the problem was developed by Fellegi and Sunter [12]. See [13] and [14] for more recent work on probabilistic record linkage.

*Practical example 1:* The HES dataset is contained in 36 CSV files spread across 11 directories. Although several keys appear repeatedly in different tables, unfortunately, the names of these keys were not always the same across tables, even when they referred to the same concepts. For example, the household identifier was sometimes given the name “Household” while in other tables was called “Clt Ref”. Additionally, each key contained different information regarding the combination of different sources. For example, “Household” identified the specific household for which monitoring took place (ID feature), “appliance code” was a number corresponding to a specific type of appliance (e.g. 182 → trouser press) and “interval id” was a number referring to the type of monitoring for a given appliance (e.g. 1 for monitoring conducted over one month at two minute intervals).

*Practical example 2:* The Tundra dataset presents an interesting table joining problem. It was necessary to combine the “Tundra Traits Team database”, which contained different measurements from plants across the world, with the “CRU Time Series temperature data and rainfall data” datasets, which contained the temperature and rainfall data across the world, gridded to 0.5°, with a separate table for each month between 1950 and 2016. This process was needed since temperature and rainfall have an effect on the measured traits of the plants. The joining of both data sources was performed with a two step process for each plant:

1. Identify the year and month when the specific trait for a plant was recorded, and look for the corresponding table into the CRU catalog.
2. Check the longitude and latitude values for that plant in the Tundra dataset, and map the corresponding temperature from the CRU dataset into the extended table.

Four different keys were thus necessary in the Tundra dataset (“DayOfYear”, “Year”, “Longitude” and “Latitude”) to connect the temperature data in the CRU catalog into the extended table. **JustifyTable unioning:** This process involves aggregating together row-wise different tables that contain different entities with the same information into one extended table. While ideally concatenating several tables together should be straightforward,



ward, in many real world scenarios the structure of different tables can differ dramatically. Some common problems that arise during table unioning include: features located in different positions in two or more tables, header names changing across tables, or features being added or deleted. To address all these problems, the authors in [15] obtained a matching between the attributes in two datasets, based on the idea that the statistical *distribution* of an attribute should remain similar between the two datasets.

*Practical example 1:* In the Broadband dataset, the different annual installments distributed across different CSV files needed to be concatenated into a single extended table. An exploration of each table reveals several problems: some columns were renamed between tables, the order of the columns was not preserved, not all columns appeared in each table and some categorical columns were recoded. The union process for all these tables involved selecting a common structure for the extended dataset, and mapping every feature from each table into the corresponding feature of the extended table. Doing this process manually (instead of using the program in [15]) involved accounting for every single particular mapping across tables in the code. **Heterogeneous integration:** This process involves combining data from different structured sources (relational tables, time series, etc) and different physical locations (e.g. websites, repositories in different directories, etc.) into a single extended structure format. Data repositories can be massive, consisting of multiple sources across different locations. Getting all this information into a proper format is time consuming and sometimes not feasible. Since the data scientists might be interested only in extracting a small subset of the data that refers to their particular problem, query based systems are needed during the integration process. This parsing is often handled by an ETL (Extract, Transform and Load) procedure [16], but such code may be difficult to write and maintain. The idea of Ontology Based Data Access (OBDA; [17]) is to specify at a higher level what needs to be done, not exactly how to do it, and to make use of powerful reasoning systems that combine information from an ontology and the data to produce the desired result.

*Practical example:* The CleanEHR dataset is composed of a collection of R objects that contained demographic information about the different patients, time series measurements of the different medical tests that were performed on the patients and some CSV files with detailed information about different encodings employed in the data. Since the modelling task is related to the times of death of the patients, only parts of the time series data are needed to train the predictive models, since in a real predictive scenario future information is not available. With these considerations, only the files containing the first 10 hours of the patients' stay in the hospital would be extracted to train the model, discarding all the patients that lived less than 10 hours, in order to include as much data as possible. From those selected files, only relevant summary measures from the time-series data (mean, standard deviation and last value measured) should be combined with the demographics data during the table joining process. **Deduplication:** It is common after a data integration process that several duplicate instances containing the same or similar information exist in the extended table [11]; these duplicates need to be resolved into one in-

stance. Note that, while record linkage involves identifying matching entities across tables to create an extended table with all the available information, deduplication involves identifying matching entities in a specific table to remove the duplicate entries in the data. Similar techniques employed during the matching process in record linkage can also be employed during deduplication<sup>4</sup>

<sup>4</sup>The generic term *entity resolution* encompasses both record linkage and deduplication.

### 3.1.4 Data Transformation

Most of the time, data analysts need the data to be formatted in a  $n \times D$  table, where every instance should have  $D$  attributes. However, the original shape of the data does not always conform to this structure, and one may need to transform the “shape” of the data to achieve the desired form [18]. Furthermore, the original data source may not be tabular, but unstructured or semi-structured. In this case we need to carry out *information extraction* to put the data into tabular form. **Table transformations:** This process involves any manipulation on the data that changes the overall “shape” of the data. One of the most common table manipulations is the removal of rows or columns. There are many reasons why data scientists remove parts of the data (e.g. some rows or features being completely or almost completely empty, some information is deemed unnecessary for the analysis task, etc.). Another common table manipulation is switching the format of the table from a “wide” to a “tall” format or vice versa [18], which can happen e.g. when column headers in the data are values and not variable names. Note that the “tall” format is closely related to the one encoded in a semantic (or RDF) triple, which has the form of a (subject, predicate, object) expression; for example (patient 42, has height, 175cm).

*Practical example 1:* In the extended table of the Tundra dataset scenario, from all the possible plant traits, only a small subset of them were measured for each plant. In the original wide format (see Section 3.1.3, record linkage practical example 2), the table is extremely sparse, with many missing entries. By changing the table from a “wide” to a “tall” format and grouping all the trait names under a new feature “Traits” and the values under a new feature “Values”, a more compact table is created with the missing trait values not being explicitly represented. Additionally, the data scientist removed all observations where: a) a geographical location or year of observation was not recorded, b) a species had less than four observation sites and c) sites had less than 10 observations. Notice the new structure of the table was decided according to the analytical task at hand (other structures are possible). **Information extraction:** Sometimes the raw data may be available in unstructured or semi-structured form, such as free text. A process involving the extraction of the relevant pieces of information into multiple features, while discarding any unnecessary information is often required. Examples include named entity recognition [19] (e.g. names of people or places), or relationship extraction [20] (e.g. a person is in a partic-

ular location). Natural language processing (NLP) methods are often used to tackle such tasks.

*Practical example:* FlashExtract by Le and Gulwani [21] provides a programming-by-example approach to information extraction. A file contains a sequence of sample readings, where each sample reading lists various “analytes” and their characteristics. By highlighting the different required target fields for a few samples, a program is synthesized (from an appropriate domain specific language) which can extract the required information into tabular form.

## 3.2 Data Quality

When the data has been properly structured into the desired output format, data scientists need to carefully check it in order to fix any possible problems appearing in the data. Data quality issues involve any process where data values need to be modified without changing the underlying structure of the data. Common data cleaning operations include standardization of the data (canonicalization), resolving missing entries (missing data), correcting errors or strange values (anomalies) and detecting changes in the properties of the data (non-stationarity).

### 3.2.1 Canonicalization

Canonicalization (aka standardization or normalization) involves any process that *converts* entities that have more than one possible representation into a “canonical” format. We can identify different canonicalization problems in datasets according to the transformations needed to standardize the data. One form of canonicalization involves obtaining a common representation for each unique entity under a specific feature (e.g. U.K., UK and United Kingdom refer to the same entity under different representations.). This process usually involves a previous step of identifying which values of a given feature correspond to the same entities, which we term *cell entity resolution*. Another form of canonicalization involves obtaining a standard representation for every value under a given feature (e.g. specific formats for dates, addresses, etc.). This standard representation is often chosen by the data scientist according to the task they intend to solve. A particular case of a feature canonicalization involves standardizing the units of physical measurements across a given feature. The final goal of a canonicalization process is to obtain a table where every entity in the data is represented uniquely and all the features in the data follow a common format. **Cell entity resolution:** This process involves identifying when two or more instances of a given feature refer to the same entity. This process has many similarities with deduplication and record linkage (see Section 3.1.3). The main difference is that the goal of deduplication and record linkage is to match complete instances across the same table or across multiple tables, while cell entity resolution is only concerned about identifying when two or more instances with a different representation in a given feature refer to the same entity. A lot of variability can arise when inputting values into a dataset. Different names for the same entity, abbreviations, or syntactic mismatches during record-

ing (e.g. typos, double spaces, capitalization, etc.) lead to many different entries in a feature referring to the same underlying concept. Identifying which cells correspond to the same entity allows to repair them by matching them to a common or standard concept<sup>5</sup>

<sup>5</sup> We note that [22] argue that such cell entity resolution may not be necessary if one uses a similarity-based encoder for strings which gracefully handles morphological variants like typos. This may indeed handle variants like U.K. and UK, but it seems unlikely to group these with “United Kingdom” unless some knowledge is introduced.

. The software tool OpenRefine [23] provides some useful functionality (“clustering”) for this task.

*Practical example:* In the Tundra dataset there are two features referring to the names of the plants in the dataset: “AccSpeciesName” and “OriginalName”. While “AccSpeciesName” contains the name of the plant species, the “OriginalName” contains different names that the scientists employed to record those plants, including typos, capitalization changes, etc. (e.g. AccSpeciesName: “Betula nana” - OriginalName: [“Betula nana”, “Betula nana exilis”, “Betula nana subsp. exilis”]). **Justify Canonicalization of features:** This refers to any process that involves *representing* a specific feature type (e.g. dates, addresses, etc) with a standard format. For example, phone numbers can be encoded as “(425)-706-7709” or “416 123 4567”, dates can be represented as 25 Mar 2016 or 2016-03-25, etc. While different feature formats exist for a specific type, is it a decision of the data scientist to select the desired standard format for a feature (usually related to the task to be solved) and convert all the values in that feature to that standard format. This can often be done by writing regular expressions, but this is only possible for skilled operators. The authors in [24] developed a method for *learning* these transformers via programming-by-example. This was later made available as the Flash Fill feature in Microsoft Excel to a very wide user base.

*Practical example:* Features related with dates and time in the CleanEHR dataset occur in different formats. For example in one case both the date and time were recorded in the same feature (DAICU), and in another case date and time were recorded under two different features (DOD and TOD). Each feature needed to be dealt case-by-case by the data scientist and transformed into a common datetime Python object. **Justify Canonicalization of units:** This refers to any process that involves *transforming* the numerical values and units of a feature into a standard representation. This problem commonly arises from physical measurements being recorded with different units. For example, height can be recorded both in metres or centimetres, temperature in Celsius or Fahrenheit, etc. Different unit formats can lead to different representations appearing in the data, and the data scientist needs to standardize all of them into a single representation.

*Practical example 1:* A common unit canonicalization problem appears in the HES dataset. A feature in the dataset measured the volume of the refrigerators in each household (“Refrigerator volume”). Unfortunately, the values were recorded with different units (e.g. litres, cubic feet or no unit), which were also written in different formats (e.g. “Litres”,



“Ltr”, “L”). A process of removing the units from the feature and standardizing all the values according to a common unit (litres in this case) would be necessary.

*Practical example 2:* Several of the features in the CleanEHR dataset were recorded with different units. For example, the feature “HCM” containing the height of the patients was supposedly recorded in centimetres, but around 200 patients had their height recorded in metres. Additionally, another feature “apacheProbability”, recording the probability output of the apache test, was recorded in the range  $[0, 100]$  in some cases and in other cases between the range  $[0, 1]$ . Notice that, in this case, the units were not provided in the data, and reasoning about the meaning of the feature and its values was necessary to determine that a unit canonicalization problem was present for those features. According to the protocol description, “HCM” was encoded in centimetres and “apache-probability” in the  $[0, 1]$  range.

### 3.2.2 Missing data

This issue concerns every operation that involves detecting, understanding and imputing missing values in a dataset. Missing data is a challenging problem arising very frequently in the data wrangling process [25]. Since many machine learning models assume that the data is complete, data scientists need to detect the missing values and repair them properly. Otherwise, they would be restricted to employing prediction methods that can handle incomplete data. **JustifyDetection:** Datasets often contain missing entries. These may be denoted as “NULL”, “NaN” or “NA”, but other existing codes are widely employed like “?”, or “-99”. While codes like “NULL” or “NaN” are easily identified by a simple exploration of the data, other values encoded with the same type of the feature (e.g. “-99” for numerical values) are *disguised missing values* [26] and can only be identified by understanding the properties of the features.

*Practical example:* At first glance, all the missing values in the CleanEHR dataset seemed to be encoded as “NaN”. However, after further inspection of features “apache-probability” and “apache-score”, the analyst noticed that two supposedly positive features had a significant number of “-1” values. Since “-1” does not conform with the range of possible values of those features, these codes were inferred to represent when the apache test was not provided, and consequently, they should be treated as missing values. **JustifyUnderstanding:** The underlying process of the missing data patterns can provide additional information about the contents of the data. The book by [27] is a seminal reference on the understanding and *imputation* of missing data, classifying the missing patterns in three groups according to the generation process. a) Missing Completely At Random (MCAR), when the pattern of missingness does not depend on the data, b) Missing At Random (MAR), when the missingness only depends on observed values and c) Missing Not At Random (MNAR), when the missingness can depend both on observed and missing values.

*Practical example:* Different missing data patterns exist in the CleanEHR dataset, depending on the features. For example, the “HCM” feature seemingly had entries missing with no correlation with other values in the data (MCAR), while some of the medical tests (e.g. “CHEMIOX” or “RADIOX”) had missing entries that seemed to indicate that a specific test was not performed (MNAR). Unfortunately, these features also had entries with “0” values, indicating clearly that a test was not performed (see practical example 1 in Section 3.2.4). From a data scientist’s perspective, this means that we cannot be sure whether a missing value indicates a test not performed, or whether there were other reasons for the entry being missing (e.g. someone forgot to fill this entry). **JustifyRepair:** This process involves any operation performed on the missing data. The most common procedures are either removing any rows with missing entries (known as “complete case” analysis) or substituting those missing entries with other values according to different rules (imputation). Some imputation methods include replacing every missing entry in a feature by the mean or mode of the statistical distribution (mean/mode imputation), filling those missing entries with values sampled randomly from the observed values of the feature, or applying more sophisticated models for missing data imputation (see [25] for some classical methods and [28], [29] or [30] for recent work). Such multiple imputation methods can represent the inherent uncertainty in imputing missing data. We would like to remind the reader of the difficulty of this problem in a real world scenario: ground truth for the missing entries is not available, so a data scientist needs to be sure that whatever method they decide to use during repair will impute sensible values for those entries.

*Practical example 1:* in the Tundra extended table, the geographical location, the date of the observation and temperature features at a site were often missing. During the integration process, whenever either the location or the year was not provided, the temperature could not be joined into the extended table, resulting in a missing entry. Since these entries would become problematic for the modelling task, every plant where any of these features were missing was removed from the dataset.

*Practical example 2:* for the missing values in the HES dataset, different approaches were followed depending on the feature. For example, for the “House.age” feature, a unique missing entry with a code of “-1” exists, and it was imputed using the most common age range in the feature (mode imputation).

*Practical example 3:* a similar procedure was also employed in the CleanEHR dataset. For example, the missing entries in “HCM”, most likely presenting a MCAR pattern, were imputed using the mean of the distribution (mean imputation) after standardizing the feature (converting the metres values into centimetres, see canonicalization in Sec. 3.2.1). However, for the medical test (“CHEMIOX”, “RADIOX”, etc.) those missing values were imputed with a “0”, according to the belief that a missing entry indicated that a test was not performed.

### 3.2.3 Anomalies



An anomaly can be defined as “a pattern that does not conform to expected normal behaviour” [31]. Since anomalies can potentially bias models to wrong conclusions from the data, identifying and possibly repairing these values becomes critical during the wrangling process. Anomalies arise in the data for a variety of reasons, from systematic errors in measurement devices to malicious activity or fraud. Anomaly detection is such an important topic that in many problems the detection of anomalies in a dataset is the analytical challenge itself (e.g. fraud detection or intruder detection).

Multiple statistical approaches exist for anomaly detection, which can be grouped under the nature of the problem to be solved. *Supervised anomaly detection* requires a test dataset with labelled instances of anomalous entries. Classification machine learning algorithms are usually employed in this setting, where we consider that we are provided with an unbalanced dataset [32] (we expect a lower fraction of anomalies). *Unsupervised anomaly detection* assumes that no labels exist for the anomalous data [33]. Clustering approaches are usually employed in this setting, assuming that most of the data is normal, and that instances not fitting the distribution of the rest of the data are anomalous. Finally, *Semi-supervised anomaly detection* approaches assume that training data is normal, builds a model over it, and tests the likelihood of a new instance being generated from the learnt model [34]. **JustifyDetection:** Anomaly detection is in principle harder than missing data detection, since anomalies are not normally encoded explicitly in the data. Approaches to anomaly detection can be classified as *univariate* (based only on an individual feature) or *multivariate* (based on multiple features). At a univariate level, a cell might be anomalous for *syntactic* reasons, e.g. that the observed value “Error” is not consistent with the known type (e.g. integer) of the variable<sup>6</sup>

<sup>6</sup> In the database literature this is termed a *domain constraint*.

[9]. Another cause of anomaly is *semantic*, e.g. that for an integer field representing months only the values 1-12 are valid, and hence an entry 13 would be anomalous. A further class of anomaly is *statistical*, where a model is built for the clean distribution of a feature, and anomalies are detected by being low-probability events under the clean distribution.

For multivariate statistical anomaly detection, one should distinguish between row outlier detection (where a whole data instance is declared to be an outlier, and discarded), and cell outlier detection, where only one or more cells in the row are identified as anomalous<sup>7</sup>

<sup>7</sup>Our terminology here follows [35].

. Some classical algorithms for unsupervised row outlier detection include Isolation Forests [36] and One Class SVMs [37]. More recently deep learning models have been used for cell outlier detection, see e.g. [38], [35].

A multivariate approach to anomaly detection from the databases community makes use of rule-based *integrity constraints*, such as functional dependencies or conditional functional dependencies, see e.g. [39]. One example of such a constraint is that a postal code should entail the corresponding city or state, and one can check for inconsistencies. Any violation of an integrity constraint in the data would be identified as an error that needs to be repaired.

*Practical example:* A univariate statistical approach was followed in [2] to remove anomalous entries in the Tundra dataset. The observations were grouped by a certain taxon (e.g. species, genus or site) and then a threshold was chosen based on eight times the standard deviation of a trait under the taxon ( $8\sigma$ ), flagging as anomalous every observation that deviated from the mean of the taxon more than the threshold. This procedure was employed for all the traits except “plant height” and “leaf area”, based on the recommendations of the domain experts. **\justifyRepair:** anomaly repair techniques are similar to missing data repair. Normally, data scientists either remove the anomalous entries completely or, when locating anomalous values under a feature, they substitute those values by other *sensible* values.

*Practical example:* in the Tundra dataset, the anomalous entries detected with the approach mentioned above were removed from the data, in order to avoid introducing biases into the model.

### 3.2.4 Non-Stationarity

This issue involves detecting any *change* occurring in the data distribution over some period of time. This problem is usually referred as change point detection (CPD) in time series analysis, see e.g. [40]. However, non-stationarity problems can also arise in tabular data. In particular, a well known problem in machine learning is *dataset shift*, occurring when the distribution of the input data differs between training and test stages [41]. Additionally, a common source of non-stationarity in wrangling problems arises from a change in how the data is collected. In some cases, the protocol of data collection can change over time, e.g. the units of some measurements are changed, labels can be recoded, etc. In other cases, when a clear data collection protocol is not established, different people or institutions may collect data using different criteria, and a final combined dataset presents clear format variability that remains constant over some chunks of the data (normally related to the person or institution that collected that piece of information). **\justifyChange points:** CPD in time series is usually concerned in identifying those points in time where a specific change in the probabilistic distribution of the data occurs [40]. Changes may occur in the mean, variance, correlation or spectral density, among others. Also, a change can be defined as an abrupt change in the distribution or a drift over time over the probability distribution. We refer to [42] for a review on CPD methods and [43] for an extensive evaluation of CPD algorithms. **\justifyProtocol changes:** this problem involves any process that changes the collection of the data over a period of time. This problem is clearly related with the problem of table unioning described in Section 3.1.3. In

many cases data scientists are provided directly with a dataset that contains a combination of different tables. It is common that this combination results in the format of some features changing, new labels being added to the data [44] or measurements being recorded in different units (see Section 3.2.1). Detecting when these changes in the data collection occur is vital to solve other wrangling problems arising from these changes.

*Practical example 1:* In the CleanEHR, a patient undergoing a specific test was always encoded with “1”. However, a test not being performed on a patient had two different encodings: “0” for some groups of patients and “NaN” for other groups. These two sets of encodings follow a sequential pattern, since the data is an aggregate of datasets from different hospitals and each hospital used different encoding conventions (either “1” and “0”, or “1” and “NaN”). Without noticing this problem, a data scientist might remove some of these features from the data, assuming that NaN implies missing data.

*Practical example 2:* In the Broadband dataset, the feature indicating whether the broadband connection was in a rural or urban environment not only had different names across tables, but also some tables encoded only “Rural” and “Urban” (installments from 2013 and 2014) and others “Rural”, “Urban” and “Semi-Urban” (installments from 2015). In principle, these features could be combined easily, however, another problem is raised from the modelling perspective. There is no knowledge on whether in the “Rural-Urban” installments there were not any “Semi-Urban” instances, or whether a new encoding of the different locations was introduced at some point (non-stationarity problem). The data analyst decided to encode “Semi-Urban” instances as “Rural”, to get a binary classification problem, since the test data did not have any “Semi-Urban” instances either.

### 3.3 Feature Engineering

Once the data is relatively clean and organized in a single table, a data scientist will start to be concerned about the representation of the features in the data needed for the analytical task at hand. It is common that the raw features in the data are not suitable for the machine learning algorithm to be employed. For example, data might contain a combination of string and numerical features, while the method they intend to employ only accepts numerical values as inputs. A *feature engineering* process, where some transformations are applied to the features, or new features are created based on existing ones, is arguably one of the most important aspects of a data scientist’s work. This can be carried out based on the analyst’s knowledge or beliefs about the task at hand, and the information required to solve it. Additionally, methods employed to extract meaningful features from the data are usually domain specific. For example, when the data involves sensor readings, images or other low-level information, signal processing and computer vision techniques may be used to determine meaningful features that can be used. Also, more recently deep learning approaches have been used to *learn* appropriate features in an end-to-end fashion in such domains, given sufficient training data.

We define **feature engineering** as any manipulation of the data that involves changing the number of features contained in the data or their properties. Some common feature manipulations include: aggregating several features with the same information into a unique feature, creating new features based on already existing features in the data, deleting unnecessary features or creating one-hot encoding representations of categorical variables. Notice that some of these manipulations can also be categorized as table manipulations (see Section 3.1.4).

*Practical example 1:* in the HES dataset, redundant information in the demographics table was combined into a newly created feature “PensionerOnly”, and all the features with information already contained under “PensionerOnly” were removed. Also, “House.age” was originally encoded as a string with a range of years (e.g. 1950-1966). To encode this as a numerical feature, the difference between the midpoint of the range and 2007 was computed (which was the latest age of any house in the dataset).

*Practical example 2:* In the CleanEHR dataset, many features that were directly correlated with the time of death of the patients had to be removed (e.g. “CCL3D” recorded the number of days the patient was in the ICU), as these would “leak” information about the chosen target variable. Additionally, every patient that was admitted into the ICU already dead and every patient where no time of death was recorded was removed from the dataset, since the evaluation of the predictive model is not possible without ground truth.

Table 3: Summary of data wrangling problems.

## Data Organization

### Data Parsing

What is the original data format? How can it be read properly?

### Data Dictionary

Table description	What is the meaning of the table? Is there a header? Are there several tables in the data?
Feature description	What is the type of each feature? What are the possible ranges of values? What is the meaning of the feature?
Value description	What is the meaning of the values of a feature? Are there unexpected values in a feature?

### Data Integration

Table joining	How do we join tables containing the same entities? How do we detect common entities across tables?
Table unioning	How do we aggregate tables with common information together? Are common features consistent across tables?
Heterogeneous integration	How do we combine e.g. time series with relational data or images? How do we query multiple datasets stored in different locations?
Deduplication	How do we detect duplicate entities in the data?

### Data

### Transformation

Table transformations	Should we use a “tall” format or a “wide” format? Should we remove rows or columns?
Information extraction	Are there properties of the data contained in free text features? If so, how do we extract this information?

## Data Quality

### Canonicalization

Cell entity resolution	Do some values in a feature represent the same concept? If so, how do we group them under a common concept?
Features	Are there different formats of a feature present? What is the standard format?
Units	Are measurements recorded with the same units?

### Missing Data

Detection	Which cells are missing? Which values are used to represent missing data?
Understanding	Why is the data missing? Is it MCAR, MAR or MNAR?
Repair	Should we impute missing values? Should we delete rows or columns containing missing values?

### Anomalies

Detection	How do we identify anomalous entries across features?
Repair	Should we leave these values in the data or repair them? Should we remove rows with anomalies?

Non-Stationarity	
Change points	Does the behaviour of a time series change abruptly? Is there a meaning behind these changes?
Protocol changes	Do the properties of the data change while exploring it sequentially? Are there different feature encodings present across consecutive entities?
Feature Engineering	
Feature Engineering Are the features in the data useful for the task at hand? Do we need to concatenate or expand features? Do we need to create new features based on existing ones?	

4 Related Work

The literature on data engineering is extensive with many works addressing general problems on the field, while others only focusing on a specific data wrangling issue. We discuss here a number of other review papers on general data engineering.

The authors in [45] divide data cleaning problems into schema level and instance level. At the schema level the focus is on integrity constraints (which fall under our anomaly detection heading), while the instance level contains problems such as missing data, canonicalization, data integration, data description, etc. Note that these instance level issues are not systematically categorized in the paper, but only listed as examples (see e.g., their Table 2). The authors also distinguish single-source and multi-source problems, although the main new issue that they identify for multiple sources is that of record linkage.

The CRISP-DM framework of [46] highlights two phases relating to data engineering, which they call data understanding and data preparation. Their data understanding phase includes data description (similar to our data dictionary heading), and verification of data quality (which relates to our headings of missing data and anomalies), as well as data collection and data exploration. Their data preparation phase includes data selection and cleaning tasks (including the handling of missing data), data integration, and tasks we describe under feature engineering including the formatting of data for modelling tools, and constructing derived features. Our descriptions in Section 3 are more detailed than those provided in the CRISP-DM paper.

A taxonomy of “dirty data” is provided in [47]. At the highest level this taxonomy is split between missing data (their class 1), versus non-missing data (class 2). Class 2 is further broken down into 2.1 “wrong data” (due e.g. to violation of integrity constraints, and to failures of deduplication), and 2.2 “not wrong, but unusable data” (which include issues of canonicalization and record linkage). In our view the choice of a top-level split on missing/non-missing data creates a rather unbalanced taxonomy. Note also that the authors do not provide much discussion of the topics falling under our *data organization* heading.



In [48], the authors refined the notion of *data readiness levels* introduced by [49], to provide levels C (conceive), B (believe) and A (analyze). Level C relates mainly to our data organization issue, especially data parsing and data integration. Their level B mainly covers topics falling under our data quality heading (missing data, canonicalization) along with data dictionary and data integration (deduplication) topics from data organization. Their level A includes mainly feature engineering issues, but also includes outlier detection (which we class under anomaly detection) and a semantic description of features (see our data dictionary heading). Note also that our paper provides a fuller discussion of the issues; in [48] the topics mentioned under levels A, B and C get only one paragraph each.

In [7], the authors survey the task of *data profiling*, which is defined (following [50]) as “the activity of creating small but informative summaries of a database”. This is clearly related to our data dictionary task, but they also discuss detecting multivariate dependencies, which we mainly cover under the heading of anomaly detection.

The identification of various problems as described above leads to the question of tools to help addressing them. We have pointed out various tools to address specific problems in Section 3. However, there is also a need for systems that allow the *integration* of multiple individual tools to guide data scientists during the data engineering process. [51] provide a survey of intelligent assistants for data analysis. One prominent (commercial) system is Trifacta [52], which is based on preceding systems such as Wrangler [53]. It provides a system for interactive data transformations that suggests applicable transformations based on the current interaction with the data [54]. Wrangler provides common data transformations such as mapping operations, fold operations, sorting or aggregations among others. It also infers statistical data types and higher-level semantic types. Another tool is DATA CIVILIZER [55] which offers functionality including entity matching across multiple heterogeneous sources, handling missing values, and canonicalization.

## 5 Case studies

We showcase here the full data wrangling analysis performed in our four case studies. For each dataset X, we start by giving a description of the raw dataset, followed by: Section 5.X.1 gives a description of the analytical challenge associated with the dataset. Section 5.X.2 provides an ordered pipeline of the data engineering issues addressed in each dataset to obtain a clean version of the data. Section 5.X.3 describes the issues that arose against the headings of our classification. Finally, Section 5.X.4 describes the model employed for the associated analytical task and the final results of the analysis.

### 5.1 Tundra Traits

This use-case comprises two separate datasets:

1) The *Tundra Traits Team database*. It contains nearly 92,000 measurements of 18 plant traits. The most frequently measured traits (more than 1 000 observations each) include

plant height, leaf area, specific leaf area, leaf fresh and dry mass, leaf dry matter content, leaf nitrogen content, leaf carbon content, leaf phosphorus content, seed mass, and stem specific density. The dataset also comes with a cleaning script prepared by its originators, which we have followed.<sup>8</sup>

<sup>8</sup>Publicly available at <https://github.com/ShrubHub/TraitHub>. We were kindly granted early access to this dataset by Isla H. Myers-Smith and Anne Bjorkman of the sTUNDRA group (<https://teamshrub.wordpress.com/research/tundra-trait-team/>)

## 2) The “CRU Time Series” temperature data and rainfall data<sup>9</sup>

<sup>9</sup><http://catalogue.ceda.ac.uk/uuid/58a8802721c94c66ae45c3baa4d814d0>

. These are global datasets, gridded to 0.5°. We use only the date range 1950 to 2016.

### 5.1.1 Analytical Challenge

The challenge posed in [2] was to infer how climate affects shrub growth across a variety of measured traits. We attempt to fit a model predicting certain traits (e.g. vegetative height) from temperature, similar to the first panel of Figure 2b in [2]. Much of our approach follows [2]; however, we have made some simplifications and assumptions, and we acknowledge that we are not experts in this domain. We also do not have access to the original code.

There is some terminology to know. The measurement subjects are individual plants, and the types of measurements on a plant are called *traits*. For example, “vegetative height” is a trait. Only the species of a plant is recorded, so no identification of the same plant across different measurements of the same trait is possible; however, multiple traits on the same plant are measured and recorded together. The experimental protocol in this field, as we understand it, is to delineate, for each observational *site*, a number of individual *plots* (or *subsites*) and to record all plants within each plot, typically in a single session on a particular day. Thus, an “individual observational unit” is a single plant, within a particular plot, on a given day; the properties of the unit are the traits. Notice that the creators of the Tundra dataset provided a script (“TTT\_data\_cleaning\_script.R”) that attempts to make the raw data more consistent and interpretable, although they do not perform a complete data wrangling.

### 5.1.2 Pipeline of data engineering steps

The first five steps listed below were carried out using the early-access version of the data made available privately to us. The remaining steps apply to the publicly available version

of the data (what they call `data_raw`).

1) Loading the Tundra Traits data (DP):

- The csv of the data in wide format is loaded (DP).
- An individual ID variable is created for each plant (FE).
- Header names are renamed into more informative names (DD).

2) Data is transformed from a wide format into a tall format, where two variables are created: a “Trait” variable with the names of the traits and a “Value” variable with the corresponding values for each trait (DT).

3) A removal of untrustworthy data is performed at this stage, according to different rules (DT):

- Some observations are removed because the analysts were unsure about the units of the measurements.
- Some traits were removed because the analysts were unsure of what they meant.
- They removed plants according to their “Treatment” feature values.

4) A data dictionary process occur at this point, where additional information is added into different features (DD):

- Units are added for each trait (they create new features).
- New names for the traits are added (they create additional features).

5) A “Genus” feature is created, using only the first part of the “AccSpeciesName” feature in the data (FE).

6) At this stage, the analysts create different summary statistics from the data according to different groupings, and use them to filter part of the observations in the dataset according to different rules (DT + FE).

The list of groupings considered in the analysis are: By Trait, by Trait and “AccSpeciesName”, by Trait and Genus, by Trait, “AccSpeciesName” and “SiteName”, by Trait, Genus and “SiteName”.

The list of statistics computed in a given group, and added for each individual  $x_i$  in that group are:

- Median, standard deviation and number of elements of the group.
- Mean of the rest of the elements of the group, without considering  $x_i$ .

- Error risk of each value under the group, according to the computed a) mean and standard deviation and b) median and standard deviation. Error risk is explained further under Anomaly Detection in sec. 5.1.3.

7) After this filtering process, all unnecessary features are removed from the dataset (most of the previously computed statistics) obtaining a cleaned version of their data (DT). This is the state where, in the publicly available version of the data, the authors say that the data is clean. Note that the integration of the temperature data from the CRU dataset is not performed in the public repository.

8) Temperature data from the CRU dataset is integrated into the Tundra dataset according to the location of the plants (longitude and latitude) and the day and year when the measurements were recorded (DI).

### 5.1.3 Data Engineering Issues

**Data Dictionary:** some issues were raised during the exploration of the data.

- 1) Latitude and longitude coordinates are given for each row in the Tundra dataset, but it is not stated whether those coordinates apply to a site or to a plot. Inspection of the data seems to indicate that in fact the coordinates apply at site level, so that all plots within a site should be taken to have the same coordinates.
- 2) In the original analysis [2], the authors define temperature as “the average temperature of the warmest quarter of the year”. For simplicity our analysis fixes a particular month and uses the average temperature in that month.
- 3) Columns were renamed to a standard terminology.<sup>10</sup>

<sup>10</sup>Provided by “TTT\_data\_cleaning\_script.R”

- 4) Units for each measurement were added.<sup>11</sup>

<sup>11</sup>Also provided by “TTT\_data\_cleaning\_script.R”

**justifyData integration:** Our model requires pairs of observations, consisting of individual plant traits,  $y_i$ , and the temperature corresponding to the plot  $T_\Delta$ . There are two immediate problems: (i) The CRU temperature data does not come with plot labels; (ii) We need an average environmental temperature, not necessarily the monthly average temperature available in the CRU dataset. The CRU data is gridded: the region of interest is divided into cells whose centres are  $0.5^\circ$  apart, starting at  $-179.75^\circ\text{N}, -89.75^\circ\text{E}$  and ending at  $179.75^\circ\text{N}, 89.75^\circ\text{E}$ . Each file (apart from its header rows) gives the temperature (or precipitation) for a specific month, at a matrix of geographical locations. Thus, to determine the monthly temperature for a given plot, we must load that month’s temperature data into a matrix, convert the row and column indices into longitude and latitude, and look up the coordinates of a particular plot. **justifyData Transformation:** The original format of the Tundra dataset had one row for each observation of an individual plant, in which each possible measurement was represented by a column. However, since most observations

only include a subset of the possible measurements, there were many missing values in this format. So the table has been changed from “wide” to “tall” format: missing measurements are now simply not represented.<sup>12</sup>

<sup>12</sup>This was done following “TTT\_data\_cleaning\_script.R”

**\justifyCanonicalization:** there was an underlying cell entity resolution problem in the dataset where the same plants were recorded with different name variations (including typos). It was necessary to group the rows referring to the same plants and to provide a unique identifier for each plant (“AccSpeciesName” column). **\justifyMissing Data:** For some entries in the Tundra dataset, a temperature measurement is not available. There were two sources of missing data (1) the geographical location or the year of observation were not recorded for a specific measurement, and as such, a temperature value could not be extracted during the data integration and (b) a temperature value for a specific geographical location and year of observation was not available in the “CRU Time Series” dataset.

In both cases, the value in the matrix is replaced by a code meaning “missing”. The meta-data header rows in each file specify the value of disguised missing (−9999.999). However, the value that is actually used in the data is not the one given; it is −10000.0.

**\justifyAnomaly Detection:** There is significant identification and removal of “anomalous” data in this task. Some of it was done by the sTUNDRA team before releasing the dataset; additional filtering was done for the journal article. We have used the initial filtering exactly as given<sup>13</sup>

<sup>13</sup>provided by “TTT\_data\_cleaning\_script.R”

but our secondary filtering may be slightly different from the authors’.

Both kinds of filtering are described in the *Methods* section of [2] and both follow a similar strategy: (i) group the observations by a certain taxon (which may be species, genus, site, or particular interactions of these); (ii) choose a threshold “error risk” (multiples of the standard deviation of a trait within the taxon); (iii) remove observations further from the mean of the taxon than the threshold “error risk”. (For certain taxon, the threshold error risk depends on the count of observations.) For example, observations more than  $8\sigma$  from the mean of all observations of a particular trait are excluded (unless the trait is plant height or leaf area).

Presumably, these tactics reflect domain knowledge about how datasets like these become corrupted (for example, perhaps incorrect assumptions about units are common), although a principled strategy is not clear. **\justifyFeature Engineering:** All covariates were “centred” by subtracting their species mean.

#### 5.1.4 Modelling

After this preliminary clean-up, the analyst has a dataset of 66308 observations covering 18 traits and 528 species. For the specific challenge addressed in [2], the authors perform additional filtering, mostly to remove observations that would otherwise be difficult to integrate into the modelling.

We note that the line between “wrangling” and “analysis” is becoming rather blurred at this stage. In particular, one could imagine a modelling approach that allowed certain observations to have missing components, whilst using the data in the other components. We followed [2] by:

1. Removing all observations without a geographical location (latitude and longitude), year of observation or temperature data;
2. Removing all observations for species present in strictly fewer than four observation sites;
3. Removing all sites with fewer than 10 observations;
4. Removing species without a sufficient temperature span in their observations, where “sufficient” is defined by “those species for which traits had been measured in at least four unique locations spanning a temperature range of at least 10% of the entire temperature range.”

In this analysis, we used a modified version of the hierarchical model described in [2], with some changes in the notation. Let  $\Sigma$  range over species,  $\Delta$  range over plots, and let individual observations be identified by  $i$ . We use the following hierarchical model of the relationship between the measurement of a plant trait,  $y$ , and temperature,  $T$ :

$$\begin{aligned}\log y_i(T) \mid \Sigma, \Delta &\sim \text{Normal}(\alpha_\Sigma + \beta_\Sigma T_\Delta, \sigma) \\ \alpha_\Sigma &\sim \text{Normal}(\mu_A, \sigma_A), \beta_\Sigma \sim \text{Normal}(\mu_B, \sigma_B)\end{aligned}$$

with parameters  $\alpha_\Sigma$ ,  $\beta_\Sigma$  and  $\sigma$  and hyperparameters  $\mu_A$ ,  $\mu_B$ ,  $\sigma_A$  and  $\sigma_B$ , to be inferred from the data.

Different Bayesian models can now be fitted to the data, the analyst used Stan<sup>14</sup>

<sup>14</sup><https://mc-stan.org/>

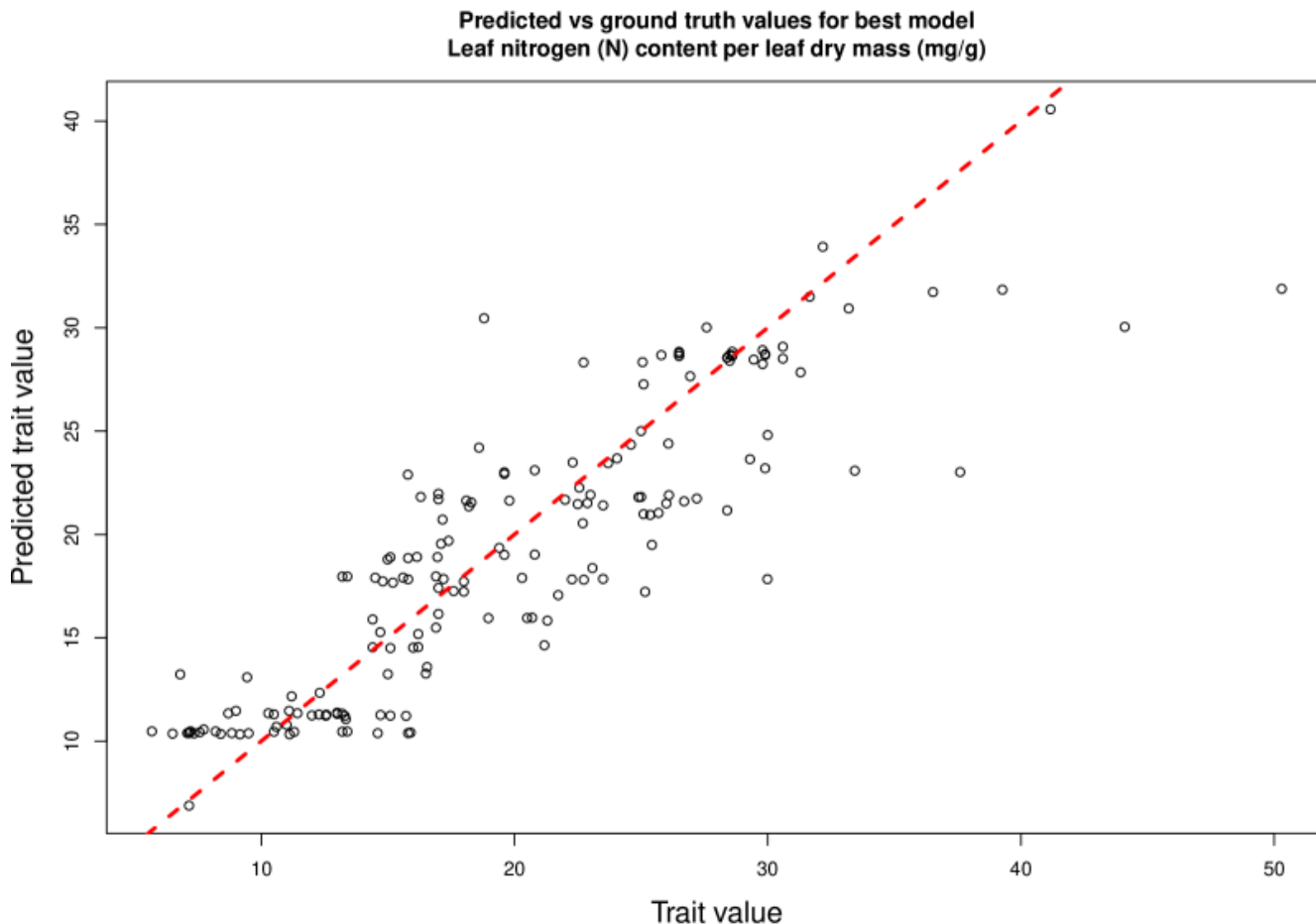
to perform this step. A variety of goodness of fit and convergence tests were performed: examination of paired plots, of trace plots, density sampled estimates vs original data, leave one out checks. The model described above was found to perform best among alternatives, as established by its  $R^2$  (coefficient of determination) calculated over the test set of 0.75.



**Results:** This model can be evaluated using goodness of fit diagnostics and held-out data. We split our dataset in two: train (80% of the total observations) and test (20% of the total) and assess the model by predicting trait values on the test set. For every data point of the test data, which consists of a species and a temperature for a given trait, 1000 parameter values were sampled from the fitted model sampling chains. These values were used to produce 1000 trait estimates as per the model described above. The mean trait value from these estimates was then taken as the prediction, and compared to ground truth.

Figure 1 shows how observations sampled from the fitted model for “Leaf nitrogen (N) content per leaf dry mass” capture at least part of the effects of temperature. The model is partially accurate in predicting trait values given site temperature and species. We omit the precipitation data, although the wrangling and modelling phases are identical and can be accomplished with no modifications to the code besides a change in the CRU dataset in use.

Figure 1: Trait “Leaf nitrogen (N) content per leaf dry mass (mg/g)” true observations compared with predicted observations from the test set. The ideal actual-predicted line is shown in red.



## 5.2 Household Electricity Survey

The Household Electricity Survey 2010–2011 (Department of Energy and Climate Change 2016), a study commissioned by the UK government, collected detailed time-series measurements of the electrical energy consumption of individual appliances across around 200 households in England. The data from that study are available from the UK Data Archive (UKDA, but only on application); an overview is publicly available from the government’s website [3].

The available data from the archive are not the raw measurements but have instead been “cleaned” by Cambridge Architectural Research Ltd (CAR). Fortunately, CAR have also provided a report describing the process of data cleaning that they undertook. In the following, we are reporting the relevant information from the provided documentation.

All households (all owner-occupied) were monitored from 2010 to 2011. Periodic measurements were taken of the power consumption of all electrical appliances in each household. The majority of households were monitored for a single month. The power drawn by appliances in these households was recorded every two-minutes. The remaining households were monitored for a full year, with measurements made every 10 minutes (every two minutes in some cases). Finally, the study also collected qualitative “diaries” from each household, in which the occupants recorded how they used each appliance. We have not made any use of these diaries here.

Within the data are three primary entities:

- *Households*: one of the 250 residences for which monitoring took place.
- *Appliances*: an electrical appliance that was monitored.
- *Profiles*: electricity load profile, where the power usage from a given appliance or group of appliances is measured at regular intervals.

The dataset consists of 36 CSV files, spread across 11 directories. For our purposes we will group 6 of these directories into one, called `appgroupdata`. The directories are then as follows:

- `small`: Metadata about appliances.
- `originalhes`: Unmodified version of the HES dataset.
- `experianhes`: Files created by Experian that give a consumer classification for each household.
- `appdata`: One file containing metadata relating to the monitored appliances.

- **anonhes:** Anonymized HES files containing demographic information and metadata about the houses.
- **appgroupdata:** Files containing the profile information for each appliance that was monitored.

There are several encodings (or keys) that appear across tables, and are necessary for combining information from multiple tables (joining the tables). These are:

- **household id:** a number that corresponds to a specific household for which monitoring took place.
- **appliance code:** a number that corresponds to a specific type of appliance (e.g., 182 -> trouser press).
- **appliance type code:** a number that corresponds to a group of appliances (e.g., 0 -> Cold Appliances).
- **interval id:** a number that refers to the type of monitoring that occurred for a given appliance (e.g., 1 -> for one month at two minute intervals).

There are some other encodings, but the four described above appear most frequently across the tables. The “important files” (defined as so by Cambridge Architectural Research in their report) are as follows: `appliance_codes.csv`, `appliance_type_codes.csv`, `appliance_types.csv`, `total_profiles.csv`, `appliance_data.csv`, `rdsap_public_anon.csv`, `ipsosanonymizedcorrected_310713.csv`, and the folder `appgroupdata` containing 6 CSV files with the profile information of each appliance.

### 5.2.1 Analytical Challenge

The dataset can be used to investigate disaggregation models, where the signal with the overall electricity consumption is used to estimate the consumption from component appliances. [56] provides an approach to the full disaggregation problem using a hidden Markov model. Since the focus of the present analysis is data wrangling, this task is overly involved for our purposes. Instead, the analyst attempted to solve a simpler problem. The different appliances in the HES data are categorised into “Appliance Groups”. Examples of appliance groups are “heating”, “audiovisual” and “cold appliances”. There are 13 such groups in total. The analyst attempted to predict the consumption of a given household in each of these appliance groups over a whole day (instead of at 2 or 10 minute intervals), based on the household information, the day and month of the observation and the total electricity consumption for that day.

### 5.2.2 Pipeline of data engineering steps

1. Loading the necessary recording files information:
  - Parsing the csv files (DP)
  - Selecting the necessary files among all folders (DD)
  - Adding header names to the profile data (DD)
  - Removing white spaces from header names (CA)
2. Record linkage where we add the appliance type code of each appliance into the profile information (DI). This appliance type code is referred as “GroupCode” in the different files.
  - Three files are linked: “appliance\_type\_codes.csv”, “appliance\_types.csv” and the profile data.
  - “appliance\_type\_codes.csv” contains “GroupCode” and “Name”, “appliance\_types.csv” contains “ApplianceCode” and “GroupCode”, and the profile data contains the “ApplianceCode” for each measurement.
  - First, each “ApplianceCode” is linked to a “Name” using the “GroupCode” as primary key.
  - Two names for “GroupCode” are “Other” and “Unknown”, so every “ApplianceCode” related to one of these appliances groups is removed (MD).
  - Lastly, each measurement in the profile data is linked to a “GroupCode”, using “ApplianceCode” as the primary key. Notice that, by removing the “ApplianceCode” linked to “Other” and “Unknown”, in the final integrated data, those “GroupCode” missing values are now stardardized to “NaN”.
3. After the DI step, we remove all rows that contain missing values in the “GroupCode” feature (DT + MD). These values correspond to temperature readings instead of power consumption readings.
4. Loading the demographic data (DP) and selecting only a subset of ten features from the data (DD + DT).

5. Now, different data wrangling challenges are tackled in the demographic data, to obtain a cleaner version:

- From “HouseholdOccupancy”, transform any “6+” code into “6” (CA).
- Create “PensionerOnly” indicator feature using “SinglePensioner” and “MultiplePensioner” (FE).
- Remove redundant features (DT).
- “Social.Grade” is an ordinal feature (e.g. A, B, C1, etc) where each category is transformed into an ordered numerical value and the only missing entry is replaced with the mode of the feature (FE + MD).
- “House.age” is transformed from a year interval (e.g. 1930-1949) into a numerical value, using the difference between the year where the measurements were taken (2010) and the middle value of the interval (FE).
  - “-1” indicates unknown, so these values are replaced with the mode of the feature (MD).
  - “2007 onwards” was encoded as “3” (2010 - 2007).

6. Creation of data  $X$  and target  $y$  variables:

- The target  $y$  is the aggregate power consumption per “groupCode” for each household and date (FE+DT).
- The data  $X$  is created through a two step process:
  - Aggregate the total consumption for each household and date (DT).
  - Link the demographic data into this aggregate data using the Household ID as primary key (DI).

7. Feature engineering processes done on both  $X$  and  $y$ :

- In  $X$ , the month and day of the week are extracted from the date, creating 2 new features: “month”, a number between 1 and 12 and “day of the week”, a one-hot encoded variable with 7 categories (FE).
- Three Fourier components are created based on the month of the recording for each household and date (FE). Afterwards, “month” is removed (DT).
- For the target, a standard  $\log(1 + x)$  transformation for non-negative target variables is applied for each “GroupCode” power consumption feature (FE).
- Numerical features are scaled (both in  $X$  and  $y$ ), dividing them by the difference between their min and max values (FE).

### 5.2.3 Data Engineering Issues

It is worth noting that many more wrangling challenges are described in the user guide for this dataset. It appears that the wrangling described in the user guide has been carried out already, so that the version available for download from UKDA has been pre-processed.

**\justifyData Dictionary:** The tables in this dataset form a rich relational structure that must be inferred by inspection of the files and using the documentation. It is sometimes unclear what the meaning of a given field is, or even the purpose of a sometimes redundant table. Example of the former: the Index column in the `monitered_appl.csv` file. Example of the latter: `appliance_attributes.csv` is actually redundant but this is not obvious immediately. Presently, this wrangling challenge is solved by spending a substantial amount of time inspecting the data, possibly missing relevant information in the process.

**\justifyData Integration:** In many of the tables, fields that are in fact referring to the same information are given different names. This makes the task of joining tables difficult. For example, the household identifier is sometimes given field name Household (e.g., in `appliance_data.csv`), but on other occasions is referred to as Clt Ref (e.g., in `rdsap_glazing_details_anon.csv`). This is an example of a key identification problem during record linkage. This challenge is again solved manually by the analyst, with the obvious costs and risks of introducing errors. An automated agent inspecting whether two columns might actually contain values from the same domain would greatly ease this inspection (primary key - foreign key matcher).

**\justifyData Transformation:** Subsets of observations in the dataset were manually identified and removed due to different problems. For example, some of the rows in the monitoring data did not correspond to electricity readings, but instead outdoor temperature measurements.

**\justifyCanonicalization:** Many examples of this problem exist in the data. For example, the Refrigerator\_volume column in `appliance_data.csv` does not have an explicit unit specified in the field name. Different entries specify different units (e.g. litres, cubic feet or no unit specified), which can themselves be written in different ways (e.g. "Litres", "L").

Another canonicalization problem is related with some columns expected to be numeric that are not so. For example Win Area in `rdsap_glazing_details_anon.csv` is not numeric because windows with area greater than 10 (the unit is not specified) have values "10+". To use this column, therefore, one would have to modify the entries that are "10+". The same problem appeared in the HouseholdOccupancy column, which was encoded as a string, and households with six or more tenants were encoded as "6+". To use this as a numerical feature, the column was cast to integer type and set "6+" to "6".

The analyst here acted on a case-by-case basis, often introducing ad-hoc rules to uniform variable names, unit of measures, as well as transforming the data as needed.

**\justifyMissing Data:** Missing entries appear in multiple tables.

Example: `ipsos-anonymized-corrected_310713.csv` has some missing entries in the survey question fields. The various diary files also have a reasonable fraction of missing values. Also, the encodings of the missing values vary across files and, more importantly, within the same attribute. For example, in the table `diary_dish_washer.csv`, the



Options column can take values NULL, N/A or N/a, all of which mean that data is not available.

The analyst here acted on a case-by-case basis. For example, the `Social.grade` column contained a single missing value, which was imputed with the most common value in the remaining rows. In the monitoring data, there was a significant number of day/house combinations for which the aggregated consumption for a given appliance group was zero. It remains unclear whether this should be considered as a genuine reading, or treated instead as missing or bad data. This was the biggest wrangling challenge for the present use case. **justify Feature Engineering:** the following original features were used during the analysis:

- `TotalUsage`: the total electricity consumption of a household on a given day.
- `HouseholdOccupancy`: the number of people living in the house.
- `HouseholdWithChildren`: a binary indicator, set to '1' if any children live in the house.
- `Social.grade`: the "social grade" of the individuals living in the house.
- Day of the week of the observation, one-hot-encoded.
- Month of the year.

Two features were added after performing some feature engineering to put them into a proper format for our model:

1. There was redundant information in the demographics table. The analyst created the `PensionerOnly` feature, and removed columns that contained information already present in other columns.
2. `House.age` was encoded as a string, e.g. "1950-1966". To encode this as a numerical feature, the difference between the midpoint of the range and 2007 was taken. There was a single missing value in this column, which was set to "-1". This was manually identified and imputed with the most common age range in the column.

#### 5.2.4 Modelling

The analyst then turned to the analytical challenge as follows. A baseline linear model performed poorly. Upon further inspection, this was found to be because a significant fraction of the electricity readings in each appliance group were zero: a linear model struggled to model these data. It is unclear whether the readings of zero are problems with data or correct measurements. Additionally, for some appliance groups, the frequency of zero readings was sufficiently high that the analyst simply dropped the appliance group, resulting in only 7 categories being predicted.

Afterwards, for each appliance group, the analyst modelled the consumption as follows:

1. Classify the house/day combination as “zero” or “not zero”, using a random forest classifier.
2. For the combinations classified as “not zero”, use a linear regression to predict the actual consumption.

This approach worked more effectively than the original approach (linear regression only). Additionally, we used the following approach for each appliance group as a baseline:

1. For each house/day combination in the holdout set, draw a binary indicator from a binomial distribution with parameter  $p$  set to the fraction of non-zero readings for this appliance group in the training set.
2. For house/day combinations where the binary indicator is 0, set the predicted consumption to zero.
3. For house/day combinations where the binary indicator is 1, set the predicted consumption to the mean consumption of non-zero readings in the training set.

The comparison of the baseline to the model is shown in Table 4. The model produces a smaller mean absolute error than the baseline for each appliance group, but is not a particularly good fit to the data.

Table 4: Comparison of baseline with model predicted energy consumption of appliance types. Overall, there were 1 546 data points.

Appliance Group	Baseline MAE	Model MAE
Showers	0.150	0.187
Heating	0.124	0.116
Water heating	0.098	0.111
Washing/drying/dishwasher	0.374	0.237
Audiovisual	0.407	0.228
Cooking	0.103	0.078
Cold appliances	0.070	0.061
Overall	<b>0.189</b>	<b>0.145</b>

### 5.3 Critical Care Health Informatics Collaborative

The CleanEHR anonymized and public dataset can be requested online. It contains records for 1978 patients (one record each) who died at a hospital (or in some cases arrived dead), with 263 fields, including 154 longitudinal fields (time-series). These fields cover patient

demographics, physiology, laboratory, and medication information for each patient/record, recorded in intensive care units across several NHS trusts in England. The full dataset, available only to selected researchers, contains 22,628 admissions from 2014 to 2016, with about 119 million data points. The dataset comes as an R data object, which can be most profitably accessed with an accompanying R package <sup>15</sup>

<sup>15</sup>Information on how to get the dataset and an introduction to it can be found in here: [https://cran.r-project.org/web/packages/cleanEHR/vignettes/cchic\\_overview.html](https://cran.r-project.org/web/packages/cleanEHR/vignettes/cchic_overview.html). The R package is available at <https://github.com/ropensci/cleanEHR>. There is also a blog post on how to use it: [https://ropensci.github.io/cleanEHR/data\\_clean.html](https://ropensci.github.io/cleanEHR/data_clean.html). A detailed explanation of each field is found in <https://github.com/ropensci/cleanEHR/wiki> under Data-set-1.0 and CCHIC-Data-Fields

We consider the dataset called ‘anon\_public\_d’ containing 1978 patient episodes. It is anonymized and only contains fatal outcomes. Some examples of the non time-series fields (demographic) found in the dataset are ADNO (Critical care local identifier), HCM (Height) and RAICU1 (Primary reason for admission to your unit). The longitudinal fields are time-series variables, that correspond to physiological/nursing measurements, laboratory tests results and drugs administered to the patient during their stay. Some examples are mean arterial blood pressure (Physiology), sodium (Laboratory) and adrenaline (Drugs).

### 5.3.1 Analytical Challenge

The analytical challenge we first set ourselves is to predict the amount of time it takes for a patient to die (in minutes), after they arrived at the hospital alive. Unfortunately, the proposed model fitted the data poorly, so we decided to shift the analysis into predicting which patients die in the first 100 hours from admission to the unit.

### 5.3.2 Pipeline of data engineering steps

1. First the analyst loads both CSVs for the demographic data and the time series statistics data (DD) and creates an extended table with the features of both tables using “ADNO” as primary key (DT).

2. Data transformations and feature engineering steps are done to the data with the analytical task in mind.
  - Remove all rows where the date of death, time of death or date of access to the ICU were not recorded (DT + MD).
  - Remove features fully missing in the data (MD).
  - Standardize dates and times into the same format (CA), creating a numerical variable based on those dates (FE).
  - A “survival class” variable is created, where patients are divided into two groups according to whether they survived for more or less than 100 hours.
  - All patients who died before arriving at the ICU were removed from the analysis (DT).
3. Creation of a numerical age feature based on other features in the data (FE).
4. Categorical variables are transformed into one-hot variables (FE). In particular, “RAICU1”, “RAICU2” and “OPCHM” features are simplified, and only the first two components are used (e.g. 2.1.2  $\rightarrow$  2.1)
5. Further rows and features were removed from the data according to different criteria (DT).
  - All patients that didn’t live for for than 10 hours were removed from the study (DT).
  - Previous versions of transformed features were removed.
  - Other variables were removed because they were heavily correlated to the target variable. For example, “CCL3D” recorded the number of days the patient was in the ICU. Other variables recorded the number of days the patients were under any type of support system. These variables disclose information about the number of days that the patients were alive, so they were removed from the analysis.
6. Missing data (MD): a) Features with more than 50% of their values missing were deleted. b) For the remaining features, missing values were replaced by “-1”.

### 5.3.3 Data Engineering Issues

There was a previous integration process done before getting access to the data we are employing in our analysis. The data coming from eleven adult ICUs at five UK teaching hospitals is passed through a pipeline that extracts, links, normalizes and anonymizes the EHR data. The resulting data is then processed using the cleanEHR toolkit, covering the most common processing and cleaning operations for this type of data (see above). Some of the most important functions in the cleanEHR package converts the various asynchro-

nous lists of time-dependent measurements into a table of measurements with a customizable binning. A second function is used to join together separate but sequential critical care admissions into a unified illness spell [57]. **\justifyData Dictionary:** The analyst started by attempting to understand the available data fields, whose contents are highly domain-specific and for which documentation is limited. Column names like DOB, WKG, HDIS or DOD were not readily understood by the data scientist. A matching process of each feature name in the dataset and a website containing the descriptions and information of the different features was necessary to understand the data.<sup>16</sup>

<sup>16</sup><https://github.com/ropensci/cleanEHR/wiki> under Data-set-1.0 and CCHIC-Data-Fields

**\justifyData Integration:** the analyst loaded the two datasets (the demographics and the time-series analysis) and linked them into a single extended table using the ADNO (admission number) field. Since the primary key (ADNO) was present in both tables, the mapping was done directly by adding the features in the time-series table to the demographics table. **\justifyData Transformation:** after the DI process, it was necessary to remove rows in the data according to two criteria: a) all rows without date and time of admission or death were removed, as their absence makes the predictive task impossible and b) all patients admitted dead (i.e. whose elapsed time to death is zero or negative) were removed. **\justifyCanonicalization:** Several fields are not standardized. For example, datetimes show a variety of encodings being used, such as: ‘1970-01-01T00:01:00’, ‘1970-01-01’ and ‘00:01:00’ (i.e. datetime, date and time). The analyst had to deal with these issues case-by-case. **\justifyMissing Data:** Several fields contain missing values. This is to be expected since many measurements are only performed in case of medical necessity. Unfortunately, an added challenge is that the analyst is never sure if a value is missing due to the measurement not being performed or due to other reasons. We expect the former case to be the most common, yet we do not know in practice.

Intuitively, NaN values usually entail a lack of observation due to a measurement deemed not important for the patient/condition at hand. Thus, it was decided to drop all columns containing more than 50% of NaN values (including some completely empty columns). The remaining NaN values were imputed with -1 to have a clear indication that this particular value was not necessary or unobserved (the default value of 0 was first considered, however there are fields where zero can be the result of a measurement). A more detailed analysis of missing values and of different imputation strategies might improve results. **\justifyNon-Stationarity:** while exploring the data the data scientists noticed that consecutive patients could be grouped under different groups according to the properties of some of the attributes. For example, when looking at HCM (height of the patients), the patients with IDs between 800-1300 had their height measured in metres, while the rest of the patients had their height measured in centimetres. According to the documentation, this attribute should have been recorded in centimetres, so a proper transformation from metres to centimetres for this attribute was necessary (related to canonicalization). We are aware that most of this non-stationarity problems are related to the preliminary integration script provided by the dataset. **\justifyFeature Engineering:** The analyst performed



the following set of operations in sequence:

- 1) Export date-times from all datetime columns, using a variety of string representations ('1970-01-01T00:01:00', '1970-01-01' and '00:01:00'. This format variability operation was performed by defining a set of rules that transformed all datetime strings into datetime Python objects (which internally abide to ISO standards).
- 2) Calculate the elapsed time to death (prediction target or dependent variable) by subtracting the time of admission from the time of death.
- 3) Calculate the age from birth and admission dates.
- 4) Transform the taxonomies used for diagnoses into dummy one-hot encoded variables ('RAICU1', 'RAICU2' and 'OCPMH' above).
- 5) Create dummy one-hot encoded variables for all remaining categorical variables.
- 6) Extract relevant statistics from time-series data. These were the mean, standard deviation, and last value measured (but more variables could be used in the future).
- 7) Drop unnecessary columns (either judged as not predictive or duplicated with dummy variables).
- 8) Drop columns that can leak the time of death (e.g. number of days on the ICU 'CCL3D'), this is a challenging step since it is not always clear when the data was recoded.

### 5.3.4 Modelling

Here it is important not to include variables that can leak asynchronous information from the target (time to death). For example, using the full time-series data from the patient to build the descriptive variables would be misleading, because in a real predictive scenario this corresponds to future information that will not be available. Taking this into consideration, only the first 10 hours of time-series data was used to build the model, and predictions are done only in patients that have lived at least those 10 hours. These choices were made in order to include as much of the data as possible, without making the model overly complex.

Two datasets were obtained from the previous wrangling steps. A first sample containing only the demographic variables and a second one with both demographic and time-series information. The sample containing both demographic and time-series data only has patients that lived at least 10 hours. The demographic only sample has all patients that arrived alive to the unit. After the data wrangling process, the demographic-only sample had 176 variables for 1730 patients. The demographic plus time-series data had 373 variables corresponding to 1586 patients. Both samples are divided in training and testing samples with a ratio of 80/20 and two models are built based on the datasets. A linear regression model with ElasticNet regularization (joint L1 and L2) [58] was implemented to predict the time (in minutes) elapsed from admission to death. However, no suitable model was found. The regression model fits the data poorly, reporting an R-squared value of 3% for the demographics only sample and 7% for the full dataset.

The analysis focus was shifted to predict which patients die in the first 100 hours from admission to the unit. Random Forests [59] were used for classification. Both samples are

split into two classes: patients that died in the first 100 hours and patients that survived for 100 hours. For the demographic-only sample 51% of the patients correspond to the first class (and 49% to the second). The demographic plus time-series sample is divided in 47% and 53% for the first and second class, respectively.

The sample with demographic-only data achieves an average classification accuracy of 53%, which is barely better than the classification baseline of predicting the most frequent class (51% based on the class balance for this sample). This result hints that this sample might not contain enough information to accurately classify patients that die in the first 100 hours from admission (see Table 5). The classification accuracy obtained by using the demographic plus time-series data (where all patients survived at least 10 hours and their previous time-series data is used in the model) is shown in Table 6. The average accuracy for this sample value is of 66%, which is a significant improvement compared to the demographic-only sample and the classification baseline of predicting the most frequent class (53%). This result shows that the time-varying fields bring important information to the system, which can be of great use in the training of a more sophisticated survival model in the future. One of the main challenges of this analysis is to know how and when some of the demographic variables are measured or computed. For example, the apache score or AMUAI variables are good predictive features but they can be asynchronous to the information available up to 10 hours after admission. In this model those features are not used, but they might be useful to increase the performance or build a more sophisticated model.

Table 5: Confusion matrix of classification of time of death within the first 100 hours from admission (demographic only sample).

Time of death (%)	< 100 hours (Pred.)	> 100 hours (Pred.)
< 100 hours (True)	0.38	0.62
> 100 hours (True)	0.30	0.70

Table 6: Confusion matrix of classification of time of death within the first 100 hours from admission (demographic plus timeseries sample).

Time of death (%)	< 100 hours (Pred.)	> 100 hours (Pred.)
< 100 hours (True)	0.75	0.25
> 100 hours (True)	0.33	0.67

## 5.4 Ofcom Consumer Broadband Performance

The UK's Office of Communications (Ofcom) conducts an annual survey of the performance of residential fixed-line broadband services<sup>17</sup>

<sup>17</sup><https://data.gov.uk/dataset/uk-fixed-line-broadband-performance>

. These data are published as a table in annual instalments: a new spreadsheet each year containing that year's data. Each row of this table corresponds to a recruited broadband user panellist. There are 1 450 rows in the 2013 dataset, 1 971 rows in the 2014 data, and 2 802 rows in the 2015 data.

### 5.4.1 Analytical Challenge

There isn't a natural challenge accompanying this data. We chose the following simplistic challenge: fit a simple model to detect whether a broadband speed corresponds to an urban or rural area based on several features from the data. We will use the annual installments from 2014 and 2015 to train our model and the installment from 2016 to test it.

### 5.4.2 Pipeline of data engineering steps

1) There are two installments from 2014 (May and November), one from 2015 and another from 2016 that needs to be loaded (DP). Some of these tables have notes at the beginning of the csv, so we need to carefully select the part of the csv that corresponds to the data.

2) Every table has different features and different names for the same features. We rename those features into a standard naming and identify the correct features (DD). Since only 6 features were deemed necessary to the analysis, we only rename those and delete the rest from the tables (DT).

3) Installments from 2014 and 2015 are concatenated into the same table (DI).

- The feature indicating whether a broadband device is in an urban or rural area changes between 2014 and 2015. A protocol change occurred in 2015, where they introduced the term "Semi-Urban" to indicate an area that is in between urban and rural (NS). The analyst decided to encode "Semi-Urban" instances as "Rural", since there were fewer instances of "Rural" in the data.

- There are several duplicates across 2014 and 2015, since some devices were measured several times at different months. The analyst decided to keep the records from the most recent measurements, removing the rest of the duplicates (DI, deduplication).

4) The analyst removed from the test set (2016) any broadband devices included both in the training and test set, using the "Id" of the device (DI).

5) Since the amount of missing data across features was less than 1%, the analyst decided to remove entries with missing values, to avoid biasing the model later (MD).

6) Training and test datasets were prepared (FE):

- The “Urban/Rural” feature was recoded, assigning 0 to rural and semi-urban areas and 1 to urban areas (FE).
- The “Id” feature was deemed unnecessary and removed from the data (DT).
- Real features were standardized (FE).

### 5.4.3 Data Engineering Issues

**Data Parsing:** Some of the CSV files contained notes in the first lines of the headers, and automatic parsing failed. The analyst needed to explore the files and identify the positions of the tables in the files to load the data properly. **justifyData Dictionary:** The columns in the data describe characteristics of the geographical region (such as whether it is rural or urban); the nature of the broadband service (for example, the provider); and measured characteristics of the broadband service (for example, the average download speed). There are roughly five fields describing properties of the region; three fields describing the service; and around 20 fields describing measured characteristics. As is often the case, this dataset is not in “normal form” but instead can usefully be thought of as a relational join of multiple tables. It is left to the analyst to determine the schema. **justifyData Integration:** Since the data comes in annual installments, it was necessary to aggregate all the tables into an extended table. Unfortunately, a common schema for the features employed during the data collection was not present, so the analysts needed to match corresponding features across tables together and do the integration manually. Some challenges they needed to address were:

1. Reaming columns to a standard name
2. Ordering columns across tables.
3. Not all features appeared in all installments.
4. Recoding some categorical features, so as to use the same encoding in all installments (CA).

Additionally, it was necessary to remove duplicate devices measured across different installments. **justifyMissing Data:** There were some features with missing data across installments. The analyst needed to check every feature and treat the missing data accordingly. In this case, since the missing values were less than 1% per feature, instances with missing values were removed from the data.

### 5.4.4 Modelling

For this task, we are trying to detect whether a broadband measurement comes from an urban or rural area based on the download and upload speed of the broadband, the latency and the web pages loading speed. These features were recorded as an average of the speed during a period of 24 hours. We will make a comparison between different classi-

fiers for this specific task, training and validating the models with the data from 2014 and 2015, and testing the results in the 2016 data.

We compare the performance of Logistic Regression (LR), Naive Bayes (NB), SVM and Random Forests (RF). A grid search for the best set of hyperparameters for each model was performed, using cross-validation with 3 folds on the training set. Table 7 shows the precision, recall, F1 score and accuracy on the 2016 dataset for the classifiers trained on the 2014 and 2015 data. All the classifiers obtain similar results, with RF performing slightly better.

Table 7: Precision, recall, F1 score and accuracy for the different classifiers

Model	Precision	Recall	F1 score	Accuracy
NB	0.8031	0.8975	0.8477	0.7666
LR	0.7933	0.9347	0.8582	0.7764
SVM	0.7718	0.9578	0.8547	0.7644
RF	0.7822	0.9774	0.8686	0.7859

## 6 Conclusions

In this paper we have identified three high-level groups of data wrangling problems, those related with obtaining a proper representation of the data (data organization), those related to assessing and improving the quality of the data (data quality), and feature engineering issues, which heavily depend on the task at hand and the model employed to solve it. Furthermore, we have presented the full analysis of four use cases, where we have provided a systematic pipeline for each of the datasets to clean them while identifying and classifying the main problems the data scientists faced during the wrangling steps. We hope that this work helps to further explore and understand the field of data engineering, and to value a part of every data scientist's work that most of the time goes unnoticed both in research and industry. Additionally, we would like to encourage practitioners to provide their raw data and the scripts necessary to clean it in order to advance the field. In future work we would like to study data engineering workflows across multiple datasets in order to identify (if possible) common structures concerning the ordering of the various wrangling operations. We note that there can be feedback loops in the process, as described e.g. in [46].

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