Responsibility in the Data Science Lifecycle

Responsible Data Science
DS-UA 202 and DS-GA 1017

Instructors: Julia Stoyanovich and George Wood

This reader contains links to online materials and excerpts from selected articles on responsibility in the data science lifecycle. For convenience, the readings are organized by course week. Please note that some excerpts end in the middle of a section. Where that is the case, the partial section is not required reading.

Week 5: Responsible data management, data profiling, data cleaning

Responsible Data Management

Julia Stoyanovich
New York University
New York, NY, USA
stoyanovich@nyu.edu

Bill Howe
University of Washington
Seattle, WA, USA
billhowe@uw.edu

H.V. Jagadish
University of Michigan
Ann Arbor, MI, USA
jag@umich.edu

ABSTRACT

The need for responsible data management intensifies with the growing impact of data on society. One central locus of the societal impact of data are Automated Decision Systems (ADS), socio-legal-technical systems that are used broadly in industry, non-profits, and government. ADS process data about people, help make decisions that are consequential to people's lives, are designed with the stated goals of improving efficiency and promoting equitable access to opportunity, involve a combination of human and automated decision making, and are subject to auditing for legal compliance and to public disclosure. They may or may not use AI, and may or may not operate with a high degree of autonomy, but they rely heavily on data.

In this article, we argue that the data management community is uniquely positioned to lead the responsible design, development, use, and oversight of ADS. We outline a technical research agenda that requires that we step outside our comfort zone of engineering for efficiency and accuracy, to also incorporate reasoning about values and beliefs. This seems high-risk, but one of the upsides is being able to explain to our children what we do and why it matters.

PVLDB Reference Format:
Julia Stoyanovich, Bill Howe, H.V. Jagadish. Responsible Data Management. *PVLDB*, 13(12): 3474 - 3488, 2020.
DOI: https://doi.org/10.14778/3415478.3415570

1. INTRODUCTION

We are in the midst of a global trend to regulate algorithms, artificial intelligence, and automated decision systems. This flurry of activity hardly comes as a surprise. As reported by the recent One Hundred Year Study on Artificial Intelligence [58]: "AI technologies already pervade our lives. As they become a central force in society, the field is shifting from simply building systems that are intelligent to building intelligent systems that are human-aware and trustworthy." In the European Union, the General Data Protection Regulation (GDPR) [66] offers protections to individuals regarding the collection, processing, and movement of their personal data, and applies broadly to the use of such data by governments and private-sector entities. Regulatory activity in several countries outside of the EU, notably, Japan [48] and Brazil [32], is in close alignment with the GDPR.

In the US, many major cities, a handful of states, and even the Federal government are establishing task forces and issuing guidelines about responsible development and use of technology, often starting with its use in government itself——rather than in the private sector——where there is, at least in theory, less friction between organizational goals and societal values. Case in point: New York City rightfully prides itself on being a trendsetter—in architecture, fashion, the performing arts and, as of late, in its very publicly made commitment to opening the black box of the government's use of technology: In May 2018, an Automated Decision Systems (ADS) Task Force was convened, the first such in the nation, and charged with providing recommendations to New York City's agencies about becoming transparent and accountable in their use of ADS. The Task Force issued its report in November 2019, making a commitment to using ADS *where* they are beneficial, reducing potential harm across their lifespan, and promoting fairness, equity, accountability, and transparency in their use [5].

Can the principles of the responsible use of ADS — of *socio-legal-technical systems* that may or may not use AI, and may or may not operate with a high degree of autonomy, but that rely heavily on data — be operationalized as a matter of policy [2]? Can this be done in the face of a crisis of trust in government, which extends to the lack of trust in the government's ability to manage modern technology in the interest of the public [73]? What will it take to instill responsible ADS practices beyond government?

In this article, we hope to convince you that the data management community should play a central role in the responsible design, development, use, and oversight of ADS. By engaging in this work, we have a critical opportunity to help make society more equitable, inclusive, and just; make government operations more transparent and accountable; and encourage public participation in ADS design and oversight. To make progress, we may need to step outside our engineering comfort zone and start reasoning in terms of values and beliefs, in addition to checking results against known ground truths and optimizing for efficiency objectives. This seems high-risk, but one of the upsides is being able to explain to our children what we do and why it matters.

Proceedings of the VLDB Endowment, Vol. 13, No. 12
ISSN 2150-8097.
DOI: https://doi.org/10.14778/3415478.3415570

Outline. In the remainder of this paper, we will first illustrate the issues under discussion with an example from the domain of hiring and employment (Section 2). We will go on to position these issues, and possible solutions, within the broader context of bias, worldviews, and equality of opportunity frameworks (Section 4). Then, we will discuss recent technical work by us and others on embedding responsibility into data lifecycle management (Sections 5) and on interpretability of data and models for a range of stakeholders (Section 6). In the technical sections, we will point out specific opportunities for contributions by the data management community. We will conclude in Section 7.

2. AUTOMATED HIRING SYSTEMS

To make our discussion concrete, let us focus on hiring and employment. Since the 1990s, and increasingly so in the last decade, commercial tools are being used by companies large and small to hire more efficiently: source and screen candidates faster and with less paperwork, and successfully select candidates who will perform well on the job. These tools are also meant to improve efficiency for the job applicants, matching them with relevant positions, allowing them to apply with a click of a button, and facilitating the interview process. According to Jenny Yang, former Commissioner of the US Equal Employment Opportunity Commission (EEOC), "Automated hiring systems act as modern gatekeepers to economic opportunity. [...] Across industries, major employers including Unilever, Hilton, and Delta Air Lines are using data-driven, predictive hiring tools." [68]

The hiring funnel. Bogen and Rieke [9] describe the hiring process from the point of view of an employer as a series of decisions that form a funnel (Figure 1): "Employers start by *sourcing* candidates, attracting potential candidates to apply for open positions through advertisements, job postings, and individual outreach. Next, during the *screening* stage, employers assess candidates—both before and after those candidates apply—by analyzing their experience, skills, and characteristics. Through *interviewing* applicants, employers continue their assessment in a more direct, individualized fashion. During the *selection* step, employers make final hiring and compensation determinations."

The hiring funnel is an example of an ADS: a socio-legal-technical system operationalized as a sequence of data-driven, algorithm-assisted steps, in which a series of decisions culminates in job offers to some candidates and rejections to others. While potentially beneficial, the use of ADS in hiring is also raising concerns that pertain, broadly speaking, to the decisions made by these systems and to the process by which these decisions are made.

Discrimination. One set of concerns relates to *discrimination.* As pointed out by Bogen and Rieke [9], "The hiring process starts well before anyone submits an actual job application, and jobseekers can be disadvantaged or rejected at any stage. Importantly, while new hiring tools rarely make affirmative hiring decisions, they often automate rejections."

Because of how impactful hiring decisions are for individuals and population groups, and because of a history of discrimination, hiring practices are subject to antidiscrimination laws in many countries. In the US, Title VII of the Civil Rights Act of 1964 broadly prohibits hiring discrimination by employers and employment agencies on the basis of *protected characteristics* that include "race, color, religion, sex, and national origin." This law is supplemented by other federal laws that extend similar protections based on age and disability status, and by a patchwork of other federal, state, and local laws.

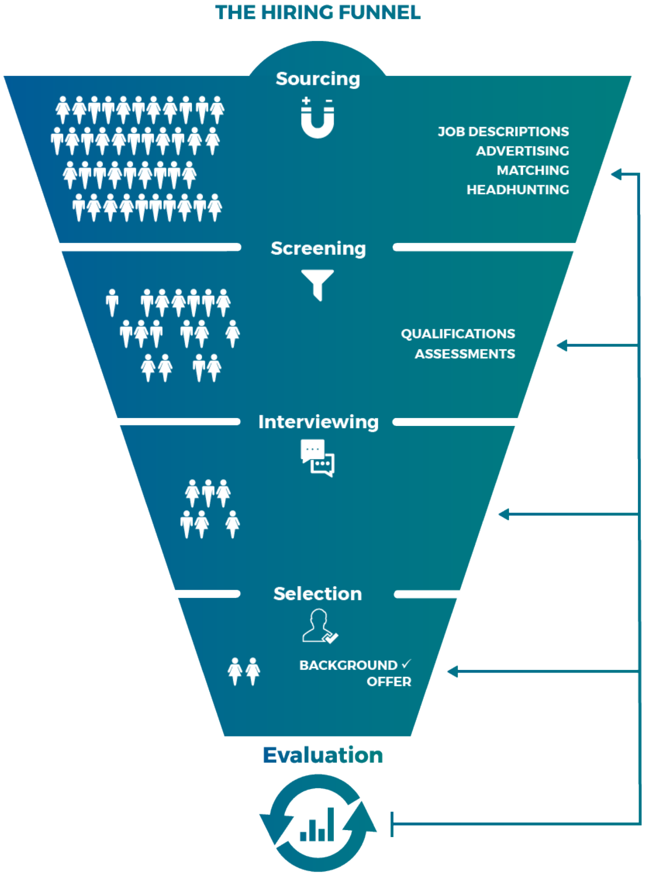


Figure 1: The hiring funnel, reproduced with permission from Bogen and Rieke [9], is an example of an Automated Decision System (ADS): a data-driven, algorithm-assisted process in which a series of decisions culminates in job offers to some applicants and rejections to others.

Are existing legal protections against discrimination sufficient today, when ADS are reshaping, streamlining, and scaling up hiring? Or is the use of ADS reviving and reinforcing historical discrimination, and giving rise to new forms of discrimination? Is discrimination going undetected, due, for example, to legal constraints on the types of demographic data that a potential employer can collected, or to applicants declining to disclose their demographic group membership? Can attempts to de-bias datasets and models be effective, or do they amount to *fairwashing*—covering up, and even legitimizing, discrimination with the help of technological solutions?

Due process. Another set of concerns relates to *due process*, also known as *procedural fairness* or *procedural regularity.* As explained by Kroll *et al.* [34]: "A baseline requirement in most contexts is procedural regularity: each participant will know that the same procedure was applied to her and that the procedure was not designed in a way that disadvantages her. This baseline requirement draws on the Fourteenth Amendment [to the US Constitution] principle of procedural due process. Ever since a seminal nineteenth century case, the [US] Supreme Court has articulated that procedural fairness or due process requires rules to be generally applicable and not designed for individual cases."

Notably, research demonstrates that, as long as a process is seen as fair, people will accept outcomes that may not benefit them. This finding is supported in numerous domains, including hiring and employment, legal dispute resolution and citizen reactions to police and political leaders, and it remains relevant when decisions are made with the assistance of algorithms [63].

Citron and Pasquale [12] discuss the need for due process safeguards in scoring systems: "The act of designating someone as a likely credit risk (or bad hire, or reckless driver) raises the cost of future financing (or work, or insurance rates), increasing the likelihood of eventual insolvency or un-employability. When scoring systems have the potential to take a life of their own, contributing to or creating the situation they claim merely to predict, it becomes a normative matter, requiring moral justification and rationale." Score-based selection and ranking are indeed in broad use at all stages of the hiring funnel, and can amount to self-fulfilling prophecy if left unchecked.

An immediate interpretation of due process for the hiring ADS is that the employer ought to be able to show that the same decision making procedure was used for all job candidates. Yet, simply stating that the same code was executed for everyone does not get to the heart of the issue, precisely because individuals and population groups may be represented differently in the data. For example, groups that are historically under-represented in the workforce will also be under-represented in the data record, which may in turn reduce generalizability of predictive models for those groups [11]. Further, values of a particular feature may be missing more frequently for one sub-population than for another (e.g., age may be unspecified for women more frequently than for men), also leading to disparate predictive accuracy. Finally, it has been documented that survey data can be noisier for minority groups than for others [28]. (Lehr and Ohm [36] give additional examples of the impact of data on discrimination and due process in machine learning.)

Feature selection. An important dimension of due process, closely linked to discrimination, is substantiating the use of particular features in decision-making. Regarding the use of predictive analytics to screen candidates, Yang [68] states: "Algorithmic screens do not fit neatly within our existing laws because algorithmic models aim to identify statistical relationships among variables in the data whether or not they are understood or job related.[...] Although algorithms can uncover job-related characteristics with strong predictive power, they can also identify correlations arising from statistical noise or undetected bias in the training data. Many of these models do not attempt to establish cause-and-effect relationships, creating a risk that employers may hire based on arbitrary and potentially biased correlations." That is, identifying features that are impacting a decision is important, but it is insufficient to alleviate due process and discrimination concerns. The employer should also show that these features are relevant for performance on the job.

An extreme case of feature selection gone wrong is when tools claim to predict job performance by analyzing an interview video for body language and speech patterns. In his recent talk, Arvind Narayanan refers to tools of this kind as "fundamentally dubious" and places them in the category of *AI snake oil* [44]. The premise of such tools, that (a) it is possible to predict social outcomes based on a person's appearance or demeanor and (b) it is ethically defensible to try, reeks of scientific racism and is at best an elaborate random number generator.

Even features that can legitimately be used for hiring may capture information differently for different individuals and groups. For example, it has been documented that the mean score of the math section of the SAT (Scholastic Assessment Test, used broadly in the US) differs across racial groups, as does the shape of the score distribution [50]. These disparities are often attributed to racial and class inequalities encountered early in life, and are thought to present persistent obstacles to upward mobility and opportunity.

Auditing and disclosure. Because of the wide-spread use of commercial ADS in hiring, and because of the discrimination and due process concerns they raise, there is a push to strengthen the accountability structure in this domain. The gist of most proposals is to develop new legal and regulatory mechanisms—and the supporting technical methods—to facilitate auditing of these systems and public disclosure.

For example, Yang [68] advocates that "A federal *explainability standard* that sets forth the parameters for what it means to explain an algorithm to different audiences (such as workers, employers, or technologists) would be valuable to ensure these considerations are built into the design of an algorithmic system from the outset." She also speaks to the importance of *the right to an explanation*—that "employers should explain the rationale for a decision in terms that a reasonable worker could understand. Standards could be established to include disclosure of the material variables considered and the types of inferences the algorithm is making to score the individuals."

As another example, New York City Commission on Technology is entertaining a bill "in relation to the sale of automated employment decision tools" that would require auditing such tools for bias and disclosing to the candidate the job qualifications or characteristics used for assessment [67].

3. WHAT IS AN ADS? AND WHY US?

We have been referring to Automated Decision Systems (ADS) throughout this paper. Yet, there is currently no consensus as to what is, and is not, an ADS. In fact, the need to define this term for the purpose of regulation has been the subject of much debate. As a representative case, Chapter 6 of the NYC ADS Task Force report [5] summarizes their months-long struggle to, somewhat ironically, define their own mandate—come up with a definition that is sufficiently broad to capture the important concerns discussed earlier in this section, yet sufficiently specific to be practically useful.

If an intentional definition is out of reach, we may attempt to define ADS by extension. An automated resume screening tool seems like a natural example of an ADS, as does a tool that matches job applicants with positions in which they are predicted to do well. But is a calculator an ADS? (No!) What about a formula in a spreadsheet? (Depends on what it's used for [23].)

The hiring funnel in Figure 1, *as well as each component of the funnel*, are ADS examples. These systems (1) process data about people, some of which may be sensitive or proprietary; (2) help make decisions that are consequential to people's lives and livelihoods; (3) are designed with the stated goals of improving efficiency and promoting, or at least not hindering, equitable access to opportunity; (4) involve a combination of human and automated decision making; and (5) are subject to auditing for legal compliance and, at least potentially, to public disclosure.

Central to this ADS definition is the placing of technical decision-making components—a spreadsheet formula, a matchmaking algorithm, or a predictive analytic—within *the lifecycle of data collection and analysis.* Much excellent work on algorithmic fairness and transparency goes on in the machine learning, data mining, and algorithms communities. Yet, a critical shortcoming of that work is their focus on the last mile of data analysis. In contrast, and precisely because of the importance of a lifecycle view of ADS, the data management community is uniquely positioned to deliver true practical impact in the responsible design, development, use, and oversight of these systems.

- Because data management technology offers a natural centralized point for enforcing policies, we can develop methodologies to transparently and explicitly enforce requirements through the ADS lifecycle.

- Because of the unique blend of theory and systems in our methodological toolkit, we can help inform regulation by studying the feasible trade-offs between different classes of legal and efficiency requirements.

- Because of our pragmatic approach, we can support compliance by developing standards for effective and efficient auditing and disclosure, and developing protocols for embedding these standards in systems.

Importantly, the ADS lifecycle discussed in this section is itself embedded within the societal context of ADS purpose and impacts. We elaborate on this point in the next section.

4. FRAMING TECHNICAL SOLUTIONS

Before diving into specific research directions, let us step back and think carefully about the role that technological interventions, such as data management solutions, can play in supporting the responsible use of ADS. This discussion is necessary to help us find a pragmatic middle ground between the harmful extremes of techno-optimism—a belief that technology can single-handedly fix deep-seated societal problems like structural discrimination in hiring, and techno-bashing—a belief that any attempt to operationalize ethics and legal compliance in ADS will amount to fairwashing and so should be dismissed outright.

4.1 Data: a Mirror Reflection of the World

We often hear that ADS, such as automated hiring systems, operate on biased data and result in biased outcomes. What is the meaning of the term "bias" in this context? Informally, data is a mirror reflection of the world. More often than not, this reflection is distorted. One reason for this may be that the mirror itself (the measurement process) is distorted: it faithfully reflects some portions of the world, while amplifying or diminishing others. Another reason may be that *even if* the mirror was perfect, it may be reflecting a distorted world — a world such as it is, and not as it could or should be. The mirror metaphor helps us make several simple but important observations, on which we will elaborate more formally (and less poetically) in Section 4.2.

1. *A reflection cannot know whether it is distorted.* Based on the reflection alone, and without knowledge about the properties of the mirror and of the world it reflects, we cannot know whether the reflection is distorted, and, if so, for what reason. That is, data alone cannot tell us whether it is a distorted reflection of a perfect world, a perfect reflection of a distorted world, or whether these distortions compound.

2. *Beauty is in the eye of the (human) beholder.* It is up to people — individuals, groups, and society at large — and not up to data or algorithms, to come to a consensus about whether the world is how it should be, or if it needs to be improved and, if so, how we should go about improving it.

3. *Changing the reflection does not change the world.* If the reflection itself is used to make important decisions, and we agree that it is distorted and explicitly state the assumed or verified nature of such distortions, then compensating for the distortions is worthwhile. But the mirror metaphor only takes us so far. We have to work much harder—usually going far beyond technological solutions—to propagate the changes back into the world, not merely brush up the reflection.

In their seminal 1996 paper, Friedman and Nissenbaum identified three types of bias that can arise in computer systems: pre-existing, technical, and emergent bias [19]. In the remainder of this section we will use this classification to structure our discussion on bias, worldviews, and mitigation strategies.

4.2 Pre-existing Bias

Pre-existing bias exists independently of an algorithm itself and has its origins in society. Often, the presence or absence of pre-existing bias cannot be scientifically verified, but rather is postulated based on a belief system. We already discussed that disparities in math SAT scores have been observed among ethnic groups [50]. If we believed that the test measures an individual's academic potential, we would not consider this an indication of pre-existing bias. If, on the other hand, we believed that standardized test scores are sufficiently impacted by preparation courses that the score itself says more about socio-economic conditions than an individual's academic potential, then we would consider the data to be biased.

Worldviews. Friedler *et al.* [18] reflect on the impossibility of a purely objective interpretation of algorithmic fairness (in the sense of a lack of bias): "In order to make fairness mathematically precise, we tease out the difference between beliefs and mechanisms to make clear what aspects of this debate are opinions and which choices and policies logically follow from those beliefs." They model the decision pipeline of a task as a sequence of mappings between three metric spaces: construct space (CS), observed space (OS), and decision space (DS), and define worldviews (belief systems) as assumptions about the properties of these mappings.

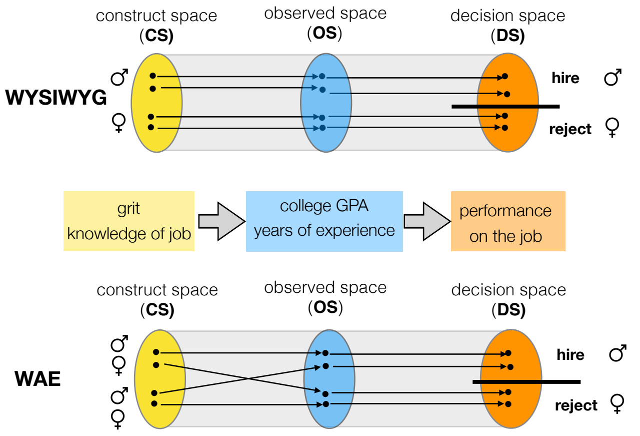


Figure 2: An illustration of worldviews from Frieder et al. [18] for hiring. "What you see is what you get" (WYSYWIG) assumes that the mapping from the construct space (*CS*) to the observed space (*OS*) shows low distortion, while "We are all equal" (WAE) assumes that this mapping shows structural bias, leading to a distortion in group structure.

The spaces and the mappings between them are illustrated in Figure 2 for the hiring ADS. Individuals are represented by points. *CS* represents the "true" properties of an individual (e.g., grit and knowledge of the job for the hiring ADS), *OS* represents the properties that we can measure (e.g., college GPA as a proxy for grit, years of experience as a proxy for knowledge of the job). *OS* is the feature space of a component in the decision pipeline, such as a classifier, a score-based selection procedure, or a human hiring manager. Finally, *DS* is the space of outcomes of that component.

When considering mappings, we are concerned with whether they preserve pair-wise distances between individuals. Importantly, because both *CS* and the mapping from *CS* to *OS* are, by definition, unobservable, a belief about the properties of the mapping has to be postulated. Friedler *et al.* [18] describe two extreme cases: WYSIWYG ("what you see is what you get") assumes low distortion from *CS* to *OS*, while WAE ("we are all equal") assumes the presence of structural bias—a systematic distortion in group structure.

While in general we cannot confirm the presence of pre-existing bias in a dataset, we are sometimes able to use another dataset, or contextual knowledge about the dataset or about the world itself, to corroborate or challenge the claim of pre-existing bias. For example, Lum and Isaac [39] showed that two areas with non-white and low-income populations in Oakland, CA experience 200 times more drug-related arrests than other areas. Yet, based on the 2011 National Survey on Drug Use and Health, the estimated number of drug users is distributed essentially uniformly across Oakland, with variation driven primarily by differences in population density. This information can be combined with our knowledge about policing practices, namely, that low-income neighborhoods are patrolled more frequently than other neighborhoods, and influence our belief about the presence of bias in the drug-related arrests dataset.

If pre-existing bias in a dataset is postulated, perhaps with corroboration from other datasources and with background knowledge about data collection practices, yet we are still interested in using this data in decision-making, then we need to identify an appropriate bias mitigation strategy. The WAE worldview justifies mitigations that enforce equality of outcomes, which are most intuitively operationalized as *statistical parity*, a requirement that the demographics of individuals receiving any outcome (positive or negative, in the case of binary classification) is the same as their demographics in the input. For example, if half of the job applicants are women, then half of those selected for in-person interviews should be women even if they appear less qualified by conventional metrics. (See Mitchell *et al.* [41] for a recent survey of fairness measures, of which statistical parity is an example.) This mitigation is simple to enact, but it's a blunt instrument: it does not tell us which women to select or, more generally, whether and how to look for useful signal in the data under the assumption of pre-existing bias. Next, we look at an alternative framework that brings more nuance into the treatment of pre-existing bias and can help inform the design of mitigation strategies.

Equality of opportunity. Heidari *et al.* [22] show an application of equality of opportunity (EOP) frameworks to algorithmic fairness. EOP emphasizes the importance of personal qualifications, and seeks to minimize the impact of circumstances and arbitrary factors on individual outcomes. "At a high level, in these models an individual's outcome/position is assumed to be affected by two main factors: his/her circumstance c and effort e. Circumstance c is meant to capture all factors that are deemed irrelevant, or for which the individual should not be held morally accountable; for instance c could specify the socio-economic status they were born into. Effort e captures all accountability factors—those that can morally justify inequality." [22]

Several conceptions of EOP have been proposed, differing in what features they consider to be relevant (or morally acceptable to use) and which they deemed irrelevant. So, libertarian EOP allows all features to be used in decision-making, while formal EOP prohibits the use of sensitive features like gender and race but can still use proxy features.

In contrast, substantive EOP, notably, Rawlsian [49] and luck egalitarian [51], seeks to offer equal opportunity in access to positions by providing fair access to the necessary qualifications for the positions. Both conceptions concede that opportunity is only equal relative to one's effort, but they differ in how effort is modeled: Rawlsian EOP asserts that equal effort should imply equal opportunity (represented as a utility distribution), regardless of circumstances. Luck egalitarian EOP considers effort relative to one's demographic group ("type" in their terms): two individuals are considered to have exercised the same level of effort if "they sit at the same quantile or rank of the effort distribution for their corresponding types." [22]

4.3 Technical Bias

Technical bias can be introduced at any stage of the ADS lifecycle, and it may exacerbate pre-existing bias. The bad news is that risks of introducing technical bias stemming from data management components abound. The good news is that, unlike with pre-existing bias, there is no ambiguity about whether a technical fix should be attempted: if technical systems we develop are introducing bias, then we should be able to instrument these systems to measure it and understand its cause. It may then be possible to mitigate this bias and to check whether the mitigation was effective.

Importantly, as we instrument our systems, we must once again take the lifecycle view. The goal is to understand how properties of individual components compose, and whether we can make guarantees about the presence or absence of technical bias in the pipeline overall based on what we know about individual components. In what follows, we discuss potential sources of technical bias in several lifecycle stages that are within our (data management) purview.

Data cleaning. Methods for missing value imputation that are based on incorrect assumptions about whether data is missing at random may distort protected group proportions. Consider a form that gives job applicants a binary choice of gender and also allows to leave gender unspecified. Suppose that about half of the users identify as men and half as women, but that women are more likely to omit gender. Then, if mode imputation (replacing a missing value with the most frequent value for the feature, the default in scikit-learn) is used, then all (predominantly female) unspecified gender values will be set to male. More generally, multi-class classification for missing value imputation typically only uses the most frequent classes as target variables [8], leading to a distortion for small population groups, because membership in these groups will never be imputed.

Next, suppose that some individuals identify as non-binary. Because the system only supports male, female, and unspecified as options, these individuals will leave gender unspecified. If mode imputation is used, then their gender will be set to male. A more sophisticated imputation method will still use values from the active domain of the feature, setting the missing values of gender to either male or female. This example illustrates that bias can arise from an incomplete or incorrect choice of data representation.

Finally, consider a form that has home address as a field. A homeless person will leave this value unspecified, and it is incorrect to attempt to impute it. While dealing with `null` values is known to be difficult and is already considered among the issues in data cleaning, the needs of responsible data management introduce new problems. As we pointed out in Section 2 under *due process*, data quality issues often disproportionately affect members of historically disadvantaged groups, and we risk compounding technical bias due to data representation with bias due to statistical concerns.

Filtering. Selections and joins can arbitrarily change the proportion of protected groups (e.g., female gender) even if they do not directly use the sensitive attribute (e.g., gender) as part of the predicate or of the join key. This change in proportion may be unintended and is important to detect, particularly when this happens during one of many preprocessing steps in the ADS pipelines.

Another potential source of technical bias is the usage of pre-trained word embeddings. For example, a pipeline may replace a textual name feature with the corresponding vector from a word embedding that is missing for rare, non-western names. If we then filter out records for which no embedding was found, we may disproportionately remove individuals from specific ethnic groups.

Ranking. Technical bias can arise when results are presented in ranked order, such as when a hiring manager is considering potential candidates to invite for in-person interviews. The main reason is the inherent position bias — the geometric drop in visibility for items at lower ranks compared to those at higher ranks, which arises because in Western cultures we read from top to bottom, and from left to right, and so items in the top-left corner of the screen attract more attention [7]. A practical implication is that, even if two candidates are equally suitable for the job, only one of them can be placed above the other, suggesting that it should be prioritized. Depending on the needs of the application and on the level of technical sophistication of the decision-maker, this problem can be addressed by suitably randomizing the ranking, showing results with ties, or plotting the score distribution.

4.4 Emergent Bias

Emergent bias arises in a context of use and may be present if a system was designed with different users in mind or when societal concepts shift over time. For ranking and recommendation in e-commerce, emergent bias arises most notably because searchers tend to trust the systems to indeed show them the most suitable items at the top positions [46], which in turn shapes a searcher's idea of a satisfactory answer, leading to a “rich-get-richer” situation.

This example immediately translates to hiring and employment. If hiring managers trust recommendations from an ADS, and if these recommendations systematically prioritize applicants of a particular demographic profile, then a feedback loop will be created, further diminishing workforce diversity over time. Bogen and Rieken [9] illustrate this problem: “For example, an employer, with the help of a third-party vendor, might select a group of employees who meet some definition of success—–for instance, those who ‘outperformed’ their peers on the job. If the employer's performance evaluations were themselves biased, favoring men, then the resulting model might predict that men are more likely to be high performers than women, or make more errors when evaluating women. This is not theoretical: One resume screening company found that its model had identified having the name ‘Jared’ and playing high school lacrosse as strong signals of success, even though those features clearly had no causal link to job performance.”

4.5 Summary

In summary, (1) We must clearly state the beliefs against which we are validating fairness. Technical interventions to improve fairness should be consistent with these beliefs. Beliefs cannot be checked empirically or falsified, as they are not hypotheses; they can only be stated axiomatically. (2) We cannot fully automate responsibility, particularly because many of the concerns we are looking to address are themselves a consequence of automation. We embrace the idea that technical interventions are only part of an over-all mitigation strategy, and should verify that they are even an effective step — there is no guarantee that is the case. (3) We need to broaden the scope of data management research beyond manipulations of properties of either a dataset or an algorithm; ADS are datasets together with algorithms together with contexts of use: the calculator is not discriminatory, but its context of use may be.

5. MANAGING THE ADS LIFECYCLE

As we discussed in Section 3, ADS critically depend on data and so should be seen through the lens of the *data* *lifecycle* [26]. Responsibility concerns, and important decision points, arise in data sharing, annotation, acquisition, curation, cleaning, and integration. Several lines of recent work argue that opportunities for improving data quality and representativeness, controlling for bias, and allowing humans to oversee the process, are missed if we do not consider these earlier lifecyle stages [30, 36, 61].

Database systems centralize correctness constraints to simplify application development via schemas, transaction protocols, etc.; algorithmic fairness and interpretability are now emerging as first-class requirements. But unlike research in the machine learning community, we need generalized requirements and generalized solutions that work across a range of applications. In what follows, we give examples of our own recent and ongoing work that is motivated by this need. These examples underscore that tangible technical progress is possible, and also that much work remains to be done to offer systems support for the responsible management of the ADS lifecycle.

5.1 Data Acquisition

Data used for analysis is often originally created for a different purpose, and therefore is frequently not representative of the true distribution. Even if the data is explicitly collected for the purpose of analysis, it can be hard to obtain a representative sample. Consider, for example, a website with reviews of products (or restaurants or hotels or movies). The point of collecting reviews and scores is to provide users with a distribution of opinion about the product, including not only the average score, but also the variance, and other aspects in the detailed reviews. Yet, we know that not every customer leaves a review—in fact only a very small fraction do. There is no reason to believe that this small fraction is a random sample of the population. It is likely that the sample skews young and well educated, potentially leading to a substantial bias in the aggregate opinions recorded.

While bias in restaurant reviews may not be a socially critical issue, similar bias could manifest itself in many other scenarios as well. Consider the use of ADS for pre-screening employment applications. As discussed above, historical under-representation of some minorities in the workforce can lead to minorities being under-represented in the training set, which in turn could push the ADS to reject more minority applicants or, more gennerally, to exhibit disparate predictive accuracy [11]. It is worth noting that the problem here is not only that some minorities are proportionally under-represented, but also that the absolute representation of some groups is low. Having 2% African Americans in the training set is a problem when they constitute 13% of the population. But it is also a problem to have only 0.2% Native Americans in the training set, even if that is representative of their proportion in the population. Such a low number can lead to Native Americans being ignored by the ADS as a small "outlier" group.

To address the problem of low absolute representation, Asudeh *et al.* [4] proposed methods to assess the coverage of a given dataset over multiple categorical features and to mitigate inadequate coverage. An important question for the data owner is what they can do about the lack of coverage. The proposed answer is to direct the data owner to acquire more data, in a way that is cognizant of the cost of data acquisition. Further, because some combinations of features are invalid or unimportant, a human expert helps identify regions of the feature space that are of interest and sets coverage goals for these regions.

Asudeh *et al.* [4] use a threshold to determine an appropriate level of coverage. Experimental results in the paper demonstrate an improvement in classifier accuracy for minority groups when additional data is acquired. This work addresses a step in the ADS lifecycle upstream from model training, and shows how improving data representativeness can improve accuracy and fairness, in the sense of disparate predictive accuracy [11]. As we will discuss in Section 5.5, there is an opportunity to integrate coverage-enhancing interventions more closely into ADS lifecycle management, both to help orchestrate the pipelines and, perhaps more importantly, to make data acquisition task-aware, setting coverage objectives based on performance requirements for the specific predictive analytics downstream, rather than based on a global threshold.

5.2 Preprocessing for Fair Classification

Even when the acquired data satisfies representativeness requirements, it may still be subject to pre-existing bias, as discussed in Section 4.2. Further, preprocessing operations, including data cleaning, filtering, and ranking, can exhibit technical bias in subtle ways, as discussed in Section 4.3. We may thus be interested in developing fairness-enhancing interventions to mitigate these effects.

In this section, we assume that data acquisition and preprocessing are preparing data for a prediction task that involves training a classifier. In most contexts, there are many prediction tasks associated with a given dataset, each representing a separate application requiring distinct domain knowledge. We first we briefly describe *associational fairness* measures, and then present methods that use *causal models* to capture this domain knowledge, and intervene on the data at the preprocessing stage to manage unfairness for a specific downstream prediction task.

Associational fairness. Most treatments of algorithmic fairness rely on statistical correlations in the observed data. A prominent example is statistical parity (discussed in Section 4.2), a requirement that the demographics of individuals receiving any outcome is the same as their demographics in the input. *Conditional statistical parity* [13] controls for a set of admissible factors to avoid some spurious correlations.

Equalized odds requires protected and privileged groups to have the same false positive rates and the same false negative rates [21]. This notion is consistent with Rawlsian equality of opportunity (EOP), discussed in Section 4.2, under the assumption that all individuals with the same true label have the same effort-based utility. As a final example, *predictive value parity* (a weaker version of calibration [31]) requires the equality of positive and negative predictive values across different groups and is consistent with luck egalitarian EOP if the predicted label is assumed to reflect an individual's effort-based utility. (See Heidari *et al.* [22] for details.)

Associational fairness measures are based on data alone, without reference to additional structure or context [41]. Consequently, these measures can be fooled by anomalies such as Simpson's paradox [47].

Causal fairness. Avoiding anomalous correlations motivates work based on causal models [29, 35, 43, 52, 53, 74]. These approaches capture background knowledge as causal relationships between variables, usually represented as causal DAGs: directed graphs in which nodes represent variables and edges represent potential causal relationships. Discrimination is measured as the causal influence of the protected attribute on the outcome along particular causal paths that are deemed to be socially unacceptable.

An important concept in causal modeling is a *counterfactual* — an intervention where we modify the state of a set of variables $\mathbf{X}$ in the real world to some value $\mathbf{X} = \mathbf{x}$ and observe the effect on some output Y. For example, we may ask "Would this applicant have been hired if they had (or had not) been female?" Kusner *et al.* [35] define fairness in terms of counterfactuals for an individual, which in general cannot be estimated from observational data [47]. Kilbertus *et al.* [29] define fairness as equal outcome distributions for the whole population under counterfactuals for a different value of the protected attribute, however, the distributions can be equal even when there is discrimination [54].

Salimi *et al.* [54] introduced a measure called *interventional fairness* that addresses these issues, and also showed how to achieve it based on observational data, without requiring the complete causal model. The user specifies a set of *admissible* and *inadmissible* variables, indicating through which paths in the causal model influence is allowed to flow from the protected attribute to the outcome. The Markov boundary (MB) (parents, children, children's other parents) of a variable Y describes those nodes that can potentially influence Y. A key result is that, if the MB of the outcome is a subset of the MB of the admissible variables (i.e., admissible variables "shield" the outcome from the influence of sensitive and inadmissible variables), then the algorithm satisfies interventional fairness.

This condition on MB is used to design database repair algorithms, through a connection between the independence constraints encoding fairness and multi-valued dependencies (MVD). Several repair algorithms are described, and the results show that, in addition to satisfying interventional fairness, the classifier trained on repaired data performs well against associational fairness metrics.

5.3 Preprocessing for Fair Ranking

In Section 5.2 we discussed fairness-enhancing interventions for classification. We now turn to ranking, another common operation in automated hiring systems. Ranking may be invoked as part of preprocessing, with results passed to a predictive analytic; alternatively, its output may be presented directly to a human decision-maker.

Algorithmic *rankers* take a collection of candidates as input and produce a ranking (permutation) of the candidates as output. The simplest kind of a ranker is *score-based*; it computes a score of each candidate independently and returns the candidates in score order (e.g., from higher to lower, with suitably specified tie-breaking). Another common kind of a ranker is *learning-to-rank* (LTR), where supervised learning is used to predict the ranking of unseen candidates. In both score-based ranking and LTR, we may output the entire permutation, or, more often, only the highest scoring k candidates, the top-k, where k is much smaller than the size of the input n. Set selection is a special case of ranking that ignores the relative order among the top-k.

Associational fairness. Yang and Stoyanovich [71] were the first to propose associational fairness measures for ranking. Their formulation is based on an adaptation of equality-of-outcomes fairness measures, such as statistical parity (see Section 4.2) to account for position bias, a kind of technical bias that is prominent in rankings (see Section 4.3). The intuition is that, because it is more likely that a higher-ranked candidate will be selected, it is also more important to achieve statistical parity at higher ranks.

For example, suppose that there is a single job opening, that half of the applicants are women, and that at most 10 of the applicants will be invited for in-person interviews. It is insufficient to guarantee that 5 women are among the top-10, because they may end up in positions 6 through 10. Rather, men and women should alternate at the top-10, and it is particularly important to see both genders in equal proportion in earlier prefixes. To operationalize this intuition, Yang and Stoyanovich [71] place proportional representation fairness within the NDCG framework [27], imposing proprotionality constraint over every prefix of the ranking and accounting for position bias with a logarithmic discount.

Fairness measures of this kind can be used in supervised learning to train a fair LTR model. They can also be used to formulate a fairness objective that a ranking—score-based or learned—must meet to be legally or ethically admissible. Asudeh *et al.* [3] develop methods to *design fair score-based rankers* that rely on such fairness objectives. These methods query a fairness oracle that, given a ranking, returns true if it meets fairness criteria. If the ranking is found inadmissible, an alternative ranking is suggested that is both fair and close to the original, in the sense of being generated by a score-based ranker with similar feature weights.

For example, if a job applicant's score is computed as $0.5x_1 + 0.5x_2$, where x_1 is their years of experience and x_2 is their college GPA (both suitably normalized), and the resulting ranking turns out to be unfair, then the system may suggest to the hiring manager a satisfactory ranking, computed as $0.55x_1 + 0.45x_2$ instead.

Causal intersectional fairness. Much previous research on algorithmic fairness, including also on fairness in raking, considers a single sensitive attribute, such as either gender *or* race, or allows constraints on the combinations of sensitive attribute values. In all these cases, the set of sensitive attribute values induces a partitioning on the set of candidates. However, this treatment may be insufficient because we often need to impose fairness constraints on gender *and* on race, *and* on some combinations of gender and race. For example, we may be interested in detecting discrimination with respect to women, Blacks, and Black women. This is because, as noted by Crenshaw [14], it is possible to give the appearance of being fair with respect to each sensitive attribute such as race and gender separately, while being unfair with respect to *intersectional* subgroups.

Yang *et al.* [70] developed a causal framework for intersectionally fair ranking. Consider the task of selecting (and ranking) job applicants at a moving company (this example is inspired by Datta *et al.* [15]), and the corresponding causal model in Figure 3. Applicants are hired based on their qualification score Y, computed from weight-lifting ability X, and affected by gender G and race R, either directly or through X. By representing relationships between features in a causal DAG, we gain an ability to postulate which relationships between features and outcomes are legitimate, and which are

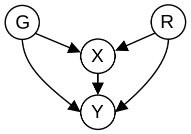


Figure 3: Causal model that includes sensitive attributes G (gender), R (race), utility score Y, other covariates $\mathbf{X}$.

potentially discriminatory.

In our example, we may state that the impact of gender G on score Y through weight-lifting ability X is legitimate (because men are on average better at lifting weights than women), but that direct impact of gender on score Y is discriminatory. Further, we may state that the impact of race R on score Y is discriminatory, both directly and through X. Technically, we can encode these constraints by treating X as a *resolving mediator* [29] for gender but not for race.

If the qualification score Y is lower for female applicants and for Blacks, then the intersectional group Black females faces greater discrimination than either the Black or the female group. The gist of the methods of Yang *et al.* [70] is to rank on counterfactual scores to achieve intersectional fairness. From the causal model, they compute model-based counterfactuals to answer the question, "What would this person's score be if they had (or had not) been a Black woman (for example)?" By ranking on counterfactual scores, they are treating every individual in the sample as though they had belonged to one specific intersectional subgroup.

This method can be justified by a connection to luck egalitarian EOP in that it considers the fine-grained impacts of group membership on the effort-based utility distribution Y.

5.4 Diversity in Set Selection and Ranking

The term *diversity* captures the quality of a collection of candidates $\mathcal{S} \subset \mathcal{C}$ of size k with regards to the variety of its constituent elements [16]. Diversity constraints on the output of an ADS may be imposed for legal reasons, such as for compliance with Title VII of the Civil Rights Act of 1964. Beyond legal requirements, benefits of diversity in hiring and elsewhere are broadly recognized [45, 65]. Further, when set selection or ranking are used as part of preprocessing, improving diversity of the training set can improve performance of the predictive analytic upstream.

A popular measure of diversity is *coverage*, which ensures representation of the demographic categories of interest in $\mathcal{S}$, or in every prefix of a ranking $\boldsymbol{\tau}(\mathcal{S})$. Coverage diversity is closely related to proportional representation fairness: a unifying formulation is to specify a lower bound ℓ_v for each sensitive attribute value v, and to enforce it as the minimum cardinality of items satisfying v in the selected set $\mathcal{S}$ [64]. If the k selected candidates need to also be ranked in the output, this formulation can be extended to specify a lower bound $\ell_{v,p}$ for every attribute v and every prefix p of the returned ranked list, with $p \leq k$ [10]. Then, at least $\ell_{v,p}$ items satisfying v should appear in the top p positions of the output. Given a set of diversity constraints, one can then seek to maximize the score utility of $\mathcal{S}$ (the sum of utility scores of the elements of $\mathcal{S}$), subject to these constraints.

Stoyanovich *et al.* [64] consider *on-line set selection.* Their work extends the classic Secretary problem [17, 37], and it's more recent k-choice variant [6], to account for diversity over a single sensitive attribute. In on-line set selection, candidates are interviewed one-by-one, their utility is revealed during the interview, the decision is made to hire or reject the candidate, and this decision is irreversible. The goal is to hire k candidates to maximize the *expected utility* of the selected set. The strategy is to (1) estimate the expected scores by observing and, initially, not hiring any candidates; then (2) hire candidates whose utility meets or exceeds the estimate. Stoyanovich *et al.* [64] estimate expected scores independently for different demographic groups to meet the ℓ_v constraints, thus deriving a relative view of utility, which is consistent with luck egalitarian EOP.

Table 1: 12 candidates with sensitive attributes `race` and `gender`. Each cell lists an individual's id, and score in parentheses.

	Male		**Female**	
White	A (99)	B (98)	C (96)	D (95)
Black	E (91)	F (91)	G (90)	H (89)
Asian	I (87)	J (87)	K (86)	L (83)

Yang *et al.* [69] also take a relative view of utility. They consider set selection and ranking in presence of *multiple* sensitive attributes, with diversity constraints on each. They observe an intersectional issue — that utility loss is non-uniform across groups, and that groups with systematically lower scores suffer the loss disproportionately. They address this by placing additional constraint on the selection procedure, balancing utility loss across groups.

For example, consider 12 candidates in Table 1 who are applying for $k = 4$ positions, and suppose that we wish to hire two candidates of each gender, and at least one candidate from each race. The set that maximizes utility while satisfying diversity is {A, B, G, K} (utility 373). This outcome selects the highest-scoring male and White candidates (A and B), but misses the highest-scoring Black (E and F) and Asian (I and J) candidates. This type of unfairness is unavoidable, but it can be distributed this unfairness in a more balanced way: the set {A, C, E, K} (utility 372) contains the top female, male, White, and Black candidates.

5.5 Holistic View of the Pipeline

In Sections 5.1-5.4, we discussed fairness and diversity considerations at different lifecycle stages. We now show how components such as these can be treated holistically.

Schelter *et al.* [56] developed FairPrep, a design and evaluation framework for fairness-enhancing interventions in machine learning pipelines that treats data as a first-class citizen. The framework implements a modular data lifecycle, enables re-use of existing implementations of fairness metrics and interventions, and integration of custom feature transformations and data cleaning operations from real world use cases. FairPrep pursues the following goals:

- Expose a *developer-centered design* throughout the lifecycle, which allows for low effort customization and composition of the framework's components.

- Surface *discrimination* and *due process* concerns, including disparate error rates, failure of a model to fit the data, and failure of a model to generalize.

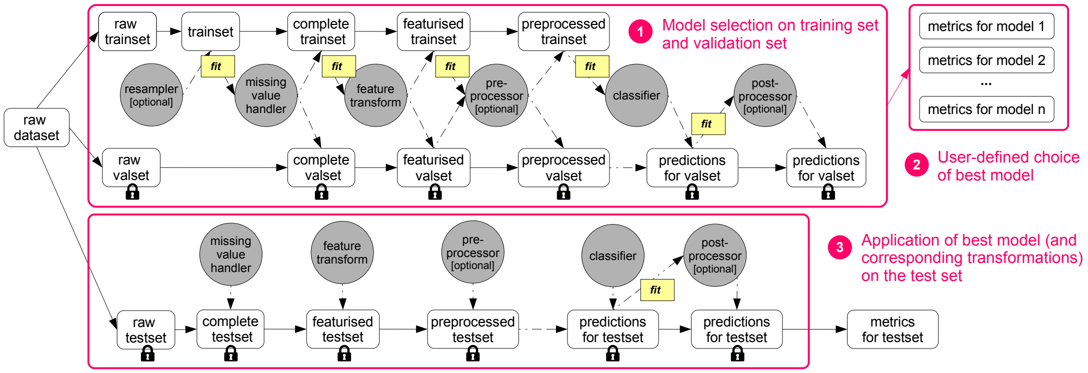


Figure 4: Data life cycle in FairPrep [56], designed to enforce isolation of test data, and to allow for customization through user-provided implementations of different components. An evaluation run consists of three different phases: (1) Learn different models, and their corresponding data transformations, on the training set; (2) Compute performance / accuracy-related metrics of the model on the validation set, and allow the user to select the 'best' model according to their setup; (3) Compute predictions and metrics for the user-selected best model on the held-out test set.

- Follow software engineering and machine learning best practices to reduce the *technical debt* of incorporating fairness-enhancing interventions into an already complex development and evaluation scenario [55, 57].

Figure 4 summarizes the architecture of FairPrep that is based on three main principles: *Data isolation* — to avoid target leakage, user code should only interact with the training set, and never be able to access the held-out test set. *Componentization* — different data transformations and learning operations should be implementable as single, exchangable standalone components; the framework should expose simple interfaces to users, supporting low effort customization. *Explicit modeling of the data lifecycle* — the framework defines an explicit, standardized data lifecycle that applies a sequence of data transformations and model training in a predefined order.

FairPrep currently focuses on data cleaning (including different methods for data imputation), and model selection and validation (including hyperparameter tuning), and can be extended to accommodate earlier lifecycle stages, such as data acquisition, integration, and curation. Schelter *et al.* [56] measured the impact of sound best practices, such as hyperparameter tuning and feature scaling, on the fairness and accuracy of the resulting classifiers, and also showcased how FairPrep enables the inclusion of incomplete data into studies and helps analyze the effects.

6. INTERPRETABILITY

Interpretability—allowing people to understand the process and the decisions of an ADS—is critical to responsibility. Interpretability is needed because it allows people, including software developers, decision-makers, auditors, regulators, individuals who are affected by ADS decisions, and members of the public, to *exercise agency* by accepting or challenging algorithmic decisions and, in the case of decision-makers, to *take responsibility* for these decisions.

Making ADS interpretable is difficult, both because they are complex (multiple steps, models with implicit assumptions), and because they rely on datasets that are often re-purposed—used outside of the original context for which they were intended. For these reasons, humans need to be able to determine the "fitness for use" of a given model or dataset, and to assess the methodology that was used to produce it.

To address this need, we have been developing interpretability tools based on the concept of a *nutritional label*, drawing an analogy to the food industry, where simple, standard labels convey information about the ingredients and production processes [60, 72]. Short of setting up a chemistry lab, the consumer would otherwise have no access to this information. Similarly, consumers of data products cannot be expected to reproduce the computational procedures just to understand fitness for their use. Nutritional labels, in contrast, are designed to support specific decisions rather than provide complete information.

6.1 Properties of a Nutritional Label

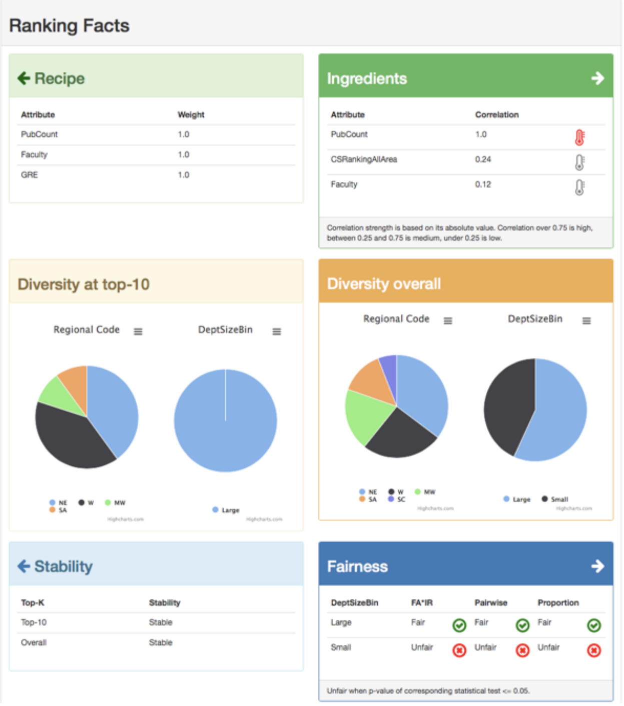
The data management community has been studying systems and standards for metadata, provenance, and transparency for decades [24, 1, 42]. We are now seeing renewed interest in these topics, and clear opportunities for this community to contribute.

Several recent projects, including the Dataset Nutrition Label project [25], Datasheets for Datasets [20], and Model Cards [40], are proposing to use metadata to support interpretability. Notably, all these method rely on manually constructed annotations. In contrast, our goal is to *generate labels automatically or semi-automatically* as a side effect of the computational process itself, embodying the paradigm of *interpretability-by-design.*

To differentiate a nutritional label from more general forms of metadata, we articulate several properties.

- *Comprehensible*: The label is not a complete (and therefore overwhelming) history of every processing step applied to produce the result. This approach has its place and has been extensively studied in the literature on scientific workflows, but is unsuitable for the applications we target. The information on a nutritional label must be short, simple, and clear.

- *Consultative*: The label should provide actionable information, not just descriptive metadata. Based on this information, consumers may cancel unused credit



Ranking Facts

← Recipe

Attribute	Weight
PubCount	1.0
Faculty	1.0
GRE	1.0

Ingredients →

Attribute	Correlation
PubCount	1.0
CSRankingAllArea	0.24
Faculty	0.12

Correlation strength is based on its absolute value. Correlation over 0.75 is high, between 0.25 and 0.75 is medium, under 0.25 is low.

Diversity at top-10

Diversity overall

← Stability

Top-K	Stability
Top-10	Stable
Overall	Stable

Fairness →

DeptSizeBin	FA*IR	Pairwise	Proportion
Large	Fair ✓	Fair ✓	Fair ✓
Small	Unfair ✗	Unfair ✗	Unfair ✗

Unfair when p-value of corresponding statistical test <= 0.05.

Figure 5: Ranking Facts for the CS departments dataset.

cards to improve their credit score and job applicants may take a certification exam to improve their chances of being hired.

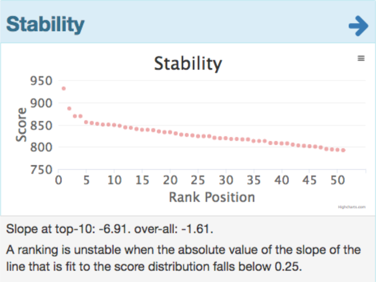
- *Comparable*: Labels should enable comparisons between related products, implying a standard. The IEEE is developing a series of ethics standards, known as the IEEE P70xx series, as part of its Global Initiative on Ethics of Autonomous and Intelligent Systems. These standards include "IEEE P7001: Transparency of Autonomous Systems" and "P7003: Algorithmic Bias Considerations" [33]. The work on nutritional labels is synergistic with these efforts.

- *Concrete*: The label must contain more than just general statements about the source of the data; such statements do not provide sufficient information to make technical decisions about fitness for use.

- *Computable*: Although primarily intended for human consumption, nutritional labels should be machine-readable to enable data discovery, integration, and automated warnings of potential misuse.

- *Composable*: Datasets are frequently integrated to construct training data; the nutritional labels must be similarly integratable. In some situations, the composed label is simple to construct: the union of sources. In other cases, the biases may interact in complex ways: a group may be sufficiently represented in each source dataset, but underrepresented in their join.

- *Concomitant*: The label should be carried with the dataset; systems should be designed to propagate labels through pipelines, modifying them as appropriate.



Stability →

Slope at top-10: -6.91. over-all: -1.61.

A ranking is unstable when the absolute value of the slope of the line that is fit to the score distribution falls below 0.25.

Figure 6: Stability: detailed widget.

6.2 A Nutritional Label for Rankings

To make our discussion more concrete, we now describe Ranking Facts, a system that automatically derives nutritional labels for rankings, developed by Yang *et al.* [72].

Figure 5 presents Ranking Facts that explains a ranking of Computer Science departments. Ranking Facts is made up of a collection of visual widgets. Each widget addresses an essential aspect of interpretability, and is based on our recent technical work on fairness, diversity, and stability in algorithmic rankers. We spoke about fairness and diversity in Section 5.3, and will now briefly describe the remaining components of the tool.

Features and methodology. The Recipe and Ingredients widgets help explain the ranking methodology. Recipe succinctly describes the ranking algorithm. For example, for a linear scoring formula, each attribute would be listed together with its weight. Ingredients lists attributes most material to the ranked outcome, in order of importance. For example, for a linear model, this list could present the attributes with the highest learned weights. Put another way, the explicit intentions of the designer of the scoring function about which attributes matter, and to what extent, are stated in the Recipe, while Ingredients may show attributes that are actually associated with high rank. Such associations can be derived with linear models or with other methods, such as rank-aware similarity in our prior work [59].

Stability. The Stability widget explains whether the ranking methodology is robust on the given dataset. An unstable ranking is one where slight changes to the data (e.g., due to uncertainty or noise), or to the methodology (e.g., by slightly adjusting the weights in a score-based ranker) could lead to a significant change in the output. This widget can report whether the ranking is sufficiently stable according to some pre-specified criterion, or give a score that indicates the extent of the change required for the ranking to change.

A detailed Stability widget complements the overview widget. An example is shown in Figure 6, where the stability of a ranking is quantified as the slope of the line that is fit to the score distribution, at the top-10 and over-all. A score distribution is unstable if scores of items in adjacent ranks are close to each other, and so a very small change in scores will lead to a change in the ranking. In this example the score distribution is considered unstable if the slope is 0.25 or lower. Alternatively, stability can be computed with respect to each scoring attribute, or it can be assessed using a model of uncertainty in the data. In these cases, stability quantifies the extent to which a ranked list will change as a result of small *changes to the underlying data*. A complementary notion of stability, quantifies the magnitude of change as a result of small changes to the ranking model.

Asudeh *et al.* [3] develped methods for quantifying and improving the stability of a score-based ranker with respect to a given dataset, and focused on a notion of stability that quantifies whether the output ranking will change due to a small change in the attribute weights. This notion of stability is natural for consumers of a ranked list (i.e., those who use the ranking to prioritize items and make decisions), who should be able to assess the magnitude of the *region in the weight space* that produces the observed ranking. If this region is large, then the same ranked order would be obtained for many choices of weights, and the ranking is stable. But if this region is small, then we know that only a few weight choices can produce the observed ranking. This may suggest that the ranking was "cherry-picked" by the producer to obtain a specific outcome.

6.3 Interpretability in the Service of Trust

Interpretability means different things to different stakeholders, including individuals being affected by decisions, individuals making decisions with the help of algorithmic tools, policy-makers, regulators, auditors, vendors, data scientists who develop and deploy the systems, and members of the general public. Stoyanovich *et al.* [63] proposed a framework that connects interpretability of ADS with *trust*, which was one of the starting points of our discussion in Section 1. Indeed, remarkably little is known about how humans perceive and evaluate algorithms and their outputs, what makes a human trust or mistrust an algorithm, and how we can empower humans to exercise agency —– to adopt or challenge an algorithmic decision.

The authors argued that designers of nutritional labels should explicitly consider *what* they are explaining, *to whom*, and *for what purpose*. Further, to design effective explanations, it will be helpful to rely on concepts from social psychology such as procedural justice (that links with due process, discussed in Section 2), moral cognition, and social identity. Finally, it is necessary to experimentally validate the effectiveness of explanations, because information disclosure does not always have the intended effect.

For example, although the nutritional and calorie labelling for food are in broad use today, the information conveyed in the labels does not always affect calorie consumption. A plausible explanation is that "When comparing a $3 Big Mac at 540 calories with a similarly priced chicken sandwich with 360 calories, the financially strapped consumer [. . .] may well conclude that the Big Mac is a better deal in terms of calories per dollar" [38]. It is therefore important to understand, with the help of experimental studies, what kinds of disclosure are effective, and for what purpose.

7. CONCLUSIONS

In this article, we gave a perspective on the role that the data management research community can play in the responsible design, development, use, and oversight of Automated Decision Systems (ADS). We intentionally grounded our discussion in automated hiring tools, a specific use case that gave us ample opportunity to both appreciate the potential benefits of data science and AI in an important domain, and to get a sense of the ethical and legal risks.

We also intentionally devoted half of this paper to setting the stage — bringing in concepts from law, philosophy and social science, and grounding them in data management questions, before discussing technical research. This breakdown underscores that we (technologists) must think carefully about where in the ADS lifecycle a technical solution is appropriate, and where it simply won't do.

On a related note, an important thread that runs through this paper is that we *cannot fully automate responsibility*. While some of the duties of carrying out the task of, say, legal compliance can in principle be assigned to an algorithm, the accountability for the decisions being made by an ADS always rests with a person. This person may be a decision maker or a regulator, a business leader or a software developer. For this reason, we see our role as researchers in helping build systems that "expose the knobs" or responsibility to people, for example, in the form of explicit fairness constrains or interpretability mechanisms.

Those of us in academia have an additional responsibility to teach students about the social implications of the technology they build. A typical student is driven to develop technical skills and has an engineer's desire to build useful artifacts, such as a classification algorithm with low error rates. A typical student may not have the awareness of historical discrimination, or the motivation to ask hard questions about the choice of a model or of a metric. This typical student will soon become a practising data scientist, influencing how technology companies impact society. It is critical that the students we send out into the world have at least a rudimentary understanding of responsible data science and AI.

Towards this end, we are developing educational materials on responsible data science. Jagadish launched the first Data Science Ethics MOOC on the EdX platform in 2015 (`https://www.edx.org/course/data-science-ethics`). This course has since been ported to Coursera (`https://www.coursera.org/learn/data-science-ethics`) and to Futurum, and has been taken by thousands of students worldwide. More importantly, individual videos, including case study videos, have been individually licensed under Creative Commons and can be freely incorporated in your own teaching where appropriate.

Stoyanovich has a highly visible technical course on Responsible Data Science [62], with all materials publicly available online. In a pre-course survey, in response to the prompt, "Briefly state your view of the role of data science and AI in society", one student wrote: "It is something we cannot avoid and therefore shouldn't be afraid of. I'm glad that as a data science researcher, I have more opportunities as well as more responsibility to define and develop this 'monster' under a brighter goal." Another student responded, "Data Science [DS] is a powerful tool and has the capacity to be used in many different contexts. As a responsible citizen, it is important to be aware of the consequences of DS/AI decisions and to appropriately navigate situations that have the risk of harming ourselves or others."

8. ACKNOWLEDGEMENTS

The work of Julia Stoyanovich was supported in part by NSF Grants No. 1926250, 1934464, and 1922658. The work of Bill Howe was supported in part by NSF Grants No. 1740996 and 1934405. The work of H.V. Jagadish was supported in part by NSF Grants No. 1741022 and 1934565.

9. REFERENCES

[1] Open provenance. https://openprovenance.org. [Online; accessed 14-August-2019].

[2] S. Abiteboul and J. Stoyanovich. Transparency, fairness, data protection, neutrality: Data management challenges in the face of new regulation. *J. Data and Information Quality*, 11(3):15:1–15:9, 2019.

[3] A. Asudeh, H. V. Jagadish, G. Miklau, and J. Stoyanovich. On obtaining stable rankings. *PVLDB*, 12(3):237–250, 2018.

[4] A. Asudeh, Z. Jin, and H. V. Jagadish. Assessing and remedying coverage for a given dataset. In *35th IEEE International Conference on Data Engineering, ICDE 2019, Macao, China, April 8-11, 2019*, pages 554–565. IEEE, 2019.

[5] Automated Decision Systems Task Force. New York City Automated Decision Systems Task Force Report. https://www1.nyc.gov/assets/adstaskforce/downloads/pdf/ADS-Report-11192019.pdf, 2019. [Online; accessed 14-August-2019].

[6] M. Babaioff, N. Immorlica, D. Kempe, and R. Kleinberg. Online auctions and generalized secretary problems. *SIGecom Exchanges*, 7(2), 2008.

[7] R. Baeza-Yates. Bias on the web. *Commun. ACM*, 61(6):54–61, 2018.

[8] F. Biessmann, D. Salinas, S. Schelter, P. Schmidt, and D. Lange. Deep learning for missing value imputation in tables with non-numerical data. In *Proceedings of the 27th ACM International Conference on Information and Knowledge Management*, pages 2017–2025. ACM, 2018.

[9] M. Bogen and A. Rieke. Help wanted: An examination of hiring algorithms, equity, and bias. *Upturn*, 2018.

[10] L. E. Celis, D. Straszak, and N. K. Vishnoi. Ranking with fairness constraints. In *45th International Colloquium on Automata, Languages, and Programming, ICALP*, pages 28:1–28:15, 2018.

[11] I. Y. Chen, F. D. Johansson, and D. A. Sontag. Why is my classifier discriminatory? In S. Bengio, H. M. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, 3-8 December 2018, Montréal, Canada*, pages 3543–3554, 2018.

[12] D. K. Citron and F. A. Pasquale. The scored society: Due process for automated predictions. *Washington Law Review*, 89, 2014.

[13] S. Corbett-Davies, E. Pierson, A. Feller, S. Goel, and A. Huq. Algorithmic decision making and the cost of fairness. In *Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, Halifax, NS, Canada, August 13 - 17, 2017*, pages 797–806. ACM, 2017.

[14] K. Crenshaw. Demarginalizing the intersection of race and sex: A black feminist critique of antidiscrimination doctrine, feminist theory and antiracist politics. *University of Chicago Legal Forum*, (1):139–167, 1989.

[15] A. Datta, S. Sen, and Y. Zick. Algorithmic transparency via quantitative input influence: Theory and experiments with learning systems. In *IEEE Symposium on Security and Privacy, SP 2016, San Jose, CA, USA, May 22-26, 2016*, pages 598–617. IEEE Computer Society, 2016.

[16] M. Drosou, H. V. Jagadish, E. Pitoura, and J. Stoyanovich. Diversity in big data: A review. *Big Data*, 5(2):73–84, 2017.

[17] E. Dynkin. The optimum choice of the instant for stopping a markov process. *Sov. Math. Dokl.*, 4, 1963.

[18] S. A. Friedler, C. Scheidegger, and S. Venkatasubramanian. On the (im)possibility of fairness. *CoRR*, abs/1609.07236, 2016.

[19] B. Friedman and H. Nissenbaum. Bias in computer systems. *ACM Trans. Inf. Syst.*, 14(3):330–347, 1996.

[20] T. Gebru, J. Morgenstern, B. Vecchione, J. W. Vaughan, H. M. Wallach, H. D. III, and K. Crawford. Datasheets for datasets. *CoRR*, abs/1803.09010, 2018.

[21] M. Hardt, E. Price, and N. Srebro. Equality of opportunity in supervised learning. In D. D. Lee, M. Sugiyama, U. von Luxburg, I. Guyon, and R. Garnett, editors, *Advances in Neural Information Processing Systems 29: Annual Conference on Neural Information Processing Systems 2016, December 5-10, 2016, Barcelona, Spain*, pages 3315–3323, 2016.

[22] H. Heidari, M. Loi, K. P. Gummadi, and A. Krause. A moral framework for understanding fair ML through economic models of equality of opportunity. In *Proceedings of the Conference on Fairness, Accountability, and Transparency, FAT* 2019, Atlanta, GA, USA, January 29-31, 2019*, pages 181–190. ACM, 2019.

[23] T. Herndon, M. Ash, and R. Pollin. Does high public debt consistently stifle economic growth? a critique of Reinhart and Rogof. *Political Economy Research Institute working Paper Series*, (322), 2013.

[24] M. Herschel, R. Diestelkämper, and H. Ben Lahmar. A survey on provenance: What for? what form? what from? *VLDB J.*, 26(6):881–906, 2017.

[25] S. Holland, A. Hosny, S. Newman, J. Joseph, and K. Chmielinski. The dataset nutrition label: A framework to drive higher data quality standards. *CoRR*, abs/1805.03677, 2018.

[26] H. V. Jagadish, J. Gehrke, A. Labrinidis, Y. Papakonstantinou, J. M. Patel, R. Ramakrishnan, and C. Shahabi. Big data and its technical challenges. *Commun. ACM*, 57(7):86–94, 2014.

[27] K. Järvelin and J. Kekäläinen. Cumulated gain-based evaluation of IR techniques. *ACM Trans. Inf. Syst.*, 20(4):422–446, 2002.

[28] J. Kappelhof. *Total Survey Error in Practice*, chapter Survey Research and the Quality of Survey Data Among Ethnic Minorities. 2017.

[29] N. Kilbertus, M. R. Carulla, G. Parascandolo, M. Hardt, D. Janzing, and B. Schölkopf. Avoiding discrimination through causal reasoning. In *Advances in Neural Information Processing Systems*, pages 656–666, 2017.

[30] K. Kirkpatrick. It's not the algorithm, it's the data. *Commun. ACM*, 60(2):21–23, 2017.

[31] J. M. Kleinberg, S. Mullainathan, and M. Raghavan. Inherent trade-offs in the fair determination of risk scores. In C. H. Papadimitriou, editor, *8th Innovations in Theoretical Computer Science Conference, ITCS 2017, January 9-11, 2017, Berkeley, CA, USA*,

volume 67 of *LIPIcs*, pages 43:1–43:23. Schloss Dagstuhl - Leibniz-Zentrum für Informatik, 2017.

[32] R. Koch. What is the LGPD? Brazil's version of the GDPR. `https://gdpr.eu/gdpr-vs-lgpd/`, 2018. [Online; accessed 14-August-2019].

[33] A. R. Koene, L. Dowthwaite, and S. Seth. IEEE p7003$^{\text{TM}}$ standard for algorithmic bias considerations: work in progress paper. In *Proceedings of the International Workshop on Software Fairness, FairWare@ICSE 2018, Gothenburg, Sweden, May 29, 2018*, pages 38–41, 2018.

[34] J. A. Kroll, J. Huey, S. Barocas, E. W. Felten, J. R. Reidenberg, D. G. Robinson, and H. Yu. Accountable algorithms. *University of Pennsylvania Law Review*, 165, 2017.

[35] M. J. Kusner, J. R. Loftus, C. Russell, and R. Silva. Counterfactual fairness. In I. Guyon, U. von Luxburg, S. Bengio, H. M. Wallach, R. Fergus, S. V. N. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, 4-9 December 2017, Long Beach, CA, USA*, pages 4066–4076, 2017.

[36] D. Lehr and P. Ohm. Playing with the data: What legal scholars should learn about machine learning. *UC Davis Law Review*, 51(2):653–717, 2017.

[37] D. V. Lindley. Dynamic programming and decision theory. *Journal of the Royal Statistical Society*, 10(1):39–51, 03 1961.

[38] G. Loewenstein. Confronting reality: pitfalls of calorie posting. *The American Journal of Clinical Nutrition*, 93(4):679–680, 2011.

[39] K. Lum and W. Isaac. To predict and serve? *Significance*, 13(5), 2016.

[40] M. Mitchell, S. Wu, A. Zaldivar, P. Barnes, L. Vasserman, B. Hutchinson, E. Spitzer, I. D. Raji, and T. Gebru. Model cards for model reporting. In *Proceedings of the Conference on Fairness, Accountability, and Transparency, FAT* 2019, Atlanta, GA, USA, January 29-31, 2019*, pages 220–229, 2019.

[41] S. Mitchell, E. Potash, S. Barocas, A. D'Amour, and K. Lum. Prediction-based decisions and fairness: A catalogue of choices, assumptions, and definitions. *CoRR*, abs/1811.07867, 2020.

[42] L. Moreau, B. Ludäscher, I. Altintas, R. S. Barga, S. Bowers, S. P. Callahan, G. C. Jr., B. Clifford, S. Cohen, S. C. Boulakia, S. B. Davidson, E. Deelman, L. A. Digiampietri, I. T. Foster, J. Freire, J. Frew, J. Futrelle, T. Gibson, Y. Gil, C. A. Goble, J. Golbeck, P. T. Groth, D. A. Holland, S. Jiang, J. Kim, D. Koop, A. Krenek, T. M. McPhillips, G. Mehta, S. Miles, D. Metzger, S. Munroe, J. Myers, B. Plale, N. Podhorszki, V. Ratnakar, E. Santos, C. E. Scheidegger, K. Schuchardt, M. I. Seltzer, Y. L. Simmhan, C. T. Silva, P. Slaughter, E. G. Stephan, R. Stevens, D. Turi, H. T. Vo, M. Wilde, J. Zhao, and Y. Zhao. Special issue: The first provenance challenge. *Concurrency and Computation: Practice and Experience*, 20(5):409–418, 2008.

[43] R. Nabi and I. Shpitser. Fair inference on outcomes. In S. A. McIlraith and K. Q. Weinberger, editors, *Proceedings of the Thirty-Second AAAI Conference on Artificial Intelligence, (AAAI-18), the 30th innovative Applications of Artificial Intelligence (IAAI-18), and the 8th AAAI Symposium on Educational Advances in Artificial Intelligence (EAAI-18), New Orleans , Louisiana, USA, February 2-7, 2018*, pages 1931–1940. AAAI Press, 2018.

[44] A. Narayanan. How to recognize ai snake oil. `https://www.cs.princeton.edu/~arvindn/talks/MIT-STS-AI-snakeoil.pdf`, 2019. Arthur Miller lecture on science and ethics, MIT.

[45] S. E. Page. *The Difference: How the Power of Diversity Creates Better Groups, Firms, Schools, and Societies-New Edition*. Princeton University Press, 2008.

[46] B. Pan, H. Hembrooke, T. Joachims, L. Lorigo, G. Gay, and L. Granka. In google we trust: Users' decisions on rank, position, and relevance. *Journal of computer-mediated communication*, 12(3):801–823, 2007.

[47] J. Pearl. *Causality: Models, Reasoning and Inference*. Cambridge University Press, USA, 2nd edition, 2009.

[48] Personal Information Protection Commission, Japan. Amended Act on the Protection of Personal Information. 2016.

[49] J. Rawls. *A theory of justice*. Harvard University Press, 1971.

[50] R. V. Reeves and D. Halikias. Race gaps in sat scores highlight inequality and hinder upward mobility. `https://www.brookings.edu/research/race-gaps-in-sat-scores-highlight-inequality\-and-hinder-upward-mobility`, 2017. [Online; accessed 14-August-2019].

[51] J. E. Roemer. Equality of opportunity: a progress report. *Social Choice and Welfare*, 19(2):405–471, 2002.

[52] C. Russell, M. J. Kusner, J. Loftus, and R. Silva. When worlds collide: integrating different counterfactual assumptions in fairness. In *Advances in Neural Information Processing Systems*, pages 6414–6423, 2017.

[53] B. Salimi, H. Parikh, M. Kayali, L. Getoor, S. Roy, and D. Suciu. Causal relational learning. In *Proceedings of the 2020 International Conference on Management of Data, SIGMOD Conference 2020, June 14-19, 2020*, pages 241–256. ACM, 2020.

[54] B. Salimi, L. Rodriguez, B. Howe, and D. Suciu. Interventional fairness: Causal database repair for algorithmic fairness. In P. A. Boncz, S. Manegold, A. Ailamaki, A. Deshpande, and T. Kraska, editors, *Proceedings of the 2019 International Conference on Management of Data, SIGMOD Conference 2019, Amsterdam, The Netherlands, June 30 - July 5, 2019*, pages 793–810. ACM, 2019.

[55] S. Schelter, F. Biessmann, T. Januschowski, D. Salinas, S. Seufert, G. Szarvas, M. Vartak, S. Madden, H. Miao, A. Deshpande, et al. On challenges in machine learning model management. *IEEE Data Eng. Bull.*, 41(4):5–15, 2018.

[56] S. Schelter, Y. He, J. Khilnani, and J. Stoyanovich. Fairprep: Promoting data to a first-class citizen in studies on fairness-enhancing interventions. In A. Bonifati, Y. Zhou, M. A. V. Salles, A. Böhm, D. Olteanu, G. H. L. Fletcher, A. Khan, and B. Yang,

editors, *Proceedings of the 23nd International Conference on Extending Database Technology, EDBT 2020, Copenhagen, Denmark, March 30 - April 02, 2020*, pages 395–398. OpenProceedings.org, 2020.

[57] D. Sculley, G. Holt, D. Golovin, E. Davydov, T. Phillips, D. Ebner, V. Chaudhary, M. Young, J.-F. Crespo, and D. Dennison. Hidden technical debt in machine learning systems. In *Advances in neural information processing systems*, pages 2503–2511, 2015.

[58] P. Stone, R. Brooks, E. Brynjolfsson, R. Calo, O. Etzioni, G. Hager, J. Hirschberg, S. Kalyanakrishnan, E. Kamar, S. Kraus, K. Leyton-Brown, D. Parkes, W. Press, A. A. Saxenian, J. Shah, M. Tambe, and A. Teller. One hundred year study on artificial intelligence: Report of the 2015-2016 study panel. *Stanford University*, 2016.

[59] J. Stoyanovich, S. Amer-Yahia, and T. Milo. Making interval-based clustering rank-aware. In A. Ailamaki, S. Amer-Yahia, J. M. Patel, T. Risch, P. Senellart, and J. Stoyanovich, editors, *EDBT 2011, 14th International Conference on Extending Database Technology, Uppsala, Sweden, March 21-24, 2011, Proceedings*, pages 437–448. ACM, 2011.

[60] J. Stoyanovich and B. Howe. Nutritional labels for data and models. *IEEE Data Eng. Bull.*, 42(3):13–23, 2019.

[61] J. Stoyanovich, B. Howe, S. Abiteboul, G. Miklau, A. Sahuguet, and G. Weikum. Fides: Towards a platform for responsible data science. In *Proceedings of the 29th International Conference on Scientific and Statistical Database Management, Chicago, IL, USA, June 27-29, 2017*, pages 26:1–26:6. ACM, 2017.

[62] J. Stoyanovich and A. Lewis. Teaching responsible data science: Charting new pedagogical territory. *CoRR*, abs/1912.10564, 2019.

[63] J. Stoyanovich, J. J. Van Bavel, and T. V. West. The imperative of interpretable machines. *Nature Machine Intelligence*, 2:197–199, 2020.

[64] J. Stoyanovich, K. Yang, and H. V. Jagadish. Online set selection with fairness and diversity constraints. In M. H. Böhlen, R. Pichler, N. May, E. Rahm, S. Wu, and K. Hose, editors, *Proceedings of the 21th International Conference on Extending Database Technology, EDBT 2018, Vienna, Austria, March 26-29, 2018*, pages 241–252. OpenProceedings.org, 2018.

[65] J. Surowiecki. *The wisdom of crowds.* Anchor, 2005.

[66] The European Union. Regulation (EU) 2016/679: General Data Protection Regulation (GDPR). 2016.

[67] The New York City Council. A local law to amend the administrative code of the city of new york, in relation to the sale of automated employment decision tools. `https://legistar.council.nyc.gov/LegislationDetail.aspx?ID=4344524&GUID=B051915D-A9AC-451E-81F8-6596032FA3F9`, 2020.

[68] J. Yang. The future of work: Protecting workres' civil rights in the digital age. *Testimony before the Education and Labor Committee, United States House of Representatives*, 2020.

[69] K. Yang, V. Gkatzelis, and J. Stoyanovich. Balanced ranking with diversity constraints. In S. Kraus, editor, *Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence, IJCAI 2019, Macao, China, August 10-16, 2019*, pages 6035–6042. ijcai.org, 2019.

[70] K. Yang, J. R. Loftus, and J. Stoyanovich. Causal intersectionality for fair ranking. *CoRR*, abs/2006.08688, 2020.

[71] K. Yang and J. Stoyanovich. Measuring fairness in ranked outputs. In *Proceedings of the 29th International Conference on Scientific and Statistical Database Management, Chicago, IL, USA, June 27-29, 2017*, pages 22:1–22:6. ACM, 2017.

[72] K. Yang, J. Stoyanovich, A. Asudeh, B. Howe, H. V. Jagadish, and G. Miklau. A nutritional label for rankings. In G. Das, C. M. Jermaine, and P. A. Bernstein, editors, *Proceedings of the 2018 International Conference on Management of Data, SIGMOD Conference 2018, Houston, TX, USA, June 10-15, 2018*, pages 1773–1776. ACM, 2018.

[73] B. Zhang and A. Dafoe. Artificial intelligence: American attitudes and trends. *Center for the Governance of AI, Future of Humanity Institute, University of Oxford*, 2019.

[74] J. Zhang and E. Bareinboim. Fairness in decision-making - the causal explanation formula. In S. A. McIlraith and K. Q. Weinberger, editors, *Proceedings of the Thirty-Second AAAI Conference on Artificial Intelligence, (AAAI-18), the 30th innovative Applications of Artificial Intelligence (IAAI-18), and the 8th AAAI Symposium on Educational Advances in Artificial Intelligence (EAAI-18), New Orleans, Louisiana, USA, February 2-7, 2018*, pages 2037–2045. AAAI Press, 2018.

IN DETAIL

To predict and serve?

Predictive policing systems are used increasingly by law enforcement to try to prevent crime before it occurs. But what happens when these systems are trained using biased data? **Kristian Lum** and **William Isaac** consider the evidence – and the social consequences

Main image: Maciej Bledowski/Bigstock.com

Kristian Lum, PhD is the lead statistician at the Human Rights Data Analysis Group

William Isaac, MPP is a doctoral candidate in the Department of Political Science at Michigan State University

In late 2013, Robert McDaniel – a 22-year-old black man who lives on the South Side of Chicago – received an unannounced visit by a Chicago Police Department commander to warn him not to commit any further crimes. The visit took McDaniel by surprise. He had not committed a crime, did not have a violent criminal record, and had had no recent contact with law enforcement. So why did the police come knocking?

It turns out that McDaniel was one of approximately 400 people to have been placed on Chicago Police Department's "heat list". These individuals had all been forecast to be potentially involved in violent crime, based on an analysis of geographic location and arrest data. The heat list is one of a growing suite of predictive "Big Data" systems used in police departments across the USA and in Europe to attempt what was previously thought impossible: to stop crime before it occurs.[1]

This seems like the sort of thing citizens would want their police to be doing. But predictive policing software – and the policing tactics based on it – has raised serious concerns among community activists, legal scholars, and sceptical police chiefs. These concerns include: the apparent conflict with protections against unlawful search and seizure and the concept of reasonable suspicion; the lack of transparency from both police departments and private firms regarding how predictive policing models are built; how departments utilise their data; and whether the programs unnecessarily target specific groups more than others.

But there is also the concern that police-recorded data sets are rife with systematic bias. Predictive policing software is designed to learn and reproduce patterns in data, but if biased data is used to train these predictive models, the models will reproduce and in some cases amplify those same biases. At best, this renders the predictive models ineffective. At worst, it results in discriminatory policing.

Bias in police-recorded data

Decades of criminological research, dating to at least the nineteenth century, have shown that police databases are not a complete census of all criminal offences, nor do they constitute a representative random sample.[2–5] Empirical evidence suggests that police officers – either implicitly or explicitly – consider race and ethnicity in their determination of which persons to detain and search and which neighbourhoods to patrol.[6,7]

If police focus attention on certain ethnic groups and certain neighbourhoods, it is likely that police records will systematically over-represent those groups and neighbourhoods. That is, crimes that occur in locations frequented by police are more likely to appear in the database simply because that is where the police are patrolling.

Bias in police records can also be attributed to levels of community trust in police, and the desired amount of local policing – both of which can be expected to vary according to geographic location and the demographic make-up of communities. These effects manifest as unequal crime reporting rates throughout a precinct. With many of the crimes in police databases being citizen-reported, a major source of

What is predictive policing?

According to the RAND Corporation, predictive policing is defined as "the application of analytical techniques – particularly quantitative techniques – to identify likely targets for police intervention and prevent crime or solve past crimes by making statistical predictions".[13] Much like how Amazon and Facebook use consumer data to serve up relevant ads or products to consumers, police departments across the United States and Europe increasingly utilise software from technology companies, such as PredPol, Palantir, HunchLabs, and IBM to identify future offenders, highlight trends in criminal activity, and even forecast the locations of future crimes.

What is a synthetic population?

A synthetic population is a demographically accurate individual-level representation of a real population – in this case, the residents of the city of Oakland. Here, individuals in the synthetic population are labelled with their sex, household income, age, race, and the geo-coordinates of their home. These characteristics are assigned so that the demographic characteristics in the synthetic population match data from the US Census at the highest geographic resolution possible.

How do we estimate the number of drug users?

In order to combine the NSDUH survey with our synthetic population, we first fit a model to the NSDUH data that predicts an individual's probability of drug use within the past month based on their demographic characteristics (i.e. sex, household income, age, and race). Then, we apply this model to each individual in the synthetic population to obtain an estimated probability of drug use for every synthetic person in Oakland. These estimates are based on the assumption that the relationship between drug use and demographic characteristics is the same at the national level as it is in Oakland. While this is probably not completely true, contextual knowledge about the local culture in Oakland leads us to believe that, if anything, drug use is even more widely and evenly spread than indicated by national-level data. While some highly localised "hotspots" of drug use may be missed by this approach, we have no reason to believe the location of those should correlate with the locations indicated by police data.

bias may actually be community-driven rather than police-driven. How these two factors balance each other is unknown and is likely to vary with the type of crime. Nevertheless, it is clear that police records do not measure crime. They measure some complex interaction between criminality, policing strategy, and community–police relations.

Machine learning algorithms of the kind predictive policing software relies upon are designed to learn and reproduce patterns in the data they are given, regardless of whether the data represents what the model's creators believe or intend. One recent example of intentional machine learning bias is Tay, Microsoft's automated chatbot launched earlier this year. A coordinated effort by the users of 4chan – an online message board with a reputation for crass digital pranks – flooded Tay with misogynistic and otherwise offensive tweets, which then became part of the data corpus used to train Tay's algorithms. Tay's training data quickly became unrepresentative of the type of speech its creators had intended. Within a day, Tay's Twitter account was put on hold because it was generating similarly unsavoury tweets.

A prominent case of unintentionally unrepresentative data can be seen in Google Flu Trends – a near real-time service that purported to infer the intensity and location of influenza outbreaks by applying machine learning models to search volume data. Despite some initial success, the models completely missed the 2009 influenza A–H1N1 pandemic and consistently over-predicted flu cases from 2011 to 2014. Many attribute the failure of Google Flu Trends to internal changes to Google's recommendation systems, which began suggesting flu-related queries to people who did not have flu.[8] In this case, the cause of the biased data was self-induced rather than internet hooliganism. Google's own system had seeded the data with excess flu-related queries, and as a result Google Flu Trends began inferring flu cases where there were none.

In both examples the problem resides with the data, not the algorithm. The algorithms were behaving exactly as expected – they reproduced the patterns in the data used to train them. Much in the same way, even the best machine learning algorithms trained on police data will reproduce the patterns and unknown biases in police data. Because this data is collected as a by-product of police activity, predictions made on the basis of patterns learned from this data do not pertain to future instances of crime on the whole. They pertain to future instances of *crime that becomes known to police*. In this sense, predictive policing (see "What is predictive policing?") is aptly named: it is predicting future policing, not future crime.

To make matters worse, the presence of bias in the initial training data can be further compounded as police departments use biased predictions to make tactical policing decisions. Because these predictions are likely to over-represent areas that were already known to police, officers become increasingly likely to patrol these same areas and observe new criminal acts that confirm their prior beliefs regarding the distributions of criminal activity. The newly observed criminal acts that police document as a result of these targeted patrols then feed into the predictive policing algorithm on subsequent days, generating increasingly biased predictions. This creates a feedback loop where the model becomes increasingly confident that the locations most likely to experience further criminal activity are exactly the locations they had previously believed to be high in crime: selection bias meets confirmation bias.

Predictive policing case study

How biased are police data sets? To answer this, we would need to compare the crimes recorded by police to a complete record of all crimes that occur, whether reported or not. Efforts such as the National Crime Victimization Survey provide national estimates of crimes of various sorts, including unreported crime. But while these surveys offer some insight into how much crime goes unrecorded nationally, it is still difficult to gauge any bias in police data at the local level because there is no "ground truth" data set containing a representative sample of local crimes to which we can compare the police databases.

We needed to overcome this particular hurdle to assess whether our claims about the effects of data bias and feedback in predictive policing were grounded in reality. Our solution was to combine a demographically representative *synthetic population* of Oakland, California (see "What is a synthetic population?") with survey data from the 2011 National Survey on Drug Use and Health (NSDUH). This approach allowed us to obtain high-resolution *estimates* of illicit drug use from a non-criminal justice, population-based data source (see "How do we estimate the number of drug users?") which we could then compare with police records. In doing so, we find that drug crimes known to police are not a representative sample of all drug crimes.

While it is likely that estimates derived from national-level data do not *perfectly* represent drug use at the local level, we still believe these estimates paint a more accurate picture of drug use in Oakland than the arrest data for several reasons. First, the US Bureau of Justice Statistics – the government body responsible for compiling and analysing criminal justice data – has used data from the NSDUH as a more representative measure of drug use than police reports.[2] Second, while arrest data is collected as a by-product of police activity, the NSDUH is a well-funded survey designed using best practices for obtaining a statistically representative sample. And finally, although there is evidence that some drug users do conceal illegal drug use from public health surveys, we believe that any incentives for such concealment apply much more strongly to police records of drug use than to public health surveys, as public health officials are not empowered (nor inclined) to arrest those who admit to illicit drug use. For these reasons, our analysis continues under the assumption that our public health-derived estimates of drug crimes represent a ground truth for the purpose of comparison.

Figure 1(a) shows the number of drug arrests in 2010 based on data obtained from the Oakland Police Department; Figure 1(b) shows the estimated number of drug users by grid square. From comparing these figures, it is clear that police databases and public health-derived estimates tell dramatically different stories about the pattern of drug use in Oakland. In Figure 1(a), we see that drug arrests in the police database appear concentrated in neighbourhoods around West Oakland (1) and International Boulevard (2), two areas with largely non-white and low-income populations. These neighbourhoods experience about 200 times more drug-related arrests than areas outside of these clusters. In contrast, our estimates (in Figure 1(b)) suggest that drug crimes are much more evenly distributed across the city. Variations in our estimated number of drug users are driven primarily by differences in population density, as the estimated rate of drug use is relatively uniform across the city. This suggests that while drug crimes exist everywhere, drug arrests tend to only occur in very specific locations – the police data appear to disproportionately represent crimes committed in areas with higher populations of non-white and low-income residents.

To investigate the effect of police-recorded data on predictive policing models, we apply a recently published predictive policing algorithm to the drug crime records in Oakland.[9] This algorithm was developed by PredPol, one of the largest vendors of predictive policing systems in the USA and one of the few companies to publicly release its algorithm in a peer-reviewed journal. It has been described by its founders

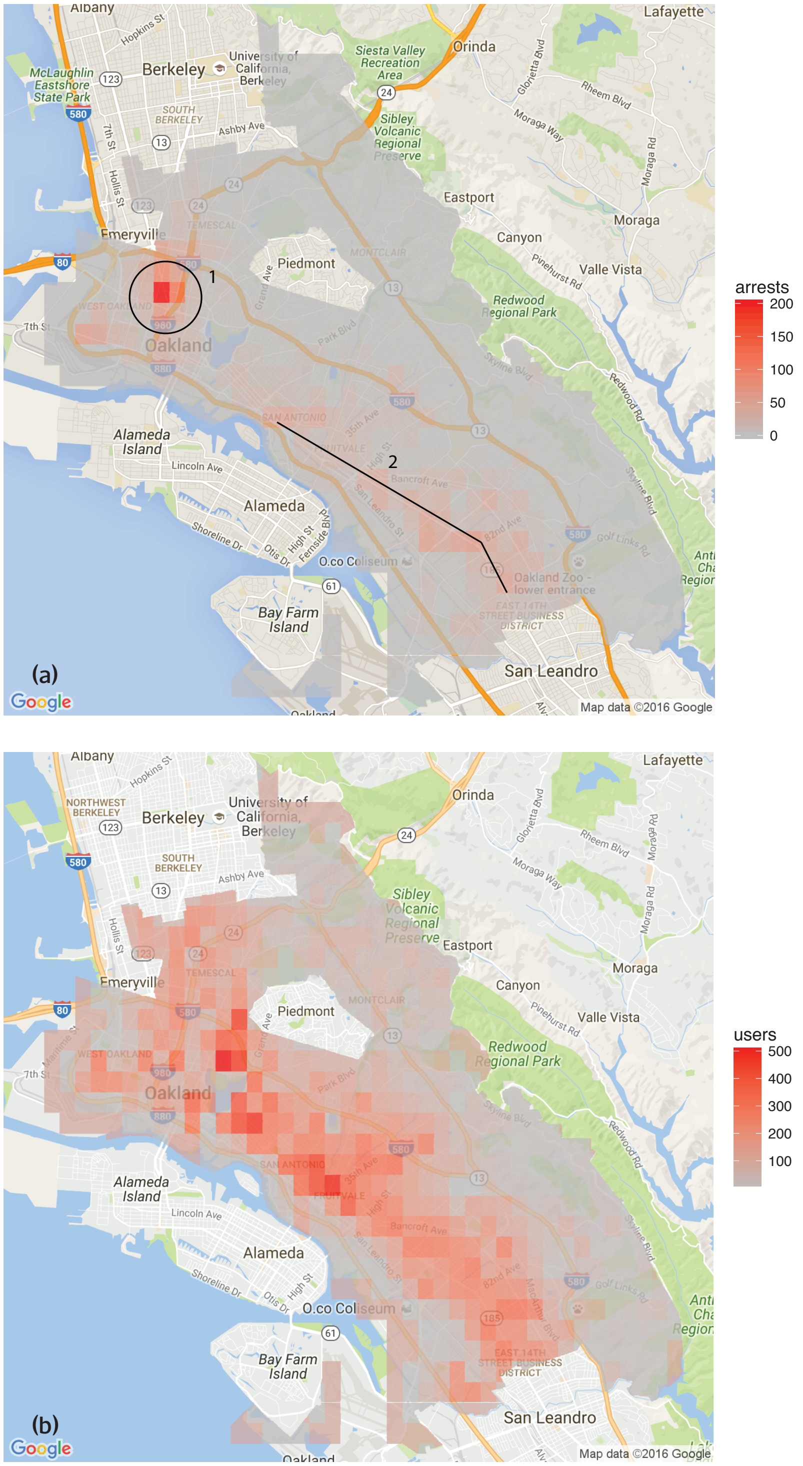


FIGURE 1 (a) Number of drug arrests made by Oakland police department, 2010. (1) West Oakland, (2) International Boulevard. (b) Estimated number of drug users, based on 2011 National Survey on Drug Use and Health

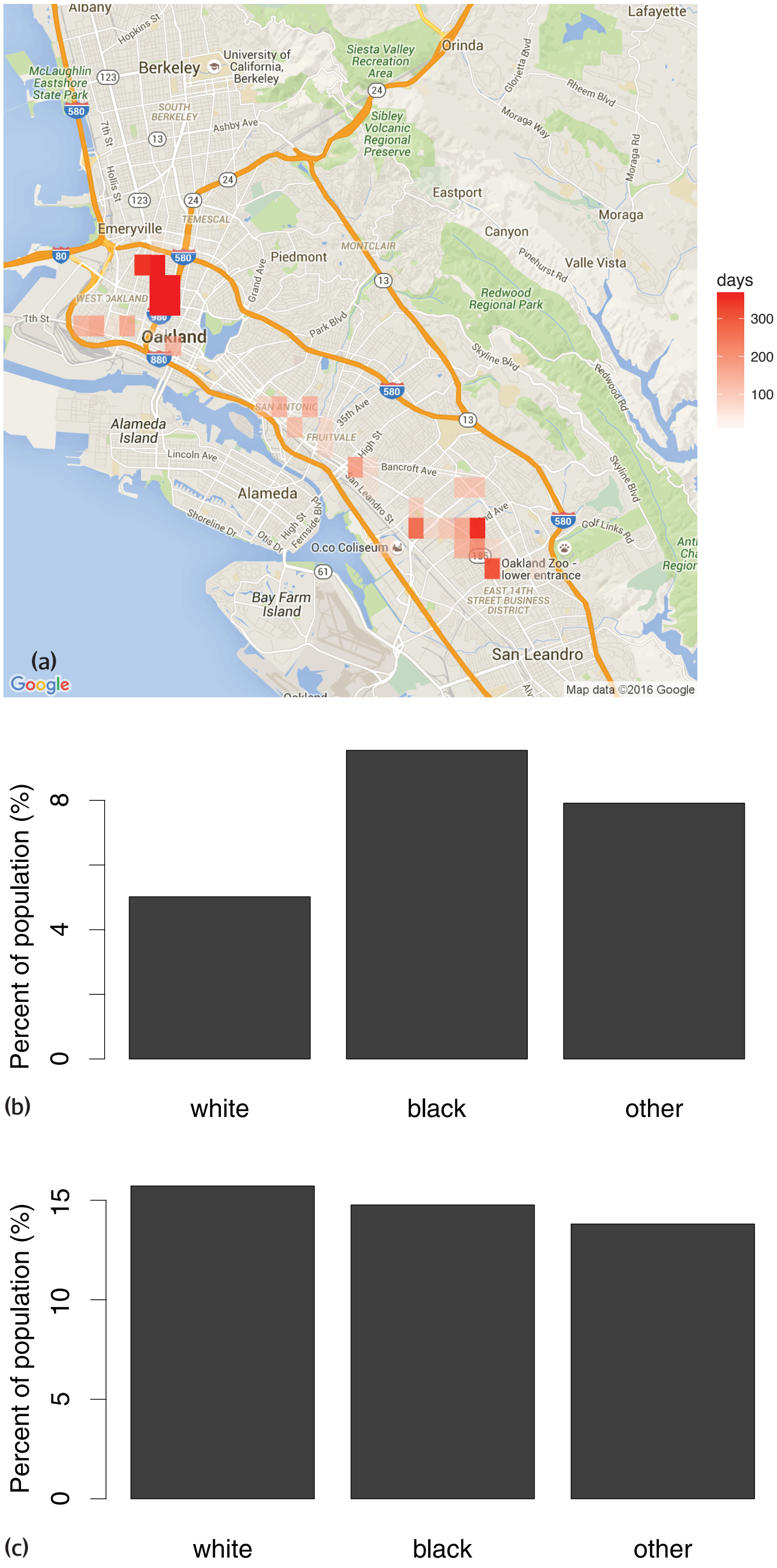


FIGURE 2 (a) Number of days with targeted policing for drug crimes in areas flagged by PredPol analysis of Oakland police data. (b) Targeted policing for drug crimes, by race. (c) Estimated drug use by race

as a parsimonious race-neutral system that uses "only three data points in making predictions: past type of crime, place of crime and time of crime. It uses no personal information about individuals or groups of individuals, eliminating any personal liberties and profiling concerns." While we use the PredPol algorithm in the following demonstration, the broad conclusions we draw are applicable to any predictive policing algorithm that uses unadjusted police records to predict future crime.

The PredPol algorithm, originally based on models of seismographic activity, uses a sliding window approach to produce a one-day-ahead prediction of the crime rate across locations in a city, using only the previously recorded crimes. The areas with the highest predicted crime rates are flagged as "hotspots" and receive additional police attention on the following day. We apply this algorithm to Oakland's police database to obtain a predicted rate of drug crime for every grid square in the city for every day in 2011. We record how many times each grid square would have been flagged by PredPol for targeted policing. This is shown in Figure 2(a).

We find that rather than correcting for the apparent biases in the police data, the model reinforces these biases. The locations that are flagged for targeted policing are those that were, by our estimates, already over-represented in the historical police data. Figure 2(b) shows the percentage of the population experiencing targeted policing for drug crimes broken down by race. Using PredPol in Oakland, black people would be targeted by predictive policing at roughly twice the rate of whites. Individuals classified as a race other than white or black would receive targeted policing at a rate 1.5 times that of whites. This is in contrast to the estimated pattern of drug use by race, shown in Figure 2(c), where drug use is roughly equivalent across racial classifications. We find similar results when analysing the rate of targeted policing by income group, with low-income households experiencing targeted policing at disproportionately high rates. Thus, allowing a predictive policing algorithm to allocate police resources would result in the disproportionate policing of low-income communities and communities of colour.

The results so far rely on one implicit assumption: that the presence of additional policing in a location does not change the number of crimes that are discovered in that location. But what if police officers have incentives to increase their productivity as a result of either internal or external demands? If true, they might seek additional opportunities to make arrests during patrols. It is then plausible that the more time police spend in a location, the more crime they will find in that location.

We can investigate the consequences of this scenario through simulation. For each day of 2011, we assign targeted policing according to the PredPol algorithm. In each location where targeted policing is sent, we increase the number of crimes observed by 20%. These additional simulated crimes then become part of the data set that is fed into PredPol on subsequent days and are factored into future forecasts. We study this phenomenon by considering the ratio of the predicted daily crime rate for targeted locations to that for non-targeted locations. This is shown in Figure 3, where large values indicate that many more crimes are predicted in the targeted locations relative to the non-targeted locations. This is shown separately for the original data (baseline) and the described simulation. If the additional crimes that were found as a result of targeted policing did not affect future predictions, the lines for both scenarios would follow the same trajectory. Instead, we find that this process causes the PredPol algorithm to become increasingly confident that most of the crime is contained in the targeted bins. This illustrates the feedback loop we described previously.

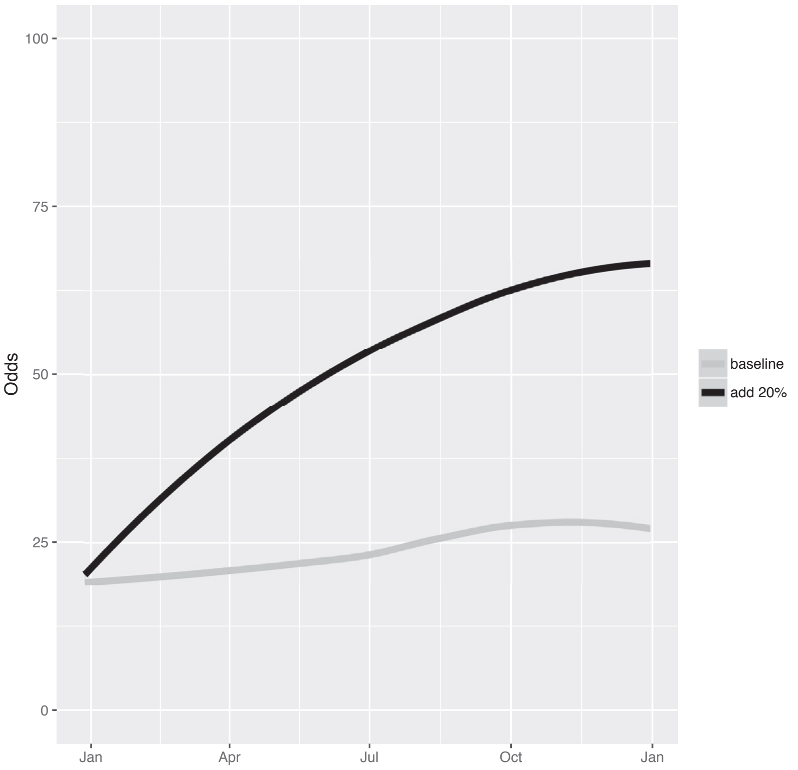


FIGURE 3 Predicted odds of crime in locations targeted by PredPol algorithm, relative to non-targeted locations. 'Baseline' is original Oakland police data. 'Add 20%' simulates the effect of additional crimes being observed in targeted locations

Discussion

We have demonstrated that predictive policing of drug crimes results in increasingly disproportionate policing of historically over-policed communities. Over-policing imposes real costs on these communities. Increased police scrutiny and surveillance have been linked to worsening mental and physical health;[10,11] and, in the extreme, additional police contact will create additional opportunities for police violence in over-policed areas.[12] When the costs of policing are disproportionate to the level of crime, this amounts to discriminatory policy.

In the past, police have relied on human analysts to allocate police resources, often using the same data that would be used to train predictive policing models. In many cases, this has also resulted in unequal or discriminatory policing. Whereas before, a police chief could reasonably be expected to justify policing decisions, using a computer to allocate police attention shifts accountability from departmental decision-makers to black-box machinery that purports to be scientific, evidence-based and race-neutral. Although predictive policing is simply reproducing and magnifying the same biases the police have historically held, filtering this decision-making process through sophisticated software that few people understand lends unwarranted legitimacy to biased policing strategies.

The impact of poor data on analysis and prediction is not a new concern. Every student who has taken a course on statistics or data analysis has heard the old adage "garbage in, garbage out". In an era when an ever-expanding array of statistical and machine learning algorithms are presented as panaceas to large and complex real-world problems, we must not forget this fundamental lesson, especially when doing so can result in significant negative consequences for society. ■

Note

The authors would like to thank Bobbi Isaac, Corwin Smidt, Eric Juenke, James Johndrow, Jim Hawdon, Matt Grossman, Michael Colaresi, Patrick Ball and the members of the HRDAG policing team for insightful conversations on this topic and comments on this article.

References

1. Gorner, J. (2013) Chicago police use "heat list" as strategy to prevent violence. *Chicago Tribune*, 21 August.

2. Langan, P. A. (1995) The racial disparity in U.S. drug arrests. bit.ly/29B2pQu

3. Levitt, S. D. (1998) The relationship between crime reporting and police: Implications for the use of Uniform Crime Reports. *Journal of Quantitative Criminology*, **14**(1), 61–81.

4. Morrison, W. D. (1897) The interpretation of criminal statistics. *Journal of the Royal Statistical Society*, **60**(1), 1–32.

5. Mosher, C. J., Miethe, T. D. and Hart, T. C. (2010) *The Mismeasure of Crime*. Thousand Oaks, CA: Sage Publications.

6. Gelman, A., Fagan, J., & Kiss, A. (2007) An analysis of the New York City Police Department's "stop-and-frisk" policy in the context of claims of racial bias. *Journal of the American Statistical Association*, **102**(479), 813–823.

7. Lange, J. E., Johnson, M. B. and Voas, R. B. (2005) Testing the racial profiling hypothesis for seemingly disparate traffic stops on the New Jersey Turnpike. *Justice Quarterly*, **22**(2), 193–223.

8. Lazer, D., Kennedy, R., King, G. and Vespignani, A. (2014) The parable of Google flu: traps in big data analysis. *Science*, **343**(6176), 1203–1205.

9. Mohler, G. O., Short, M. B., Malinowski, S., Johnson, M., Tita, G. E., Bertozzi, A. L. and Brantingham, P. J. (2015) Randomized controlled field trials of predictive policing. *Journal of the American Statistical Association*, **110**(512), 1399–1411.

10. Sewell, A. A. and Jefferson, K. A. (2016) Collateral Damage: The Health Effects of Invasive Police Encounters in New York City. *Journal of Urban Health*, **93**(1), 42–67.

11. Sewell, A. A., Jefferson, K. A. and Lee, H. (2016) Living under surveillance: gender, psychological distress, and stop-question-and-frisk policing in New York City. *Social Science & Medicine*, **159**, 1–13.

12. Lerman, A. E. and Weaver, V. (2014) Staying out of sight? Concentrated policing and local political action. *Annals of the American Academy of Political and Social Science*, **651**(1), 202–219.

13. Perry, W. L. (2013) *Predictive Policing: The Role of Crime Forecasting in Law Enforcement Operations*. Santa Monica, CA: Rand Corporation.

The VLDB Journal (2015) 24:557–581
DOI 10.1007/s00778-015-0389-y

REGULAR PAPER

Profiling relational data: a survey

Ziawasch Abedjan[1] · Lukasz Golab[2] · Felix Naumann[3]

Received: 1 August 2014 / Revised: 5 May 2015 / Accepted: 13 May 2015 / Published online: 2 June 2015

Abstract Profiling data to determine metadata about a given dataset is an important and frequent activity of any IT professional and researcher and is necessary for various use-cases. It encompasses a vast array of methods to examine datasets and produce metadata. Among the simpler results are statistics, such as the number of null values and distinct values in a column, its data type, or the most frequent patterns of its data values. Metadata that are more difficult to compute involve multiple columns, namely correlations, unique column combinations, functional dependencies, and inclusion dependencies. Further techniques detect conditional properties of the dataset at hand. This survey provides a classification of data profiling tasks and comprehensively reviews the state of the art for each class. In addition, we review data profiling tools and systems from research and industry. We conclude with an outlook on the future of data profiling beyond traditional profiling tasks and beyond relational databases.

✉ Felix Naumann
felix.naumann@hpi.de

Ziawasch Abedjan
abedjan@csail.mit.edu

Lukasz Golab
lgolab@uwaterloo.ca

[1] MIT CSAIL, Cambridge, MA, USA

[2] University of Waterloo, Waterloo, Canada

[3] Hasso Plattner Institute, Potsdam, Germany

1 Data profiling: finding metadata

Data profiling is the set of activities and processes to determine the metadata about a given dataset. Profiling data is an important and frequent activity of any IT professional and researcher. We can safely assume that any reader of this article has engaged in the activity of data profiling, at least by eye-balling spreadsheets, database tables, XML files, etc. Possibly, more advanced techniques were used, such as keyword searching in datasets, writing structured queries, or even using dedicated data profiling tools.

Johnson gives the following definition: “Data profiling refers to the activity of creating small but informative summaries of a database” [79]. Data profiling encompasses a vast array of methods to examine datasets and produce metadata. Among the simpler results are statistics, such as the number of null values and distinct values in a column, its data type, or the most frequent patterns of its data values. Metadata that are more difficult to compute involve multiple columns, such as inclusion dependencies or functional dependencies. Also of practical interest are approximate versions of these dependencies, in particular because they are typically more efficient to compute. In this survey we preclude these and concentrate on exact methods.

Like many data management tasks, data profiling faces three challenges: *(i)* managing the input, *(ii)* performing the computation, and *(iii)* managing the output. Apart from typical data formatting issues, the first challenge addresses the problem of specifying the expected outcome, i.e., determining which profiling tasks to execute on which parts of the data. In fact, many tools require a precise specification of what to inspect. Other approaches are more open and perform a wider range of tasks, discovering all metadata automatically.

The second challenge is the main focus of this survey and that of most research in the area of data profiling: The computational complexity of data profiling algorithms depends on the number or rows, with a sort being a typical operation, but also on the number of columns. Many tasks need to inspect all column combinations, i.e., they are exponential in the number of columns. In addition, the scalability of data profiling methods is important, as the ever-growing data volumes demand disk-based and distributed processing.

The third challenge is arguably the most difficult, namely meaningfully interpreting the data profiling results. Obviously, any discovered metadata refer only to the given data instance and cannot be used to derive schematic/semantic properties with certainty, such as value domains, primary keys, or foreign key relationships. Thus, profiling results need interpretation, which is usually performed by database and domain experts.

Tools and algorithms have tackled these challenges in different ways. First, many rely on the capabilities of the underlying DBMS, as many profiling tasks can be expressed as SQL queries. Second, many have developed innovative ways to handle the individual challenges, for instance using indexing schemes, parallel processing, and reusing intermediate results. Third, several methods have been proposed that deliver only approximate results for various profiling tasks, for instance by profiling samples. Finally, users may be asked to narrow down the discovery process to certain columns or tables. For instance, there are tools that verify inclusion dependencies on user-suggested pairs of columns, but cannot automatically check inclusion between all pairs of columns or column sets.

Systematic data profiling, i.e., profiling beyond the occasional exploratory SQL query or spreadsheet browsing, is usually performed with dedicated tools or components, such as IBM's Information Analyzer, Microsoft's SQL Server Integration Services (SSIS), or Informatica's Data Explorer.[1] These approaches follow the same general procedure: A user specifies the data to be profiled and selects the types of metadata to be generated. Next, the tool computes the metadata in batch mode, using SQL queries and/or specialized algorithms. Depending on the volume of the data and the selected profiling results, this step can last minutes to hours. Results are usually displayed in a vast collection of tabs, tables, charts, and other visualizations to be explored by the user. Typically, discoveries can then be translated to constraints or rules that are then enforced in a subsequent cleansing/integration phase. For instance, after discovering that the most frequent pattern for phone numbers is `(ddd)ddd-dddd`, this pattern can be promoted to a *rule* stating that all phone numbers must be formatted accordingly. Most data cleansing tools can then either transform differently formatted numbers or mark them as improper.

We focus our discussion on relational data, the predominant format of traditional data profiling methods, but we do cover data profiling for other data models in Sect. 7.2.

1.1 Use-cases for data profiling

Data profiling has many traditional use-cases, including the data exploration, data cleansing, and data integration scenarios. Statistics about data are also useful in query optimization. Finally we describe several domain-specific use-cases, such as scientific data management and big data analytics.

Data exploration Database administrators, researchers, and developers are often confronted with new datasets, about which they know nothing. Examples include data files downloaded from the Web, old database dumps, or newly gained access to some DBMS. In many cases, such data have no known schema, no or old documentation, etc. Even if a formal schema is specified, it might be incomplete, for instance specifying only the primary keys but no foreign keys. A natural first step is to understand how the data are structured, what they are about, and how much of them there are.

Such manual data exploration, or data gazing[2], can and should be supported with data profiling techniques. Simple, ad hoc SQL queries can reveal some insight, such as the number of distinct values, but more sophisticated methods are needed to efficiently and systematically discover metadata. Furthermore, we cannot always expect an SQL expert as the explorer, but rather "data enthusiasts" without formal computer science training [68]. Thus, automated data profiling is needed to provide a basis for further analysis. Morton et al. [107] recognize that a key challenge is overcoming the current assumption of data exploration tools that data are "clean and in a well-structured relational format." Often data cannot be analyzed and visualized as is.

Database management A basic form of data profiling is the analysis of individual columns in a given table. Typically, the generated metadata include various counts, such as the number of values, the number of unique values, and the number of non-null values. These metadata are often part of the basic statistics gathered by a DBMS. An optimizer uses them to estimate the selectivity of operators and perform other optimization steps. Mannino et al. [99] give a survey of statistics collection and its relationship to database optimization. More advanced techniques use histograms of value distributions, functional dependencies, and unique column combinations to optimize range queries [118] or for dynamic reoptimization [80].

[1] See Sect. 6 for a more comprehensive list of tools.

[2] "Data gazing involves looking at the data and trying to reconstruct a story behind these data. […] Data gazing mostly uses deduction and common sense." [104]

Database reverse engineering Given a "bare" database instance, the task of schema and database reverse engineering is to identify its relations and attributes, as well as domain semantics, such as foreign keys and cardinalities [103, 116]. Hainaut et al. [66] call these metadata "implicit constructs," i.e., those that are not explicitly specified by DDL statements. However, possible sources for reverse engineering are DDL statements, data instances, data dictionaries, etc. The result of reverse engineering might be an entity-relationship model or a logical schema to assist experts in maintaining, integrating, and querying the database.

Data integration Often, the datasets to be integrated are unfamiliar and the integration expert wants to explore the datasets first: How large are they? What data types are needed? What are the semantics of columns and tables? Are there dependencies between tables and among databases?, etc. The vast abundance of (linked) *open data* and the desire and potential to integrate them with local data has amplified this need.

A concrete use-case for data profiling is that of *schema matching*, i.e., finding semantically correct correspondences between elements of two schemata [44]. Many schema matching systems perform data profiling to create attribute features, such as data type, average value length, and patterns, to compare feature vectors and align those attributes with the best matching ones [98, 109].

Scientific data management and integration have created additional motivation for efficient and effective data profiling: When importing raw data, e.g., from scientific experiments or extracted from the Web, into a DBMS, it is often necessary and useful to profile the data and then devise an adequate schema. In many cases, scientific data are produced by non-database experts and without the intention to enable integration. Thus, they often come with no adequate schematic information, such as data types, keys, or foreign keys.

Apart from exploring individual sources, data profiling can also reveal how and how well two datasets can be integrated. For instance, inclusion dependencies across tables from different sources suggest which tables might reasonably be combined with a join operation. Additionally, specialized data profiling techniques can reveal how much two relations overlap in their intent and extent. We discuss these challenges in Sect. 7.1.

Data quality / data cleansing The need to profile a new or unfamiliar set of data arises in many situations, in general to prepare for some subsequent task. A typical use-case is profiling data to prepare a *data cleansing* process. Commercial data profiling tools are usually bundled with corresponding data quality / data cleansing software.

Profiling as a data quality assessment tool reveals data errors, such as inconsistent formatting within a column, missing values, or outliers. Profiling results can also be used to measure and monitor the general quality of a dataset, for instance by determining the number of records that do not conform to previously established constraints [81, 117]. Generated constraints and dependencies also allow for rule-based data imputation.

Big data analytics "Big data," with its high volume, high velocity, and high variety [90], are data that cannot be managed with traditional techniques. Thus, data profiling gains a new importance. Fetching, storing, querying, and integrating big data are expensive, despite many modern technologies: Before exposing an infrastructure to Twitter's firehose, it might be worthwhile to know about properties of the data one is receiving; before downloading significant parts of the linked data cloud, some prior sense of the integration effort is needed; before augmenting a warehouse with text mining results an understanding of its data quality is required. In this context, leading researchers have noted "*If we just have a bunch of datasets in a repository, it is unlikely anyone will ever be able to find, let alone reuse, any of these data. With adequate metadata, there is some hope, but even so, challenges will remain*[…] [7]."

Many big data and related data science scenarios call for data mining and machine learning techniques to explore and mine data. Again, data profiling is an important preparatory task to determine which data to mine, how to import it into the various tools, and how to interpret the results [120].

Further use-cases Knowledge about data types, keys, foreign keys, and other constraints supports data modeling and helps keep data consistent, improves query optimization, and reaps all the other benefits of structured data management. Others have mentioned query formulation and indexing [126] and scientific discovery [75] as further motivation for data profiling. Also, compression techniques internally perform basic data profiling to optimize the compression ratio. Finally, the areas of data governance and data life-cycle management are becoming more and more relevant to businesses trying to adhere to regulations and code. Especially concerned are financial institutions and health care organizations. Again, data profiling can help ascertain which actions to take on which data.

1.2 Article overview and contributions

Data profiling is an important and practical topic that is closely connected to several other data management areas. It is also a timely topic and is becoming increasingly important given the recent trends in data science and big data analytics [108]. While it may not yet be a mainstream term in the database community, there already exists a large body of work that directly and indirectly addresses various aspects of data profiling. The goal of this survey is to classify and describe this body of work and illustrate its relevance to database research and practice. We also show that data profiling is far from a "done deal" and identify several promising directions for future work in this area.

The remainder of this paper is organized as follows. In Sect. 2, we outline and define data profiling based on a new taxonomy of profiling tasks. Sections 3, 4, and 5 survey the state of the art of the three main research areas in data profiling: analysis of individual columns, analysis of multiple columns, and detection of dependencies between columns, respectively. Section 6 surveys data profiling tools from research and industry. We provide an outlook of data profiling challenges in Sect. 7 and conclude this survey in Sect. 8.

2 Profiling tasks

This section presents a classification of data profiling tasks. Figure 1 shows our classification, which includes single-column tasks, multi-column tasks and dependency detection. While dependency detection falls under multi-column profiling, we chose to assign a separate profiling class to this large, complex, and important set of tasks. The classes are discussed in the following subsections. We also highlight additional dimensions of data profiling, such as the type of storage, the approximation of profiling results, as well as the relationship between data profiling and data mining.

Collectively, a set of results of these tasks is called the *data profile* or *database profile*. In general, we assume the dataset itself as our only input, i.e., we cannot rely on query logs, schema, documentation.

2.1 Single-column profiling

A basic form of data profiling is the analysis of individual columns in a given table. Typically, the generated metadata comprise various counts, such as the number of values, the number of unique values, and the number of non-null values. These metadata are often part of the basic statistics gathered by the DBMS. In addition, the maximum and minimum values are discovered and the data type is derived (usually restricted to string versus numeric versus date). More advanced techniques create histograms of value distributions and identify typical patterns in the data values in the form of regular expressions [122]. Data profiling tools display such results and can suggest actions, such as declaring a column with only unique values to be a key candidate or suggesting to enforce the most frequent patterns. As another exemplary use-case, query optimizers in database management systems also make heavy use of such statistics to estimate the cost of an execution plan.

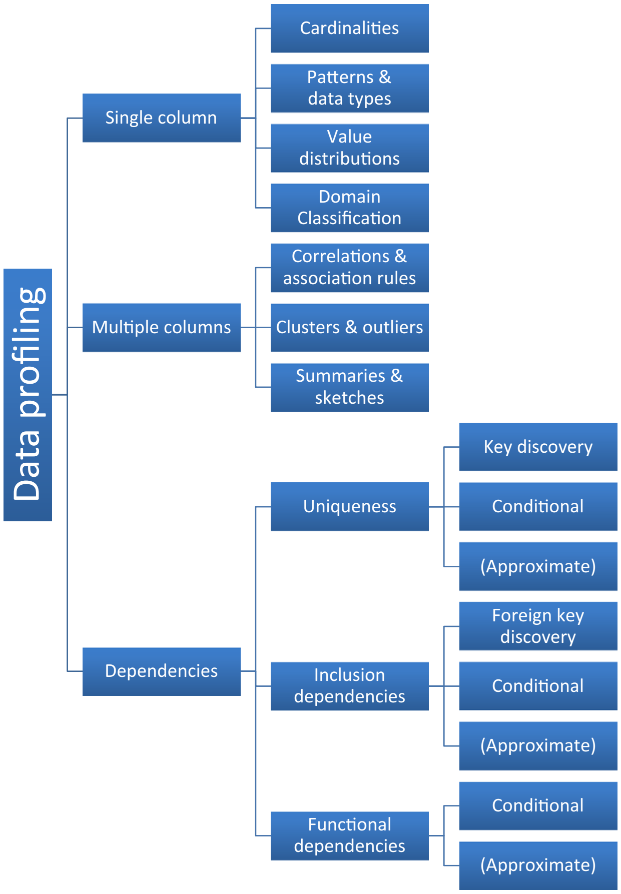


Fig. 1 A classification of traditional data profiling tasks

Table 1 lists the possible and typical metadata as a result of single-column data profiling. Some tasks are self-evident while others deserve more explanation. In Sect. 3, we elaborate on the more interesting tasks, their implementation, and their use.

2.2 Multi-column profiling

The second class of profiling tasks covers multiple columns simultaneously. Multi-column profiling generalizes profiling tasks on single columns to multiple columns and also identifies intervalue dependencies and column similarities. One task is to identify correlations between values through frequent patterns or association rules. Furthermore, clustering approaches that consume values of multiple columns as features allow for the discovery of coherent subsets of data records and outliers. Similarly, generating summaries and sketches of large datasets relates to profiling values across columns.

Table 1 Overview of selected single-column profiling tasks (see Sect. 3 for details)

Category	Task	Description
Cardinalities	num-rows	Number of rows
	value length	Measurements of value lengths (minimum, maximum, median, and average)
	null values	Number or percentage of null values
	distinct	Number of distinct values; sometimes called "cardinality"
	uniqueness	Number of distinct values divided by the number of rows
Value distributions	histogram	Frequency histograms (equi-width, equi-depth, etc.)
	constancy	Frequency of most frequent value divided by number of rows
	quartiles	Three points that divide the (numeric) values into four equal groups
	first digit	Distribution of first digit in numeric values; to check Benford's law
Patterns, data types, and domains	basic type	Generic data type, such as numeric, alphabetic, alphanumeric, date, time
	data type	Concrete DBMS-specific data type, such as varchar, timestamp.
	size	Maximum number of digits in numeric values
	decimals	Maximum number of decimals in numeric values
	patterns	Histogram of value patterns (Aa9…)
	data class	Semantic, generic data type, such as code, indicator, text, date/time, quantity, identifier
	domain	Classification of semantic domain, such as credit card, first name, city, phenotype

Such metadata are useful in many applications, such as data exploration and analytics. Outlier detection is used in data cleansing applications, where outliers may indicate incorrect data values.

Section 4 describes these tasks and techniques in more detail. It comprises multi-column profiling tasks that generate metadata on horizontal partitions of the data, such as values and records, instead vertical partitions, such as columns and column groups. Although the discovery of column dependencies, such as key or functional dependency discovery, also relates to multi-column profiling, we dedicate a separate section to dependency discovery as described next.

2.3 Dependencies

Dependencies are metadata that describe relationships among columns. The difficulties of automatically detecting such dependencies in a given dataset are twofold: First, pairs of columns or larger column sets must be examined, and second, the chance existence of a dependency in the data at hand does not imply that this dependency is meaningful. While much research has been invested in addressing the first challenge and is the focus of this survey, there is less work on semantically interpreting the profiling results.

A common goal of data profiling is to identify suitable keys for a given table. Thus, the discovery of *unique column combinations*, i.e., sets of columns whose values uniquely identify rows, is an important data profiling task [70]. Once unique column combinations have been discovered, a second step is to identify among them the intended primary key of a relation.

A frequent real-world use-case of multi-column profiling is the discovery of foreign keys [96,123] with the help of inclusion dependencies [14,100]. An inclusion dependency states that all values or value combinations from one set of columns also appear in the other set of columns—a prerequisite for a foreign key.

Another form of dependency that is also relevant for data quality is the functional dependency (FD). A functional dependency states that values in one set of columns functionally determine the value of another column. Again, much research has been performed to automatically detect FDs [75,139]. Section 5 surveys dependency discovery algorithms in detail.

Dependencies have many applications: An obvious use-case for functional dependencies is schema normalization. Inclusion dependencies can suggest how to join two relations, possibly across data sources. Their conditional counterparts help explore the data by focusing on certain parts of the dataset.

2.4 Conditional, partial, and approximate solutions

Real datasets usually contain exceptions to rules. To account for this, dependencies and other constraints detected by data profiling can be relaxed. We describe two relaxations below: partial and approximate.

Partial dependencies hold for only a subset of the records, for instance, for 95 % of the records or for all but 10 records. Such dependencies are especially valuable in data cleansing scenarios: They are patterns that hold for almost all records and thus should probably hold for *all* records if the data were clean. Violating records can be extracted and cleansed [129].

Once a partial dependency has been detected, it is interesting to characterize for which records it holds, i.e., if we can find a condition that selects precisely those records. *Conditional dependencies* can specify such conditions. For instance, a conditional unique column combination might state that the column street is unique for all records with city = 'NY.' Conditional inclusion dependencies (CINDs) were proposed by Bravo et al. for data cleaning and contextual schema matching [19]. Conditional functional dependencies (CFDs) were introduced in [46], also for data cleaning.

Approximate dependencies and other constraints are unconditional statements, but are not guaranteed to hold for the entire relation. Such dependencies are often discovered using sampling [76] or other summarization techniques [31]. Their approximate nature is often sufficient for certain tasks, and approximate dependencies can be used as input to the more rigorous task of detecting true dependencies. This survey does not discuss such approximation techniques.

2.5 Types of storage

Data profiling tasks are applicable to a wide range of situations in which data are provided in various forms. For instance, most commercial profiling tools assume that data reside in a relational database, make use of SQL queries and indexes. In other situations, for instance, a csv file is provided and a data profiling method needs to create its own data structures in memory or on disk. And finally, there are situations in which a mixed approach is useful: Data that were originally in the database are read once and processed further outside the database.

The discussion and distinction of such different situations is relevant when evaluating the performance of data profiling algorithms and tools. Can we assume that data are already loaded into main memory? Can we assume the presence of indices? Are profiling results, which can be quite voluminous, written to disk? Fair comparisons need to establish a level playing field with same assumptions about data storage.

2.6 Data profiling versus data mining

A clear, well-defined, and accepted distinction between data profiling and data mining does not exist. Two criteria are conceivable:

1. Distinction by the object of analysis: instance versus schema or columns versus rows
2. Distinction by the goal of the task: description of existing data versus new insights beyond existing data.

Following the first criterion, Rahm and Do distinguish data profiling from data mining by the number of columns that are examined: "Data profiling focuses on the instance analysis of individual attributes. [...] Data mining helps discover specific data patterns in large datasets, e.g., relationships holding between several attributes" [121]. While this distinction is well defined, we believe several tasks, such as IND or FD detection, belong to data profiling, even if they discover relationships between multiple columns.

We believe a different distinction along both criteria is more useful: Data profiling gathers technical metadata to support data management; data mining and data analytics discovers non-obvious results to support business management with new insights. While data profiling focuses mainly on columns, some data mining tasks, such as rule discovery or clustering, may also be used for identifying interesting characteristics of a dataset. Others, such as recommendation or classification, are not related to data profiling.

With this distinction, we concentrate on data profiling and put aside the broad area of data mining, which has already received unifying treatment in numerous textbooks and surveys. However, in Sect. 4, we address the subset of unsupervised mining approaches that can be applied on unknown data to generate metadata and hence serves the purpose of data profiling.

Classifications of data mining tasks include an overview by Chen et al., who distinguish the kinds of databases (relational, OO, temporal, etc.), the kinds of knowledge to be mined (association rules, clustering, deviation analysis, etc.), and the kinds of techniques to be used [130]. We make a similar distinction in this survey. In particular, we distinguish the different classes of data profiling tasks and then examine various techniques to perform them. We discuss profiling non-relational data in Sect. 7.

2.7 Summary

We summarize this section by connecting the various data profiling tasks with the use-cases mentioned in the introduction. Conceivably, any task can be useful for any use-case, depending on the context, the properties of the data at hand,

Table 2 Data profiling tasks and their primary use-cases

	Database management	Data integration	Data cleansing	Database reverse engineering	Data exploration	Data analytics	Scientific data management
Single-column							
Cardinalities	✓				✓	✓	
Patterns and data types		✓	✓	✓			
Value distributions	✓		✓		✓	✓	
Domain classification		✓	✓	✓			✓
Multi-column							
Correlations					✓	✓	✓
Association rules						✓	✓
Clustering		✓			✓	✓	✓
Outliers			✓				✓
Summaries and sketches			✓		✓	✓	
Dependencies							
Unique column combinations	✓		✓	✓			
Inclusion dependencies	✓	✓		✓	✓		✓
Conditional inclusion dependencies		✓			✓	✓	✓
Functional dependencies	✓		✓	✓	✓		
Conditional functional dependencies			✓		✓	✓	

etc. Table 2 lists the profiling tasks and their primary use-cases.

3 Column analysis

The analysis of the values of individual columns is usually a straightforward task. Table 1 lists the typical metadata that can determined for a given column. The following sections describe each category of tasks in more detail, mentioning possible uses of the respective results. In [104], a book addressing practitioners, several of these tasks are discussed in more detail.

3.1 Cardinalities

Cardinalities or counts of values in a column are the most basic form of metadata. The number of rows in a table (num-rows) reflects how many entities (e.g., customers, orders, items) are represented in the data, and it is relevant to data management systems, for instance to estimate query costs or to assign storage space.

Information about the length of values in terms of characters (value length), including the length of the longest and shortest value and the average length, is useful for schema reverse engineering (e.g., to determine tight data type bounds), outlier detection (e.g., single-character first names), and formatting (dates have the same min-, max- and average length).

The number of empty cells, i.e., cells with null values or empty strings (null values), indicates the (in-)completeness of a column. The number of distinct values (distinct) allows query optimizers to estimate selectivity of selection or join operations: The more distinct values there are, the more selective such operations are. To users, this number can indicate a candidate key by comparing it with the number of rows. Alternatively, this number simply illustrates how many different values are present (e.g., how many customers have ordered something or how many cities appear in an address table).

Determining the number of rows, metadata about value lengths, and the number of null values is straightforward and can be performed in a single pass over the data. Determining the number of *distinct values* is more involved: Either hashing or sorting all values is necessary. When hashing, the number of non-empty buckets must be counted, taking into account hash collisions, which further add to the count. When sorting, a pass through the sorted data counts the number of values, where groups of same values are counted only once.

From the number of distinct values the *uniqueness* can be calculated, which is typically defined as the number of unique values divided by the number of rows. Note that the number of distinct values can also be estimated using the minHash technique discussed in Sect. 4.3.

Apart from determining the exact number of distinct values, query optimization is a strong incentive to *estimate* those counts in order to predict query execution plan costs without actually reading the entire data. Because approximate profiling is not the focus of this survey, we give only two exemplary pointers. Haas et al. [65] base their estimation on data samples and describe and empirically compare various estimators from the literature. Other works do scan the entire data but use only a small amount of memory to hash the values and estimate the number of distinct values, an early example being [11].

3.2 Value distribution

Value distributions are more fine-grained cardinalities, namely the cardinalities of groups of values. *Histograms* are among the most common profiling results. A histogram stores frequencies of values within well-defined groups, usually by dividing the ordered set of values into a fixed set of buckets. The buckets of equi-width histograms span value ranges of same length, while the buckets of equi-depth (or equi-height) histograms each represent the same number of value occurrences. A common special case of an equi-depth histogram is dividing the data into four *quartiles*. A more general concept is *biased histograms*, which can adapt their accuracy for different regions[33]. Histograms are used for database optimization as a rough probability distribution to avoid a uniform distribution assumption and thus provide better cardinality estimations [77]. In addition, histograms are interpretable by humans, as their visual representation is easy to comprehend.

The *constancy* of a column is defined as the ratio of the frequency of the most frequent value (possibly a pre-defined default value) and the overall number of values. It thus represents the proportion of some constant value compared with the entire column.

A particularly interesting distribution is the first digit distribution for numeric values. Benford's law [15] states that in naturally occurring numbers the distribution of the first digit d of a number approximately follows $P(d) = \log_{10}(1 + \frac{1}{d})$. Thus, the 1 is expected to be the most frequent leading digit, followed by 2, etc. Benford and others have observed this behavior in many sets of numbers, such as molecular weights, building sizes, and electricity bills. In fact, the law has been used to uncover accounting fraud and other fraudulently created numbers.

Determining the above distributions usually involves a single pass over the column, except for equi-depth histograms (i.e., with fixed bucket sizes) and quartiles, which determine bucket boundaries through sorting. In the same manner or through hashing the most frequent value can be discovered to determine constancy.

Finally, many more things can be counted and aggregated in a column. For instance, some profiling tools and methods determine among others the frequency distribution of soundex code, n-grams, and others, the inverse frequency distribution, i.e., the distribution of the frequency distribution, or the entropy of the frequency distribution of the values in a column [82].

3.3 Types and patterns

The profiling tasks of this section are ordered by increasing semantic richness (see also Table 1). We start with the most simple observable properties, move on to specific patterns of the values of a column, and end with the semantic domain of a column.

Discovering the *basic type* of a column, i.e., classifying it as numeric, alphabetic, alphanumeric, date, or time, is fairly simple: The presence or absence of numeric and non-numeric characters already distinguishes the first three. The latter two can usually be recognized by the presence of numbers only within certain ranges, and by numbers separated in regular patterns by special symbols. Recognizing the actual data type, for instance among the SQL types, is similarly easy. In fact, data of many data types, such as timestamp, boolean, or int, must follow a fixed, sometimes DBMS-specific pattern. When classifying columns into data types, one should choose the most specific data type—in particular avoiding the catchalls char or varchar if possible. For the data types decimal, float, and double, one can additionally extract the maximum number of digits and decimals to determine the metadata size and decimals.

A common and useful data profiling result is the extraction of frequent *patterns* observed in the data of a column. Then, data that do not conform to such a pattern are likely erroneous or ill-formed. For instance, a pattern for phone numbers might be informally encoded as `+dd (ddd) ddd dddd` or as a simple regular expression `\(\d3\)\ − \d3\ − \d4)`.[3] A challenge when determining frequent patterns is to find a good balance between generality and specificity. The regular expression `.*` is the most general and matches any string. On the other hand, the expression `data` allows only that one single string. For the Potter's Wheel tool, Raman and Hellerstein [122] suggest finding the data pattern with the minimal description length (MDL). They model description length as a combination of precision, recall, and conciseness and provide an algorithm to enumerate all possible patterns. The RelIE system was designed

[3] A more detailed regular expression, taking into account different formatting options and different restrictions (e.g., phone numbers cannot begin with a 1), can easily reach 200 characters in length.

for information extraction from textual data [92]. It creates regular expressions based on training data with positive and negative examples by systematically, greedily transforming regular expressions. Finally, Fernau [51] provides a good characterization of the problem of learning regular expressions from data and presents a learning algorithm for the task. This work is also a good starting point for further reading

The semantic *domain* of a column describes not the syntax of its values but their meaning. While a regular expression might characterize a column, labeling it as "phone number" provides a concrete domain. Clearly, this task cannot be fully automated, but some work has been done for common-place domains about persons, places, etc. Zhang et al. take a first step by clustering columns that have the same meaning across the tables of a database [144], which they extend to the particularly difficult area of numeric values in [142]. In [133] the authors take the additional step of matching columns to pre-defined semantics from the person domain. Knowledge of the domain is not only of general data profiling interest, but also of particular interest to schema matching, i.e., the task of finding semantic correspondences between elements of different database schemata.

3.4 Data completeness

Explicit missing data are simple to characterize: For each column, we report the number of tuples with a null or a default value. However, datasets may contain *disguised* missing values. For example, Web forms often include fields whose values must be chosen from pull-down lists. The first value from the pull-down list may be pre-populated on the form, and some users may not replace it with a proper or correct value due to lack of time or privacy concerns. Specific examples include entering 99999 as the zip code of an address or leaving "Alabama" as the pre-populated state (in the US, Alabama is alphabetically the first state). Of course, for some records, Alabama may be the true state.

Detecting disguised default values is difficult. One heuristic solution is to examine each column at a time, and, for each possible value, compute the distribution of the other attribute values [74]. For example, if Alabama is indeed a disguised default value, we expect a large subset of tuples with state = `Alabama` (i.e., those whose true state is different) to form an unbiased sample of the whole relation.

Another instance in which profiling missing data is not trivial involves timestamped data, such as measurement or transaction data feeds. In some cases, tuples are expected to arrive regularly, e.g., in datacenter monitoring, every machine may be configured to report its CPU utilization every minute. However, measurements may be lost en route to the database, and overloaded or malfunctioning machines may not report any measurements at all. [60]. In contrast to detecting missing attribute values, here we are interested in estimating the number of missing tuples. Thus, the profiling task may be to single out the columns identified as being of type timestamp, and, for those that appear to be distributed uniformly across a range, infer the expected frequency of the underlying data source and estimate the number of missing tuples. Of course, some timestamp columns correspond to application timestamps with no expectation of regularity, rather than data arrival timestamps. For instance, in an online retailer database, order dates and delivery dates are generally not expected to be scattered uniformly over time.

4 Multi-column analysis

Profiling tasks over a single column can be generalized to projections of multiple columns. For example, there has been work on computing multi-dimensional histograms for query optimization [41,119]. Multi-column profiling also plays an important role in data cleansing, e.g., in assessing and explaining data glitches, which often occur in column combinations [40].

In the remainder of this section, we discuss statistical methods and data mining approaches for generating metadata based on co-occurrences and dependencies of values across attributes. We focus on correlation and rule mining approaches as well as unsupervised clustering and learning approaches; machine learning techniques that require training data or detailed knowledge of the data are beyond the scope of data profiling.

4.1 Correlations and association rules

Correlation analysis reveals related numeric columns, e.g., in an Employees table, age and salary may be correlated. A straightforward way to do this is to compute pairwise correlations among all pairs of columns. In addition to column-level correlations, value-level *associations* may provide useful data profiling information.

Traditionally, a common application of association rules has been to find items that tend to be purchased together based on point-of-sale transaction data. In these datasets, each row is a list of items purchased in a given transaction. An association rule `{bread}` → `{butter}`, for example, states that if a transaction includes bread, it is also likely to include butter, i.e., customers who buy bread also buy butter. A set of items is referred to as an *itemset*, and an association rule specifies an itemset on the left-hand side and another itemset on the right-hand side.

Algorithms for generating association rules from data decompose the problem into two steps [8]:

1. Discover all frequent itemsets, i.e., those whose frequencies in the dataset (i.e., their *support*) exceed some

threshold. For instance, the itemset {`bread`, `butter`} may appear in 800 out of a total of 50,000 transactions for a support of 1.6 %.

2. For each frequent itemset a, generate association rules of the form $l \rightarrow a - l$ with $l \subset a$, whose *confidence* exceeds some threshold. Confidence is defined as the frequency of a divided by the frequency of l, i.e., the conditional probability of l given $a - l$. For example, if the frequency of {`bread`, `butter`} is 800 and the frequency of {`bread`} alone is 1000, then the confidence of the association rule {`bread`} → {`butter`} is 0.8. That is, if bread is purchased, there is an 80 % chance that butter is also purchased in the same transaction.

In the context of relational data profiling, association rules denote relationships or patterns between attribute values among columns. Consider an Employees table with fields name, employee number, department, position, and allowance. We may find a frequent itemset of the form {department = `finance`, position = `assistant manager`, allowance = `$1000`} and a corresponding association rule of the form {department = `finance`, position = `assistant manager`} → {allowance = `$1000`}. This would be the case if most or all assistant managers in the finance department were assigned an allowance budget of $1000.

While the second step mentioned above is straightforward (generating association rules from frequent itemsets), the first step is computationally expensive due to the large number of possible frequent itemsets (or patterns of values) [72]. Popular algorithms for efficiently discovering frequent patterns include Apriori [8], Eclat [141], and FP-Growth [67].

The Apriori algorithm exploits the observation that all subsets of a frequent itemset must also be frequent. In the first iteration, Apriori finds all frequent itemsets of size one, i.e., those containing one item or one attribute value. In the next iteration, only the frequent itemsets of size one are expanded to find frequent itemsets of size two, and so on.

There are also several optimized versions of Apriori, such as DHP [115] and RARM [35]. FP-Growth discovers frequent itemsets without a candidate generation step. It transforms the database into an extended prefix tree of frequent patterns (FP-tree). The FP-Growth algorithm traverses the tree and generates frequent itemsets by pattern growth in a depth-first manner. Finally, Eclat is based on intersecting transaction-id (TID) sets of associated itemsets and is best suited for dealing with large frequent itemsets. Eclat's strategy for identifying frequent itemsets is similar to Apriori.

Negative correlation rules, i.e., those that identify attribute values that *do not* co-occur with other attribute values, may also be useful in data profiling to find anomalies and outliers [21]. However, discovering negative association rules is more difficult, because *infrequent* itemsets cannot be pruned in the same way as frequent itemsets, and therefore, novel pruning rules are required [135].

Finally, we note that in addition to using existing techniques, such as correlations and association rules for profiling, extensions have been proposed, such as discovering linear dependencies between columns [25].

However, in this approach, the user has to choose the subset of attributes to be analyzed. We discuss dependency discovery in more detail in Sect. 5.

4.2 Clustering and outlier detection

Another useful profiling task is to segment the records into homogeneous groups using a clustering algorithm; furthermore, records that do not fit into any cluster may be flagged as outliers. Cluster analysis can identify groups of similar records in a table, while outliers may indicate data quality problems. For example, Dasu and Johnson [36] cluster numeric columns and identify outliers in the data. Furthermore, based on the assumption that data glitches occur across attributes and not in isolation [16], statistical inference has been applied to measure glitch recovery in [39].

Another example of clustering in the context of data profiling is ProLOD++, which applies k-means clustering to RDF relations [1]. We refer the reader to surveys by Jain et al. [78] and Xu and Wunsch II [137] for more details on clustering algorithms for relational data.

4.3 Summaries and sketches

Besides clustering, another way to describe data is to create summaries or sketches [23]. This can be done by sampling or hashing data values to a smaller domain. Sketches have been widely applied to answering approximate queries, data stream processing and estimating join sizes [37,54,111]. Cormode et al. [31] give an overview of sketching and sampling for approximate query processing.

Another interesting task is to assess the similarity of two columns, which can be done using multi-column hashing techniques. The *Jaccard similarity* of two columns A and B is $|A \cap B|/|A \cup B|$, i.e., the number of distinct values they have in common divided by the total number of distinct values appearing in them. This gives the relative number of values that appear in both A and B. Since semantically similar values may have different formats, we can also compute the Jaccard similarity of the n-gram distributions in A and B. If the distinct value sets of columns A and B are not available, we can estimate the Jaccard similarity using their *MinHash signatures* [38].

Table 3 Dependency discovery algorithms

Dependency	**Algorithms**
Uniques	HCA [3], GORDIAN [126], DUCC [70], SWAN [5]
Functional dependencies	TANE [75], FUN [110], FD_Mine [139], Dep-Miner [95], FastFDs [136], FDEP [52], DFD[6]
Conditional functional dependencies	[24], [59], CTANE [47], CFUN [42], FACD [91], FastCFD [47]
Inclusion dependencies	[101], [87], SPIDER [14], ZigZag [102]
Conditional inclusion dependencies	[61], CINDERELLA [13], PLI [13]
Foreign keys	[123], [143]
Denial constraints	FastDC [29]
Differential dependencies	[128]
Sequential dependencies	[57]

5 Dependency detection

We now survey various formalisms for detecting dependencies among columns and algorithms for mining them from data, including keys and unique column combinations (Sect. 5.1), functional dependencies (Sect. 5.2), inclusion dependencies (Sect. 5.3), and other types of dependencies that are relevant to data profiling (Sect. 5.4). Table 3 lists the algorithms that are discussed.

We use the following symbols: R and S denote relational schemata, with r and s denoting instances of R and S, respectively. The number of columns in R is $|R|$ and the number of tuples in r is $|r|$. We refer to tuples of r and s as r_i and s_j, respectively. Subsets of columns are denoted by uppercase X, Y, Z (with $|X|$ denoting the number of columns in X) and individual columns by uppercase A, B, C. Furthermore, we define $\pi_X(r)$ and $\pi_A(r)$ as the projection of r on the attribute set X or attribute A, respectively; thus, $|\pi_X(r)|$ denotes the count of district combinations of the values of X appearing in r. Accordingly, $r_i[A]$ indicates the value of the attribute A of tuple r_i and $r_i[X] = \pi_X(r_i)$. We refer to an attribute value of a tuple as a *cell*.

The number of potential dependencies in r can be exponential in the number of attributes $|R|$; see Fig. 2 for an illustration of all possible subsets of the attributes in Table 4. This means that any dependency discovery algorithm has a worst-case exponential time complexity. There are two classes of heuristics that have appeared in the literature. Column-based or top-down approaches start with "small" dependencies (in terms of the number of attributes they reference) and work their way to larger dependencies, pruning candidates along the way whenever possible. Row-based or bottom-up approaches attempt to avoid repeated scanning of the entire relation during candidate generation. While these approaches cannot reduce the worst-case exponential complexity of dependency discovery, experimental studies have shown that column-based approaches work well on tables containing a very large number of rows and row-based approaches work well for wide tables [6,113]. For more details on the computational complexity of various Fd and Ind discovery algorithms, we refer the interested reader to [94].

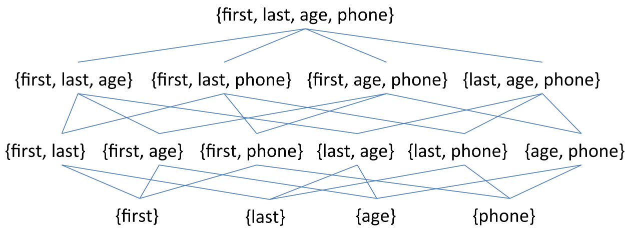


Fig. 2 Powerset lattice for the example Table 4

Table 4 Example dataset

Tuple id	First	Last	Age	Phone
1	Max	Payne	32	1234
2	Eve	Smith	24	5432
3	Eve	Payne	24	3333
4	Max	Payne	24	3333

5.1 Unique column combinations and keys

Given a relation R with instance r, a *unique column combination* (a "unique") is a set of columns $X \subseteq R$ whose projection on r contains only unique value combinations.

Definition 1 (*Unique*) A column combination $X \subseteq R$ is a *unique*, iff $\forall r_i, r_j \in r, i \neq j : r_i[X] \neq r_j[X]$.

Analogously, a set of columns $X \subseteq R$ is a *non-unique column combination* (a "non-unique"), iff its projection on r contains at least one duplicate value combination.

Definition 2 (*Non-unique*) A column combination $X \subseteq R$ is a *non-unique*, iff $\exists r_i, r_j \in r, i \neq j : r_i[X] = r_j[X]$.

Each superset of a unique is also unique while each subset of a non-unique is also a non-unique. Therefore, discovering all uniques and non-uniques can be reduced to the discovery of minimal uniques and maximal non-uniques:

Definition 3 (*Minimal Unique*) A column combination $X \subseteq R$ is a *minimal unique*, iff $\forall X' \subset X : X'$ is a non-unique.

Definition 4 (*Maximal Non-Unique*) A column combination $X \subseteq R$ is a *maximal non-unique*, iff $\forall X' \supset X : X'$ is a unique.

A *primary key* is a unique that was explicitly chosen to be the unique record identifier while designing the table schema. Since the discovered uniqueness constraints are only valid for a relational instance at a specific point of time, we refer to uniques and non-uniques instead of keys and non-keys. A further distinction can be made in terms of possible keys and certain keys when dealing with uncertain data and NULL values [86].

The problem of discovering a minimal unique of size $k \leq n$ is NP-complete [97]. To discover all minimal uniques and maximal non-uniques of a relational instance, in the worst case, one has to visit all subsets of the given relation, no matter the strategy (breadth-first or depth-first) or direction (bottom-up or top-down). Thus, the discovery of all minimal uniques and maximal non-uniques of a relational instance is an NP-hard problem and even the solution set can be exponential [64].

Given $|R|$, there can be $\binom{|R|}{\frac{|R|}{2}} \geq 2^{\frac{|R|}{2}}$ minimal uniques in the worst case, as all combinations of size $\frac{|R|}{2}$ can simultaneously be minimal uniques.

5.1.1 Gordian*: row-based discovery*

Row-based algorithms require multiple runs over all column combinations as more and more rows are considered. They benefit from the intuition that non-uniques can be detected without considering every row. A recursive unique discovery algorithm that works this way is Gordian [126]. The algorithm consists of three parts: *(i)* Pre-organize the data in form of a prefix tree, *(ii)* find maximal non-uniques by traversing the prefix tree, *(iii)* compute minimal uniques from maximal non-uniques.

The prefix tree is stored in main memory. Each level of the tree represents one column of the table, whereas each branch stands for one distinct tuple. Tuples that have the same values in their prefix share the corresponding branches. For example, all tuples that have the same value in the first column share the same node cells. The time to create the prefix tree depends on the number of rows; therefore, this can be a bottleneck for very large datasets.

The traversal of the tree is based on the cube operator [63], which computes aggregate functions on projected columns. Non-unique discovery is performed by a depth-first traversal of the tree for discovering maximum repeated branches, which constitute maximal non-uniques.

After discovering all maximal non-uniques, Gordian computes all minimal uniques by generating minimal combinations that are not covered by any of the maximal non-uniques. In [126] it is stated that this complementation step needs only quadratic time in the number of minimal uniques, but the presented algorithm implies cubic runtime: For each non-unique, the updated set of minimal uniques must be *simplified* by removing redundant uniques. This simplification requires quadratic runtime in the number of uniques. As the number of minimal uniques is bound linearly by the number s of maximal non-uniques, the runtime of the unique generation step is $O(s^3)$.

Gordian exploits the intuition that non-uniques can be discovered faster than uniques. Non-unique discovery can be aborted as soon as one repeated value is discovered among the projections. The prefix structure of the data facilitates this analysis. It is stated that the algorithm is polynomial in the number of tuples for data with a Zipfian distribution of values. Nevertheless, in the worst case, Gordian has exponential runtime.

The generation of minimal uniques from maximal non-uniques can be a bottleneck if there are many maximal non-uniques. Experiments showed that in most cases the unique generation dominates the runtime [3]. Furthermore, the approach is limited by the available main memory. Although data may be compressed because of the prefix structure of the tree, the amount of processed data may still be too large to fit in main memory.

5.1.2 Column-based traversal of the column lattice

The problem of finding minimal uniques is comparable to the problem of finding frequent itemsets [8]. The well-known Apriori approach is applicable to minimal unique discovery, working bottom-up as well as top-down. With regard to the powerset lattice of a relational schema, the Apriori algorithms generate all relevant column combinations of a certain size and verify those at once. Figure 2 illustrates the powerset lattice for the running example in Table 4. The effectiveness and theoretical background of those algorithms is discussed by Giannela and Wyss [55]. They presented three breadth-first traversal strategies: a bottom-up, a top-down, and a hybrid traversal strategy.

Bottom-up unique discovery traverses the powerset lattice of the schema R from the bottom, beginning with all 1-*combinations* toward the top of the lattice, which is the $|R|$-*combination*. The prefixed number k of *k-combination* indicates the size of the combination. The same notation applies for *k-candidates*, *k-uniques*, and *k-non-uniques*. To generate the set of *2-candidates*, we generate all pairs of

1-non-uniques. *k-candidates* with $k > 2$ are generated by extending the $(k-1)$-*non-uniques* by another non-unique column. After the candidate generation, each candidate is checked for uniqueness. If it is identified as a non-unique, the *k-candidate* is added to the list of *k-non-uniques*.

If the candidate is verified as unique, its minimality has to be checked. The algorithm terminates when $k = |1\text{-}non\text{-}uniques|$. A disadvantage of this candidate generation technique is that redundant uniques and duplicate candidates are generated and tested.

The Apriori idea can also be applied to the top-down approach. Having the set of identified *k-uniques*, one has to verify whether the uniques are minimal. Therefore, for each *k-unique*, all possible $(k-1)$-*subsets* have to be generated and verified. The hybrid approach generates the kth and $(n-k)$th levels simultaneously. Experiments have shown that in most datasets, uniques usually occur in the lower levels of the lattice, which favors bottom-up traversal [3].

HCA is an improved version of the bottom-up Apriori technique [3]. HCA optimizes the candidate generation step, applies statistical pruning and considers functional dependencies that have been inferred on the fly. In terms of candidate generation, HCA applies the optimized join that was introduced for frequent itemset mining [8]. HCA generates candidates by combining only $(k-1)$-*non-uniques* that share the first $k-2$ elements. If no such two non-uniques exist, no candidates are generated and the algorithm terminates before reaching the last level of the powerset lattice. Further pruning can be achieved by considering value histograms and distinct counts that can be retrieved on the fly in previous levels. For example, consider the *1-non-uniques* last and age from Table 4. The column combination {last,age} cannot be a unique based on the value distributions. While the value "`Payne`" occurs three times in last, the column age contains only two distinct values. That means at least two of the rows containing the value "`Payne`" also have a duplicate value in the age column. Using the count distinct values, HCA detects functional dependencies on the fly and leverages them to avoid unnecessary uniqueness checks.

While HCA improves existing bottom-up approaches, it does not perform the early identification of non-uniques in a row-based manner done by GORDIAN. Thus, GORDIAN is faster on datasets with many non-uniques, but HCA works better on datasets with many minimal uniques.

5.1.3 DUCC: traversing the lattice via random walk

While the breadth-first approach for discovering minimal uniques gives the most pruning, a depth-first approach might work well if there are relatively few minimal uniques that are scattered on different levels of the powerset lattice. Depth-first detection of unique column combinations resembles the problem of identifying the most promising paths through the lattice to discover existing minimal uniques and avoid unnecessary uniqueness checks. DUCC is a depth-first approach that traverses the lattice back and forth based on the uniqueness of combinations [70]. Following a random walk principle by randomly adding columns to non-uniques and removing columns from uniques, DUCC traverses the lattice in a manner that resembles the border between uniques and non-uniques in the powerset lattice of the schema.

DUCC starts with a seed set of *2-non-uniques* and picks a seed at random. Each k-combination is checked using the superset/subset relations and pruned if any of them subsumes the current combination. If no previously identified combination subsumes the current combination DUCC performs uniqueness verification. Depending on the verification, DUCC proceeds with an unchecked $(k-1)$-subset or $(k-1)$-superset of the current k-combination. If no seeds are available, it checks whether the set of discovered minimal uniques and maximal non-uniques correctly complement each other. If so, DUCC terminates; otherwise, a new seed set is generated by complementation.

DUCC also optimizes the verification of minimal uniques by using a position list index (PLI) representation of values of a column combination. In this index, each position list contains the tuple ids that correspond to the same value combination. Position lists with only one tuple id can be discarded, so that the position list index of a unique contains no position lists. To obtain the PLI of a column combination, the position lists in PLIs of all contained columns have to be cross-intersected. In fact, DUCC intersects two PLIs in a similar way in which a hash join operator would join two relations. As a result of using PLIs, DUCC can also apply row-based pruning, because the total number of positions decreases with the size of column combinations. Intuitively, combining columns makes the contained combination values more specific and therefore more likely to be distinct.

DUCC has been experimentally compared to HCA, a column-based approach, and GORDIAN, a row-based unique discovery algorithm. Since DUCC combines row-based and column-based pruning, it performs significantly better [70]. Experiments on smaller datasets showed that while HCA outperforms GORDIAN on low-dimensional data with many uniques, GORDIAN outperforms HCA on datasets with many attributes but few uniques [3].

Furthermore the random walk strategy allows a distributed application of DUCC for better scalability.

5.1.4 SWAN: an incremental approach

SWAN maintains a set of indexes to efficiently find the new sets of minimal uniques and maximal non-uniques after inserting or deleting tuples [5]. SWAN builds such indexes based on existing minimal uniques and maximal non-uniques in a way that avoids a full table scan. SWAN consists of two main components: the *Inserts Handler* and the *Deletes Handler*. The Inserts Handler takes as input a set of inserted tuples, checks all minimal uniques for uniqueness, finds the new sets of minimal uniques and maximal non-uniques, and updates the repository of minimal uniques and maximal non-uniques accordingly. Similarly, the Deletes Handler takes as input a set of deleted tuples, searches for duplicates in all maximal non-uniques, finds the new sets of minimal uniques and maximal non-uniques, and updates the repository accordingly.

5.2 Functional dependencies

A *functional dependency* (FD) over R is an expression of the form $X \rightarrow A$, indicating that $\forall r_i, r_j \in r$ if $r_i[X] = r_j[X]$; then, $r_i[A] = r_j[A]$. That is, any two tuples that agree on X must also agree on A. We refer to X as the left-hand side (LHS) and A as the right-hand side (RHS). Given r, we are interested in finding all non-trivial and minimal FDs $X \rightarrow A$ that hold on r, with non-trivial meaning $A \cap X = \emptyset$ and minimal meaning that there must not be any FD $Y \rightarrow A$ for any $Y \subset X$. A naive solution to the FD discovery problem is as follows.

```
For each possible RHS $A$
    For each possible LHS $X \in R \backslash A$
        For each pair of tuples $r_i$ and $r_j$
            If $r_i[X] = r_j[X]$ and $r_i[A] \neq r_j[A]$ Break
    Return $X \rightarrow A$
```

This algorithm is prohibitively expensive: For each of the $|R|$ possibilities for the RHS, it tests $2^{(|R|-1)}$ possibilities for the LHS, each time having to scan r multiple times to compare all pairs of tuples. However, notice that for $X \rightarrow A$ to hold, the number of distinct values of X must be the same as the number of distinct values of XA—otherwise at least one combination of values of X that is associated with more than one value of A, thereby breaking the FD [75]. Thus, if we precompute the number of distinct values of each combination of one or more columns, the algorithm simplifies to:

```
For each possible RHS $A$
    For each possible LHS $X \in R \backslash A$
        If $|\pi_X(r)| = |\pi_{XA}(r)|$
            Return $X \rightarrow A$
```

Recall Table 4. We have $|\pi_{\text{phone}}(r)| = |\pi_{\text{age,phone}}(r)| = |\pi_{\text{last,phone}}(r)|$. Thus, phone → age and phone → last hold. Furthermore, $|\pi_{\text{last,age}}(r)| = |\pi_{\text{last,age,phone}}(r)|$, implying $\{\text{last,age}\} \rightarrow \text{phone}$.

The above algorithm is still inefficient due to the need to compute distinct value counts and test all possible column combinations. As was the case with unique discovery, FD discovery algorithms employ row-based (bottom-up) and column-based (top-down) optimizations, as discussed below. Figure 3 lists the algorithms that are discussed, along with their extensions to conditional FD discovery, which are covered in Sect. 5.2.4. An extensive experimental evaluation of various FD discovery algorithms on different datasets, scaling in both the number of rows and the number of columns, is presented in [113].

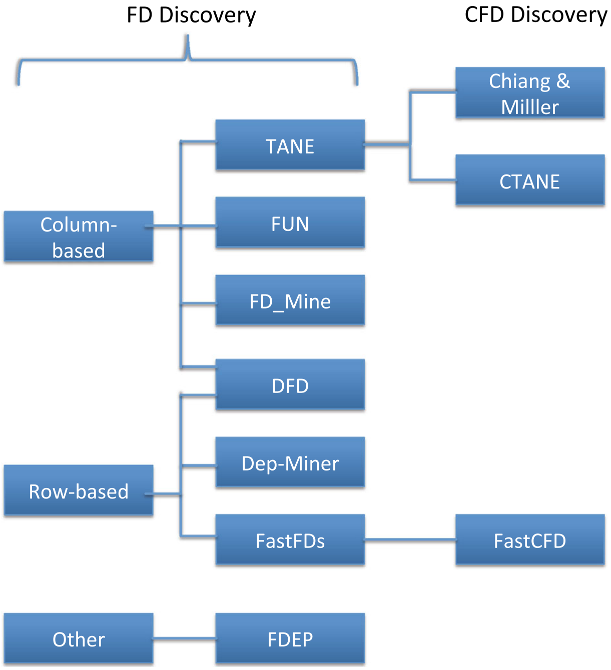


Fig. 3 Classification of algorithms for functional dependency discovery and their extensions to conditional functional dependencies

5.2.1 Column-based algorithms

As was the case with uniques, Apriori-like approaches can help prune the space of FDs that need to be examined, thereby optimizing the first two lines of the above straightforward algorithms. TANE [75], FUN [110], and FD_Mine [139] are three algorithms that follow this strategy, with FUN and FD_Mine introducing additional pruning rules beyond TANE's based on the properties of FDs. They start with sets of single columns in the LHS and work their way up the powerset lattice in a *level-wise* manner. Since only minimal FDs need to be returned, it is not necessary to test possible FDs whose LHS is a superset of an already found FD with the same RHS. For instance, in Table 4, once we find that *phone* → *age* holds, we do not need to consider {first,phone} → age, {last,phone} → age, etc.

Additional pruning rules may be formulated from Armstrong's axioms, i.e., we can prune from consideration those FDs that are logically implied by those we have found so far. For instance, if we find that $A \rightarrow B$ and $B \rightarrow A$, then we can prune all LHS column sets including B, because A

and B are equivalent [139]. Another pruning strategy is to ignore columns sets that have the same number of distinct values as their subsets [110]. Returning to Table 4, observe that phone → first does not hold. Since $|\pi_{\text{phone}}(r)| = |\pi_{\text{last,phone}}(r)| = |\pi_{\text{age,phone}}(r)| = |\pi_{\text{last,age,phone}}(r)|$, we know that adding last and/or age to the LHS cannot lead to a valid FD with first on the RHS. To determine these cardinalities the approaches use a so-called partition data structure, which is similar to the PLIs of Sect. 5.1.3.

5.2.2 *Row-based algorithms*

Row-based algorithms examine pairs of tuples to determine LHS candidates. Dep-Miner [95] and FastFDs [136] are two examples; the FDEP algorithm [52] is also row-based, but the way it ultimately finds FDs that hold is different.

The idea behind row-based algorithms is to compute the so-called difference sets for each pair of tuples, which are the columns on which the two tuples differ. Table 5 enumerates the difference sets in the data from Table 4. Next, we can find candidate LHS's from the difference sets as follows. Pick a candidate RHS, say, phone. The difference sets that include phone, with phone removed are as follows: {first,last,age}, {first,age}, {age}, {last} and {first,last}. This means that there exist pairs of tuples with different values of phone and also with different values of these five difference sets. Next, we find minimal subsets of columns that have a non-empty intersection with each of these difference sets. Such subsets are exactly the LHS's of minimal FDs with phone as the RHS: If two tuples have different values of phone, they are guaranteed to have different values of the columns in the above minimal subsets, and therefore, they do not cause FD violations. Here, there is only one such minimal subset, {last,age}, giving {last,age} → phone. If we repeat this process for each possible RHS, and compute minimal subsets corresponding to the LHS's, we obtain the set of minimal FDs. The main difference among row-based FD discovery algorithms is in how they find the minimal subsets.

A recent approach to FD discovery is DFD, which adapts the column-based and row-based pruning of the unique discovery approach DUCC to the problem of FD discovery [6]. DFD decomposes the attribute lattice into $|R|$ lattices, considering each attribute as a possible RHS of an FD. For the remaining $|R| - 1$ attributes, DFD applies a random walk approach by pruning supersets of FD LHS's and subsets of non-FD LHS's.

Table 5 Difference sets computed from Table 4

Tuple ID pair	Difference set
(1,2)	first, last, age, phone
(1,3)	first, age, phone
(1,4)	age, phone
(2,3)	last, phone
(2,4)	first, last, phone
(3,4)	first

DFD has been experimentally compared to TANE, which is a column-based approach, and FastFDs, which is row-based [6]. The experiments confirm that row-based approaches work well on high-dimensional tables with a relatively small number of tuples, while column-based approaches, such as TANE, perform better on low-dimensional tables with a large number of rows. DFD, which benefits from row-based and column-based pruning, performs significantly better than TANE and FastFDs, unless the table has very many tuples and very few columns or vice versa.

5.2.3 *Partial and approximate functional dependencies*

While FDs were meant for schema design and were enforced by the database management system, there are many instances in which a database may not satisfy some FDs exactly. For example, the application semantics may have changed over time and FD enforcement was disabled, or the database may have been created by integrating conflicting data sources. As a result, it is useful to discover *partial* or *soft* FDs, i.e., those which "almost hold," perhaps with a few exceptions.

A common definition of "almost holding" or "confidence" is the relative size of the largest subset of r on which a given FD holds exactly divided by $|r|$ [58,85]. For example, if we remove tuple 1 from Table 4, the FD *last* → *phone* holds exactly, and therefore, its confidence is $\frac{3}{4}$. The CORDS system for finding soft FDs uses a slightly different definition: The confidence of $X \to A$ is $\frac{|\pi_X(r)|}{|\pi_{XA}(r)|}$ [76]. Other definitions involve computing the number of tuples or tuple pairs that do not violate the FD divided by $|r|$ or $|r|^2$, respectively [85].

A related notion is that of *approximate* FD inference, in which partial or exact FDs are generated from a sample of a relation [76,85]. Of course, even if an FD holds exactly on a subset of a relation, it may hold partially on the whole relation. Approximate FD inference is appealing from a computational standpoint as it requires only a sample of the data.

5.2.4 *Conditional functional dependencies*

Conditional functional dependencies (CFDs), proposed in [46], encode FDs that hold only on well-defined subsets of r. For instance, {first,last} → age does not hold on the entire relation in Table 4, but it does hold on a subset of it where first = Eve. Formally, a CFD consists of two parts: an embedded FD $X \to A$ and an accompanying *pattern tuple* with attributes XA. Each cell of a pattern tuple contains a value from the corresponding attribute's domain or a wildcard symbol "_". A pattern tuple identifies a subset of a relation instance in a natural way: A tuple r_i matches a pattern tuple if it agrees on all of its non-wildcard attributes. In the above example, we can formulate a CFD with an embedded FD {first,last} → age and a pattern tuple (Eve, _, _), meaning that the embedded FD holds only on tuples which match the pattern, i.e., those with first = Eve. We define the *support* of a pattern tuple as the fraction of tuples in r that it matches; for example, the support of (Eve, _, _) in Table 4 is $\frac{2}{4}$.

An important special case occurs when the pattern tuple has no wildcards. For example, the following (admittedly accidental) CFD holds on Table 4: age → phone with a pattern tuple (32, 1234). In other words, if age = 32, then phone = 1234. These special cases, which resemble instance-level association rules (that have 100 % *confidence*), are referred to as *constant* CFDs.

Additionally, as was the case with traditional FDs, we can define approximate CFDs as those that hold on the subset specified by the pattern tableau with some exceptions. For the case of confidence defined as the minimum number of tuples that must be removed to make the CFD hold, [32] gives algorithms for computing summaries that allow the confidence of a CFD to be estimated with guaranteed accuracy.

CFD discovery involves a larger search space than FD discovery: In addition to detecting embedded FDs, we must also find the pattern tuples. CFD discovery algorithms typically extend existing FD discovery algorithms: For example, CTANE [47] and the algorithm from [24] extend TANE, while FastCFD [47] extends FastFDs (see Fig. 3).

Additionally, two simpler problems have been studied. The first is to discover pattern tuples given an embedded FD [59]. The output of this technique is an (approximately) smallest set of pattern tuples, each leading to an approximate CFD with a confidence exceeding a user-supplied confidence threshold, the union of which has a support that exceeds a user-supplied support threshold. The second problem is to report only the constant CFDs. For this problem, CFDMiner has been proposed CFDs [47], which is based on frequent itemset mining, as well as FACD [91], which includes more pruning rules. Also, CFUN, an extension of FUN to generating *frequent* constant CFDs that exceed a given support threshold, has been proposed in [42].

5.3 Inclusion dependencies

An *inclusion dependency* (IND) between column A of relation R and column B of relation S, written $R.A \subseteq S.B$, or $A \subseteq B$ when the relations are clear from context, asserts that each value of A appears in B. Similarly, for two sets of columns X and Y, we write $R.X \subseteq S.Y$, or $X \subseteq Y$, when each distinct combinations of values in X appears in Y. We refer to $R.A$ or $R.X$ as the left-hand side (LHS) and $S.B$ or $S.Y$ as the right-hand side (RHS). INDs with a single-column LHS and RHS are referred to as *unary* and those with multiple columns in the LHS and RHS are called *n-ary*.

A naive solution to IND discovery in relation instances r and s is to try to match each possible LHS with each possible RHS, as shown below.

```
For each column combination $X$ in $R$
  For each column combination $Y$ in $S$
  with $|Y| = |X|$
    If $\forall x \in \pi_X(r)\ \exists y \in \pi_Y(s)$ such that $x = y$
      Return $X \subseteq Y$
```

Note that for any considered X and Y, we can stop as soon as we find a value combination of X that does not appear in Y. Still, this is not an efficient approach as it repeatedly scans r and s when testing the possible LHS and RHS combinations.

5.3.1 Generating unary inclusion dependencies

For the special case of unary INDs, a common approach is to preprocess the data to speed up the subsequent IND discovery. De Marchi et al. [101] propose a technique that scans the database and builds value indices, which are similar to inverted indices. Table 6 shows excerpts of two relations instances, one with columns A and B and the other with columns C and D, and the corresponding value index. The index contains an entry for each value occurring in the database, followed by a list of columns in which this value appears. It is now straightforward to find the INDs: For each possible LHS column, we check if there exists another column that occurs in every row of the value index that contains the LHS column. In Table 6, we have $A \subseteq C$ (whenever A appears in the value index, so does B) and $D \subseteq B$.

The SPIDER algorithm [14] is another example, which preprocesses the data by sorting the values of each column and writing them to disk. Next, each sorted stream, corresponding to the values of one particular attribute, is consumed in parallel in a cursor-like manner, and an IND $A \subseteq B$ can be discarded as soon as we detect a value in A that is not present in B.

Table 6 Excerpts of two relation instances and the corresponding value index

A	B	C	D	Value	Columns
1	3	1	3	1	A, C
1	4	2	3	2	A, C
2	3	4	4	3	B, D
1	5	7	4	4	B, D
				5	B
				7	C

5.3.2 Generating n-ary inclusion dependencies

Once all unary INDs have been discovered, De Marchi et al. [101] give a level-wise algorithm, similar to the TANE algorithm for FD discovery, which constructs INDs with i columns from those with $i-1$ columns and prunes INDs that cannot be true. Additionally, hybrid algorithms have been proposed in [87,102] that combine bottom-up and top-down traversal for additional pruning.

The BINDER algorithm uses divide and conquer principles to handle larger datasets than related work [114]. In the divide step, it splits the input dataset horizontally into partitions and vertically into buckets with the goal to fit each partition into main memory. In the conquer step, BINDER then validates the set of all possible inclusion dependency candidates, which are created in the same fashion as in [101], against the partitions. Processing one partition after another, the validation constructs two indexes on each partition, a dense index and an inverted index, and uses them to efficiently prune invalid candidates from the result set.

5.3.3 Partial and approximate inclusion dependencies

Similar to partial FDs, partial INDs have been defined as those that almost hold. Using the notion of removing the fewest tuples so that the remainder satisfies the IND exactly, we can define the strength or confidence of a partial IND $X \subseteq Y$ as $\frac{|\pi_X(r)|-|\pi_X(r)/\pi_Y(r)|}{|\pi_X(r)|}$ [96,101]. That is, the confidence is the number of distinct values of X that appear in Y divided by the number of distinct values of X. An equivalent bag-semantics version of this definition is to divide the number of tuples whose X-values appear in Y by the total number of tuples [61]. According to both definitions, the confidence of $B \subseteq D$ in Table 6 is $\frac{3}{4}$. Most of the algorithms discussed above can be extended to discover partial INDs.

5.3.4 Conditional inclusion dependencies

Similar to CFDs, *conditional inclusion dependencies* (CINDs) represent INDs that hold only on well-defined subsets of relations [19]. A CIND consists of an embedded standard IND $R.X \subseteq S.Y$ and an accompanying pattern tuple with attributes $R.X_p$ and $S.Y_p$, where $X \cap X_p = \emptyset$ and $Y \cap Y_p = \emptyset$. A CIND specifies that for the subset of R that matches the X_p-values of the pattern tuple, all the X-values must appear in Y, and furthermore, the Y_p values of these tuples in S must match the Y_p-values of the pattern tuple.

For example, suppose a business maintains a Customers table, keyed by cid, and including a column class indicating the class of the customer (e.g., gold or silver). Furthermore, suppose a Services table maintains the services that customers subscribe to, including a service id (sid), a cid and the type of service (e.g., hardware or software). Let Services.cid $\subseteq$ Customers.cid be the embedded IND and let (Services.type $=$ `software`, Customers.class $=$ `gold`) be a pattern tuple. This CIND asserts that the customer ids in the Services table must be drawn from the customer ids in the Customers table, and moreover, gold customers can obtain only software services. On the other hand, a pattern tuple Services.type $=$ `software` implies that only the software services must have customer ids drawn from those in the Customers table (e.g., perhaps hardware services are provided to customers stored in a different table).

Given an embedded IND, the algorithm from [61], which also applies to CFDs, finds pattern tuples that lead to partial CINDs with a confidence satisfying a user-supplied threshold. Similarly, Bauckmann et al. [13] start with a set of approximate INDs and find pattern tuples to turn these into CINDs; however, in contrast to [61], they are not constrained to a single embedded IND. The authors present two algorithms: CINDERELLA, which is based on the Apriori algorithm for association rule mining and employs a breadth-first traversal of the powerset lattice, and PLI, which employs a depth-first traversal instead.

5.3.5 Generating foreign keys

IND discovery is a precursor to foreign key detection: A foreign key must satisfy the corresponding inclusion dependency but not all INDs are foreign keys. For example, multiple tables may contain auto-increment columns that serve as surrogate keys, and while inclusion dependencies among them may exist, they are not foreign keys. Once INDs have been discovered, additional heuristics have been proposed, which essentially rank the discovered INDs according to their likelihood of being foreign keys [96,123,143]. A very simple rule may be that if the LHS and RHS have similar names, then A may be a foreign key. It is also useful to examine the set of discovered INDs as a whole: For instance, foreign keys usually are not also primary keys that serve as foreign keys for other tables, and furthermore, a primary key is often referenced by multiple foreign keys in multiple tables, meaning that a primary key should appear in the RHS of multiple INDs, with the LHS's being the foreign keys. More complex rules may reference value distributions; for example, the values in a foreign key column should form a random sample of the values in the corresponding primary key column.

5.4 Other dependencies

Having outlined the algorithms for discovering traditional dependencies and their extensions, we now discuss other types of dependencies related to data profiling. Recently, an extension of FastFDs called FastDC was proposed for discovering *denial constraints*, which are universally quantified first-order logic formulas that subsume FDs, CFDs, INDs and many others [29].

Also, functional dependencies have recently been generalized to *differential dependencies* in [128]. A differential dependency $X \rightarrow Y$ states that if two tuples have "close" values of X (say, the edit distance between them is small), then their A values must also be close.[4] For example, in a financial database, it may be true that if two tuples have similar values of date (e.g., within seven days), then their price values must also be similar (e.g., within 100 dollars). Row- and column-based approaches to discovering differential dependencies were given in [128].

Another interesting class of dependencies involve *order*. For instance, it may be useful to discover that if r is sorted on some attribute A, it is also sorted on B, which gives an order dependency between A and B [56]. This concept was generalized in [57], which proposed *sequential dependencies* (SDs). An SD states that when sorted on A, any two consecutive values of B must be within a predefined range. Given a complete SD, including the attributes A and B as well as the range, [57] gives an algorithm for discovering ranges of values of A in which the SD is approximately satisfied. To the best of our knowledge, the general problem of SD discovery from data is open.

5.5 Summary and discussion

Dependency discovery has been a popular research area in data management. Many of the algorithms and techniques for dependency discovery are based upon classical data mining solutions, such as the Apriori algorithm for efficient generation of association rules. Additional technical challenges arise in the context of conditional dependencies, and novel search space pruning strategies have been developed based on the properties of the given dependencies.

Data profiling results can be not only complex, but also very large. For instance, it is not uncommon to find thousands of functional dependencies in a given dataset. To handle this and focus users on the most important, interesting, or surprising ones, ranking profiling results can help, as Chu et al. [29] show for denial constraints. They suggest two functions, namely succinctness and coverage, to assess their interestingness. Similar interestingness functions for CFDs are given by Chiang and Miller [24]. Additionally, Andritsos et al. [9] show how to rank FDs according to their information content. Furthermore, as we discussed earlier, post-processing methods have been proposed to determine which of the discovered inclusion dependencies are likely to be foreign keys; however, we are not aware of corresponding techniques for uniques and FDs.

6 Profiling tools

Whenever data are too voluminous to fit on a screen or a sheet of paper, data profiling is performed. Even lacking explicit profiling tools, much can already be done with data management tools, such as spreadsheet software, SQL queries, search capabilities of text editors or simply by "eyeballing" the data. Such methods to become acquainted with a new set of data are probably familiar to most readers. The simple method of *sorting* the values of a column can already reveal minimum and maximum values, and scrolling through that sorted data intuits the value distribution, including the number of null values, which are typically sorted to the very beginning or end, and the uniqueness of a column. Finding the median or average values requires additional calculations, whereas it is infeasible to detect dependencies with such simple means.

To allow a more powerful and integrated approach to data profiling, software companies have developed data profiling tools, mostly to profile data residing in relational databases. Most tools discussed in this survey are part of a larger software suite, either for data integration or for data cleansing. We first give an overview of tools that were created in the context of a research project (see Table 7 for a listing). Then, we give a brief glimpse of the vast set of commercial tools with profiling capabilities (see Table 8 for a listing).

6.1 Research tools

In the research literature, data profiling tools are often embedded in data cleaning systems. For example, the Bellman [38] data quality browser supports column analysis (counting the number of rows, distinct values, and NULL values, finding the most frequently occurring values, etc.), and key detection (up to four columns). It also provides a column similarity functionality that finds columns whose value or n-gram distributions are similar; this is helpful for discovering potential foreign keys and join paths. Furthermore, an interesting application of Bellman was to profile the evolution of a database using value distributions and correlations [37]: Which tables change over time and in what ways (insertions, deletions, modifications), and which groups of tables tend to change in the same way. The Potters Wheel tool [122] also supports column analysis, in particular, detecting data types and syntactic structures/patterns.

Data profiling functionality is also included in the MADLib toolkit for scalable in-database analytics [71], including column statistics, such as count, count distinct,

[4] Differential dependencies also generalize *matching dependencies* [49] (if two tuples have close values of X, their A values must be exactly the same) and *metric functional dependencies* [89] (if two tuples have the same values of X, their A values must be close).

Table 7 Research tools with data profiling capabilities

Tool	Main goal	Profiling capabilities
Bellman [38]	Data quality browser	Column statistics, column similarity, candidate key discovery
Potters Wheel [122]	Data quality, ETL	Column statistics (including value patterns)
Data Auditor [58]	Rule discovery	CFD and CIND discovery
RuleMiner [28]	Rule discovery	Denial constraint discovery
MADLib [71]	Machine learning	Simple column statistics

Table 8 Commercial data profiling tools/components with their primary capabilities and application areas

Vendor and product	Features → Focus
Attacama DQ Analyzer	Statistics, patterns, uniques → Data exploration, ETL
IBM InfoSphere Information Analyzer	Statistics, patterns, multi-column dependencies → Data exchange, integration, cleansing
Informatica Data Quality	Structure, completeness, anomalies, dependencies → Business rules, cleansing
Microsoft SQL Server Data Profiling Task	Statistics, patterns, dependencies → ETL, cleansing
Oracle Enterprise Data Quality	Statistics, patterns, multi-column dependencies, text profiling → Quality assessment, business rules, cleansing
Paxata Adaptive Data Preparation	Statistics, histograms, semantic data types → Exploration, cleansing, sharing
SAP Information Steward	Statistics, patterns, semantic data types, dependencies → ETL, modeling, cleansing
Splunk Enterprise / Hunk	Patterns, data mining → Search, analytics, visualization
Talend Data Profiler	Statistics, patterns, dependencies → ETL, cleansing
Trifacta	Statistics, patterns → Quality assessment, data transformation

minimum and maximum values, quantiles, and the *k* most frequently occurring values.

Recent data quality tools are dependency-driven: Classical dependencies, such as FDs and INDs, as well as their conditional extensions, may be used to express the intended data semantics, and dependency violations may indicate possible data quality problems. Most research systems require users to supply data quality rules and dependencies, such as GDR [138], Nadeef [34], Semandaq [45] and StreamClean [84]. These systems focus on languages for specifying rules and generating repairs. However, data quality rules are not always known Apriori in unfamiliar and undocumented datasets, in which case data profiling, and dependency discovery in particular, is an important prerequisite to data cleaning. Notably, many of these systems perform a focused profiling of counting the number of inconsistent tuples with respect to the given rules.

There are at least two research prototype systems that perform rule discovery to some degree: Data Auditor [58] and RuleMiner [28]. Data Auditor requires an FD as input and generates corresponding CFDs from the data. Additionally, Data Auditor considers FDs similar to the one that is provided by the user and generates corresponding CFDs. The idea is to see if a slightly modified FD can generate a more suitable CFD for the given relation instance. On the other hand, RuleMine does not require any rules as input and instead it is designed to generate all reasonable rules from a given dataset. RuleMiner expresses the discovered rules as *denial constraints*, which are universally quantified first-order logic formulas that subsume FDs, CFDs, INDs and many others. Some of the rules it finds are instance-specific and therefore more general than those a typical data profiling tool would find; for example, in a database of income tax records, RuleMiner might find that if one person, A, has a higher salary than another, B, then Person A must have a higher tax rate than Person B.

6.2 Commercial tools

Because data profiling is such an important capability for many data management tasks, there are various commercial data profiling applications. In many cases, they are a part of a data quality / data cleansing tool suite, to support the use-case of profiling for frequent patterns or rules and then cleaning those records that violate them. In addition, most Extract–Transform–Load tools have some profiling capabilities.

Table 8 mentions prominent examples of current commercial tools, together with their capabilities and application focus, based on the respective product documentations. It is beyond the scope of this survey to provide a market overview or compile feature matrices. We also deliberately refrain from providing static URLs for the various products, because commercial Web sites are too fickle.

Finally, and as mentioned before, every database management system collects and maintains base statistics about the tables it manages. However, they do not readily expose those metadata, the metadata are not always up-to-date and sometimes based only on samples, and their scope is usually limited to simple counts and cardinalities.

7 Next generation profiling

Recent trends in data management have added new challenges but also opportunities for data profiling. First, under the *big data* umbrella, industry and research have turned their attention to data that they do not own or have not made use of yet. Data profiling can help assess which data might be useful and reveals the yet unknown characteristics of such new data. Second, much of the data that shall be exploited is of non-traditional type for data profiling, i.e., non-relational, non-structured (textual), and heterogeneous. And it is often truly "big," both in terms of schema and in terms of data. Many existing profiling methods cannot adequately handle that kind of data: Either they do not scale well, or there simply are no methods yet. Third, different and new data management architectures and frameworks have emerged, including distributed systems, key-value stores, multi-core- or main-memory-based servers, column-oriented layouts, streaming input, etc. We discuss some of these trends and their implications toward data profiling. A more elaborate overview of upcoming challenges of data profiling is in [108].

7.1 Profiling for integration

An important use-case of traditional data profiling methods is data integration. Knowledge about the properties of different data sources is important to create correct schema mappings and data transformations, and to correctly standardize and cleanse the data. For instance, knowledge of inclusion dependencies might hint upon ways to join two yet unrelated tables.

However, data profiling can reach beyond such supportive tasks and assess the *integrability* or ease of integration of datasets and thus also indicate the necessary integration effort, which is vital to project planning. Integration effort might be expressed in terms of similarity, but also in terms of manmonths or in terms of which tools are needed.

Like integration projects themselves, integrability has two dimensions, namely schematic fit and data fit. *Schematic fit* is the degree to which two schemata complement and overlap each other and can be determined using schema matching techniques [44]. Smith et al. [127] have recognized that schema matching techniques often play the role of profiling tools: Rather than using them to derive schema mappings and perform data transformation, they might assess project feasibility. Finally, the mere matching of schema elements might not suffice as a profiling-for-integration result: Additional column metadata can provide further details about the integration difficulty.

Data fit is the (estimated) number of real-world objects that are represented in both datasets, or that are represented multiple times in a single dataset and how different they are. Such multiple representations are typically identified using entity matching methods (also known as record linkage, duplicate detection, etc.) [27]. However, estimating the number of matches without actually performing the matching on the entire dataset is an open problem.

7.2 Profiling non-relational data

With the rapid growth of the World Wide Web, semi-structured data, such as XML and RDF data, and non-structured data, such as text document corpora, have become more important. The more flexible structure of non-relational datasets opens new challenges for profiling algorithms. So far, most methods apply only to or were developed for relational data. Below, we give an overview of both existing work that applies traditional profiling algorithms, as well as existing work about data-model-specific profiling approaches, to non-relational data. We focus on the three most relevant non-relational data formats: XML, RDF, and text documents.

7.2.1 XML

XML is the quasi-standard for exchanging data on the Web. Many applications, especially Web services, provide their results as XML documents. Because the XML structure explicitly contains markup and schema information, different profiling approaches have to be considered. Apart from that, Web services themselves are accessible through XML documents, such as WSDL and SOAP files, which are also worth profiling for Web service inspection and categorization.

There has already been a number of research approaches and proposals with a focus on statistical analysis of XML-formatted data. They concentrate either on the DTD structure, the XSD schema structure, or the inherent structure of XML documents. The analysis concentrates on gathering statistics about the number of root elements, attributes, the depth of content models, etc. [26,105,106,124].

Further approaches focus on algorithms that identify traditional relational dependencies in XML data. While Vincent et al. extend the notion of FDs to XML data [132], Yu et al.s [140] present an approach for discovering redundancies based on identified XML FD. There have also been adaptations of unique and key discovery concepts and algorithms to XML data [22]. Due to the more relaxed structure of XML, these approaches identify approximate keys [62] or validate the consistency of the identified keys against XSD definitions [10].

As many XML documents do not refer to a specific schema, a relevant application of profiling approaches is to support the process of schema extraction [17,69]. Additionally, the vast amount of existing documents do not always comply to specified syntactical rules [88], which can be identified via appropriate profiling techniques.

7.2.2 RDF

Although profiling tasks for XML data can easily be adapted to RDF datasets and vice versa, the requirement for RDF data to be machine readable and its important use-case Linked Open Data (LOD) give rise to RDF-specific challenges for data profiling. There are already some tools that generate metadata for a given RDF dataset. For example, LODStats is a stream-based approach for gathering comprehensive statistics about RDF datasets [12].

ProLOD++ provides additional functionalities by applying clustering and rule mining techniques [1]. When profiling RDF data, there are many interesting metadata beyond simple statistics and patterns of RDF statement elements, including synonymously used properties [4], inverse relationships of properties, the conformity and consistence of RDF structured data to the corresponding ontology [2], and the distribution of literals and de-referenceable resource URIs from different namespaces.

Because of the heterogeneity of interlinked sources, it is vital to identify where specific facts come from and how reliable they are. Therefore, another interesting task for profiling RDF data is provenance analysis [18].

7.2.3 Text

Many text analysis approaches and applications can be regarded as text profiling tasks. Statistical methods are used for tasks, such as information extraction [125], part-of-speech tagging [20], and text categorization [83].

Specifically, in the field of author attribution, there has been research on defining interesting features, such as word-length distributions, average number of syllables [73].

Additionally, linguistic metrics, such as distinctiveness, type-token ratio, and Simpson's index have been proposed to measure the style and diversity of text documents. The task of profiling can target single documents, such as a paper or a book, as well as sets of documents, such as Web document corpora, product reviews, or user comments. More sophisticated applications that use metadata generated through profiling include sentiment analysis and opinion mining [93,112].

7.3 Profiling dynamic data

Data profiling describes an instance of a dataset at a particular time. Since many applications work on frequently changing data, it is desirable to re-profile a dataset after a change, such as a deletion, insertion, or update, in order to obtain up-to-date metadata. Simple aggregates are easy to maintain incrementally, but many statistics needed for column analysis, such as distinct value counts, cannot be maintained exactly using limited space and time. For these aggregates, stream sketching techniques [53] may be used to maintain approximate answers. There are also techniques for continuously updating discovered association rules [131] and clusters [43].

Dependency detection may be too time-consuming for repeated execution on the entire dataset. Thus, it is necessary to incrementally update the metadata without processing the complete dataset again. One example is SWAN, an approach for unique discovery on dynamic datasets with insertions and deletions [5] as reported in Sect. 5.1.4. Also, Wang et al. present an approach for maintaining discovered FDs after data deletions [134]. From a data cleaning standpoint, there are solutions for incremental detection of FD and CFD violations [50], and incremental data repairing with respect to FDs and CFDs [30]. In general, incremental solutions for FDs, CFDs, INDs, and CINDs on growing and changing datasets remain challenges for future research.

7.4 Profiling on new architectures

There are at least two database architecture trends that affect profiling. The first is column versus row storage. Column-store systems appear to have a natural computational advantage, at least in terms of the column analysis tasks we discussed in Sect. 3, since they can directly fetch the column of interest and compute statistics on it. However, if all columns are to be profiled, the entire dataset must be read and the only remaining advantage of column stores may be their potential compression. The second trend is that of distributed and cloud data management. This introduces additional profiling challenges, such as combining statistics from multiple nodes into final per-column analysis. There has been some work on detecting FD and CFD violations in a distributed database [48,50], but many other problems in this space, such as efficient dependency detection in distributed data, remain open.

7.5 Visualization

Because data profiling mostly targets human users, effectively visualizing any profiling results is of utmost importance. Only then can users interpret results and react to them. A suggestion for a visual data profiling tool is the Profiler system by Kandel et al. [81]. A strong cooperation between the database community, which produces the data and metadata to be visualized, and the visualization community, which enables users to understand and make use of the data, is needed.

8 Summary

In this article, we provided a comprehensive survey of the state of the art in data profiling: the set of activities and processes to determine metadata about a given database. We discussed single-column profiling tasks such as identifying data types, value distributions and patterns, and multi-column tasks such as detecting various kinds of dependencies. As the amount of data and users who require access to data increase, efficient and effective data profiling will continue to be an important data management problem in research and practice. While many data profiling algorithms have been proposed and implemented in research prototypes and commercial tools, further work is needed, especially in the context of profiling new types of data, supporting and leveraging new data management architectures, and interpreting and visualizing data profiling results.

References

1. Abedjan, Z., Grütze, T., Jentzsch, A., Naumann, F.: Mining and profiling RDF data with ProLOD++. In: Proceedings of the International Conference on Data Engineering (ICDE), pp. 1198–1201 (2014). Demo
2. Abedjan, Z., Lorey, J., Naumann, F.: Reconciling ontologies and the web of data. In: Proceedings of the International Conference on Information and Knowledge Management (CIKM), pp. 1532–1536 (2012)
3. Abedjan, Z., Naumann, F.: Advancing the discovery of unique column combinations. In: Proceedings of the International Conference on Information and Knowledge Management (CIKM), pp. 1565–1570 (2011)
4. Abedjan, Z., Naumann, F.: Synonym analysis for predicate expansion. In: Proceedings of the Extended Semantic Web Conference (ESWC), pp. 140–154 (2013)
5. Abedjan, Z., Quiané-Ruiz, J.-A., Naumann, F.: Detecting unique column combinations on dynamic data. In: Proceedings of the International Conference on Data Engineering (ICDE), pp. 1036–1047 (2014)
6. Abedjan, Z., Schulze, P., Naumann, F.: DFD: efficient functional dependency discovery. In: Proceedings of the International Conference on Information and Knowledge Management (CIKM), pp. 949–958 (2014)
7. Agrawal, D., Bernstein, P., Bertino, E., Davidson, S., Dayal, U., Franklin, M., Gehrke, J., Haas, L., Halevy, A., Han, J., Jagadish, H.V., Labrinidis, A., Madden, S., Papakonstantinou, Y., Patel, J.M., Ramakrishnan, R., Ross, K., Shahabi, C., Suciu, D., Vaithyanathan, S., Widom, J.: Challenges and opportunities with Big Data. Technical report, Computing Community Consortium. http://cra.org/ccc/docs/init/bigdatawhitepaper.pdf (2012)
8. Agrawal, R., Srikant, R.: Fast algorithms for mining association rules in large databases. In: Proceedings of the International Conference on Very Large Databases (VLDB), pp. 487–499 (1994)
9. Andritsos, P., Miller, R.J., Tsaparas, P.: Information-theoretic tools for mining database structure from large data sets. In: Proceedings of the International Conference on Management of Data (SIGMOD), pp. 731–742 (2004)
10. Arenas, M., Daenen, J., Neven, F., Ugarte, M., Van den Bussche, J., Vansummeren, S.: Discovering XSD keys from XML data. In: Proceedings of the International Conference on Management of Data (SIGMOD), pp. 61–72 (2013)
11. Astrahan, M.M., Schkolnick, M., Kyu-Young, W.: Approximating the number of unique values of an attribute without sorting. Inf. Syst. **12**(1), 11–15 (1987)
12. Auer, S., Demter, J., Martin, M., Lehmann, J.: LODStats—an extensible framework for high-performance dataset analytics. In: Proceedings of the International Conference on Knowledge Engineering and Knowledge Management (EKAW), pp. 353–362 (2012)
13. Bauckmann, J., Abedjan, Z., Müller, H., Leser, U., Naumann, F.: Discovering conditional inclusion dependencies. In: Proceedings of the International Conference on Information and Knowledge Management (CIKM), pp. 2094–2098 (2012)
14. Bauckmann, J., Leser, U., Naumann, F., Tietz, V.: Efficiently detecting inclusion dependencies. In: Proceedings of the International Conference on Data Engineering (ICDE), pp. 1448–1450 (2007)
15. Benford, F.: The law of anomalous numbers. Proc. Am. Philos. Soc. **78**(4), 551–572 (1938)
16. Berti-Equille, L., Dasu, T., Srivastava, D.: Discovery of complex glitch patterns: a novel approach to quantitative data cleaning. In: Proceedings of the International Conference on Data Engineering (ICDE), pp. 733–744 (2011)
17. Bex, G.J., Neven, F., Vansummeren, S.: Inferring XML schema definitions from XML data. In: Proceedings of the International Conference on Very Large Databases (VLDB), pp. 998–1009 (2007)
18. Böhm, C., Lorey, J., Naumann, F.: Creating void descriptions for web-scale data. J. Web Semant. **9**(3), 339–345 (2011)
19. Bravo, L., Fan, W., Ma, S.: Extending dependencies with conditions. In: Proceedings of the International Conference on Very Large Databases (VLDB), pp. 243–254 (2007)
20. Brill, E.: Transformation-based error-driven learning and natural language processing: a case study in part-of-speech tagging. Comput. Linguist. **21**(4), 543–565 (1995)
21. Brin, S., Motwani, R., Silverstein, C.: Beyond market baskets: generalizing association rules to correlations. SIGMOD Rec. **26**(2), 265–276 (1997)
22. Buneman, P., Davidson, S.B., Fan, W., Hara, C.S., Tan, W.C.: Reasoning about keys for XML. Inf. Syst. **28**(8), 1037–1063 (2003)
23. Chandola, V., Kumar, V.: Summarization—compressing data into an informative representation. Knowl. Inf. Syst. **12**(3), 355–378 (2007)
24. Chiang, F., Miller, R.J.: Discovering data quality rules. Proc. VLDB Endow. **1**, 1166–1177 (2008)
25. Chiang, R.H.L., Cecil, C.E.H., Lim, E.-P.: Linear correlation discovery in databases: a data mining approach. Data Knowl. Eng. **53**(3), 311–337 (2005)

26. Choi, B.: What are real DTDs like? In: Proceedings of the ACM SIGMOD Workshop on the Web and Databases (WebDB), pp. 43–48 (2002)
27. Christen, P.: Data Matching. Springer, Berlin (2012)
28. Chu, X., Ilyas, I., Papotti, P., Ye, Y.: RuleMiner: data quality rules discovery. In: Proceedings of the International Conference on Data Engineering (ICDE), pp. 1222–1225 (2014)
29. Chu, X., Ilyas, I.F., Papotti, P.: Discovering denial constraints. Proc. VLDB Endow. **6**(13), 1498–1509 (2013)
30. Cong, G., Fan, W., Geerts, F., Jia, X., Ma, S.: Improving data quality: consistency and accuracy. In: Proceedings of the International Conference on Very Large Databases (VLDB), pp. 315–326 (2007)
31. Cormode, G., Garofalakis, M., Haas, P.J., Jermaine, C.: Synopses for massive data: samples, histograms, wavelets, sketches. Found. Trends Databases **4**(13), 1–294 (2011)
32. Cormode, G., Golab, L., Flip, K., McGregor, A., Srivastava, D., Zhang, X.: Estimating the confidence of conditional functional dependencies. In: Proceedings of the International Conference on Management of Data (SIGMOD), pp. 469–482 (2009)
33. Cormode, G., Korn, F., Muthukrishnan, S., Srivastava, D.: Space- and time-efficient deterministic algorithms for biased quantiles over data streams. In: Proceedings of the Symposium on Principles of Database Systems (PODS), pp. 263–272 (2006)
34. Dallachiesa, M., Ebaid, A., Eldawy, A., Elmagarmid, A., Ilyas, I.F., Ouzzani, M., Tang, N.: NADEEF: a commodity data cleaning system. In: Proceedings of the International Conference on Management of Data (SIGMOD), pp. 541–552 (2013)
35. Das, A., Ng, W.-K., Woon, Y.-K.: Rapid association rule mining. In: Proceedings of the International Conference on Information and Knowledge Management (CIKM), pp. 474–481 (2001)
36. Dasu, T., Johnson, T.: Hunting of the snark: finding data glitches using data mining methods. In: Proceedings of the International Conference on Information Quality (IQ), pp. 89–98 (1999)
37. Dasu, T., Johnson, T., Marathe, A.: Database exploration using database dynamics. IEEE Data Eng. Bull. **29**(2), 43–59 (2006)
38. Dasu, T., Johnson, T., Muthukrishnan, S., Shkapenyuk, V.: Mining database structure; or, how to build a data quality browser. In: Proceedings of the International Conference on Management of Data (SIGMOD), pp. 240–251 (2002)
39. Dasu, T., Loh, J.M.: Statistical distortion: consequences of data cleaning. Proc. VLDB Endow. **5**(11), 1674–1683 (2012)
40. Dasu, T., Loh, J.M., Srivastava, D.: Empirical glitch explanations. In: Proceedings of the International Conference on Knowledge Discovery and Data Mining (SIGKDD), pp. 572–581 (2014)
41. Deshpande, A., Garofalakis, M., Rastogi, R.: Independence is good: dependency-based histogram synopses for high-dimensional data. In: Proceedings of the International Conference on Management of Data (SIGMOD), pp. 199–210 (2001)
42. Diallo, T., Novelli, N., Petit, J.-M.: Discovering (frequent) constant conditional functional dependencies. Int. J. Data Min. Model. Manag. **4**(3), 205–223 (2012)
43. Ester, M., Kriegel, H.-P., Sander, J., Wimmer, M., Xu, X.: Incremental clustering for mining in a data warehousing environment. In: Proceedings of the International Conference on Very Large Databases (VLDB), pp. 323–333 (1998)
44. Euzenat, J., Shvaiko, P.: Ontology Matching, 2nd edn. Springer, Berlin (2013)
45. Fan, W., Geerts, F., Jia, X.: Semandaq: a data quality system based on conditional functional dependencies. Proc. VLDB Endow. **1**(2), 1460–1463 (2008)
46. Fan, W., Geerts, F., Jia, X., Kementsietsidis, A.: Conditional functional dependencies for capturing data inconsistencies. ACM Trans. Database Syst. **33**(2), 1–48 (2008)
47. Fan, W., Geerts, F., Li, J., Xiong, M.: Discovering conditional functional dependencies. IEEE Trans. Knowl. Data Eng. **23**(4), 683–698 (2011)
48. Fan, W., Geerts, F., Ma, S., Müller, H.: Detecting inconsistencies in distributed data. In: Proceedings of the International Conference on Data Engineering (ICDE), pp. 64–75 (2010)
49. Fan, W., Jia, X., Li, J., Ma, S.: Reasoning about record matching rules. Proc. VLDB Endow. **2**(1), 407–418 (2009)
50. Fan, W., Li, J., Tang, N., Yu, W.: Incremental detection of inconsistencies in distributed data. In: Proceedings of the International Conference on Data Engineering (ICDE), pp. 318–329 (2012)
51. Fernau, H.: Algorithms for learning regular expressions from positive data. Inf. Comput. **207**(4), 521–541 (2009)
52. Flach, P.A., Savnik, I.: Database dependency discovery: a machine learning approach. AI Commun. **12**(3), 139–160 (1999)
53. Ganguly, S.: Counting distinct items over update streams. Theor. Comput. Sci. **378**(3), 211–222 (2007)
54. Garofalakis, M., Keren, D., Samoladas, V.: Sketch-based geometric monitoring of distributed stream queries. Proc. VLDB Endow. **6**(10), 937–948 (2013)
55. Giannella, C., Wyss, C.: Finding minimal keys in a relation instance (1999). http://citeseerx.ist.psu.edu/viewdoc/summary?doi=?doi=10.1.1.41.7086
56. Ginsburg, S., Hull, R.: Order dependency in the relational model. Theor. Comput. Sci. **26**, 149–195 (1983)
57. Golab, L., Karloff, H., Korn, F., Saha, A., Srivastava, D.: Sequential dependencies. Proc. VLDB Endow. **2**(1), 574–585 (2009)
58. Golab, L., Karloff, H., Korn, F., Srivastava, D.: Data auditor: exploring data quality and semantics using pattern tableaux. Proc. VLDB Endow. **3**(1–2), 1641–1644 (2010)
59. Golab, L., Karloff, H., Korn, F., Srivastava, D., Bei, Y.: On generating near-optimal tableaux for conditional functional dependencies. Proc. VLDB Endow. **1**(1), 376–390 (2008)
60. Golab, L., Korn, F., Srivastava, D.: Discovering pattern tableaux for data quality analysis: a case study. In: Proceedings of the International Workshop on Quality in Databases (QDB), pp. 47–53 (2011)
61. Golab, L., Korn, F., Srivastava, D.: Efficient and effective analysis of data quality using pattern tableaux. IEEE Data Eng. Bull. **34**(3), 26–33 (2011)
62. Grahne, G., Zhu, J.: Discovering approximate keys in XML data. In: Proceedings of the International Conference on Information and Knowledge Management (CIKM), pp. 453–460 (2002)
63. Gray, J., Chaudhuri, S., Bosworth, A., Layman, A., Reichart, D., Venkatrao, M., Pellow, F., Pirahesh, H.: Data cube: a relational aggregation operator generalizing group-by, cross-tab, and sub totals. Data Min. Knowl. Discov. **1**(1), 29–53 (1997)
64. Gunopulos, D., Khardon, R., Mannila, H., Sharma, R.S.: Discovering all most specific sentences. ACM Trans. Database Syst. **28**, 140–174 (2003)
65. Haas, P.J., Naughton, J.F., Seshadri, S., Stokes, L.: Sampling-based estimation of the number of distinct values of an attribute. In: Proceedings of the International Conference on Very Large Databases (VLDB), pp. 311–322 (1995)
66. Hainaut, J.-L., Henrard, J., Englebert, V., Roland, D., Hick, J.-M.: Database reverse engineering. In: Liu, L., Tamer Özsu, M. (eds.) Encyclopedia of Database Systems, pp. 723–728. Springer, Heidelberg (2009)
67. Han, J., Pei, J., Yin, Y.: Mining frequent patterns without candidate generation. SIGMOD Rec. **29**(2), 1–12 (2000)
68. Hanrahan, P.: Analytic database technology for a new kind of user—the data enthusiast (keynote). In: Proceedings of the International Conference on Management of Data (SIGMOD), pp. 577–578 (2012)
69. Hegewald, J., Naumann, F., Weis, M.: XStruct: efficient schema extraction from multiple and large XML databases. In: Proceed-

ings of the International Workshop on Database Interoperability (InterDB) (2006)
70. Heise, A., Quiané-Ruiz, J.-A., Abedjan, Z., Jentzsch, A., Naumann, F.: Scalable discovery of unique column combinations. Proc. VLDB Endow. **7**(4), 301–312 (2013)
71. Hellerstein, J.M., Ré, C., Schoppmann, F., Wang, D.Z., Fratkin, E., Gorajek, A., Ng, K.S., Welton, C., Feng, X., Li, K., Kumar, A.: The MADlib analytics library or MAD skills, the SQL. Proc. VLDB Endow. **5**(12), 1700–1711 (2012)
72. Hipp, J., Güntzer, U., Nakhaeizadeh, G.: Algorithms for association rule mining—a general survey and comparison. SIGKDD Explor. **2**(1), 58–64 (2000)
73. Holmes, D.I.: Authorship attribution. Comput. Humanit. **28**, 87–106 (1994)
74. Hua, M., Pei, J.: Cleaning disguised missing data: a heuristic approach. In: Proceedings of the International Conference on Knowledge Discovery and Data Mining (SIGKDD), pp. 950–958 (2007)
75. Huhtala, Y., Kärkkäinen, J., Porkka, P., Toivonen, H.: TANE: an efficient algorithm for discovering functional and approximate dependencies. Comput. J. **42**(2), 100–111 (1999)
76. Ilyas, I.F., Markl, V., Haas, P.J., Brown, P., Aboulnaga, A.: CORDS: automatic discovery of correlations and soft functional dependencies. In: Proceedings of the International Conference on Management of Data (SIGMOD), pp. 647–658 (2004)
77. Ioannidis, Y.: The history of histograms (abridged). In: Proceedings of the International Conference on Very Large Databases (VLDB), pp. 19–30 (2003)
78. Jain, A.K., Narasimha Murty, M., Flynn, P.J.: Data clustering: a review. ACM Comput. Surv. **31**(3), 264–323 (1999)
79. Johnson, T.: Encyclopedia of Database Systems, chapter Data Profiling. Springer, Heidelberg (2009)
80. Kache, H., Han, W.-S., Markl, V., Raman, V., Ewen, S.: POP/FED: progressive query optimization for federated queries in DB2. In: Proceedings of the International Conference on Very Large Databases (VLDB), pp. 1175–1178 (2006)
81. Kandel, S., Parikh, R., Paepcke, A., Hellerstein, J., Heer, J.: Profiler: integrated statistical analysis and visualization for data quality assessment. In: Proceedings of Advanced Visual Interfaces (AVI), pp. 547–554 (2012)
82. Kang, J., Naughton, J.F.: On schema matching with opaque column names and data values. In: Proceedings of the International Conference on Management of Data (SIGMOD), pp. 205–216 (2003)
83. Keim, D.A., Oelke, D.: Literature fingerprinting: a new method for visual literary analysis. In: Proceedings of Visual Analytics Science and Technology (VAST), pp. 115–122 (2007)
84. Khoussainova, N., Balazinska, M., Suciu, D.: Towards correcting input data errors probabilistically using integrity constraints. In: Proceedings of the ACM International Workshop on Data Engineering for Wireless and Mobile Access (MobiDE), pp. 43–50 (2006)
85. Kivinen, J., Mannila, H.: Approximate inference of functional dependencies from relations. In: Proceedings of the International Conference on Database Theory (ICDT), pp. 129–149 (1995)
86. Koehler, H., Leck, U., Link, S., Prade, H.: Logical foundations of possibilistic keys. In: Fermé, E., Leite, J. (eds.) Logics in Artificial Intelligence, volume 8761 of Lecture Notes in Computer Science, pp. 181–195. Springer, Heidelberg (2014)
87. Koeller, A., Rundensteiner, E.A.: Heuristic strategies for the discovery of inclusion dependencies and other patterns. J. Data Semant. V. **3870**, 185–210 (2006)
88. Korn, F., Saha, B., Srivastava, D., Ying, S.: On repairing structural problems in semi-structured data. Proc. VLDB Endow. **6**(9), 601–612 (2013)
89. Koudas, N., Saha, A., Srivastava, D., Venkatasubramanian, S.: Metric functional dependencies. In: Proceedings of the International Conference on Data Engineering (ICDE), pp. 1275–1278 (2009)
90. Laney, D.: 3D data management: controlling data volume, velocity and variety. Technical report, Gartner (2001)
91. Li, J., Liu, J., Toivonen, H., Yong, J.: Effective pruning for the discovery of conditional functional dependencies. Comput. J. **56**(3), 378–392 (2013)
92. Li, Y., Krishnamurthy, R., Raghavan, S., Vaithyanathan, S., Jagadish, H.V.: Regular expression learning for information extraction. In: Proceedings of the Conference on Empirical Methods in Natural Language Processing (EMNLP), pp. 21–30 (2008)
93. Liu, B.: Sentiment analysis and subjectivity. Handbook of Natural Language Processing, 2nd edn. Chapman and Hall/CRC, London (2010)
94. Liu, J., Li, J., Liu, C., Chen, Y.: Discover dependencies from data—a review. IEEE Trans. Knowl. Data Eng. **24**(2), 251–264 (2012)
95. Lopes, S., Petit, J.-M., Lakhal, L.: Efficient discovery of functional dependencies and Armstrong relations. In: Proceedings of the International Conference on Extending Database Technology (EDBT), pp. 350–364 (2000)
96. Lopes, S., Petit, J.-M., Toumani, F.: Discovering interesting inclusion dependencies: application to logical database tuning. Inf. Syst. **27**(1), 1–19 (2002)
97. Lucchesi, C.L., Osborn, S.L.: Candidate keys for relations. J. Comput. Syst. Sci. **17**(2), 270–279 (1978)
98. Madhavan, J., Bernstein, P.A., Rahm, E.: Generic schema matching with Cupid. In: Proceedings of the International Conference on Very Large Databases (VLDB), pp. 49–58 (2001)
99. Mannino, M.V., Chu, P., Sager, T.: Statistical profile estimation in database systems. ACM Comput. Surv. **20**(3), 191–221 (1988)
100. De Marchi, F., Lopes, S., Petit, J.-M.: Efficient algorithms for mining inclusion dependencies. In: Proceedings of the International Conference on Extending Database Technology (EDBT), pp. 464–476 (2002)
101. De Marchi, F., Lopes, S., Petit, J.-M.: Unary and n-ary inclusion dependency discovery in relational databases. J. Intell. Inf. Syst. **32**, 53–73 (2009)
102. De Marchi, F. , Petit, J.-M.: Zigzag: a new algorithm for mining large inclusion dependencies in databases. In: Proceedings of the IEEE International Conference on Data Mining (ICDM), pp. 27–34 (2003)
103. Markowitz, V.M., Makowsky, J.A.: Identifying extended entity-relationship object structures in relational schemas. IEEE Trans. Softw. Eng. **16**(8), 777–790 (1990)
104. Maydanchik, A.: Data Quality Assessment. Technics Publications, New Jersey (2007)
105. Mignet, L., Barbosa, D., Veltri, P.: The XML web: a first study. In: Proceedings of the International World Wide Web Conference (WWW), pp. 500–510 (2003)
106. Mlynkova, I., Toman, K., Pokorný, J.: Statistical analysis of real XML data collections. In: Proceedings of the International Conference on Management of Data (COMAD), pp. 15–26 (2006)
107. Morton, K., Balazinska, M., Grossman, D., Mackinlay, J.: Support the data enthusiast: challenges for next-generation data-analysis systems. Proc. VLDB Endow. **7**(6), 453–456 (2014)
108. Naumann, F.: Data profiling revisited. SIGMOD Rec. **42**(4), 40–49 (2013)
109. Naumann, F., Ho, C.-T., Tian, X., Haas, L., Megiddo, N.: Attribute classification using feature analysis. In: Proceedings of the International Conference on Data Engineering (ICDE), p 271 (2002)
110. Novelli, N., Cicchetti, R.: FUN: an efficient algorithm for mining functional and embedded dependencies. In: Proceedings of the

International Conference on Database Theory (ICDT), pp. 189–203 (2001)
111. Ntarmos, N., Triantafillou, P., Weikum, G.: Distributed hash sketches: scalable, efficient, and accurate cardinality estimation for distributed multisets. ACM Trans. Comput. Syst. **27**(1), 1–53 (2009)
112. Pang, B., Lee, L.: Opinion mining and sentiment analysis. Found. Trends Inf. Retr. **2**(1–2), 1–135 (2008)
113. Papenbrock, T., Ehrlich, J., Marten, J., Neubert, T., Rudolph, J.-P., Schönberg, M., Zwiener, J., Naumann, F.: Functional dependency discovery: an experimental evaluation of seven algorithms. Proc. VLDB Endow. **8**(10) (2015)
114. Papenbrock, T., Kruse, S., Quiané-Ruiz, J.-A., Naumann, F.: Divide & conquer-based inclusion dependency discovery. Proc. VLDB Endow. **8**(7), 774–785 (2015)
115. Park, J.S., Chen, M.-S., Yu, P.S.: Using a hash-based method with transaction trimming for mining association rules. IEEE Trans. Knowl. Data Eng. **9**, 813–825 (1997)
116. Petit, J.-M., Kouloumdjian, J., Boulicaut, J.-F., Toumani, F.: Using queries to improve database reverse engineering. In: Proceedings of the International Conference on Conceptual Modeling (ER), pp. 369–386 (1994)
117. Pipino, L., Lee, Y., Wang, R.: Data quality assessment. Commun. ACM **4**, 211–218 (2002)
118. Poosala, V., Haas, P.J., Ioannidis, Y.E., Shekita, E.J.: Improved histograms for selectivity estimation of range predicates. In: Proceedings of the International Conference on Management of Data (SIGMOD), pp. 294–305 (1996)
119. Poosala, V., Ioannidis, Y.E.: Selectivity estimation without the attribute value independence assumption. In: Proceedings of the International Conference on Very Large Databases (VLDB), pp. 486–495 (1997)
120. Pyle, D.: Data Preparation for Data Mining. Morgan Kaufmann, Burlington (1999)
121. Rahm, E., Do, H.-H.: Data cleaning: problems and current approaches. IEEE Data Eng. Bull. **23**(4), 3–13 (2000)
122. Raman, V., Hellerstein, J.M.: Potters wheel: an interactive data cleaning system. In: Proceedings of the International Conference on Very Large Databases (VLDB), pp. 381–390 (2001)
123. Rostin, A., Albrecht, O., Bauckmann, J., Naumann, F., Leser, U.: A machine learning approach to foreign key discovery. In: Proceedings of the ACM SIGMOD Workshop on the Web and Databases (WebDB) (2009)
124. Sahuguet, A., Azavant, F.: Building light-weight wrappers for legacy Web data-sources using W4F. In: Proceedings of the International Conference on Very Large Databases (VLDB), pp. 738–741 (1999)
125. Sarawagi, S.: Information extraction. Found. Trends Databases **1**(3), 261–377 (2008)
126. Sismanis, Y., Brown, P., Haas, P.J., Reinwald, B.: GORDIAN: efficient and scalable discovery of composite keys. In: Proceedings of the International Conference on Very Large Databases (VLDB), pp. 691–702 (2006)
127. Smith, K.P., Morse, M., Mork, P., Li, M.H., Rosenthal, A., Allen, M.D., Seligman, L.: The role of schema matching in large enterprises. In: Proceedings of the Conference on Innovative Data Systems Research (CIDR) (2009)
128. Song, S., Chen, L.: Differential dependencies: reasoning and discovery. ACM Trans. Database Syst. **36**(3), 16:1–16:41 (2011)
129. Stonebraker, M., Bruckner, D., Ilyas, I.F., Beskales, G., Cherniack, M., Zdonik, S., Pagan, A., Xu, S.: Data curation at scale: the Data Tamer system. In: Proceedings of the Conference on Innovative Data Systems Research (CIDR) (2013)
130. Chen, M., Hun, J., Yu, P.S.: Data mining: an overview from a database perspective. IEEE Trans. Knowl. Data Eng. **8**, 866–883 (1996)
131. Tsai, P.S.M., Lee, C.-C., Chen, A.L.P.: An efficient approach for incremental association rule mining. Methodologies for Knowledge Discovery and Data Mining. volume 1574 of Lecture Notes in Computer Science, pp. 74–83. Springer, Heidelberg (1999)
132. Vincent, M.W., Liu, J., Liu, C.: Strong functional dependencies and their application to normal forms in XML. ACM Trans. Database Syst. **29**(3), 445–462 (2004)
133. Vogel, T., Naumann, F.: Instance-based "one-to-some" assignment of similarity measures to attributes. In: Proceedings of the International Conference on Cooperative Information Systems (CoopIS), pp. 412–420 (2011)
134. Wang, S.-L., Tsou, W.-C., Lin, J.-H., Hong, T.-P.: Maintenance of discovered functional dependencies: incremental deletion. Intelligent Systems Design and Applications, volume 23 of Advances in Soft Computing, pp. 579–588. Springer, Heidelberg (2003)
135. Xindong, W., Zhang, C., Zhang, S.: Efficient mining of both positive and negative association rules. ACM Trans. Inf. Syst. **22**(3), 381–405 (2004)
136. Wyss, C., Giannella, C., Robertson, E.L.: FastFDs: a heuristic-driven, depth-first algorithm for mining functional dependencies from relation instances. In: Proceedings of the International Conference on Data Warehousing and Knowledge Discovery (DaWaK), pp. 101–110 (2001)
137. Xu, R., Wunsch II, D.C.: Survey of clustering algorithms. IEEE Trans. Neural Netw. **16**(3), 645–678 (2005)
138. Yakout, M., Elmagarmid, A.K., Neville, J., Ouzzani, M.: GDR: a system for guided data repair. In: Proceedings of the International Conference on Management of Data (SIGMOD), pp. 1223–1226 (2010)
139. Yao, H., Hamilton, H.J.: Mining functional dependencies from data. Data Min. Knowl. Discov. **16**(2), 197–219 (2008)
140. Yu, C., Jagadish, H.V.: Efficient discovery of XML data redundancies. In: Proceedings of the International Conference on Very Large Databases (VLDB), pp. 103–114 (2006)
141. Zaki, M.J.: Scalable algorithms for association mining. IEEE Trans. Knowl. Data Eng. **12**(3), 372–390 (2000)
142. Zhang, M., Chakrabarti, K.: InfoGather+: semantic matching and annotation of numeric and time-varying attributes in web tables. In: Proceedings of the International Conference on Management of Data (SIGMOD), pp. 145–156 (2013)
143. Zhang, M., Hadjieleftheriou, M., Ooi, B.C., Procopiuc, C.M., Srivastava, D.: On multi-column foreign key discovery. Proc. VLDB Endow. **3**(1–2), 805–814 (2010)
144. Zhang, M., Hadjieleftheriou, M., Ooi, B.C., Procopiuc, C.M., Srivastava, D.: Automatic discovery of attributes in relational databases. In: Proceedings of the International Conference on Management of Data (SIGMOD), pp. 109–120 (2011)

Quantitative Data Cleaning for Large Databases

Joseph M. Hellerstein*
EECS Computer Science Division
UC Berkeley
http://db.cs.berkeley.edu/jmh

February 27, 2008

1 Introduction

Data collection has become a ubiquitous function of large organizations – not only for record keeping, but to support a variety of data analysis tasks that are critical to the organizational mission. Data analysis typically drives decision-making processes and efficiency optimizations, and in an increasing number of settings is the *raison d'etre* of entire agencies or firms.

Despite the importance of data collection and analysis, data *quality* remains a pervasive and thorny problem in almost every large organization. The presence of incorrect or inconsistent data can significantly distort the results of analyses, often negating the potential benefits of information-driven approaches. As a result, there has been a variety of research over the last decades on various aspects of *data cleaning*: computational procedures to automatically or semi-automatically identify – and, when possible, correct – errors in large data sets.

In this report, we survey data cleaning methods that focus on errors in *quantitative* attributes of large databases, though we also provide references to data cleaning methods for other types of attributes. The discussion is targeted at computer practitioners who manage large databases of quantitative information, and designers developing data entry and auditing tools for end users. Because of our focus on quantitative data, we take a statistical view of data quality, with an emphasis on intuitive outlier detection and exploratory data analysis methods based in *robust statistics* [Rousseeuw and Leroy, 1987, Hampel et al., 1986, Huber, 1981]. In addition, we stress algorithms and implementations that can be easily and efficiently implemented in very large databases, and which are easy to understand and visualize graphically. The discussion mixes statistical intuitions and methods, algorithmic building blocks, efficient relational database implementation strategies, and user interface considerations. Throughout the discussion, references are provided for deeper reading on all of these issues.

1.1 Sources of Error in Data

Before a data item ends up in a database, it typically passes through a number of steps involving both human interaction and computation. Data errors can creep in at every step of the process from initial data acquisition to archival storage. An understanding of the sources of data errors can be useful both in designing data collection and curation techniques that mitigate

*This survey was written under contract to the United Nations Economic Commission for Europe (UNECE), which holds the copyright on this version.

the introduction of errors, and in developing appropriate post-hoc data cleaning techniques to detect and ameliorate errors. Many of the sources of error in databases fall into one or more of the following categories:

- **Data entry errors:** It remains common in many settings for data entry to be done by humans, who typically extract information from speech (e.g., in telephone call centers) or by keying in data from written or printed sources. In these settings, data is often corrupted at entry time by typographic errors or misunderstanding of the data source. Another very common reason that humans enter "dirty" data into forms is to provide what we call *spurious integrity*: many forms require certain fields to be filled out, and when a data-entry user does not have access to values for one of those fields, they will often invent a default value that is easy to type, or that seems to them to be a typical value. This often passes the crude data integrity tests of the data entry system, while leaving no trace in the database that the data is in fact meaningless or misleading.

- **Measurement errors:** In many cases data is intended to measure some physical process in the world: the speed of a vehicle, the size of a population, the growth of an economy, etc. In some cases these measurements are undertaken by human processes that can have errors in their design (e.g., improper surveys or sampling strategies) and execution (e.g., misuse of instruments). In the measurement of physical properties, the increasing proliferation of sensor technology has led to large volumes of data that is never manipulated via human intervention. While this avoids various human errors in data acquisition and entry, data errors are still quite common: the human design of a sensor deployment (e.g., selection and placement of sensors) often affects data quality, and many sensors are subject to errors including miscalibration and interference from unintended signals.

- **Distillation errors:** In many settings, raw data are preprocessed and summarized before they are entered into a database. This data distillation is done for a variety of reasons: to reduce the complexity or noise in the raw data (e.g., many sensors perform smoothing in their hardware), to perform domain-specific statistical analyses not understood by the database manager, to emphasize aggregate properties of the raw data (often with some editorial bias), and in some cases simply to reduce the volume of data being stored. All these processes have the potential to produce errors in the distilled data, or in the way that the distillation technique interacts with the final analysis.

- **Data integration errors:** It is actually quite rare for a database of significant size and age to contain data from a single source, collected and entered in the same way over time. In almost all settings, a database contains information collected from multiple sources via multiple methods over time. Moreover, in practice many databases evolve by merging in other pre-existing databases; this merging task almost always requires some attempt to resolve inconsistencies across the databases involving data representations, units, measurement periods, and so on. Any procedure that integrates data from multiple sources can lead to errors.

1.2 Approaches to Improving Data Quality

The "lifetime" of data is a multi-step and sometimes iterative process involving collection, transformation, storage, auditing, cleaning and analysis. Typically this process includes people and equipment from multiple organizations within or across agencies, potentially over large spans of time and space. Each step of this process can be designed in ways that can encourage data quality. While the bulk of this report is focused on post-hoc data auditing and cleaning, here we mention a broad range of approaches that have been suggested for maintaining or improving data quality:

- **Data entry interface design.** For human data entry, errors in data can often be mitigated through judicious design of data entry interfaces. Traditionally, one key aspect of this was the specification and maintenance of database *integrity constraints*, including data type checks, bounds on numeric values, and referential integrity (the prevention of references to non-existent data). When these integrity constraints are enforced by the database, data entry interfaces prevent data-entry users from providing data that violates the constraints. An unfortunate side-effect of this *enforcement* approach is the spurious integrity problem mentioned above, which frustrates data-entry users and leads them to invent dirty data. An alternative approach is to provide the data-entry user with convenient affordances to understand, override and explain constraint violations, thus discouraging the silent injection of bad data, and encouraging annotation of surprising or incomplete source data. We discuss this topic in more detail in Section 7.

- **Organizational management.** In the business community, there is a wide-ranging set of principles regarding organizational structures for improving data quality, sometimes referred to as *Total Data Quality Management*. This work tends to include the use of technological solutions, but also focuses on organizational structures and incentives to help improve data quality. These include streamlining processes for data collection, archiving and analysis to minimize opportunities for error; automating data capture; capturing metadata and using it to improve data interpretation; and incentives for multiple parties to participate in the process of maintaining data quality [Huang et al., 1999].

- **Automated data auditing and cleaning.** There are a host of computational techniques from both research and industry for trying to identify and in some cases rectify errors in data. There are many variants on this theme, which we survey in Section 1.3.

- **Exploratory data analysis and cleaning.** In many if not most instances, data can only be cleaned effectively with some human involvement. Therefore there is typically an interaction between data cleaning tools and data visualization systems. Exploratory Data Analysis [Tukey, 1977] (sometimes called Exploratory Data Mining in more recent literature [Dasu and Johnson, 2003]) typically involves a human in the process of understanding properties of a dataset, including the identification and possible rectification of errors. Data *profiling* is often used to give a big picture of the contents of a dataset, alongside metadata that describes the possible structures and values in the database. Data visualizations are often used to make statistical properties of the data (distributions, correlations, etc.) accessible to data analysts.

In general, there is value to be gained from all these approaches to maintaining data quality. The prioritization of these tasks depends upon organizational dynamics: typically the business management techniques are dictated from organizational leadership, the technical analyses must be chosen and deployed by data processing experts within an Information Technology (IT) division, and the design and rollout of better interfaces depends on the way that user tools are deployed in an organization (e.g., via packaged software, downloads, web-based services, etc.) The techniques surveyed in this report focus largely on technical approaches that can be achieved within an IT organization, though we do discuss interface designs that would involve user adoption and training.

1.3 Data Cleaning: Types and Techniques

Focusing more specifically on post-hoc data cleaning, there are many techniques in the research literature, and many products in the marketplace. (The KDDNuggets website [Piatetsky-Shapiro, 2008] lists a number of current commercial data cleaning tools.) The space of techniques and products can be categorized fairly neatly by the types of data that they target. Here we provide a brief overview of data cleaning techniques, broken down by data type.

- **Quantitative data** are integers or floating point numbers that measure quantities of interest. Quantitative data may consist of simple sets of numbers, or complex arrays of data in multiple dimensions, sometimes captured over time in *time series*. Quantitative data is typically based in some unit of measure, which needs to be uniform across the data for analyses to be meaningful; unit conversion (especially for volatile units like currencies) can often be a challenge. Statistical methods for *outlier detection* are the foundation of data cleaning techniques in this domain: they try to identify readings that are in some sense "far" from what one would expect based on the rest of the data. In recent years, this area has expanded into the more recent field of data mining, which emerged in part to develop statistical methods that are efficient on very large data sets.

- **Categorical data** are names or codes that are used to assign data into categories or groups. Unlike quantitative attributes, categorical attributes typically have no natural ordering or distance between values that fit quantitative definitions of outliers. One key data cleaning problem with categorical data is the mapping of different category names to a uniform namespace: e.g., a "razor" in one data set may be called a "shaver" in another, and simply a "hygiene product" (a broader category) in a third. Another problem is identifying the miscategorization of data, possibly by the association of values with "lexicons" of known categories, and the identification of values outside those lexicons [Raman and Hellerstein, 2001]. Yet another problem is managing data entry errors (e.g. misspellings and typos) that often arise with textual codes. There are a variety of techniques available for handling misspellings, which often adapt themselves nicely to specialized domains, languages and lexicons [Gravano et al., 2003].

- **Postal Addresses** represent a special case of categorical data that is sufficiently important to merit its own software packages and heuristics. While postal addresses are often free text, they typically have both structure and intrinsic redundancy. One challenge in handling postal address text is to make sure any redundant or ambiguous aspects are consistent and complete – e.g. to ensure that street addresses and postal codes are consistent, and that the street name is distinctive (e.g., "100 Pine, San Francisco" vs. "100 Pine Street, San Francisco".). Another challenge is that of *deduplication*: identifying duplicate entries in a mailing list that differ in spelling but not in the actual recipient. This involves not only canonicalizing the postal address, but also deciding whether two distinct addressees (e.g. "J. Lee" and "John Li") at the same address are actually the same person. This is a fairly mature area, with commercial offerings including Trillium, QAS, and others [Piatetsky-Shapiro, 2008], and a number of approaches in the research literature (e.g., [Singla and Domingos, 2006], [Bhattacharya and Getoor, 2007], [Dong et al., 2005]). The U.S. Bureau of the Census provides a survey article on the topic [Winkler, 2006].

- **Identifiers** or *keys* are another special case of categorical data, which are used to uniquely name objects or properties. In some cases identifiers are completely arbitrary and have no semantics beyond being uniquely assigned to a single object. However, in many cases identifiers have domain-specific structure that provides some information: this is true of telephone numbers, UPC product codes, United States Social Security numbers, Internet Protocol addresses, and so on. One challenge in data cleaning is to detect the reuse of an identifier across distinct objects; this is a violation of the definition of an identifier that requires resolution. Although identifiers should by definition uniquely identify an object in some set, they may be repeatedly stored within other data items as a form of *reference* to the object being identified. For example, a table of taxpayers may have a unique tax ID per object, but a table of tax payment records may have many entries per taxpayer, each of which contains the tax ID of the payer to facilitate linking the payment with information about the payer. *Referential integrity* is the property of ensuring that all references of this form contain values that actually appear in the set of objects to which they refer. Identifying referential integrity failures is an example of finding *inconsistencies* across data items in a data set. More general integrity failures can be defined using the relational database theory of functional dependencies. Even when such dependencies (which include referential integrity as a subclass) are not enforced, they can be "mined" from data, even in the presence of failures [Huhtala et al., 1999].

This list of data types and cleaning tasks is not exhaustive, but it does cover many of the problems that have been a focus in the research literature and product offerings for data cleaning.

Note that typical database data contains a mixture of attributes from all of these data types, often within a single database table. Common practice today is to treat these different attributes separately using separate techniques. There are certainly settings where the techniques can complement each other, although this is relatively unusual in current practice.

1.4 Emphasis and Outline

The focus of this report is on post-hoc data cleaning techniques for quantitative attributes. We begin in Section 2 by considering outlier detection mechanisms for single quantitative attributes based on robust statistics. Given that background, in Section 3 we discuss techniques for handling multiple quantitative attributes together, and in Section 4 we discuss quantitative data in timeseries. Section 5 briefly presents alternative methodologies to the robust estimators presented previously, based on the idea of resampling. In Section 6, we shift from the identification of outlying values, to outlying counts or frequencies: data values that are repeated more frequently than normal. In Section 7 we turn our attention to softer issues in the design of interfaces for both data entry and the exploratory side of data cleaning. Throughout, our focus is on data cleaning techniques that are technically accessible and feasibly implemented by database professionals; we also provide algorithms and implementation guidelines and discuss how to integrate them with modern relational databases. While keeping this focus, we also provide references to additional foundational and recent methods from statistics and data mining that may be of interest for further reading.

2 Univariate Outliers: One Attribute at a Time

The simplest case to consider – and one of the most useful – is to analyze the set of values that appear in a single column of a database table. Many sources of dirty quantitative data are discoverable by examining one column at a time, including common cases of mistyping and the use of extreme default values to achieve spurious integrity on numeric columns.

This single-attribute, or *univariate*, case provides an opportunity to introduce basic statistical concepts in a relatively intuitive setting. The structure of this section also sets the tone for the next two sections to follow: we develop a notion of outliers based on some intuitive statistical properties, and then describe analogs to those properties that can remain "robust" even when significant errors are injected into a large fraction of the data.

2.1 A Note on Data, Distributions, and Outliers

Database practitioners tend to think of data in terms of a collection of information intentionally input into a computer for record-keeping purposes. They are often interested in *descriptive statistics* of the data, but they tend to make few explicit assumptions about why or how the values in the data came to be.

By contrast, statisticians tend to think of a collection of data as a *sample* of some data-generating process. They often try to use the data to find a statistical description or *model* of that process that is simple, but fits the data well. For example, one standard statistical model is *linear regression*, which in the simple two-dimensional case attempts to "fit a line" to the data (Figure 1). Given such a model, they can describe the likelihood (or the "surprise") of a data point with respect to that model in terms of probabilities. They can also use the model to provide probabilities for values that have not been measured: this is useful when data is missing (e.g., in data *imputation*), or has yet to be generated (e.g., in *forecasting*). Model-based approaches are often called *parametric*, since the parameters of a mathematical model describe the data concisely. Approaches that do not require a model are sometimes called *nonparametric* or *model-free*.

Outlier detection mechanisms have been developed from both these points of view, and model-free approaches that may appeal to database practitioners often have natural analogs in statistical models, which can be used to provide additional probabilistic tools.

In practice, most database practitioners do not implicitly view data in a strictly model-free fashion. They often use summary statistics like means and standard deviations when analyzing data sets for outliers. As we discuss shortly in Section 2.2, this assumes a model based on the *normal* distribution, which is the foundation for much of modern statistics.

We will see below that outlier detection techniques can be attacked using both model-free and model-based approaches. We will move between the two fairly often during our discussion, bringing up the distinctions as we go.

2.2 Characterizing a Set of Values: Center and Dispersion

It can be difficult to define the notion of an outlier crisply. Given a set of values, most data analysts have an intuitive sense of when some of the values are "far enough" from "average" that they deserve extra scrutiny. There are various ways to make this notion concrete, which rest on defining specific metrics for the *center* of the set of values (what is "average") and the *dispersion* of the set (which determines what is "far" from average, in a relative sense).

The center, or core, of a set of values is some "typical" value that may or may not appear in the set. The most familiar center metric is the *mean* (average) of the values, which typically is not one of the values in the set[1]. We will discuss other choices of center metrics in the remainder of this report.

[1] In statistical terminology, the average of the set of data values is called a *sample mean*; the true mean is defined with respect to the statistical distribution of the model generating those data values. Similarly below, when we speak of the standard deviation, it is the sample standard deviation we are discussing.

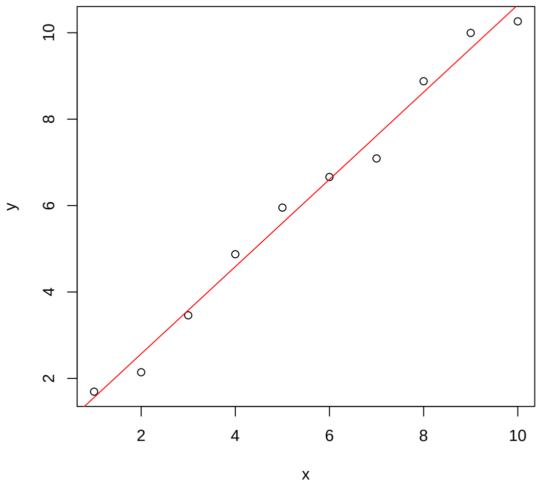


Figure 1: Linear regression applied to a simple two-dimensional dataset.

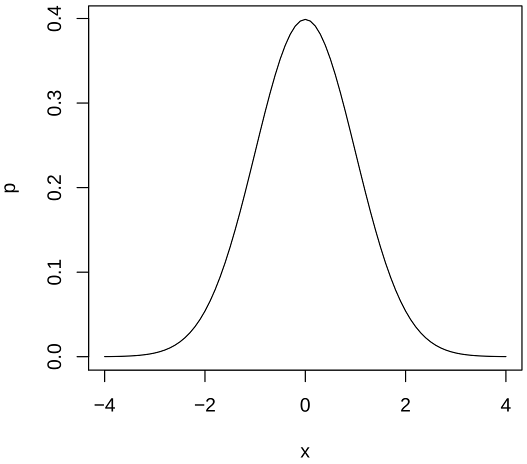


Figure 2: Probability density function for a normal ("Gaussian") distribution with mean 0 and standard deviation 1. The y axis shows the probability of each x value; the area under the curve sums to 1.0 (100%).

The dispersion, or spread, of values around the center gives a sense of what kinds of deviation from the center are common. The most familiar metric of dispersion is the *standard deviation*, or the *variance*, which is equal to the standard deviation squared. Again, we will discuss other metrics of dispersion below.

Our "center/dispersion" intuition about outliers defines one of the most familiar ideas in statistics: the *normal distribution*, sometimes called a *Gaussian distribution*, and familiarly known as the *bell curve* (Figure 2.) Normal distributions are at the heart of many statistical techniques, especially those that focus on measuring the variation of errors. The normal distribution is defined by a *mean* value μ and a standard deviation σ, and has the probability density function

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

Plotting that equation yields a characteristic bell curve like that of Figure 2, where the vertical axis roughly shows the probability of each value on the horizontal axis occurring[2]. While the normal distribution is not a good model for all data, it is a workhorse of modern statistics due both to certain clean mathematical properties, and the fact (based on the famous Central Limit Theorem of statistics) that it arises when many small, independent effects are added together – a very common occurrence.

Beyond the center and dispersion, a third class of metrics that is often discussed is the *skew* of the values, which describes how symmetrically the data is dispersed around the center. In very skewed data, one side of the center has a much longer "tail" than the other. We will return

[2] Technically, a continuous probability density function like the normal should be interpreted in terms of the *area* under the curve in a *range* on the horizontal axis – i.e., the probability that a sample of the distribution falls within that range.

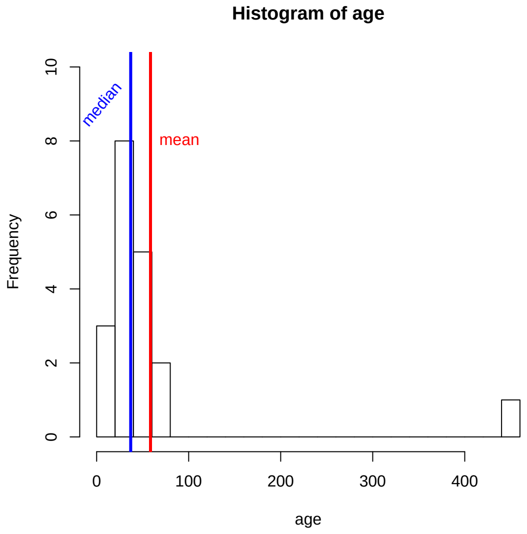


Figure 3: Histogram for example ages; median and mean points are labeled.

to the notion of skew in Section 6.

2.3 Intuition on Outliers and Robust Statistics

Our motivation in defining metrics for the center and dispersion of a data set is to identify *outliers*: values that are "far away" from the center of the data, where distance is measured in terms of the dispersion. For example, a typical definition of an outlier is any value that is more than 2 standard deviations from the mean. But this definition raises a basic question. If the mean and standard deviation are themselves computed over the entire data set, then aren't they "dirtied" to some degree by the very outliers we are using them to detect?

To get some quick intuition on this problem, consider the following set of numbers, corresponding to the ages of employees in a U.S. company:

12 13 14 21 22 26 33 35 36 37 39 42 45 47 54 57 61 68 450

A histogram of the data is shown in Figure 3.

Our knowledge about U.S. child labor laws and human life expectancy might suggest to us that the first three and last one of these numbers are errors. But an automatic procedure does not have the benefit of this knowledge. The mean of these numbers is approximately 59, and the standard deviation approximately 96. So a simple procedure that flags values more than 2 standard deviations from the mean would exclude data outside the range $[96-2*59, 96+2*59] = [-22, 214]$. It would *not* flag the first three values as outliers. This effect is called "masking": the magnitude of one outlier shifts the center and spread metrics enough to mask other outliers. This is a critical problem in data cleaning, where values can easily be off by orders of magnitude due to data entry errors (pressing a key twice instead of once), incorrect use of units, and other effects.

Robust Statistics is a subfield that considers the effect of corrupted data values on distributions, and develops estimators that are robust to such corruptions. Robust estimators can capture important properties of data distributions in a way that is stable in the face of many corruptions of the data, even when these corruptions result in arbitrarily bad values. When the percentage of corruptions in a data set exceeds a threshold called the *breakdown point* of an estimator, the estimator can produce arbitrarily erroneous results. Note that the mean described above can break down with a single bad value. However, the breakdown points for robust estimators can have high breakdown points – as high as 50% of the data. (When more than half the data is corrupted, it is not possible to distinguish true data from outliers.) A main theme in the remainder of this report will be the use of robust estimators for detecting outliers.

2.4 Robust Centers

To avoid the masking effect we saw with computing means and standard deviations, we turn our attention to robust estimators. We begin with robust metrics of the center or "core" of the data.

The *median* of a data set is that item for which half the values are smaller, and half are larger. (For data sets with an even number of values $2n$, the median is defined to be the average of the two "middle" values – those two values for which $n-1$ are smaller and $n-1$ are larger.) The median is an optimally robust statistic: it has a breakdown point of 50%, meaning that more than half of the data have to be corrupted before the median is shifted by an arbitrary amount. Returning to our previous example of employee ages, the median value was 37, which seems a lot more representative than the mean value of 96. Now, consider what happens when we "repair" the data by getting the true values of the outliers (12, 13, 14, 450), which should have been (21,31,41,45) respectively. The resulting set of ages is:

21 21 22 26 31 33 35 36 37 39 41 42 45 45 47 54 57 61 68

The new mean is about 40, and the new median is 39. Clearly the median was more stable with respect to the corruptions. To understand this, notice that the choice of the median element was affected by the *positions* of the outliers in the sort order (whether they were lower or higher than the median before and after being repaired). It was *not* affected by the values of the outliers. In particular suppose that the original value 450 had instead been 450,000,000 – the behavior of the median before and after data repair would not have changed, whereas the mean would have grown enormously before repair[3].

Another popular robust center metric is the *trimmed mean*. The k% trimmed mean is computed by discarding the lowest and highest k% of the values, and computing the mean of the remaining values[4]. The breakdown point of the k% trimmed mean is k%: when more than k% of the values are set to be arbitrarily bad, then one of those values can affect the trimmed

[3] The robust estimators we consider in this report are all based on position or *rank* in this way; they are referred to as L-estimators in the Robust Statistics literature. Another popular class of robust statistics are called M-estimators, which are based on model-based maxiumum-likelihood techniques not unlike our linear regression discussion in Section 2.1. These are somewhat less intuitive for most database professionals, and less natural to implement over SQL databases, but widely studied and used in the statistics community. There are a number of other classes of robust estimators as well. The interested reader is referred to textbooks on Robust Statistics for a more thorough discussion of these estimators [Rousseeuw and Leroy, 1987, Hampel et al., 1986, Huber, 1981].

[4] When k% of the dataset's size is not an integer, the trimmed mean is often computed by finding the two nearest trimmed means (the next lower and higher values of k that produce integers) and averaging the result. For example, the 15% trimmed mean of 10 numbers is computing by averaging the 10% trimmed mean and the 20% trimmed mean. Alternatively, one can round to an integer number of values to trim.

mean arbitrarily. A variant of the trimmed mean is the *winsorized* mean, in which the extreme values are not dropped, they are instead set to be the value of the lowest (or highest) included value. Observe that trimming or winsorizing with $k \approx 50\%$ is equivalent to computing the median: only the median value remains after trimming or winsorizing, and the resulting mean is equal to the median value.

Looking at our original "dirty" age data, the 10% trimmed mean is a bit more than 39.4, and the 10% winsorized mean is a bit more than 39.5.

It should be clear that these center metrics are more robust to outliers than the mean. A more difficult question is to decide which of these metrics to choose in a given scenario. As a rule of thumb, one can remember that (a) the median is the "safest" center metric, due to its 50% breakdown point, but (b) smaller-k trimmed/winsorized means are computed from more data than the median, and hence when they do not break down they are more tightly fit to the data.

As regards the choice between trimming and winsorization, winsorizing does put more weight on the edges of the distribution. This makes it a better choice for normally-distributed (bell-curve) datasets, whereas skewed datasets with "long tails" are more safely handled by trimming, since winsorizing can amplify the influence of unwinsorized outlying values in the tails.

2.4.1 Special Cases: Rates and Indexes

In any discussion of center metrics, there are a few special cases to keep in mind. We discuss two important ones here.

Given a collection of rates or (normalized) indexes, it can be misleading to use traditional center metrics. For example, suppose the rate of inflation of a currency over a series of years is:

$$1.03 \quad 1.05 \quad 1.01 \quad 1.03 \quad 1.06$$

Given an object worth 10 units of the currency originally, its final value would be:

$$10 * 1.03 * 1.05 * 1.01 * 1.03 * 1.06 = 11.926 \text{ units}$$

Now, in computing a center metric μ for numbers like rates, it would be natural to pick one that would lead to the same answer if it were substituted in for the actual rates above:

$$10 * \mu * \mu * \mu * \mu * \mu = 10\mu^5 = 11.926$$

This is not true of the traditional (arithmetic) mean, as one can verify on the example. The *geometric mean* is defined by this desired property: given n numbers $k_1 \ldots k_n$, the geometric mean is defined as the nth root of the product of the numbers:

$$\sqrt[n]{\left(\prod_{i=1}^{n} k_i\right)}$$

In practice, the geometric mean is not greatly affected by outlier values on the high end. However it is sensitive to values close to 0, which can pull the geometric mean down arbitrarily; as a result, the geometric mean is not a robust statistic in general.

In some computations of rates, the *harmonic mean* is the appropriate center metric. The canonical example is when computing average speeds over a fixed distance. Supposing you take a trip, traveling 50 kilometers at 10 kph, and 50 kilometers at 50 kph; you will travel 100 kilometers in 6 hours (5 hours at 10kph, one hour at 50 kph). One would like the "average" speed μ of the 100k trip to be computed as 100k/6hr = 16.67kph. The general form of this computation on values $k_1 \dots k_n$ is the harmonic mean:

$$\frac{n}{\sum_{i=1}^{n} \frac{1}{k_i}}$$

i.e. the reciprocal of the average of reciprocals of the speeds ($\frac{2}{1/10+1/50}$ in our example). Harmonic means are also useful for representing "average" sample sizes across experiments. In general, they are appropriate when the numbers being aggregated have weights associated with them; indeed, the harmonic mean is equivalent to a weighted arithmetic mean with each value's weight being the reciprocal of the value. Like geometric means, harmonic means are sensitive to values close to 0, and are not robust.

In order to make the geometric and harmonic means more robust, trimming can be used. Winsorization does not translate directly to these measures, as the weight of the values being "substituted in" depends on the value. Instead, different substitution rules have been proposed. For geometric means, some practitioners propose substituting in the value 1 (100%), or some value that represents 1/2 of the smallest measurable value, depending on the application. Clearly these approaches can affect estimations significantly, and need to be chosen carefully – they are not well suited to automatic data cleaning scenarios.

In general, a useful rule to know is that for any set of numbers, the harmonic mean is always less than or equal to the geometric mean, which in turn is always less than or equal to the arithmetic mean. So in the absence of domain information, it can be instructive to compute all three (or a robust version of all three).

2.5 Robust Dispersion

Having established some robust metrics for the "center" or "core" of a distribution, we also would like robust metrics for the "dispersion" or "spread" of the distribution as well.

Recall that the traditional standard deviation is defined in terms of each value's distance from the (arithmetic) mean:

$$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(k_i - \mu)^2}.$$

where μ is the arithmetic mean of the values $k_1 \dots k_n$.

When using the median as a center metric, a good robust metric of dispersion is the *Median Absolute Deviation* or *MAD*, which is a robust analogy to the standard deviation: it measures the median distance of all the values from the median value:

$$\underset{i}{\mathrm{MAD}}\{k_i\} = \underset{i}{\mathrm{median}}\{|k_i - \underset{j}{\mathrm{median}}\{k_j\}|\}$$

When using the trimmed (resp. winsorized) mean as the center metric, the natural dispersion metric is the trimmed (winsorized) standard deviation, which is simply the standard deviation of the trimmed (winsorized) data.

2.6 Putting It All Together: Robust Univariate Outliers

Having defined robust definitions of center and dispersion metrics, we can now fairly naturally come up with robust definitions of an *outlier*: a value that is too far away (as defined by the robust dispersion metric) from the center (as defined by the robust center metric).

The median and MAD lead to a robust outlier detection technique known as *Hampel X84* which is considered quiet reliable in the face of many outliers because it can be shown to have an ideal breakdown point of 50%. A simple version of Hampel X84 labels as outliers any data points that are more than $1.4826x$ MADs away from the median, where x is the number of standard deviations away from the mean one would have used in the absence of outliers[5]. For example, we used 2 standard deviations from the mean in Section 2.3, so we would want to look $1.4826 * 2 = 2.9652$ MADs from the median. Recall the example data:

12 13 14 21 22 26 33 35 36 37 39 42 45 47 54 57 61 68 450

The median is 39, and the MAD is 15. So the Hampel x84 outliers are numbers outside the range $[39 - 2.9652 * 15, 39 + 2.9652 * 15.] = [-5.478, 83.478]$. This still does not pick up the first three outliers. But if we compare it to the mean/standard-deviation range of Section 2.3, which was $[-22, 214]$, the robust methods cover many fewer unlikely ages. To emphasize this, consider the case of one standard deviation, corresponding to 1.4826 MADs. The non-outlier range using Hampel X84 is $[39 - 1.4826 * 15, 39 + 1.4826 * 15] = [16.761, 61.239]$, while the mean/standard-deviation range is $[37, 155]$. In this case, both techniques catch the outliers, but the robust estimators flag only one non-outlier incorrectly (68), while the mean/standard-deviation approach flags six non-outliers incorrectly $(21, 22, 26, 33, 35, 36)$.

Another approach is to trim or winsorize the data and compute means and standard deviations on the result. To briefly consider trimming our example, note that we have 19 values, so trimming the bottom and top value corresponds to approximately a 5% trim. The trimmed mean and standard deviation that result are approximately 38.24 and 16.05. Two standard deviations from the mean gives us the range $[6.14, 70.34]$; one standard deviation from the mean gives us the range $[22.19, 54.29]$.

2.7 Database Implementations of Order Statistics

Relational databases traditionally offer data *aggregation* facilities in the SQL language. The built-in SQL aggregation functions include:

- `MAX`, the maximum value in a column,
- `MIN`, the minimum value in a column,
- `COUNT`, the count of rows,
- `SUM`, the sum of the values in a column,
- `AVG`, the (sample) mean of all values in a column,
- `STDEVP`, the (sample) standard deviation of all values in a column,
- `VARP`, the (sample) variance of all values in a column,
- `STDEV`, the (sample) standard deviation of a random sample of values in a column,
- `VAR`, the (sample) variance of a random sample of values in a column

[5] The constant 1.4826 is used because for a normal distribution, one standard deviation from the mean is about 1.4826 MADs.

Obviously these aggregation functions allow outlier detection via traditional metrics such as the mean and standard deviation. Unfortunately, standard SQL offers no robust statistics as aggregate functions built into the standard language. In this section we discuss various approaches for implementing robust estimators in a relational database.

2.7.1 Median in SQL

We begin by discussing "vanilla" SQL expressions to compute the median. Later we will consider using somewhat less standard extensions of SQL to improve performance.

The basic idea of the median can be expressed declaratively in SQL by its definition: that value for which the number of values that are lower is the same as the number of values that are higher. For a column `c` of table `T`, a simple version is as follows:

```
-- A naive median query
SELECT c AS median
  FROM T
 WHERE (SELECT COUNT(*) from T AS T1 WHERE T1.c < T.c)
     = (SELECT COUNT(*) from T AS T2 WHERE T2.c > T.c)
```

Unfortunately that definition requires there to be an odd number of rows in the table, and it is likely to be slow: the straightforward execution strategy rescans `T` two times *for every row of* `T`, an $O(n^2)$ algorithm that is infeasible on a fair-sized dataset. A more thorough approach [Rozenshtein et al., 1997] gathers distinct values by using SQL's `GROUP BY` syntax, and (by joining `T` with itself) for each distinct value of `c` computes the number of rows with values less or greater, accounting for the case with an even number of rows by returning the lower of the two "middle" values:

```
-- a general-purpose median query
SELECT c as median
FROM T x, T y
GROUP BY x.c
HAVING
   SUM(CASE WHEN y.c <= x.c THEN 1 ELSE 0 END) >= (COUNT(*)+1)/2
AND
   SUM(CASE WHEN y.c >= x.c THEN 1 ELSE 0 END) >= (COUNT(*)/2)+1
```

This approach is also somewhat more efficient than the previous, since the naive execution strategy scans `T` only once per row of `T`. However, this is still an $O(n^2)$ algorithm, and remains infeasible on even modest-sized tables.

2.7.2 Sort-Based Schemes using SQL

The obvious algorithm for any order statistic is to sort the table by column `c`, count the rows, and identify the values at the appropriate position. Clearly this can be done by code running outside the database, issuing multiple queries. Psuedo-code for median might look like the following:

```
// find the median of a column
// first find the number of rows
cnt = exec_sql("SELECT count(*) FROM T");
```

```
if (cnt % 2 == 1)
  // odd number of rows: find the middle value
  results = exec_sql("SELECT c FROM T
                      ORDER BY c
                      LIMIT 1
                     OFFSET " + cnt/2);
  median = results.next();
else
  // even number: average the two middle values
  median = exec_sql("SELECT c FROM T
                    ORDER BY c
                    LIMIT 2
                    OFFSET " + cnt/2);
  median = (results.next() + results.next())/2;
```

In some database systems, including recent editions of Microsoft SQL Server, this can be achieved in a single SQL statement that results in roughly the same execution:

```
SELECT MEDIAN(c)
  FROM T
```

While this latter query looks simple, the performance will be about as bad as the previous pseudocode, due to the need to perform a sort of the table to compute the median. Any sorting-based approach takes $O(n \log n)$ operations. In practice, for a table larger than main memory, sorting requires at least 2 disk passes of the table; for tables larger than the square of the size of available memory, it requires yet more passes [Ramakrishnan and Gehrke, 2002, pp. 100-101].

2.7.3 One-Pass Approximation and User-Defined Aggregates

For very large tables and/or scenarios where efficiency is critical, there are algorithms in the database research literature that can, in a single pass of a massive data set, compute *approximate* values for the median or any other quantile, using limited memory. The approximation is in terms of the rank order: rather than returning the desired value (median, quantile, etc.), it will return some value from the data set that is within ϵN ranks of the desired value. The two most-cited algorithms [Manku et al., 1998, Greenwald and Khanna, 2001] differ slightly in their implementation and guarantees, but share the same general approach. Both work by scanning the column of data and storing copies of the values in memory along with a weight per value; during the scan, certain rules are used to discard some of the values in memory and update the weights of others. At the end of the scan, the surviving values and weights are used to produce an estimate of the median (or quantiles).

Again, these algorithms can be implemented by code running outside the database engine to manage the discard and weighting process. Unfortunately that approach will transfer every value from the database table over to the program running the algorithm which can be very inefficient, particularly if the median-finding program is running across a network from the server. To avoid this, and provide better software modularity, some modern databases allow *user-defined aggregate* (UDA) functions to be registered with the database. Once a UDA is registered, it can be invoked conveniently from SQL and executed within the server during query processing. To register a UDA, one must write three “stored procedures” or “user-defined functions”: one to initialize any data structures needed during aggregation, one to process the next tuple in the scan and update the data structures, and one to take the final state of the data structures to produce a single answer. This approach, pioneered in the open-source Postgres database system [Stonebraker, 1986], is a natural fit to the approximation algorithms mentioned above, and is a sensible choice for a scalable outlier detection scheme in a modern database system. Having registered a UDA called my_approx_median, it can be invoked in a query naturally:

```
SELECT my_approx_median(c)
  FROM T
```

Another important practical advantage of the one-pass approximate schemes is queries like the following, that compute medians over multiple columns:

```
SELECT my_approx_median(c1),
       my_approx_median(c2),
       ...
       my_approx_median(cn)
FROM T
```

Using the one-pass approximate approach, all the medians can be computed simultaneously in a single pass of the table. By contrast, the exact median algorithms (including the built-in median aggregate) require sorting the table repeatedly, once per column. Hence even for moderately large tables, the approximate schemes are very attractive.

2.7.4 From Medians to Other Robust Estimators

While the previous discussion focused on the median, all the same techniques apply quite naturally for finding any desired quantile – including the approximation techniques. Given that fact, it is fairly easy to see how to compute the other robust estimators above.

For example, consider computing trimmed means. In this example, assume we use a one-pass approximation approach based on a UDA called my_approx_quantile that takes two arguments: the desired percentile and the column being aggregated. Then the 5% trimmed mean and standard deviation can be computed in SQL as:

```
-- 5% trimming
SELECT AVG(c), STDDEVP(c)
  FROM T,
       (SELECT my_approx_quantile(5,c) AS q5,
               my_approx_quantile,(95,c) AS q95
          FROM T AS T2) AS Quants
 WHERE T.c > Quants.q5
   AND T.c < Quants.q95
```

The 5% winsorized mean and standard deviation can be computed by a similar query:

```
-- 5% winsorization
SELECT AVG(CASE WHEN T.c < Quants.q5 THEN Quants.q5
                WHEN T.c > Quants.q95 THEN Quants.q95
           ELSE T.c),
       STDDEVP(CASE WHEN T.c < Quants.q5 THEN Quants.q5
                    WHEN T.c > Quants.q95 THEN Quants.q95
               ELSE T.c)
  FROM T,
       (SELECT my_approx_quantile(5,c) AS q5,
               my_approx_quantile,(95,c) AS q95
          FROM T AS T2) AS Quants
```

Finally, given that we have functions for the median, we would like to calculate the MAD as well. For an exact median, this is straightforward:

```
   SELECT median(abs(T.c - T2.median))
     FROM T,
          (SELECT median(c) AS median
             FROM T) AS T2
```

It is possible to replace the median aggregate in this query with an approximation algorithm expressed as a UDF; the error bounds for the resulting MAD appear to be an open research question. However, note that even with a one-pass approximation of the median, this query requires two passes: one to compute the median, and a second to compute absolute deviations from the median. An interesting open question is whether there is a direct one-pass, limited-memory approximation algorithm for the MAD.

2.8 Non-Normal Distributions

Much of our discussion was built on intuitions based in normal distributions. Of course in practice, not all data sets are normally distributed. In many cases, the outlier detection schemes we consider will work reasonably well even when the distribution is not normally distributed. However, it is useful to be aware of two commonly occurring cases of distributions that are not normal:

- **Multimodal Distributions:** In some cases, a data set appears to have many “peaks”; such distributions are typically referred as being *multimodal.* In some cases these distributions can be described via superimposed “bell curves”, known as *mixtures of Gaussians.*
- **Zipfian Distributions:** In many settings with data that varies in popularity, a large fraction of the data is condensed into a small fraction of values, with the remainder of the data spread across a “long tail” of rare values. The Zipfian distribution has this quality; we discuss it in more detail in Section 6.2.

In applying data cleaning methods, it can be useful to understand whether one’s data is more or less based in a normal distribution or not. For univariate data, the standard way to do this is to plot a histogram of the data, and overlay it with a normal curve. A Q-Q plot [Barnett, 1975] can also be used to “eyeball” a data set for normality, as we illustrate in Section 7.1. In addition, there are a variety of formal statistical tests for normality [Chakravarti and Roy, 1967, C.E. and W., 1949, Frieden, 2004, Shapiro and Wilk, 1965, D’Agostino and Pearson, 1974]. However, at least one source suggests that these tests are “less useful than you’d guess” [Software, 2008], and cites D’Agostino and Stephens who are also equivocal, saying

> Attempting to make final recommendations [for normality tests] is an unwelcome and near impossible task involving the imposition of personal judgements. . . . A detailed

> graphical analysis involving normal probability plotting should always accompany a formal test of normality [D'Agostino and Pearson, 1974, pp. 405-406].

Note also that outliers can have significant effects on some normality tests; Hartigan and Hartigan's *dip* statistic is a commonly-cited robust normality test [Hartigan, 1985].

Suppose one decides via some combination of looking at plots (D'Agostino and Stephen's "detailed graphical analysis") and examining statistical tests that a data set is in fact not unimodal. What is to be done at that point to remove outliers? Four approaches are natural:

1. *Use outlier tests based on the normality assumption.* One option that is easy to adopt is simply to ignore the non-normality in the data, and use the outlier detection tests we describe in the subsequent sections that are based in normal assumptions. For multimodal distributions, these tests will continue to identify outliers that are at the extremes of the distrbution. They will not identify outliers that fall "between the bells" of multiple normal curves. They also may incorrectly label data in the edges of the outermost "bells" as being outliers, when they would not be so labeled if each bell were examined alone. However, that kind of concern is always present in outlier detection depending on the setting of threshholds: how much of the data at the "edges" is truly outlying? The answer to this question is always domain-specific and judged by an analyst. With respect to Zipfian distributions, normality assumptions will tend to arbitrarily pick points in the "long tail" as outlying, even though in many cases those points are no more likely to be outliers than points in the tail that are closer to the mean. An analyst's interpretation of these outlying points may be clouded as well, since by definition the "strange" or "unpopular" values are many, and likely to surprise even people familiar with the domain. Knowing that the tail is indeed long can help the analyst exercise caution in that setting.

2. *Model the data and look for outliers in the residuals.* Another approach is to choose a model other than a normal distribution to model the data. For example, if one believes that data is Zipfian, one can try to fit a Zipfian distribution to the data. Given such a model, the distribution of the data can be compared to the model; the differences between the empirical data and the model are called *residuals*. Residuals of well-chosen models are quite often normally distributed, so standard outlier detection techniques can be applied to the set of residuals, rather than the data – points with outlying residuals represent potential outliers from a model-based point of view. The various techniques in this paper can be applied to residuals quite naturally.

3. *Data partitioning* schemes can either manually or automatically partition a data set into subsets, in hopes that the subsets are more statistically homogeneous and more likely to be normal. Subsequently, outlier detection techniques can be run within each subset, and the subsets themselves examined to see if an entire partition is outlying. This approach is particularly natural for multimodal distributions. Unfortunately Zipfian distributions are "self-similar" – their subsets are also Zipfian. Data partitioning can be done using a variety of manual, automatic and semi-automatic schemes. The standard manual scheme for partitioning database data is to use *OLAP* or so-called *data cube* tools to help an analyst manually partition data into sensible "bins" by "drilling down" along multiple attributes. Sarawagi introduced semi-automatic techniques for identifying "interesting" regions in the data cube, which may help the analyst decide how to partition the data [Sarawagi, 2001]. Johnson and Dasu introduce an interesting multidimensional clustering technique called *data spheres* that build on the notion of quantiles in multiple dimensions [Johnson

and Dasu, 1998]. The standard fully-automated scheme for partitioning data statistically is called *clustering*, and there are a wide range of techniques in the literature on efficient and scalable clustering schemes [Berkhin, 2002].

4. *Non-parametric outlier detection.* Another option available for data that deviates significantly from normality is to use non-parametric "model-free" approaches to outlier detection. We survey a number of these techniques in Section 3.3. These techniques have drawbacks and fragilities of their own, which we also discuss.

Clearly, handling outlier detection with non-normal data presents a number of subtleties. The most important conclusion from this discussion is that in *all* settings, outlier detection should be a human-driven process, with an analyst using their judgment and domain knowledge to validate information provided by algorithms. In particular, if an analyst is convinced (e.g., via graphical tests) that a data set is not normal, they need to be particularly careful to choose outlier approaches that accomodate their non-normality. Many experienced data analysts agree that automated techniques should be accompanied by data visualizations before conclusions are drawn. In fact, the choice and parameterization of data cleaning methods is often aided by visualization-driven insights, and it is useful to consider the use of visualizations, analyses, and data cleaning transformations to be integrated into an iterative process [Raman and Hellerstein, 2001].

3 Multivariate Outliers

In the previous section, we considered methods to detect outliers in a set of numbers, as one might find in a column of a database table. In statistical nomenclature, this is the *univariate* (or *scalar*) setting. Univariate techniques can work quite well in many cases. However, there is often a good deal more information available when one considers multiple columns at a time – the *multivariate* case.

As an example, consider a table of economic indicators for various countries, which has a column for average household income, and another column for average household expenditures. In general, incomes across countries may range very widely, as would expenditures. However, one would expect that income and expenditures are positively correlated: the higher the income in a country, the higher the expenditures. So a row for a country with a low per-capita average income but a high per-capita average expenditure is very likely an error, *even though* the numbers taken individually may be well within the normal range. Multivariate outlier detection can flag these kinds of outliers as suspicious.

Multivariate techniques are analogous in some ways to ideas we saw in the univariate case, but the combinations of variables make things both more complicated to define and interpret, and more time-consuming to compute. In this section we extend our basic measures of center and dispersion to the multivariate setting, and discuss some corresponding robust metrics and outlier detection techniques.

3.1 Intuition: Multivariate Normal Distributions

In the univariate case, we based our intuition on the mean and standard deviation of a set of data, leading to the normal or "bell curve" shown in Figure 2.

Extending this in a simple way to two dimensions, one might define some (x, y) pair as the mean, and a single standard deviation number to define the dispersion around the mean. This (means, medians, etc.) have different known sampling distributions, and hence different rules for computing the mean and variance.

Resampling can be used for more complex summary statistics than simple means and variances of the original data. For example, in bivariate (two-dimensional) data, resampling can be used in conjunction with linear regression to identify outliers from the regression model [Martin and Roberts, 2006].

6 Cleaning Up Counts: Frequency Outliers

In some scenarios, the specific values in a column are less important than the number of times each value is repeated in the column – the *frequency* of the values. Frequency statistics can be important not only for quantitative attributes, but for *categorical* attributes that do not have an inherent numerical interpretation. For categorical attributes, the "names" of the data values are relevant, but the ordering of values is not. For example, in a database of animal sightings, a "species code" column may be numeric, but it is usually irrelevant whether the code number assigned to iguanas is closer to the code for tigers than it is to the code for mice. For categorical data, the statistical distribution of values is important in terms of the frequencies of occurrence of each value – the number of mice, tigers, and iguanas observed. As a result, the techniques for outlier detection in previous sections are not a natural fit for cleaning dirty data in a key column.

In this section we discuss outlier methods that focus on two extremes of frequencies: "distinct" attributes where nearly every value has frequency 1, and attributes that have high frequency "spikes" at some value.

6.1 Distinct Values and Keys

It is quite common for a data set to have *key* columns that provide a unique identifier for each row. A key can be made up of a single column (e.g., a taxpayer ID number), or of a concatenation of columns (e.g., <cityname,countrycode>). We return to multi-column "composite" keys in Section 6.1.1

In a key with perfect integrity, the frequency of each value is equal to 1, and hence the number of distinct values in the key columns should be the same as the number of rows. However, it is often the case in dirty data that a would-be key contains some duplicated values, due either to data entry errors, or repeated use of some value as a code for "unknown".

There are two scenarios when identifying dirty key columns is important. The simple scenario is one of data repair, where one has knowledge about the column(s) that form a key, and is trying to determine which entries in the key column(s) need to be cleaned. Identifying the potentially dirty rows amounts to identifying duplicated key values, and returning all rows with those key values.

The somewhat more complex scenario is "key discovery", where one is trying to discover which columns might actually be intended as keys, despite the fact that there may be some dirty data. This problem requires coming up with a metric for how "close" a column is to being a key. One intuitive measure for dirty keys is what we call the *unique row ratio*: the ratio of distinct values in the column to the total number of rows in the table. If this is close to 1.0, the column may be flagged as a potential dirty key. This is the approach used proposed by Dasu and Johnson [Dasu et al., 2002] However, this test is not robust to "frequency outliers": scenarios where there are a small number of values with very high frequency. This problem often occurs due to the spurious integrity problem mentioned in Section 1.1, which lead data-entry users to use common "dummy" values like 00000 or 12345 as a default. A more robust measure is what we call the *unique value ratio*: the ratio of "unique" values (values with frequency one) to the total number of distinct values in the key column(s).

SQL's aggregation functionality provides language features to compute basic frequency statistics fairly easily. For example, here is a query to compute the unique value ratio mentioned above:

```
SELECT UniqueCount.cnt / DistinctValues.cnt
  FROM
        -- Unique values with frequency 1
        (SELECT COUNT(Uniques.c) AS cnt
         FROM (SELECT c FROM T
               GROUP BY c HAVING COUNT(c) = 1) AS Uniques) AS UniqueCount,
        -- Number of distinct values
        (SELECT COUNT(DISTINCT c) AS cnt FROM T) AS DistinctValues;
```

Unfortunately, this query – or any other deterministic scheme for computing frequencies – can be very resource-intensive and time-consuming. The main problem arises in large tables with columns with contain many distinct values. Counting the number of distinct values requires some scheme to bring all copies of each value together – this is expressed by the GROUP BY and DISTINCT clauses in the SQL query above. This is typically implemented (either in a database engine or application code) by either sorting the table, or using a hashing scheme with one hash "bucket" per distinct value. In either case this requires multiple passes over the data for large tables with many distinct values.

However, there are a number of elegant one-pass approximation schemes for computing frequencies that can be implemented naturally as user-defined aggregates in a relational database. The Flajolet-Martin (FM) Sketch [Flajolet and Martin, 1985] is an important tool here, providing a one-pass approximation to the number of distinct values. The FM sketch is a bitmap that is initialized to zeros at the beginning of a scan. Each bit in the bitmap is associated with a random binary hash function chosen carefully from a family of such functions. As each value is scanned during a pass of the table, the hash function for each bit is evaluated on that value, and if it evaluates to 1 then the corresponding bit in the sketch is turned on. At the end of the scan, the resulting bitmap can be used to estimate the number of distinct values within a factor of ϵ, where ϵ is a function of the number of bits in the sketch.

FM sketches can be used directly to compute an approximate unique row ratio in a single pass. FM sketches can also be used to compute the denominator of the unique value ratio. However, the numerator is a specific form of what is called an *Iceberg* or *Heavy Hitter* Query: a query that looks for values with frequency above some threshold [Fang et al., 1998, Hershberger et al., 2005]. Unfortunately, the desired threshold for the unique value ratio is extremely low (1 row, or equivalently a $\frac{1}{N}$ fraction of the N rows in the table). The various approximation algorithms for iceberg queries [Fang et al., 1998, Manku and Motwani, 2002, Hershberger et al., 2005] do not perform well for such low thresholds.

The literature does not appear to contain a one-pass solution to key detection that is robust to frequency outliers. But there is a natural two-pass approach akin to a trimmed unique row ratio. First, an approximate iceberg technique like that of [Manku and Motwani, 2002] is used to identify the set of values S that have frequencies above some sizable threshold – say 1% of the rows (assuming a table much larger than 100 rows). Then, a second pass uses FM sketches to compute the unique value ratio of those rows that are not in the set of "iceberg" values.

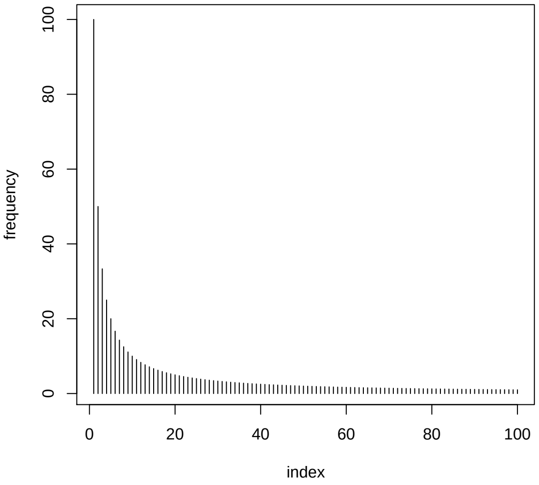


Figure 6: A Zipf Distribution, $1/x$.

To our knowledge, the question of analyzing the breakdown points of the unique value ratio or the trimmed unique row ratio are open research questions.

6.1.1 Composite Keys

We have identified a number of metrics for evaluating the likelihood of a column being a key. Any of these metrics can be applied to evaluate the likelihood of a set of columns forming a composite key as well. The problem that arises is that there are exponentially many possible sets of columns to evaluate, and even with one-pass approximations this is infeasibly slow.

Tane is an efficient algorithm for discovering approximate composite keys; it can be used with any of the metrics we describe above. The core of Tane is an efficient algorithm for deciding which combination of columns to text for "key-ness" next, based on the combinations previously tested.

It is not uncommon to uncommon to couple an algorithm like Tane with some heuristics about which combinations of columns could be keys. For example, the Bellman data cleaning system only considers composite keys with 3 or fewer columns. A recent related algorithm called Gordian [Sismanis et al., 2006] was proposed for discovering exact keys (with no duplicates in them); it seems plausible to extend Gordian to handle dirty data, but this is an open question.

6.2 Frequent Values and Zipfian Distributions

In many data sets, it is useful to identify values that have unusually high frequencies [Cormode and Muthukrishnan, 2003, Manku and Motwani, 2002, Hershberger et al., 2005]. It is often useful to report the heavy hitters in a data set – both because they are in some sense "representative" of an important fraction of the data, and because if they are indeed contaminated, they can have a significant effect on the quality of the data overall.

As noted above, heavy hitters frequently arise due to spurious integrity effects in manual data entry settings. They also arise in automatic measurement settings, when devices fall back to default readings in the face of errors or uncertainty. In these contexts, the heavy hitters often include erroneous values that should be cleaned.

Heavy hitters also become noticeable in data that follows Zipfian [Zipf, 1949] or other power-law distributions [Mitzenmacher, 2004] (Figure 6.2). In popular terminology these are sometimes referred to as "80-20" distributions, and they form the basis of "the long tail" phenomenon recently popularized in a well-known book [Anderson, 2006]. Examples of data that follow these distributions include the frequency of English words used in speech (Zipf's original example [Zipf, 1949]), the popularity of web pages, and many other settings that involve sharp distinctions between what is "hot" and what is not, in terms of frequency. An interesting property of Zipfian distributions is that they are *self-similar*: removing the heavy hitters results in a Zipfian distribution on the remaining values. As a result, in these distributions it is difficult using the techniques discussed earlier to identify when/if the data is "clean": frequency outliers are endemic to the definition of a Zipfian distribution, and removing them results in a new Zipfian which again has a few "hot" items.

Instead, in scenarios where the data is known to be Zipfian, a natural statistical approach is to fit a Zipfian model to the data, and study the *residuals*: the differences between observed frequencies, and what the best-fitting model predicts. Residuals often fall into a normal distribution, so robust mechanisms can be used to identify outliers among the residuals, which indicate outlying frequencies (outlying with respect to the Zipfian assumption, anyway). The approach of using models and identifying outliers among the residuals is quite common, though the standard models employed in the literature are usually based on linear regression. The interested reader is referred to [Rousseeuw and Leroy, 1987] to learn more about these model-based approaches.

In recent years there have been a number of approximate, one-pass heavy hitter algorithms that use limited memory; Muthukrishnan covers them in his recent survey article on data streams [Muthukrishnan, 2005].

7 Notes on Interface Design

Data cleaning can be influenced greatly by the thoughtful design of computer interfaces. This is true at all stages in the "lifetime" of data, from data collection and entry, through transformation and analysis. The field of human-computer interaction with quantitative information is rich and growing; it is the subject of numerous books and research papers. Despite this fact, there is very little work on interface design for data entry and data cleaning. This section touches briefly on both data visualization and data entry. In addition to surveying a few of the leading data visualization techniques used in data cleaning, we provide a less scholarly discussion of some the key design principles in data entry that seem to be both important and largely overlooked.

7.1 Cleaning Data Via Exploratory Data Analysis

The human visual system is a sophisticated data analysis engine, and data visualization has been a rich area of research in both statistics and computer science. A few classical techniques stand out for their utility in data cleaning; we them briefly survey here.

Histograms are a natural way to visualize the density of data points across values of a single dimension. The basic idea of a histogram is to partition the data set into bins, and plot the count or probability of items in each bin. *Equi-width* histograms partition the domain of an attribute (the set of possible values) into bins, and the heights of the bars illustrate the frequencies of the

References

Chris Anderson. *The Long Tail: Why the Future of Business is Selling Less of More*. Hyperion, 2006.

V. Barnett. Probability plotting methods and order statistics. *Applied Statistics*, 24, 1975.

S. D. Bay and M. Schwabacher. Mining distance-based outliers in near linear time with randomization and a simple pruning rule. In *Proc. ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, 2003.

Pavel Berkhin. Survey of clustering data mining techniques. Technical report, Accrue Software, San Jose, CA, 2002. `http://citeseer.ist.psu.edu/berkhin02survey.html`.

I. Bhattacharya and L. Getoor. Collective entity resolution in relational data. *ACM Transactions on Knowledge Discovery from Data (TKDD)*, 1(1), 2007.

A. M. Bianco, M. Garca Ben, E. J. Martnez, and V. J. Yohai. Outlier detection in regression models with arima errors using robust estimates. *Journal of Forecasting*, 20(8), 2001.

George Box, Gwilym M. Jenkins, and Gregory Reinsel. *Time Series Analysis: Forecasting & Control (3rd Edition)*. Prentice Hall, 1994.

M. M. Breunig, H.-P. Kriegel, R. T. Ng, and J. Sander. Lof: Identifying density-based local outliers. In *Proc. ACM SIGMOD International Conference on Management of Data*, 2000.

Shannon C.E. and Weaver W. *The Mathematical Theory of Communication*. University of Illinois Press, Urbana and Chicago, 1949.

Laha Chakravarti and Roy. *Handbook of Methods of Applied Statistics, Volume I*. John Wiley and Sons, 1967.

A. D. Chapman. Principles and methods of data cleaning primary species and species-occurrence data, version 1.0. Technical report, Report for the Global Biodiversity Information Facility, Copenhagen, 2005. `http://www.gbif.org/prog/digit/data_quality/DataCleaning`.

William S. Cleveland. *Visualizing Data*. Hobart Press, 1993.

Graham Cormode and S. Muthukrishnan. What's hot and what's not: Tracking most frequent items dynamically. In *In Proc. ACM Principles of Database Systems (PODS)*, 2003.

R.B. D'Agostino and E.S. Pearson. Tests for depature from normality: Empirical results for the distributions of b_2 and $\sqrt{b}_1$. *Biometrika*, 60, 1974.

Tamraparni Dasu and Theodore Johnson. *Exploratory Data Mining and Data Cleaning*. Wiley, 2003.

Tamraparni Dasu, Theodore Johnson, S. Muthukrishnan, and Vladislav Shkapenyuk. Mining database structure; or, how to build a data quality browser. In *Proc. ACM SIGMOD International Conference on Management of Data*, 2002.

Xin Dong, Alon Halevy, and Jayant Madhavan. Reference reconciliation in complex information spaces. In *Proc. ACM SIGMOD international conference on Management of data*, 2005.

Min Fang, Narayanan Shivakumar, Hector Garcia-Molina, Rajeev Motwani, and Jeffrey D Ullman. Computing iceberg queries efficiently. In *Proc. International Conference on Very Large Databases (VLDB)*, 1998.

Stephen Few. *Show Me the Numbers: Designing Tables and Graphs to Enlighten.* Analytics Press, 2004.

David F. Findley, Brian C. Monsell, William R. Bell, Mark C. Otto, and Bor-Chung Chen. New capabilities and methods of the x-12-arima seasonal-adjustment program. *Journal of Business & Economic Statistics*, 16(2), 1998.

Philippe Flajolet and G. Nigel Martin. Probabilistic counting algorithms for data base applications. *Journal of Computer and Systems Sciences*, 31(2), 1985.

B. Roy Frieden. *Science from Fisher Information.* Cambridge University Press, 2004.

Minos N. Garofalakis and Phillip B. Gibbons. Approximate query processing: Taming the terabytes. In *International Conference on Very Large Data Bases (VLDB)*, 2001. Tutorial. Slides available online at `http://www.cs.berkeley.edu/~minos/Talks/vldb01-tutorial.ppt`.

Minos N. Garofalakis, Johannes Gehrke, and Rajeev Rastogi. Querying and mining data streams: You only get one look. In *ACM-SIGMOD International Conference on Management of Data*, 2002. Tutorial. Slides available online at `http://www.cs.berkeley.edu/~minos/Talks/streams-tutorial02.pdf`.

Luis Gravano, Panagiotis G. Ipeirotis, Nick Koudas, and Divesh Srivastava. Text joins for data cleansing and integration in an rdbms. In *Proc. International Conference on Data Engineering (ICDE)*, 2003.

Michael Greenwald and Sanjeev Khanna. Space-efficient online computation of quantile summaries. In *Proc. ACM SIGMOD International Conference on Management of Data*, 2001.

Frank R. Hampel, Elvezio M. Ronchetti, Peter J. Rousseeuw, and Werner A. Stahel. *Robust Statistics - The Approach Based on Influence Functions.* Wiley, 1986.

P. M. Hartigan. Computation of the dip statistic to test for unimodality. *Applied Statistics*, 34 (3), 1985.

John Hershberger, Nisheeth Shrivastava, Subhash Suri, and Csaba D. Tóth. Space complexity of hierarchical heavy hitters in multi-dimensional data streams. In *Proc. ACM SIGMOD-SIGACT-SIGART Symposium on Principles of Database Systems (PODS)*, 2005.

Kuan-Tsae Huang, Yang W. Lee, and Richard Y. Wang. *Quality Information and Knowledge Management.* Prentice Hall, 1999.

Peter. J. Huber. *Robust Statistics.* Wiley, 1981.

Ykä Huhtala, Juha Kärkkäinen, Pasi Porkka, and Hannu Toivonen. TANE: An efficient algorithm for discovering functional and approximate dependencies. *The Computer Journal*, 42 (2):100–111, 1999.

Yannis Ioannidis. The history of histograms (abridged). In *Proc. International Conference on Very Large Data Bases (VLDB)*, 2003.

Michele G. Jarrell. Multivariate outliers. review of the literature. In *Proc. Annual Meeting of Mid-South Educational Research Association*, 1991. http://www.eric.ed.gov/ERICDocs/data/ericdocs2sql/content_storage_01/0000019b/80/23/61/0b.pdf.

Theodore Johnson and Tamraparni Dasu. Comparing massive high-dimensional data sets. In *Knowledge Discovery and Data Mining*, 1998.

Regina Kaiser and Agustín Maravall. Seasonal outliers in time series. Banco de España Working Papers 9915, Banco de España, 1999. available at http://ideas.repec.org/p/bde/wpaper/9915.html.

E. M. Knorr and R. T. Ng. Finding intensional knowledge of distance-based outliers. In *Proc. International Conference on Very Large Data Bases*, 1999.

G. Kollios, D. Gunopulos, N. Koudas, and S. Berchtold. Efficient biased sampling for approximate clustering and outlier detection in large data sets. *IEEE Transactions on Knowledge and Data Engineering*, 15(5), 2003.

Regina Y. Liu, Jesse M. Parelius, and Kesar Singh. Multivariate analysis by data depth: descriptive statistics, graphics and inference. *Annals of Statistics*, 27(3), 1999.

J.F. MacGregor and T.J. Harris. The exponentially weighted moving variance. *Journal of Quality Technology*, 25(2), 1993.

G.S. Maddala and C.R. Rao. *Handbook of Statistics 15: Robust Inference.* Elsevier, 1997.

Gurmeet Singh Manku and Rajeev Motwani. Approximate frequency counts over data streams. In *Proc. International Conference on Very Large Data Bases (VLDB)*, 2002.

Gurmeet Singh Manku, Sridhar Rajagopalan, and Bruce G. Lindsay. Approximate medians and other quantiles in one pass and with limited memory. In *Proc. ACM SIGMOD International Conference on Management of Data*, 1998.

R. Maronna and R. Zamar. Robust estimation of location and dispersion for high-dimensional data sets. *Technometrics*, 44(4), 2002.

Michael Martin and Steven Roberts. An evaluation of bootstrap methods for outlier detection in least squares regression. *Journal of Applied Statistics*, 33(7), 2006.

M. Mitzenmacher. A brief history of generative models for power law and lognormal distributions. *Internet Mathematics*, 1(2), 2004.

S. Muthukrishnan. Data streams: Algorithms and applications. *Foundations and Trends in Theoretical Computer Science*, 1(1), 2005.

M.C. Otto and W.R. Bell. Two issues in time series outlier detection using indicator variables. In *Proc. American Statistical Association, Business and Economics Statistics Section*, 1990.

Gregory Piatetsky-Shapiro. Kdnuggets : Solutions : Data providers and data cleaning, 2008. http://www.kdnuggets.com/solutions/data-cleaning.html.

R Project. The R project for statistical computing, 2008. http://www.r-project.org/.

Raghu Ramakrishnan and Johannes Gehrke. *Database Management Systems, 4th Edition.* McGraw-Hill, 2002.

Vijayshankar Raman and Joseph M. Hellerstein. Potter's wheel: An interactive data cleaning system. In *Proc. International Conference on Very Large Data Bases (VLDB)*, 2001.

S. Ramaswamy, R. Rastogi, and K. Shim. Efcient algorithms for mining outliers from large data sets. In *Proc. ACM SIGMOD International Conference on Management of Data*, 2000.

P. J. Rousseeuw and K. Van Driessen. A fast algorithm for the minimum covariance determinant estimator. *Technometrics*, 41(3), 1999.

Peter J. Rousseeuw and Annick M. Leroy. *Robust Regression and Outlier Detection.* Wiley, 1987.

David Rozenshtein, Anatoly Abramovich, and Eugene Birger. *Optimizing Transact-SQL : Advanced Programming Techniques.* SQL Forum Press, 1997.

S. Sarawagi. User-cognizant multidimensional analysis. *The VLDB Journal*, 10(2), 2001.

S. S. Shapiro and M. B. Wilk. An analysis of variance test for normality (complete samples). *Biometrika*, 52(3 and 4), 1965.

P. Singla and P. Domingos. Entity resolution with markov logic. In *IEEE International Conference on Data Mining (ICDM)*, 2006.

Yannis Sismanis, Paul Brown, Peter J. Haas, and Berthold Reinwald. Gordian: efficient and scalable discovery of composite keys. In *Proc. International Conference on Very Large Data Bases (VLDB)*, 2006.

Graphpad Software. Normality tests, 2008. `http://www.graphpad.com/index.cfm?cmd=library.page&pageID=24&categoryID=4`.

Michael Stonebraker. Inclusion of new types in relational data base systems. In *Proc. International Conference on Data Engineering*, 1986.

Gilbert Strang. *Introduction to Linear Algebra, Third Edition.* SIAM, 2003.

Valentin Todorov. Robust location and scatter estimators for multivariate analysis. In *useR!, The* R *User Conference*, 2006. `http://www.r-project.org/user-2006/Slides/Todorov.pdf`.

Ruey S. Tsay. Outliers, level shifts, and variance changes in time series. *Journal of Forecasting*, 7(1), 1988.

Edward R. Tufte. *The Visual Display of Quantitative Information, 2nd Edition.* Graphics Press, 2001.

Edward R. Tufte. *Envisioning Information.* Graphics Press, 1990.

Edward R. Tufte. *Beautiful Evidence.* Graphics Press, 2006.

John Tukey. *Exploratory Data Analysis.* Addison-Wesley, 1977.

William E. Winkler. Overview of record linkage and current research directions. Technical report, Statistical Research Division, U.S. Census Bureau, 2006. `http://www.census.gov/srd/papers/pdf/rrs2006-02.pdf`.

George K. Zipf. *Human Behaviour and the Principle of Least-Effort.* Addison-Wesley, 1949.

Week 6: Taming technical bias

Taming Technical Bias in Machine Learning Pipelines [*]

Sebastian Schelter
University of Amsterdam & Ahold Delhaize
Amsterdam, The Netherlands
s.schelter@uva.nl

Julia Stoyanovich
New York University
New York, NY, USA
stoyanovich@nyu.edu

Abstract

Machine Learning (ML) is commonly used to automate decisions in domains as varied as credit and lending, medical diagnosis, and hiring. These decisions are consequential, imploring us to carefully balance the benefits of efficiency with the potential risks. Much of the conversation about the risks centers around bias — a term that is used by the technical community ever more frequently but that is still poorly understood. In this paper we focus on technical bias — a type of bias that has so far received limited attention and that the data engineering community is well-equipped to address. We discuss dimensions of technical bias that can arise through the ML lifecycle, particularly when it's due to preprocessing decisions or post-deployment issues. We present results of our recent work, and discuss future research directions. Our over-all goal is to support the development of systems that expose the knobs of responsibility to data scientists, allowing them to detect instances of technical bias and to mitigate it when possible.

1 Introduction

Machine Learning (ML) is increasingly used to automate decisions that impact people's lives, in domains as varied as credit and lending, medical diagnosis, and hiring. The risks and opportunities arising from the wide-spread use of predictive analytics are garnering much attention from policy makers, scientists, and the media. Much of this conversation centers around *bias* — a term that is used by the technical community ever more frequently but that is still poorly understood.

In their seminal 1996 paper, Friedman and Nissenbaum identified three types of bias that can arise in computer systems: pre-existing, technical, and emergent [9]. We briefly discuss these in turn, see Stoyanovich et al. [33] for a more comprehensive overview.

- *Pre-existing bias* has its origins in society. In ML applications, this type of bias often exhibits itself in the input data; detecting and mitigating it is the subject of much research under the heading of algorithmic fairness [5]. Importantly, the presence or absence of pre-existing bias cannot be scientifically verified, but rather is postulated based on a belief system [8, 12]. Consequently, the effectiveness — or even the validity — of a technical attempt to mitigate pre-existing bias is predicated on that belief system.

Bulletin of the IEEE Computer Society Technical Committee on Data Engineering

[*] This work was supported in part by NSF Grants No. 1926250, 1934464, and 1922658, and by Ahold Delhaize. All content represents the opinion of the authors, which is not necessarily shared or endorsed by their respective employers and/or sponsors.

- *Technical bias* arises due to the operation of the technical system itself, and can amplify pre-existing bias. The bad news is that, as we argue in the remainder of this paper, the risks of introducing technical bias in ML pipelines abound. The good news is that, unlike with pre-existing bias, there is no ambiguity about whether a technical fix should be attempted: if technical systems we develop are introducing bias, then we should be able to instrument these systems to measure it and understand its cause. It may then be possible to mitigate this bias and to check whether the mitigation was effective.
- *Emergent bias* arises in the context of use of the technical system. In Web ranking and recommendation in e-commerce, a prominent example is "rich-get-richer": searchers tend to trust the systems to indeed show them the most suitable items at the top positions, which in turn shapes a searcher's idea of a satisfactory answer.

In this paper, we focus on technical bias, — a type of bias that has so far received limited attention, particularly when it's due to preprocessing decisions or post-deployment issues, and that the data engineering community is well-equipped to address. Our over-all goal is to support the development of systems that *expose the knobs of responsibility to data scientists*, allowing them to detect instances of technical bias, and to mitigate it when possible.

Running example. We illustrate the need for taming technical bias with an example from the medical domain. Consider a data scientist who implements a Python pipeline that takes demographic and clinical history data as input, and trains a classifier to identify patients at risk for serious complications. Further, assume that the data scientist is under a legal obligation to ensure that the resulting ML model works equally well for patients across different gender and age groups. This obligation is operationalized as an intersectional fairness criterion, requiring equal false negatives rates for groups of patients identified by a combination of gender and age group.

Consider Ann, a data scientist who is developing this classifier. Following her company's best practices, Ann will start by splitting her dataset into training, validation, and test sets. Ann will then use `pandas`, `scikit-learn` [19], and their accompanying data transformers to explore the data and implement data preprocessing, model selection, tuning, and validation. Ann starts preprocessing by computing value distributions and correlations for the features in her dataset, and by identifying missing values. She will fill these in using a default interpolation method in scikit-learn, replacing missing values with the mode value for that feature. Finally, following the accepted best practices at her company, Ann implements model selection and hyperparameter tuning. As a result of this step, Ann will select a classifier that shows acceptable performance according to her company's standard metrics: it has sufficient accuracy, while also exhibiting sufficiently low variance. When Ann considers the accuracy of her classifier closely, she observes a disparity: accuracy is lower for middle-aged women. Ann is now faced with the challenge of figuring out why this is the case, whether any of her technical choices during pipeline construction contributed to this model bias, and what she can do to mitigate this effect. We will revisit this example, and also discuss issues that may arise after the model is deployed, in the remainder of this paper.

Roadmap. The rest of this paper is organized as follows. In Section 2, we outline the dimensions of technical bias as they relate to two lifecycle views of ML applications: the data lifecycle and the lifecycle of design, development, deployment, and use. Then, in Section 3 we present our recent work on helping data scientists responsibly develop ML pipelines, and validate them post-deployment. We conclude in Section 4 with directions for future research.

2 Dimensions of Technical Bias

There are many different ways in which Ann (or her colleagues who deploy her model) could accidentally introduce technical bias. Some of these relate to the view of ML model development through the lens of the *data lifecycle*. As argued in Stoyanovich et al. [33], responsibility concerns, and important decision points, arise in data sharing, annotation, acquisition, curation, cleaning, and integration. Thus, opportunities for improving data quality and representativeness, controlling for bias, and allowing humans to oversee the process, are missed if we do not consider these earlier data lifecycle stages. We discuss these dimensions of technical bias in Section 2.1. Additional challenges, and opportunities to introduce technical bias, arise after a model is deployed. We discuss these in Section 2.2.

Note that, in contrast to Bower et al. [4] and Dwork et al. [7], who study fairness in ML pipelines in which multiple models are composed, we focus on complex — and typical — pipelines in which bias may arise due to the composition of data preprocessing steps, or to data distribution shifts past deployment.

2.1 Model Development Stage

There are several subtle ways in which data scientists can accidentally introduce data-related bias into their models during the development stage. Our discussion in this section is inspired by the early influential work by Barocas and Selbst [1], and by Lehr and Ohm [15], who highlighted the issues that we will make more concrete.

Data cleaning. Methods for missing value imputation that are based on incorrect assumptions about whether data is missing at random may distort protected group proportions. Consider a form that gives patients a binary choice of gender and also allows to leave gender unspecified. Suppose that about half of the users identify as men and half as women, but that women are more likely to omit gender. Then, if mode imputation (replacing a missing value with the most frequent value for the feature, a common choice in `scikit-learn`) is used, then all (predominantly female) unspecified gender values will be set to male. More generally, multi-class classification for missing value imputation typically only uses the most frequent classes as target variables [3], leading to a distortion for small population groups, because membership in these groups will never be imputed. Next, suppose that some individuals identify as non-binary. Because the system only supports male, female, and unspecified as options, these individuals will leave gender unspecified. If mode imputation is used, then their gender will be set to male. A more sophisticated imputation method will still use values from the active domain of the feature, setting the missing values of gender to either male or female. This example illustrates that bias can arise from an incomplete or incorrect choice of data representation.

Finally, consider a form that has home address as a field. A homeless person will leave this value unspecified, and it is incorrect to attempt to impute it. While dealing with `null` values is known to be difficult and is already considered among the issues in data cleaning, the needs of responsible data management introduce new problems. Further, data quality issues often disproportionately affect members of historically disadvantaged groups [14], and so we risk compounding technical bias due to data representation with pre-existing bias.

Data filtering. Selections and joins can arbitrarily change the proportion of protected groups (e.g., for certain age groups) even if they do not directly use the sensitive attribute (e.g., age) as part of the predicate or of the join key. This change in proportion may be unintended and is important to detect, particularly when this happens during one of many preprocessing steps in the ML pipeline. During model development, Ann might have filtered the data by zip code or county to get a sample that is easier to work with. Demographic attributes such as age and income are highly correlated with places of residency, so such a seemingly innocent filtering operation might have heavily biased the data.

Another potential source of technical bias is the increasingly common usage of pre-trained word embeddings. For example, Ann's code might replace a textual name feature with the corresponding vector from a word embedding that is missing for rare, non-western names (due to lack of data representation in the training corpus). If we then filter out records for which no embedding was found, we may disproportionately remove individuals from specific ethnic groups.

Unsound experimentation. Design and evaluation of ML models is a difficult and tedious undertaking and requires data scientists to strictly follow a set of best practices. During this process, it is unfortunately easy to make subtle mistakes that can heavily impact the quality of the resulting model. In previous research, we found that even expert users violate such best practices in highly cited studies [29]. Common mistakes include hyperparameter selection on the test set instead of the validation set, lack of hyperparameter tuning for baseline learners, lack of proper feature normalisation, or ignoring problematic data subsets during training.

While unsound experimentation is a general issue, ignoring problematic data subsets can specifically affect performance for minority and underrepresented groups, because their data might be prone to data quality issues, as we already discussed under *data filtering* above.

2.2 Model Deployment Stage

After the design of a model is finished, the model is deployed into production and produces predictions on unseen data. We outline a set of circumstances which can introduce technical bias at this stage.

Data errors introduced through integration. In modern information infrastructures, data is stored in different environments (e.g., in relational databases, in 'data lakes' on distributed file systems, or behind REST APIs), and it comes in many different formats. Many such data sources do not support integrity constraints and data quality checks, and often there is not even an accompanying schema available as the data is consumed in a 'schema-on-read' manner, where a particular application takes care of the interpretation. Additionally, there is a growing demand for applications consuming semi-structured data such as text, videos, and images. Due to these circumstances, every real world ML application has to integrate data from multiple sources, and errors in the data sources or during integration may lead to errors in downstream ML models that consume the data.

In our running example in Section 1, it may be the case that patient data is integrated from data sources of different healthcare providers. If one of these providers accidentally changes their schema, or introduces bugs in their data generation procedure, this may negatively impact the predictions for the corresponding patients when their data is used as input to Ann's model.

Distribution shifts. The maintenance of ML applications remains challenging [21], due in large part to unexpected shifts in the distribution of serving data. These shifts originate from changes in the data generating process in the real world, and the problem is exacerbated in situations where different parties are involved in the provision of the data and the training of the model. Many engineering teams, especially in smaller companies, lack ML expert knowledge, and therefore often outsource the training of ML models to data science specialists or cloud ML services. In such cases, the engineering team provides the input data and retrieves predictions, but might not be familiar with details of the model. While ML experts have specialized knowledge to debug models and predictions in such cases [16], there is a lack of automated methods for non-ML expert users to decide whether they can rely on the predictions of an ML model on unseen data. In Ann's case, her final deployed model might work well until new regulations for health care providers change the shape and contents of the patient data that they produce. If her model is not retrained on proper data, its prediction quality may quickly deteriorate.

In the following section we will introduce three software libraries that we developed in recent research to help data scientists like Ann in detecting and mitigating technical bias during model development and deployment.

3 Taming Technical Bias during Model Development and Deployment

In Schelter et al. [29] we described `FairPrep`, a design and evaluation framework for fairness-enhancing interventions in machine learning pipelines that treats data as a first-class citizen. The framework implements a modular data lifecycle, enables re-use of existing implementations of fairness metrics and interventions, and integration of custom feature transformations and data cleaning operations from real world use cases. `FairPrep` pursues the following goals: (i) Expose a developer-centered design throughout the lifecycle, which allows for low effort customization and composition of the framework's components; (ii) Surface discrimination and due process concerns, including disparate error rates, failure of a model to fit the data, and failure of a model to generalize. (iii) Follow software engineering and machine learning best practices to reduce the technical

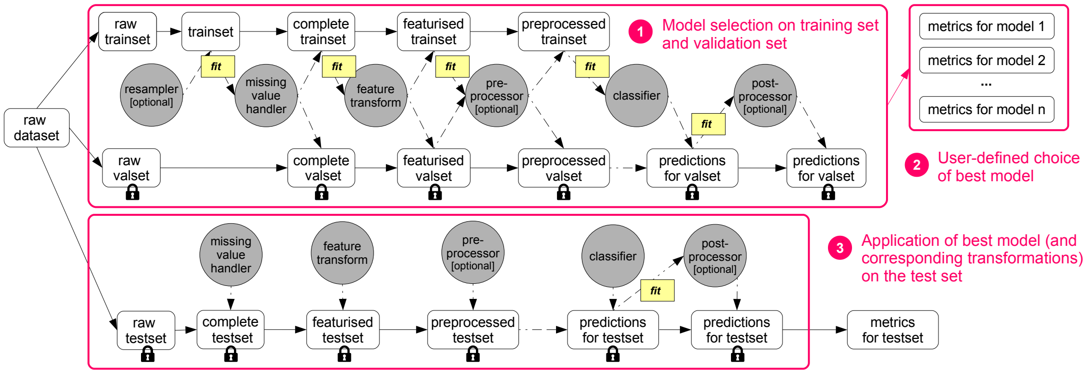


Figure 1: Data life cycle in `FairPrep`, designed to enforce isolation of test data, and to allow for customization through user-provided implementations of different components. An evaluation run consists of three different phases: (1) Learn different models, and their corresponding data transformations, on the training set; (2) Compute performance / accuracy-related metrics of the model on the validation set, and allow the user to select the 'best' model according to their setup; (3) Compute predictions and metrics for the user-selected best model on the held-out test set.

debt of incorporating fairness-enhancing interventions into an already complex development and evaluation scenario [26, 31].

Figure 1 summarizes the architecture of `FairPrep`, which is based on three main principles:

1. Data isolation: to avoid target leakage, user code should only interact with the training set, and never be able to access the held-out test set.

2. Componentization: different data transformations and learning operations should be implementable as single, exchangeable standalone components; the framework should expose simple interfaces to users, supporting low effort customization.

3. Explicit modeling of the data lifecycle: the framework defines an explicit, standardized data lifecycle that applies a sequence of data transformations and model training in a predefined order.

`FairPrep` currently focuses on data cleaning, including different methods for data imputation, and model selection and validation, including hyperparameter tuning, and can be extended to accommodate earlier lifecycle stages, such as data acquisition, integration, and curation. Schelter et al. [29] measured the impact of sound best practices, such as hyperparameter tuning and feature scaling, on the fairness and accuracy of the resulting classifiers, and also showcased how `FairPrep` enables the inclusion of incomplete data into studies and helps analyze the effects.

If Ann wants to ensure that she follows sound experimentation practices during model development, she can use the `FairPrep` library as a runtime platform for experiments, for example to compute various fairness related metrics for the predictions of her classifier. Furthermore, she can leverage the component architecture of `FairPrep` to evaluate different missing value imputation techniques and fairness enhancing interventions to see whether these help with mitigating the low accuracy that she encountered in her model for the predictions for middle-aged women, as discussed in our running example in Section 1.

Source code. A prototype implementation of FairPrep is available at `https://github.com/DataResponsibly/FairPrep`.

3.1 Detecting Data Distribution Bugs Introduced in Preprocessing

In our recent work on the *mlinspect* library [10], we focus on helping data scientists diagnose and mitigate problems to which we collectively refer as *data distribution bugs*. These types of bugs are often introduced during preprocessing, for reasons we outlined in Section 2. For example, preprocessing operations that involve filters or joins can heavily change the distribution of different groups in the training data [35], and missing value imputation can also introduce skew [28]. Recent ML fairness research, which mostly focuses on the use of learning algorithms on static datasets [5] is therefore insufficient, because it cannot address such technical bias originating from the data preparation stage. In addition, we should detect and mitigate such bias as close to its source as possible.

Unfortunately, such data distribution issues are difficult to catch. In part, this is because different pipeline steps are implemented using different libraries and abstractions, and the data representation often changes from relational data to matrices during data preparation. Further, preprocessing in the data science ecosystem [23] often combines relational operations on tabular data with *estimator/transformer pipelines*,[1] a composable and nestable abstraction for combining operations on array data, which originates from `scikit-learn` [19] and has been adopted by popular libraries like `SparkML` [18] and `Tensorflow Transform`. In such cases, tracing problematic featurised entries back to the pipeline's initial human-readable input is tedious work. Finally, complex estimator/transformer pipelines are hard to inspect because they often result in nested function calls not obvious to the data scientist.

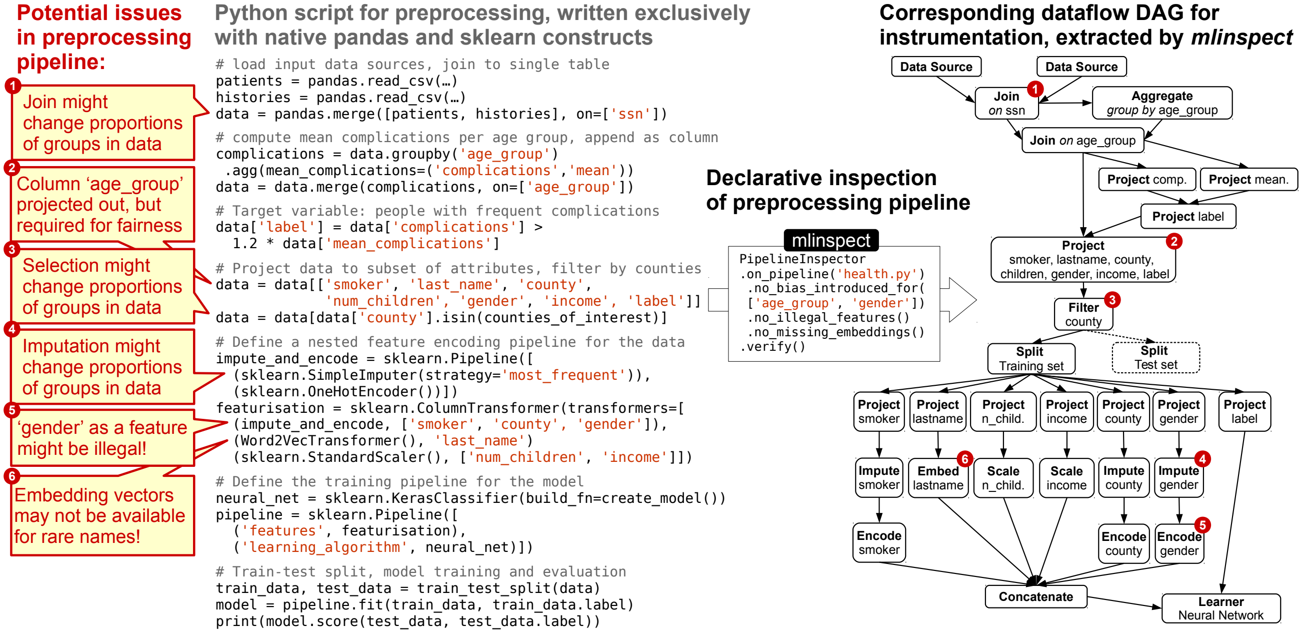
Due to time pressure in their day-to-day activities, most data scientists will not invest the necessary time and effort to manually instrument their code or insert logging statements for tracing as required by model management systems [34, 36]. This calls for the development of tools that support *automated inspection of ML pipelines*, similar to the inspections used by modern IDEs to highlight potentially problematic parts of a program, such as the use of deprecated code or problematic library functions calls. Once data scientists are pointed to such issues, they can use data debuggers like `Dagger` [17] to drill down into the specific intermediate pipeline outputs and explore the root cause of the issue. Furthermore, to be most beneficial, automated inspections need to work with code natively written with popular ML library abstractions.

Lightweight inspection with `mlinspect`. To enable lightweight pipeline inspection, we designed and implemented `mlinspect` [10], a library that helps data scientists automatically detect data distribution issues in their ML pipelines, such as the accidental introduction of statistical bias, and provides linting for best practices. The `mlinspect` library extracts logical query plans, modeled as directed acyclic graphs (DAGs) of preprocessing operators from ML pipelines that use popular libraries like `pandas` and `scikit-learn`, and combine relational operations and estimator/transformer pipelines. These plans are then used to automatically instrument the code and trace the impact of operators on properties like the distribution of sensitive groups in the data.

Importantly, `mlinspect` implements a library-independent interface to propagate annotations such as the lineage of tuples across operators from different libraries, and introduces only constant overhead per tuple flowing through the DAG. Thereby, the library offers a general runtime for pipeline inspection, and allows us to integrate many issue detection techniques that previously required custom code, such as automated model validation on data slices [22], the identification of distortions with respect to protected group membership in the training data [35], or automated sanity checking for ML datasets [13].

Identifying data distribution bugs in our running example. Figure 2 shows a preprocessing pipeline and potential data distribution bugs for our running example from Section 1. The pipeline first reads two CSV files, which contain patient demographics and their clinical histories, respectively. Next, these dataframes are joined on the `ssn` column. This join may introduce a data distribution bug (as indicated by issue ❶) if a large percentage of the records of some combination of gender and age group do not have matching entries in the clinical history dataset. Next, the pipeline computes the average number of complications per age group and adds the binary

[1] `https://scikit-learn.org/stable/modules/compose.html`



Potential issues in preprocessing pipeline:
1 Join might change proportions of groups in data
2 Column 'age_group' projected out, but required for fairness
3 Selection might change proportions of groups in data
4 Imputation might change proportions of groups in data
5 'gender' as a feature might be illegal!
6 Embedding vectors may not be available for rare names!
Python script for preprocessing, written exclusively with native pandas and sklearn constructs

```
# load input data sources, join to single table
patients = pandas.read_csv(…)
histories = pandas.read_csv(…)
data = pandas.merge([patients, histories], on=['ssn'])

# compute mean complications per age group, append as column
complications = data.groupby('age_group')
 .agg(mean_complications=('complications','mean'))
data = data.merge(complications, on=['age_group'])

# Target variable: people with frequent complications
data['label'] = data['complications'] >
  1.2 * data['mean_complications']

# Project data to subset of attributes, filter by counties
data = data[['smoker', 'last_name', 'county',
             'num_children', 'gender', 'income', 'label']]
data = data[data['county'].isin(counties_of_interest)]

# Define a nested feature encoding pipeline for the data
impute_and_encode = sklearn.Pipeline([
  (sklearn.SimpleImputer(strategy='most_frequent')),
  (sklearn.OneHotEncoder())])
featurisation = sklearn.ColumnTransformer(transformers=[
  (impute_and_encode, ['smoker', 'county', 'gender']),
  (Word2VecTransformer(), 'last_name')
  (sklearn.StandardScaler(), ['num_children', 'income']])

# Define the training pipeline for the model
neural_net = sklearn.KerasClassifier(build_fn=create_model())
pipeline = sklearn.Pipeline([
  ('features', featurisation),
  ('learning_algorithm', neural_net)])

# Train-test split, model training and evaluation
train_data, test_data = train_test_split(data)
model = pipeline.fit(train_data, train_data.label)
print(model.score(test_data, test_data.label))
```

```
PipelineInspector
.on_pipeline('health.py')
 .no_bias_introduced_for(
 ['age_group', 'gender'])
 .no_illegal_features()
 .no_missing_embeddings()
.verify()
```

Figure 2: ML pipeline for our running example that predicts which patients are at a higher risk of serious complications, under the requirement to achieve comparable false negative rates across intersectional groups by gender and age group. On the left, we highlight potential issues identified by `mlinspect`. On the right, we show the corresponding dataflow graph, extracted to instrument the code and pinpoint the issues.

target label to the dataset, indicating which patients had a higher than average number of complications compared to their age group. The data is then projected to a subset of the attributes, to be used by the classification model. This leads to the second issue ❷ in the pipeline: the data scientist needs to ensure that the model achieves comparable accuracy across different age groups, but the age group attribute is projected out here, making it difficult to catch data distribution bugs later in the pipeline. The data scientist additionally filters the data to only contain records from patients within a given set of counties. This may lead to issue ❸: a data distribution bug may be introduced if populations of different counties systematically differ in age.

Next, the pipeline creates a feature matrix from the dataset by applying common feature encoders with `ColumnTransformer` from `scikit-learn`, before training a neural network on the features. For the categorical attributes `smoker`, `county`, and `gender`, the pipeline imputes missing values with mode imputation (using the most frequent attribute value), and subsequently creates one-hot-encoded vectors from the data. The `last_name` is replaced with a corresponding vector from a pretrained word embedding, and the numerical attributes `num_children` and `income` are normalized. This feature encoding part of the pipeline introduces several potential issues: ❹ the imputation of missing values for the categorical attributes may introduce statistical bias, as it may associate records with a missing value in the gender attribute with the majority gender in the dataset; ❺ depending on the legal context (i.e., if the disparate treatment doctrine is enforced), it may be forbidden to use `gender` as an input to the classifier; ❻ we may not have vectors for rare non-western names in the word embedding, which may in turn lead to lower model accuracy for such records. As illustrated by this example, preprocessing can give rise to subtle data distribution bugs that are difficult to identify manually, motivating the development of automatic inspection libraries such as `mlinspect`, which will hint the data scientist towards these issues.

Source code. A prototype implementation of `mlinspect`, together with a computational notebook that shows how `mlinspect` can be used to address the issues outlined in the ML pipeline in Figure 2, is available at `https://github.com/stefan-grafberger/mlinspect`.

3.2 Validating Serving Data with Data Unit Tests

Machine learning (ML) techniques are very sensitive to their input data, as the deployed models rely on strong statistical assumptions about their inputs [32], and subtle errors introduced by changes in the data distribution can be hard to detect [20]. At the same time, there is ample evidence that the volume of data available for training is often a decisive factor for a model's performance [11]. How errors in the data affect performance, and fairness of deployed machine learning models is an open and pressing research question, especially in cases where the data describing protected groups has a higher likelihood of containing errors or missing values [29].

Unit tests for data with `Deequ`. As discussed in Section 2.2, accidental errors during data integration can heavily impact the prediction quality of downstream ML models. We therefore postulate that there is a pressing need for increased automation of data validation. To respond to this need, Schelter et al. [30] presented `Deequ`, a data unit testing library. The library centers around the vision that users should be able to write 'unit-tests' for data, analogous to established testing practices in software engineering, and is built on the following principles:

1. Declarativeness: allowing data scientist to spend time on thinking about *what* their data should look like, and not about *how* to implement the quality checks. `Deequ` offers a declarative API that allows users to define checks on their data by composing a variety of available constraints.

2. Flexibility: allowing users to leverage external data and custom code for validation (e.g., call a REST service for some data and write a complex function that compares the result to some statistic computed on the data).

3. Continuous integration: explicitly supporting the incremental computation of quality metrics on growing datasets [27], and allowing users to run anomaly detection algorithms on the resulting historical time series of quality metrics.

4. Scalability: scaling seamlessly to large datasets, by translating the data metrics computations to aggregation queries, which can be efficiently executed at scale with a distributed dataflow engine such as `Apache Spark` [37].

Unit testing serving data in our running example. A prime use case of `Deequ` in ML deployments is to test new data to be sent to the model for prediction. When Ann deploys her model for real world usage, she wants to make sure that it will only consume well-formed data. She can use `Deequ` to write down her assumptions about the data as a declarative data unit test, and have this test integrated into the pipeline that feeds data to the deployed model. If any assumptions are violated, the pipeline will stop processing, the data will be quarantined, and a data engineer will be prompted to investigate the root cause of the failure.

Listing 1 shows what a data unit test may look like. We precompute certain expected statistics for the data such as the number patients to predict for, the valid age groups, and expected distributions by gender and age group. Next, we write down our assumptions about the data, similar to integrity constraints in relational databases. We declare the following checks: we assume that the size of the data corresponds to the expected number of patients, we expect social security numbers (the `ssn` attribute) to be unique, and we expect no missing values for the `lastname`, `county`, and `age_group` attributes. We furthermore assume that the values of the `smoker` attribute are Boolean, while in the `num_children` attribute comprises of integers, and we expect the `age_group` attribute to only contain valid age group values, as defined beforehand. We also expect values of the `num_children` attribute to be non-negative. Finally, we compare the distribution of age groups and gender in serving data to their expected distribution via the `histogramSatisfies` constraint. The user-defined function `notDiverged` compares the categorical distributions of these columns and returns a Boolean value.

```
// Computed in advance
val expectedNumPatients = ...
val validAgeGroups = ...
val expectedGenderDist = ...
val expectedAgeGroupDist = ...

// Assumptions about data to predict on
val validationResultForTestData = VerificationSuite ()
  .onData(expectedNumPatients)
  .addCheck()
    .hasSize(numPatients)
    .isUnique("ssn")
    .isComplete("lastname", "county", "age_group")
    .hasDataType("smoker", Boolean)
    .hasDataType("num_children", Integral)
    .isNonNegative("num_children")
    .isContainedIn("age_group", validAgeGroups)
    .histogramSatisfies("age_group", { ageGroupDist =>
      notDiverged(ageGroupDist, expectedAgeGroupDist) })
    .histogramSatisfies("gender", { genderDist =>
      notDiverged(genderDist, expectedGenderDist) })
  .run()

if (validationResultForTestData.status != Success) {
  // Abort pipeline, notify data engineers
}
```

Listing 1: Example of a data unit test.

During the execution of the test, Deequ identifies the statistics required for evaluating the constraints and generates queries in SparkSQL with custom designed aggregation functions to compute them. For performance reasons, it applies multi-query optimization to enable scan-sharing for the aggregation queries, minimizing the number of passes over the input data. Once the data statistics are computed, Deequ invokes the validation functions and returns the evaluation results to the user.

Source code. Deequ is available under an open source license at https://github.com/awslabs/deequ. It for example forms the basis of Amazon's recent Model Monitor service[2] for concept drift detection in the SageMaker machine learning platform.

4 Conclusions and Future Research Directions

In this paper we discussed dimensions of technical bias that can arise through the lifecycle of machine learning applications, both during model development and after deployment. We outlined several approaches to detect and mitigate such bias based on our recent work, and will now discuss promising directions for future research, where the data engineering community has the potential to make significant impact. We see the overarching goal of this line of research not in mechanically scrubbing data or algorithms of bias, but rather in equipping data scientists with tools that can help them identify technical bias, understand any trade-offs, and thoughtfully enact interventions.

Integrating technical bias detection into general software development tooling. Data science is rapidly becoming an important part of the toolbox of a "general software engineer", and so methods for detection and mitigation of technical bias need to become part of that toolbox as well. The scope of these methods must be extended beyond binary classification, and they must embrace human-in-the-loop elements by providing visualisations and allowing end-users to control experiments with low effort. To achieve practical impact, it is important to integrate these methods into common computational notebooks such as Jupyter, and into general IDE's such as PyCharm.

[2] https://aws.amazon.com/blogs/aws/amazon-sagemaker-model-monitor-fully-managed-automatic-monitoring-for-your-machine-learning-models/

Automating data quality monitoring. The arising challenge of automating the operation of deployed ML applications is gaining a lot of attention recently, especially with respect to monitoring the quality of their input data [25]. As outlined in Sections 2 and 3, data quality issues and the choice of a data cleaning technique can be a major source of technical bias. Existing approaches [2, 30] for this problem have not yet reached broad adoption, in part because they rely on substantial domain knowledge needed, for example, to define "data unit tests" and the corresponding similarity metrics, and to set thresholds for detecting data distribution shifts. Additionally, it is very challenging to test data during the earlier pipeline stages (e.g., data integration) without explicit knowledge of how an ML model will transform this data at the later stages.

We thus see a dire need for automated or semi-automated approaches to quantify and monitor data quality in ML pipelines. A promising direction is to treat historical data (for which no system failures were recorded and no negative user feedback has been received) as "positive" examples, and to explore anomaly detection-based methods to identify future data that heavily deviates from these examples. It is important to integrate a technical bias perspective into these approaches, for example, by measuring data quality separately for subsets of the data that correspond to historically disadvantaged or minority groups, since these groups tend to be more heavily hit by data quality issues [6].

Integrating technical bias detection into continuous integration systems for ML. Continuous integration is an indispensable step of modern best practices in software engineering to control the quality of deployed software, typically by automatically ensuring that software changes pass a set of unit and integration tests before deployment. There is ongoing work to adapt and reinvent continuous integration for the machine learning engineering process [24], which also exposes a lifecycle similar to the software engineering lifecycle, as discussed in Section 2. We see the need to make detection techniques for technical bias, such as automated inspections and data unit tests, first-class citizen in ML-specific continuous integration systems.

References

[1] Solon Barocas and Andrew D. Selbst. Big data's disparate impact. *California Law Review*, 104(3):671–732, 2016.

[2] Denis Baylor, Eric Breck, Heng-Tze Cheng, Noah Fiedel, Chuan Yu Foo, Zakaria Haque, Salem Haykal, Mustafa Ispir, Vihan Jain, Levent Koc, et al. Tfx: A tensorflow-based production-scale machine learning platform. In *Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pages 1387–1395, 2017.

[3] Felix Biessmann, David Salinas, Sebastian Schelter, Philipp Schmidt, and Dustin Lange. Deep learning for missing value imputation in tables with non-numerical data. In *Proceedings of the 27th ACM International Conference on Information and Knowledge Management*, pages 2017–2025. ACM, 2018.

[4] Amanda Bower, Sarah N. Kitchen, Laura Niss, Martin J. Strauss, Alexander Vargas, and Suresh Venkatasubramanian. Fair pipelines. *CoRR*, abs/1707.00391, 2017.

[5] Alexandra Chouldechova and Aaron Roth. A snapshot of the frontiers of fairness in machine learning. *Commun. ACM*, 63(5):82–89, 2020.

[6] Yeounoh Chung, Tim Kraska, Neoklis Polyzotis, Ki Hyun Tae, and Steven Euijong Whang. Slice finder: Automated data slicing for model validation. In *2019 IEEE 35th International Conference on Data Engineering (ICDE)*, pages 1550–1553. IEEE, 2019.

[7] Cynthia Dwork, Christina Ilvento, and Meena Jagadeesan. Individual fairness in pipelines. In Aaron Roth, editor, *1st Symposium on Foundations of Responsible Computing, FORC 2020, June 1-3, 2020, Harvard*

University, Cambridge, MA, USA (virtual conference), volume 156 of *LIPIcs*, pages 7:1–7:22. Schloss Dagstuhl - Leibniz-Zentrum für Informatik, 2020.

[8] Sorelle A. Friedler, Carlos Scheidegger, and Suresh Venkatasubramanian. On the (im)possibility of fairness. *CoRR*, abs/1609.07236, 2016.

[9] Batya Friedman and Helen Nissenbaum. Bias in computer systems. *ACM Trans. Inf. Syst.*, 14(3):330–347, 1996.

[10] Stefan Grafberger, Julia Stoyanovich, and Sebastian Schelter. Lightweight inspection of data preprocessing in native machine learning pipelines. In *CIDR*, 2021.

[11] Alon Halevy, Peter Norvig, and Fernando Pereira. The unreasonable effectiveness of data. *IEEE Intelligent Systems*, 24(2):8–12, 2009.

[12] Hoda Heidari, Michele Loi, Krishna P. Gummadi, and Andreas Krause. A moral framework for understanding fair ML through economic models of equality of opportunity. In *Proceedings of the Conference on Fairness, Accountability, and Transparency, FAT* 2019, Atlanta, GA, USA, January 29-31, 2019*, pages 181–190. ACM, 2019.

[13] Nick Hynes, D Sculley, and Michael Terry. The data linter: Lightweight, automated sanity checking for ml data sets. *NIPS MLSys Workshop*, 2017.

[14] Joost Kappelhof. *Total Survey Error in Practice*, chapter Survey Research and the Quality of Survey Data Among Ethnic Minorities. 2017.

[15] David Lehr and Paul Ohm. Playing with the data: What legal scholars should learn about machine learning. *UC Davis Law Review*, 51(2):653–717, 2017.

[16] Zachary Lipton, Yu-Xiang Wang, and Alexander Smola. Detecting and correcting for label shift with black box predictors. In *International Conference on Machine Learning*, pages 3122–3130, 2018.

[17] Samuel Madden, Mourad Ouzzani, Nan Tang, and Michael Stonebraker. Dagger: A data (not code) debugger. *CIDR*, 2020.

[18] Xiangrui Meng, Joseph Bradley, Burak Yavuz, Evan Sparks, Shivaram Venkataraman, Davies Liu, Jeremy Freeman, DB Tsai, Manish Amde, Sean Owen, et al. Mllib: Machine learning in apache spark. *JMLR*, 17(1):1235–1241, 2016.

[19] Fabian Pedregosa, Gaël Varoquaux, Alexandre Gramfort, et al. Scikit-learn: Machine learning in python. *JMLR*, 12:2825–2830, 2011.

[20] Neoklis Polyzotis, Sudip Roy, Steven Euijong Whang, and Martin Zinkevich. Data management challenges in production machine learning. In *Proceedings of the 2017 ACM International Conference on Management of Data*, pages 1723–1726, 2017.

[21] Neoklis Polyzotis, Sudip Roy, Steven Euijong Whang, and Martin Zinkevich. Data lifecycle challenges in production machine learning: A survey. *SIGMOD Record*, 47:17–28, 2018.

[22] Neoklis Polyzotis, Steven Whang, Tim Klas Kraska, and Yeounoh Chung. Slice finder: Automated data slicing for model validation. *ICDE*, 2019.

[23] Fotis Psallidas, Yiwen Zhu, Bojan Karlas, et al. Data science through the looking glass and what we found there, 2019.

[24] Cedric Renggli, Bojan Karlas, Bolin Ding, Feng Liu, Kevin Schawinski, Wentao Wu, and Ce Zhang. Continuous integration of machine learning models: A rigorous yet practical treatment. *Proceedings of SysML 2019*, 2019.

[25] Tammo Rukat, Dustin Lange, Sebastian Schelter, and Felix Biessmann. Towards automated ml model monitoring: Measure, improve and quantify data quality. 2020.

[26] Sebastian Schelter, Felix Biessmann, Tim Januschowski, David Salinas, Stephan Seufert, Gyuri Szarvas, Manasi Vartak, Samuel Madden, Hui Miao, Amol Deshpande, et al. On challenges in machine learning model management. *IEEE Data Eng. Bull.*, 41(4):5–15, 2018.

[27] Sebastian Schelter, Stefan Grafberger, Philipp Schmidt, Tammo Rukat, Mario Kiessling, Andrey Taptunov, Felix Biessmann, and Dustin Lange. Differential data quality verification on partitioned data. In *2019 IEEE 35th International Conference on Data Engineering (ICDE)*, pages 1940–1945. IEEE, 2019.

[28] Sebastian Schelter, Yuxuan He, Jatin Khilnani, and Julia Stoyanovich. Fairprep: Promoting data to a first-class citizen in studies on fairness-enhancing interventions. *EDBT*, 2019.

[29] Sebastian Schelter, Yuxuan He, Jatin Khilnani, and Julia Stoyanovich. Fairprep: Promoting data to a first-class citizen in studies on fairness-enhancing interventions. In Angela Bonifati, Yongluan Zhou, Marcos Antonio Vaz Salles, Alexander Böhm, Dan Olteanu, George H. L. Fletcher, Arijit Khan, and Bin Yang, editors, *EDBT*, pages 395–398. OpenProceedings.org, 2020.

[30] Sebastian Schelter, Dustin Lange, Philipp Schmidt, Meltem Celikel, Felix Biessmann, and Andreas Grafberger. Automating large-scale data quality verification. *Proceedings of the VLDB Endowment*, 11(12):1781–1794, 2018.

[31] David Sculley, Gary Holt, Daniel Golovin, Eugene Davydov, Todd Phillips, Dietmar Ebner, Vinay Chaudhary, Michael Young, Jean-Francois Crespo, and Dan Dennison. Hidden technical debt in machine learning systems. In *Advances in neural information processing systems*, pages 2503–2511, 2015.

[32] David Sculley, Gary Holt, Daniel Golovin, Eugene Davydov, Todd Phillips, Dietmar Ebner, Vinay Chaudhary, Michael Young, Jean-Francois Crespo, and Dan Dennison. Hidden technical debt in machine learning systems. In *Advances in neural information processing systems*, pages 2503–2511, 2015.

[33] Julia Stoyanovich, Bill Howe, and H. V. Jagadish. Responsible data management. *Proc. VLDB Endow.*, 13(12):3474–3488, 2020.

[34] Manasi Vartak and Samuel Madden. Modeldb: Opportunities and challenges in managing machine learning models. *IEEE Data Eng.*, 41:16–25, 2018.

[35] Ke Yang, Biao Huang, Julia Stoyanovich, and Sebastian Schelter. Fairness-aware instrumentation of preprocessing pipelines for machine learning. *HILDA workshop at SIGMOD*, 2020.

[36] Matei Zaharia, Andrew Chen, Aaron Davidson, Ali Ghodsi, Sue Ann Hong, Andy Konwinski, Siddharth Murching, Tomas Nykodym, Paul Ogilvie, Mani Parkhe, et al. Accelerating the machine learning lifecycle with mlflow. *IEEE Data Eng. Bull.*, 41(4):39–45, 2018.

[37] Matei Zaharia, Mosharaf Chowdhury, Tathagata Das, Ankur Dave, Justin Ma, Murphy McCauly, Michael J Franklin, Scott Shenker, and Ion Stoica. Resilient distributed datasets: A fault-tolerant abstraction for in-memory cluster computing. In *NSDI*, pages 15–28, 2012.

The VLDB Journal
https://doi.org/10.1007/s00778-021-00726-w

SPECIAL ISSUE PAPER

Data distribution debugging in machine learning pipelines

Stefan Grafberger[1] · Paul Groth[1] · Julia Stoyanovich[2] · Sebastian Schelter[1]

Received: 27 February 2021 / Revised: 9 September 2021 / Accepted: 3 December 2021

Abstract
Machine learning (ML) is increasingly used to automate impactful decisions, and the risks arising from this widespread use are garnering attention from policy makers, scientists, and the media. ML applications are often brittle with respect to their input data, which leads to concerns about their correctness, reliability, and fairness. In this paper, we describe `mlinspect`, a library that helps diagnose and mitigate technical bias that may arise during preprocessing steps in an ML pipeline. We refer to these problems collectively as *data distribution bugs*. The key idea is to extract a directed acyclic graph representation of the dataflow from a preprocessing pipeline and to use this representation to automatically instrument the code with predefined *inspections*. These inspections are based on a lightweight annotation propagation approach to propagate metadata such as lineage information from operator to operator. In contrast to existing work, `mlinspect` operates on declarative abstractions of popular data science libraries like estimator/transformer pipelines and does not require manual code instrumentation. We discuss the design and implementation of the `mlinspect` library and give a comprehensive end-to-end example that illustrates its functionality.

Keywords Data debugging · Machine learning pipelines · Data preparation for machine learning

1 Introduction

Machine learning (ML) is increasingly used to automate decisions that impact people's lives, in domains as varied as credit and lending, medical diagnosis, and hiring, with the potential to reduce costs, reduce errors, and make outcomes more equitable. Yet, despite their potential, the risks arising from the widespread use of ML-based tools are garnering attention from policy makers, scientists, and the media [52]. In large part this is because the correctness, reliability, and fairness of ML models critically depend on their training data. Preexisting bias, such as under- or over-representation of particular groups in the training data [12], and technical bias, such as skew introduced during data preparation [49], can heavily impact performance. In this work, we focus on helping diagnose and mitigate technical bias that arises during preprocessing steps in an ML pipeline. We refer to these problems collectively as *data distribution bugs*.

Data distribution bugs are often introduced during preprocessing Input data for ML applications come from a variety of data sources, and it has to be preprocessed and encoded as features before it can be used. This preprocessing can introduce skew in the data, and, in particular, it can exacerbate under-representation of historically disadvantaged groups. For example, preprocessing operations that involve filters or joins can heavily change the distribution of different groups represented in the training data [58], and missing value imputation can also introduce skew [47]. Recent ML fairness research, which mostly focuses on the use of learning algorithms on static datasets [14], is therefore insufficient because it cannot address such technical bias originating from the data preparation stage. Furthermore, it is important to detect and mitigate bias as close to its source as possible [52].

Data distribution bugs are difficult to catch In part, this is because different pipeline steps are implemented using different libraries and abstractions, and data representation often

Sebastian Schelter
s.schelter@uva.nl

Stefan Grafberger
s.grafberger@uva.nl

Paul Groth
p.t.groth@uva.nl

Julia Stoyanovich
stoyanovich@nyu.edu

[1] University of Amsterdam, Amsterdam, Netherlands

[2] New York University, New York, USA

Published online: 31 January 2022

changes from relational data to matrices during data preparation. Further, preprocessing in the data science ecosystem [44] often combines relational operations on tabular data with *estimator/transformer pipelines*.[1] These pipelines are composable and nestable abstractions for operations on array data. The approach originates from scikit-learn [37] and has been adopted by libraries like SparkML [28] and TensorFlow Transform.[2] Tracing problematic featurized entries that may be the result of nested function calls back to the pipeline's initial human-readable input is tedious work.

We need automated inspection of ML pipelines Due to the pressures of their day-to-day activities, most data scientists will not invest the necessary time and effort to manually instrument their code or insert logging statements for tracing, as required by model management systems [53,60]. We envision support for data scientists in the form of *automated inspections of their pipelines*, similar to the inspections used by modern IDEs to highlight potentially problematic parts of a program, such as the use of deprecated code. Once data scientists become aware of such issues, they can use data debuggers like Dagger [26] to drill down into the specific intermediate pipeline outputs and explore the root cause of the issue. We furthermore argue that, to be most beneficial, automated inspections need to *work with code natively written with popular ML library abstractions*.

Lightweight pipeline inspection with `mlinspect` We design and implement `mlinspect`, a library that helps data scientists automatically detect data distribution bugs in their ML pipelines. The `mlinspect` library extracts logical query plans, modeled as directed acyclic graphs (DAGs) of preprocessing operators, from pipelines that use popular libraries like pandas and scikit-learn [37], and that combine estimator/transformer pipelines and relational operators. The pipeline code is then automatically instrumented to trace the impact of operators on properties like the distribution of sensitive groups in the data. In this way, `mlinspect` empowers data scientists to automatically and comfortably check their ML pipeline code for data distribution bugs.

Importantly, `mlinspect` provides a library-independent interface to propagate annotations such as the lineage of tuples across operators from different libraries and introduces only constant overhead per tuple flowing through the DAG. Thereby, `mlinspect` offers a general runtime for pipeline inspection and allows for integration of many detection techniques for data distribution bugs that previously required custom code, such as automated model validation of data slices [42], identification of distortions with respect to protected group membership in the training data [58], and automated dataset sanity checking [21].

We proposed the initial ideas for our approach in earlier work [17]. In this paper, we give a comprehensive description of the approach and of the corresponding open source library. We explain how to instrument estimator/transformer pipelines (Sect. 3.2), provide implementation details for all our components (Sect. 4), and add an extensive discussion of related work (Sect. 6). We also present quantitative and qualitative experiments to evaluate `mlinspect` with respect to its runtime overhead and usability.
In this paper, we make the following contributions:

- We describe hard-to-identify issues in ML preprocessing pipelines with respect to the fairness and correctness of the resulting models (Sects. 2, 3.3).
- We discuss the design of `mlinspect`, which enables lightweight lineage-based inspection of ML preprocessing pipelines. The `mlinspect` library bases its analysis on declarative abstractions of popular data science libraries and does not require manual code instrumentation (Sect. 3).
- We describe how to efficiently implement the instrumentation and inspections of `mlinspect` and how to enable support for control flow (Sect. 4).
- We experimentally show that the runtime overhead of `mlinspect` is linear in the number of input and output records of instrumented operators and highlight performance trade-offs (Sect. 5).
- We provide a qualitative comparison of our approach to related libraries for experiment tracking and provenance capturing. We also conduct a user study, showing that `mlinspect` is helpful to data scientists in their data distribution debugging tasks (Sect. 5).

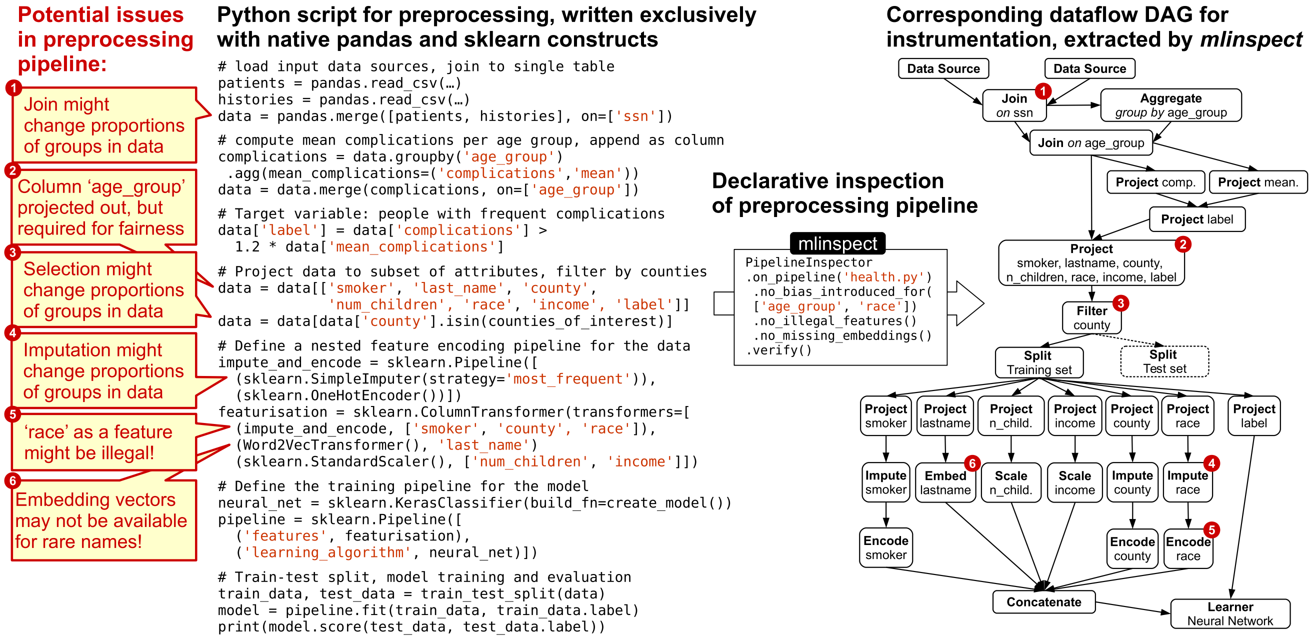
2 Data distribution bugs by example

We illustrate the need for assisting data scientists with the inspection of their preprocessing pipelines with an example from the medical domain, shown in Fig. 1. Consider a data scientist who implements a Python pipeline that takes demographic and clinical history data as input, and trains a classifier to identify patients at risk for serious complications. Further, assume that the data scientist is under a legal obligation to ensure that the resulting model works equally well for patients across different age groups and races. This obligation is operationalized as an intersectional fairness criterion, requiring equal false-negative rates for groups of patients identified by a combination of `age_group` and `race`.

The pipeline first reads two CSV files, which contain patient demographics and their clinical histories, respectively. Next, the resulting dataframes are joined on the `ssn` column. This join may introduce a data distribution bug (as indicated by issue ①) if a large percentage of the records of

[1] https://scikit-learn.org/stable/modules/compose.html.

[2] https://github.com/tensorflow/transform.


Potential issues in preprocessing pipeline:
1 Join might change proportions of groups in data
2 Column ‘age_group’ projected out, but required for fairness
3 Selection might change proportions of groups in data
4 Imputation might change proportions of groups in data
5 ‘race’ as a feature might be illegal!
6 Embedding vectors may not be available for rare names!
Python script for preprocessing, written exclusively with native pandas and sklearn constructs
Declarative inspection of preprocessing pipeline
mlinspect
Corresponding dataflow DAG for instrumentation, extracted by *mlinspect*
Data Source
Data Source
Join on ssn
Aggregate group by age_group
Join on age_group
Project comp.
Project mean.
Project label
Project smoker, lastname, county, n_children, race, income, label
Filter county
Split Training set
Split Test set
Project smoker
Project lastname
Project n_child.
Project income
Project county
Project race
Project label
Impute smoker
Embed lastname
Scale n_child.
Scale income
Impute county
Impute race
Encode smoker
Encode county
Encode race
Concatenate
Learner Neural Network

```
# load input data sources, join to single table
patients = pandas.read_csv(…)
histories = pandas.read_csv(…)
data = pandas.merge([patients, histories], on=['ssn'])

# compute mean complications per age group, append as column
complications = data.groupby('age_group')
 .agg(mean_complications=('complications','mean'))
data = data.merge(complications, on=['age_group'])

# Target variable: people with frequent complications
data['label'] = data['complications'] >
  1.2 * data['mean_complications']

# Project data to subset of attributes, filter by counties
data = data[['smoker', 'last_name', 'county',
             'num_children', 'race', 'income', 'label']]
data = data[data['county'].isin(counties_of_interest)]

# Define a nested feature encoding pipeline for the data
impute_and_encode = sklearn.Pipeline([
  (sklearn.SimpleImputer(strategy='most_frequent')),
  (sklearn.OneHotEncoder())])
featurisation = sklearn.ColumnTransformer(transformers=[
  (impute_and_encode, ['smoker', 'county', 'race']),
  (Word2VecTransformer(), 'last_name')
  (sklearn.StandardScaler(), ['num_children', 'income']])

# Define the training pipeline for the model
neural_net = sklearn.KerasClassifier(build_fn=create_model())
pipeline = sklearn.Pipeline([
  ('features', featurisation),
  ('learning_algorithm', neural_net)])

# Train-test split, model training and evaluation
train_data, test_data = train_test_split(data)
model = pipeline.fit(train_data, train_data.label)
print(model.score(test_data, test_data.label))
```

```
PipelineInspector
.on_pipeline('health.py')
 .no_bias_introduced_for(
 ['age_group', 'race'])
 .no_illegal_features()
 .no_missing_embeddings()
.verify()
```

Fig. 1 Example of an ML pipeline that predicts which patients are at a higher risk of serious complications, under the requirement to achieve comparable false-negative rates across intersectional groups by age and race. The pipeline is implemented using native constructs from the popular pandas and scikit-learn libraries. On the left, we highlight potential issues identified by `mlinspect`. On the right, we show the corresponding dataflow graph extracted by `mlinspect` to instrument the code and pinpoint issues. (Operations on the test set are omitted for readability)

some combination of age group and race do not have matching entries in the clinical history dataset.

Next, the pipeline computes the average number of complications per age group and adds the binary target label to the dataset, indicating which patients had a higher than average number of complications compared to their age group. Data is then projected to a subset of the attributes, to be used by the classification model. This leads to the second issue ② in the pipeline: the data scientist needs to ensure that the model achieves comparable accuracy across different age groups, but the age group attribute is projected out here, making it difficult to catch this data distribution bug later in the pipeline. The data scientist additionally filters the data to only contain records from patients within a given set of counties. This may lead to issue ③: a data distribution bug may be introduced if populations of different counties systematically differ in age.

Next, the pipeline creates a feature matrix from the dataset by applying feature encoders with scikit-learn's `ColumnTransformer`, before training a neural network on the features. For the categorical attributes `smoker`, `county`, and `race`, the pipeline imputes missing values with mode imputation (using the most frequent attribute value), and subsequently creates one-hot encoded vectors from the data. The `last_name` attribute is replaced with a corresponding vector from a pretrained word embedding, and we normalize the numerical attributes `num_children` and `income`.

This feature encoding part of the pipeline introduces several potential issues: ④ the imputation of missing values for the categorical attributes may introduce statistical bias by attributing records with a missing value of `race` to the majority race in the dataset; ⑤ depending on the legal context (i.e., if the disparate treatment doctrine is enforced[3]), it may be forbidden to use `race` as an input to the classifier; ⑥ we may not have vectors for rare non-western names in the word embedding, which may in turn lead to lower model accuracy for such records. As illustrated by this example, preprocessing can give rise to subtle data distribution bugs that are difficult to identify manually, motivating the development of our automatic inspection library, `mlinspect`.

3 Design of mlinspect

The analysis of Python code for data science pipelines is difficult because, in contrast to SQL queries, these pipelines are not built on top of an algebraic abstraction. Further, these pipelines operate not only on relational data but also on tensors, when converting input data to feature matrices. However, popular data science libraries expose a set of

[3] https://en.wikipedia.org/wiki/Disparate_treatment.

declarative abstractions with some algebraic properties. For example, pandas and pyspark both operate on dataframes with SQL-like operations, and scikit-learn, SparkML, and TensorFlow Transform[4] rely on (potentially nested) estimator/transformer chains.

This abstraction consists of an *estimator* that conducts an aggregation over its inputs to create a reusable *transformer*. The transformer applies a tuple-at-a-time transformation to the data based on the state computed by its corresponding estimator. This abstraction allows data scientists to build nested pipelines of estimators and transformers that combine common operations like feature transformations (like one-hot encoding of categorical variables) with model training and hyperparameter optimization (like k-fold cross-validation). The estimator/transformer abstraction can be seen as a declarative way to specify ML pipelines and has recently been the subject of database-style research to optimize execution time [50].

3.1 Overview

We propose `mlinspect`, a runtime for lightweight lineage-based inspection of python scripts that uses existing library code and does not require manual code instrumentation. In the current research prototype, we restrict ourselves to scripts that use a combination of SQL-like operations on dataframes and estimator/transformer pipelines, analogously to our example in Sect. 2. This has the potential to cover a wide range of existing ML code: According to results of a recent analysis of several million Jupyter Notebooks, more than 50% of these use pandas, and more than 25% use scikit-learn [44]. The `mlinspect` library focuses on declarative pipeline code, supports control flow, and has fallbacks for when it encounters unsupported code snippets.

The `mlinspect` library extracts a directed acyclic graph (DAG) representing the dataflow from ML pipelines with logical operators like join, selection, projection, column encoders, and missing value imputation. Based on this extracted DAG, `mlinspect` automatically instruments the code with predefined lightweight *inspections* that detect data distribution bugs in the pipeline and give hints to users.

We now give a high-level overview of how `mlinspect` executes and inspects data preprocessing operations based on the architecture shown in Fig. 2. The execution takes place as follows: (1) Users execute their data science pipeline implemented in native pandas/sklearn code via `mlinspect` and define the inspections to apply; (2) `mlinspect` automatically instruments relevant function calls (Sect. 3.2) and executes the instrumented program; (3) during the execution, `mlinspect` delegates instrumented function calls to library-specific backends, which expose the inputs, annotations, and outputs of operators to the configured inspections (Sect. 3.3); (4) `mlinspect` extracts a dataflow representation of the program (Sect. 3.4) and maps the results of the inspection to the corresponding operators. In the remainder of this section, we detail the design of each component. We will discuss implementation decisions in Sect. 4.

3.2 Instrumentation and annotation propagation

Instrumentation and DAG extraction at runtime We conduct all instrumentation necessary for inspection before the execution of the pipeline and extract the DAG at runtime during a single execution of the pipeline, as follows. During the execution of each instrumented function call, corresponding operator nodes are added to the DAG. For this, `mlinspect` generates a unique identifier for each DAG node. Whenever a dataframe object is returned from an instrumented function, `mlinspect` adds a new attribute that contains the identifier of the DAG operator that produced the dataframe. For example, when processing the `pd.merge(df_a, df_b)` call, `mlinspect` retrieves the DAG node identifiers for `df_a` and `df_b` and adds a new DAG node, in this case a `JOIN`, with nodes representing `df_a` and `df_b` as parents. There might be cases where a user pipeline contains operators that `mlinspect` cannot recognize (e.g., custom transformers in a scikit-learn pipeline). Such operators are ignored and not represented in the DAG, and execution continues with the remaining known operations. Due to this fallback, the library does not fail for pipelines where it recognizes only a subset of the relevant dataflow operations, but still applies all inspections and checks on a best-effort basis.

Handling control flow Early `mlinspect` versions [17] lacked support for control flow in pipelines; they created the DAG based on the pipeline code after execution, using module information obtained through Python's `inspect` module. This made it difficult to deal with conditional code such as loops, where the number of iterations depends on runtime variables. The current DAG extraction method supports pipelines with control flow by building up the DAG dynamically at runtime based on the actual execution of the program. If there are branches in the user code, only operators from the executed branch are contained in the DAG. As a consequence, `mlinspect` now runs and instruments pipeline code contained in custom functions, which leverage loops and branches. This approach enables easy instrumentation of relevant function calls, even if they happen indirectly (as is the case with nested scikit-learn pipelines). We refer to Sect. 4.3.2 for further details.

Annotation propagation The data flowing through the preprocessing pipeline is further enriched with user-definable "annotations" that propagate through operators and can be

[4] Note that TensorFlow Transform refers to estimators and transformers as TensorFlow Transform Analyzers and TensorFlow Ops https://www.tensorflow.org/tfx/tutorials/transform/simple?hl=en.

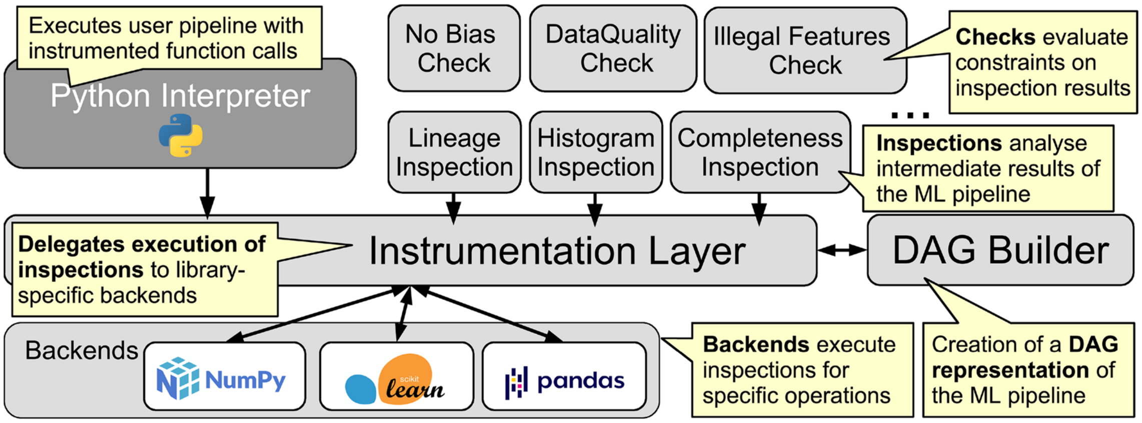

Executes user pipeline with instrumented function calls
Python Interpreter
No Bias Check
DataQuality Check
Illegal Features Check
Checks evaluate constraints on inspection results
...
Lineage Inspection
Histogram Inspection
Completeness Inspection
Inspections analyse intermediate results of the ML pipeline
Delegates execution of inspections to library-specific backends
Instrumentation Layer
DAG Builder
Backends
NumPy
learn
pandas
Backends execute inspections for specific operations
Creation of a DAG representation of the ML pipeline

Fig. 2 Architecture of `mlinspect`. We apply checks and inspections to an instrumented ML pipeline written by the user. The instrumentation layer delegates the execution of the inspections to library-specific backends and creates a DAG representation of the pipeline

created, read, and modified by the inspection code. This annotation propagation mechanism offers a simple library-independent interface to propagate annotations (e.g., for tracking the lineage of tuples) across operators from different libraries. We base the design of our *inspections* on this annotation propagation mechanism. Each inspection retains a fixed-size state that is reset after each operator and is invoked only once for each DAG operator. The inspection has access to the output tuples of the operator and the corresponding annotated inputs. The following listing details the abstract operations performed by such an inspection. At runtime, the `visit_op` method is called for each operator invocation and provided with information about the operator as well as an iterator over the annotated input rows. The inspection then produces the corresponding output annotations and can optionally annotate the logical operator in the DAG with the computed result (such as a histogram of the outputs) via the `op_annotation_after_visit` method.

```
# Abstract base class for all inspections
class Inspection:

  # Inspect intermediate data at a DAG operator, based on
  #  operator information (op_context), and an iterator
  #  over annotated input rows with the corresponding
  #  output rows (row_iterator);
  # Return computed annotations for output rows
  def visit_op(self, op_context,
               row_iterator) -> Iterable

  # Persist inspection result for the current DAG node
  def op_annotation_after_visit(self)
```

Users have to specify the inspections to apply in advance, which allows only the state that is required for the actual inspections configured by the user to be materialized. This avoids materializing arbitrary information from the pipeline.

As long as each row annotation has a fixed size limit, and each inspection only uses a fixed-size state, the overhead of the framework is constant per inspected tuple. This approach does not introduce additional memory overhead, as there is only the constant overhead of a fixed number of additional function calls per user function call.

We maintain a mapping between the input rows of an operator and their corresponding output rows and then expose this mapping along with the corresponding annotated inputs to each inspection. This input/output mapping is constructed differently depending on operator semantics. Operators like projection and transformers are guaranteed to have the same number of input and output elements, listed in the same order. For operators like selection, join, and train–test split, the mapping is maintained by generating an identifier column, which is transparently pushed through the operator and removed immediately afterward to hide it from user code. Note that only one possible source tuple (and not all possible sources) is tracked for aggregation operators and for duplicate elimination, as the performance overhead of detailed provenance tracking using the full provenance semiring framework [18] would be too significant, introducing dependencies between all input–output pairs [3].

Function call capturing To allow inspections to access the output of an operator such as a join, along with the corresponding input rows and their annotations, arguments and return values of function calls must be efficiently captured. For this, the abstract syntax tree (AST) from the Python parser is modified before compiling and executing the code. A function call is added before the user code to "monkey patch" functions from libraries like pandas and scikit-learn that are supported by `mlinspect`. Monkey patching [55] allows `mlinspect` to extend or modify functionality of third-party libraries at runtime by completely replacing the original implementation of a function. These monkey patched functions internally call the original, unpatched version of the function, delegate the execution of the inspections, and create new DAG operator nodes corresponding to the function. `mlinspect` also captures the exact function call location and source code snippet corresponding to each DAG operator. See Sect. 4.3.1 for implementation details.

Backends for popular Python libraries The mlinspect library is designed based on the semantics of preprocessing operations from popular Python frameworks like scikit-learn and pandas. The instrumentation based on captured function calls described so far is independent of the specific library. Importantly, libraries differ in their data representation choices and in what data preprocessing operations they support. So, pandas functions can be directly mapped to DAG operators, and each operation is executed eagerly. In contrast, scikit-learn encourages users to first declaratively define a nested pipeline using components like the ColumnTransformer, which allows passing specific columns to specific transformers like one-hot encoders. Once a pipeline is defined in a declarative way, data is passed to the nested pipeline object in a second, separate step. The function calls that actually process data, such as the fit/transform calls of transformers contained in scikit-learn pipeline objects, may not be directly visible in user code. The user pipeline only calls the fit method once on the final pipeline object, and the pipeline then internally calls the fit and transform functions of the transformers and estimators it contains. We introduce library-specific backends in mlinspect to handle the operations and data representations of popular libraries like scikit-learn.

Execution of inspections Each backend is responsible for hiding library implementation details from the inspections. The pandas backend, for example, is responsible for calling the inspections as necessary whenever it is alerted of a pandas function call. For this, it has access to the arguments and return values as described before. The backend then needs to map operator output rows to operator input rows and their corresponding annotations. It needs to create efficient iterators to expose the input/output rows in a specific format. Afterward, the backend stores the resulting new annotations created by the inspection in an efficient manner (e.g., as attributes of the processed dataframe in the case of pandas).

This annotation propagation functionality is enough to implement a variety of useful inspections. For example, basic fine-grained lineage tracking on the row level can be implemented with a simple inspection on top of the annotation propagation approach as follows: unique identifier annotations are generated for each row after the data source operator and are propagated forward through the DAG. For selections, projections, and transformers, annotations are directly forwarded through the DAG. For joins, combinations of identifier annotations from all join inputs are created and forwarded.

Optimizable inspections based on dataframe operators In addition to the generic interface for inspections written in Python, a second interface for inspections is supported. In this interface, inspections have to be expressed in terms of operations on dataframes. This approach is less general than the standard approach (which allows for arbitrary Python code), but is much more performant, because inspections can be jointly executed with the user code operations, and common optimizations from query processing such as scan sharing and projection pushdowns can be applied. We discuss implementation details in Sect. 4.3.2. Note, this approach is still in an experimental stage and not yet part of the open-source release.

3.3 Automatic inspections and checks

Inspections serve as the basis for detecting data distribution bugs in ML pipelines. They annotate the extracted DAG with information like computed histograms for different DAG nodes. On top of the extracted and annotated DAG, mlinspect provides *checks*, a rule-based approach to verify constraints on the DAG, for example, by comparing the change in a histogram to a threshold. Before execution, mlinspect determines which inspections are required based on the checks specified by the user. It then instruments the pipeline and executes it using a minimal set of inspections, based on what is required by the checks and directly specified by the user. After the execution of the instrumented pipeline and the DAG extraction, each check can access the final result to evaluate its constraint.

In the following, we discuss a set of more complex automatic inspections and checks for ML preprocessing pipelines that are enabled by our lineage-based annotation propagation approach.

Algorithmic fairness In recent years, problems with respect to the fairness of ML-based decision-making systems have been uncovered [52]. Such problems are often difficult to detect and are the focus of mlinspect. As discussed in the example from Sect. 2 and outlined in previous work [58], operations like join and selection can accidentally filter out records from protected groups and thereby *introduce or exacerbate under-representation of historically disadvantaged groups in the data*. The mlinspect library provides an inspection that computes histograms of operator outputs based on protected groups, and alerts the user if group membership proportions change drastically after an operator. A related problem is the low coverage of some population groups identified by a combinations of attributes [7]. For tracing group membership in coverage-related problems, mlinspect forward-propagates annotations identifying the groups of interest and materializes the annotated input and final output of the complete pipeline.

Furthermore, there are *legal restrictions on the usage of demographic features* such as gender, race, or disability status in automated decision making. One can check the operator DAG against a list of sensitive features and alert the user about the places in the code where such features are used.

ML models may also *perform particularly badly for specific demographic groups* in the data (e.g., yielding higher false-positive rates for recidivism predictions for African Americans [6]). The identification of such groups is in the focus of recent research [42]. This identification might be difficult in cases where the attribute required to identify the protected group is projected out early in the pipeline or is only available as a specific dimension of the feature matrix during feature transformation. To address this, mlinspect supports inspections that forward-propagate sensitive column annotations and then materialize the minimum amount of information needed for analyzing performance for different groups: rows only containing the predicted label and the sensitive columns.

Methodology and robustness Additionally, inexperienced data scientists may make methodological mistakes, such as fitting featurizers on the whole data instead of the training set only, forgetting to scale numerical features even though the model requires that (as in the case of L2 regularization), or selecting hyperparameters on the test set instead of the validation set. Such issues can impact fairness-related metrics as well [47]. All of these issues can be identified by analyzing the extracted operator DAG. Furthermore, there may be robustness issues in the pipeline. For example, some scikit-learn transformers cannot handle null values. One can identify such cases from the operator DAG and recommend that the user applies a simple imputation technique. Another problem that can be detected by analyzing histograms of operator outputs is *class imbalance*. The DAG can be analyzed to see whether the data scientist already addresses these with resampling or reweighing and alert her otherwise.

Data quality Data quality testing in the form of unit tests for data as offered by libraries like Deequ [48] can also be implemented using mlinspect. Data unit tests typically evaluate constraints based on aggregate statistics of the data such as the completeness (ratio of non-NULL values) of a column or the number of distinct values in a column. The mlinspect library can compute these data quality statistics over all intermediate results of a pipeline.

3.4 Algebraic definition of the mlinspect dataflow graph

Data preparation pipelines that use declarative abstractions such as pandas data slicing, scikit-learn's Column Transformer, or SparkML pipelines have a natural directed acyclic graph (DAG) representation [46]. Data sources in this DAG are typically comprised of tables or files holding relational data. The data flowing through the DAG is either collections of relational tuples or tensors. The operators are either relational operators like join, selection, and projection (consuming relational data and producing relational data), standard feature encoders like one-hot encoders (consuming relational data and producing vectors), or standard ML preprocessing operations like normalization or concatenation (consuming vectors and producing vectors). In the following, we list the operations supported by the current implementation of mlinspect in Table 1, and discuss their formalization. We would like to note that we focus on common operations from pandas and scikit-learn in our current research prototype. That said, the instrumentation approach of mlinspect is general, and extending its capabilities to support additional functions can be done with moderate engineering effort.

Dataframe algebra We introduced our operators as a mixture of relational algebra operators with estimator/transformer pipelines. However, relational algebra is insufficient to formalize mlinspect operators because it operates on unordered collections, while typical exploratory operations on dataframes (like printing the first or last n rows) assume an ordered data representation [39]. Estimator/transformer pipelines in scikit-learn also fundamentally rely on order: transformers map over a list and transform the data without changing the order (e.g., when converting categorical strings to one-hot vectors). Model training methods also assume that their inputs are ordered, by implicitly associating each featurized datapoint with its corresponding label. Furthermore, support for linear algebra is crucial for typical ML pipelines, because many operations, especially for feature processing, have a natural representation as matrix operations and are internally implemented on numerical array data structures. In addition, dataframes in libraries like pandas offer many specialized methods that do not have an equivalent in relational algebra [39]. Examples include the TRANSPOSE operation that interchanges rows and columns, and the TOLABELS operation that projects a column out to use it as a row label.

Peterson et al. [39] observed that dataframes combine operations from relational algebra, linear algebra and spreadsheets and proposed a novel dataframe algebra to unify them. We use this algebra as a basis for the abstract representation of ML pipelines, in order to formalize our approach. Because mlinspect currently focuses on ML pipelines that use relational operations and estimator/transformer operators, we only require a subset of the dataframe algebra.

Operator formalization Peterson et al. [39] define a *dataframe* as a tuple (A_{mn}, R_m, C_n, D_n), where A_{mn} is an array of entries from the domain Σ^*, R_m is a vector of row labels from Σ^*, C_n is a vector of column labels from Σ^*, and D_n is a vector of n domains from *Dom*, one per column, representing the schema of the dataframe. Each component of the tuple can be left unspecified. Since D_n can be left unspecified, there is a schema induction function $S(\cdot)$ that, when applied to a column of A_{mn}, returns its domain i. Function $p(\cdot)$ can be used to get the values of the column. This definition allows to represent matrices as dataframes with a

Table 1 Functions supported by `mlinspect` and their corresponding operators in the dataflow representation of the pipeline

Function call	Operator
`('pandas.io.parsers', 'read_csv')`	Data Source
`('pandas.core.frame', 'DataFrame')`	Data Source
`('pandas.core.frame', '__getitem__')`, arg type: strings	Projection
`('pandas.core.frame', '__getitem__')`, arg type: series	Selection
`('pandas.core.frame', 'dropna')`	Selection
`('pandas.core.frame', 'replace')`	Projection (Mod)
`('pandas.core.frame', '__setitem__')`	Projection (Mod)
`('pandas.core.frame', 'merge')`	Join
`('pandas.core.groupbygeneric', 'agg')`	Groupby/Agg
`('sklearn.compose._column_transformer', 'ColumnTransformer')`, column selection	Projection
`('sklearn.compose._column_transformer', 'ColumnTransformer')`, concatenation	Concatenation
`('sklearn.preprocessing._encoders', 'OneHotEncoder')`	Transformer
`('sklearn.preprocessing._data', 'StandardScaler')`	Transformer
`('sklearn.impute._base', 'SimpleImputer')`	Transformer
`('sklearn.preprocessing._discretization', 'KBinsDiscretizer')`	Transformer
`('sklearn.tree._classes', 'DecisionTreeClassifier')`, `('tensorflow.python.keras.wrappers.scikit_learn', 'KerasClassifier')`,...	Estimator
`('sklearn.model_selection._split', 'train_test_split')`	Split (Train/Test)
`('sklearn.preprocessing._label', 'label_binarize')`	Projection (Mod)
`('sklearn.pipeline', 'fit')`, arg: train data	Train Data
`('sklearn.pipeline', 'fit')`, arg: train labels	Train Labels

homogeneous numeric schema D_n, with *null* labels R_m and C_n. See Figure 3 in Peterson et al. [39] for an illustration.

We detail the representation of the one-hot encoder operator in this algebra as an example. Given a $DF = (A_{m,1}, R_m, C_1, D_1)$ with a categorical string column, the one-hot encoder is a map operator $MAP(DF, f)$ with the output $(A'_{mn'}, R_m, C'_{n'}, D'_{n'})$, and the function $f : D_n \rightarrow D'_{n'}$, where $A'_{mn'}$ is the result of the function f as applied to each row, $C'_{n'}$ is the resulting column labels, and $D'_{n'}$ is the resulting vector of domains. For a one-hot encoder, f is a function that transforms each categorical string into an n'-dimensional vector, where n' is the domain cardinality of D_1, with only a single nonzero entry in the dimension corresponding to the string value in a given row. The cardinality n' of the string column becomes the number of dimensions of the one-hot vectors and, thus, also the number of columns in the result dataframe. The column labels $C'_{n'}$, in this case, are generated by combining the attribute and string values.

In general, our operators map to this algebra as follows. Our DAGs start with one or multiple `Data Source` operators. In the dataframe algebra, the initial data inputs are not operators, rather, they are modeled as leaf nodes in their DAG. Our operator `Projection` has the same semantics as the PROJECTION operator in the dataframe algebra. The corresponding operator for our `Projection (Mod)` is a MAP because the dataframe algebra does not have extended projections but uses the MAP operator instead to also handle that functionality. Our `Selection` and `Join` operators work exactly like their equivalents in the dataframe algebra, SELECTION and JOIN. Our `Group by Agg` operator works like the GROUPBY operator in the dataframe algebra that can directly apply aggregation functions. Note that the GROUPBY operation in the data frame algebra is more powerful than ours, in that it offers a `collect` aggregation function that can group rows into multiple dataframes, which we do not support. The MAP function in the dataframe algebra applies a function uniformly to every row. Our `Transformers` have the same semantics as these MAPs. Our `Estimator` can also be expressed as a MAP that does not produce an output. The `Split (Train/Test)` and its two outputs can be expressed using a MAP to add a temporary column, a SELECT to filter records using this column, and a PROJECT to remove the temporary column afterward. The `Concatenation` can be used to append the columns of multiple dataframes that have the same number of records. In the dataframe algebra, this can be done using TRANSPOSE to interchange the columns and the rows, followed by a UNION of the two dataframes, and then a TRANSPOSE again.

Additionally, we enrich our DAG representation of ML pipelines with other information inferred from the pipeline code, which is potentially helpful for further analysis. Examples for this are the `Train Data` and `Train Label` DAG nodes that mark the data on which `estimator.fit` was called. Clearly, identifying the exact version of train and test data used to fit the ML model greatly simplifies the implementation of inspections. When formalizing our DAG operators, these operators can be ignored, as they result in *no-op* label nodes that do not change the semantics of the ML pipeline query but they simplify its analysis.

Discussion As we already pointed out, the major difference between the dataframe algebra and the relational algebra is order preservation. Relational algebra operates on sets of tuples, while dataframes are modeled as ordered collections of tuples, and operations on them preserve this order. This property is a fundamental obstacle for the efficient pushdown [23] of the execution of ML pipelines and inspections into relational databases, as we would either need to implement order-preserving variants of common relational operators, or introduce artificial sort columns and always sort query results based on them.

4 Implementation

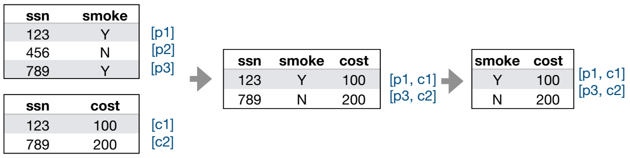
We now discuss the salient aspects of the implementation of `mlinspect` and revisit the example from Sect. 2. Our research prototype is available at: https://github.com/stefan-grafberger/mlinspect.

4.1 Overview

Our research prototype contains the core operator DAG extraction functionality, and it implements instrumentation, checks, and inspections for pandas and scikit-learn. We offer implementations of representative inspections, including an inspection that materializes the first row output by each operator, an inspection that tracks the detailed lineage of all rows flowing through the DAG, data quality inspections, and an inspection that computes histograms of operator outputs for sensitive groups. In addition, we offer implementations of checks, which evaluate a constraint on the outputs of our inspections, such as a threshold comparison of the magnitude of change in the proportions of certain groups in the data after a filter.

4.2 Inspections

Some checks only require the extracted DAG for analysis. An example for this is the `NoIllegalFeatures` check, which inspects the names of projected attributes used as features to ensure that no illegal features, such as gender or race, are used. Other checks only require simple inspections that investigate an operator in isolation. An example is the `NoMissingEmbeddings` check, which simply counts the null values in the outputs of embedding operators. Another example are inspections for data unit testing. Data unit tests typically evaluate constraints based on aggregate statistics of the data such as the completeness (ratio of non-NULL values) of a column or the number of distinct values in a column. Often, these statistics only require a single pass over the data and can therefore be pipelined with the actual execution of an operator. The `Completeness` and `NumDistinctValues` inspections compute these statistics by iterating over the values of a given column and maintaining the counts for NULL/non-NULL values (for completeness) or a hashmap containing the number of occurrences per distinct value.



ssn	smoke	
123	Y	[p1]
456	N	[p2]
789	Y	[p3]

ssn	cost	
123	100	[c1]
789	200	[c2]

ssn	smoke	cost	
123	Y	100	[p1, c1]
789	N	200	[p3, c2]

smoke	cost	
Y	100	[p1, c1]
N	200	[p3, c2]

Fig. 3 Lineage tracking by propagating identifier annotations through operators

In general, however, inspections need to work with the data annotations flowing through the operators at runtime, as described in the previous sections. In the following, we discuss two such cases in detail: lineage tracking and change detection for proportions of protected groups.

Lineage tracking It is simple to integrate lineage tracking into `mlinspect` directly using the built-in annotation propagation mechanisms. As part of lineage tracking, unique identifier annotations for all input tuples are generated and forwarded according to operator semantics (e.g., for a join, a combination of the identifier annotations of matching tuples are forwarded).

We implement lineage tracking (Fig. 3) via the lineage inspection. To illustrate our approach, we use a pandas code snippet that joins a table of patient data with a table of cost data, and projects the result to the attributes `smoke` and `cost`.

```
patient = pd.read_csv(...)
cost = pd.read_csv(...)
data = pd.merge([patient, cost], on="ssn")
data = data[["smoke", "cost"]]
```

The `visit_op(self, op_context, row_iterator)` function of the inspection is called first, as `patient` data is loaded on line 1. The inspection then checks the type of the current operator. In our example, operator type, *data source*, is contained in the `op_context`. After checking this, the inspection generates unique identifiers for each row. This process is repeated for the `cost` data source on line 2. The third call to `visit_op` corresponds to the join, which results from the `pd.merge` call on line 3. There, `visit_op` operates on five-tuples comprised of the output row from the join, the corresponding rows from the two dataframes patient and cost, and the annotations for the two input rows. The two input annotations are then combined to create the output annotation. For projection on smoke and cost on line 4, we only need to forward-propagate the existing input annotations.

One notable case not shown here is lineage inspection for the groupby operator type, where the aggregation following the groupby is treated as a new data source. We expect that the detailed lineage information from aggregations is not relevant for many ML use cases, which often mostly apply global aggregations (e.g., for normalizing features), where each tuple depends on the whole input anyways. We leave a more fine-grained treatment of aggregations for future work.

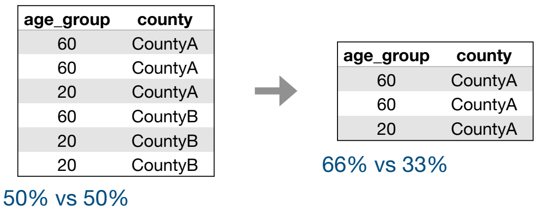
Change detection for proportions of protected groups In our running example (Fig. 1 in Sect. 2), we briefly discussed an inspection to discover the introduction of accidental changes in the proportions of protected groups. This refers to the issues ①, ②, ③ and ④ from the example and requires the histogram inspection to (*i*) trace the group membership variables age_group and race through the DAG, and handle the fact that age_group is projected out early (issue ②). We designed a custom check called NoBiasIntroducedFor for such cases. Internally, this check uses the HistogramForColumns inspection, which we will now explain. Consider the following selection statement:

```
data = data[data.county == "CountyA"]
```

Figure 4 shows how this selection might affect an example dataset flowing through it. Before the selection, the two age_groups, 60 and 20, are distributed evenly. After the selection, the majority of data points is in the age_group 60. This is an artifact of the strong correlation between the attribute county and the attribute age_group. Our simple example illustrates a common real-world trend, namely, that geographic and demographic attributes are often correlated.

To detect such distribution changes, we apply the HistogramForColumns(['age_group']) inspection that annotates both the DAG node before the selection and the selection DAG node itself with an age_group histogram of the outputs. After inspection execution and DAG extraction, the NoBiasIntroducedFor check can then look at these two annotated DAG nodes. For each sensitive attribute, it checks whether there is a significant distribution change of group memberships, and, if so, alerts the user.

We use a simple detection strategy that is easy for users to understand and configure. We start by calculating the group membership ratio compared to the overall number of people in the data. Here, this group membership ratio for people with age_group=20 is 0.5 before the selection and 0.33 after it. We compute the relative change before and after the selection as $(0.33 - 0.5)/0.5 = -0.34$. We then compare this quotient to a test threshold, set to -0.3. If the change is below that minimal threshold, as is the case in our example, we warn the user. This approach is especially sensitive to changes in the proportion of minority groups.



age_group	county
60	CountyA
60	CountyA
20	CountyA
60	CountyB
20	CountyB
20	CountyB

50% vs 50%

age_group	county
60	CountyA
60	CountyA
20	CountyA

66% vs 33%

Fig. 4 Histogram-based change detection for the proportions of protected groups in operators such as selections and joins. Here, in the beginning, the two age groups are distributed evenly, with a drastic change after the operator application

What is not encountered in this example is the removal of a group membership attribute. If projection is used to remove the attribute age_group, we annotate each row with its corresponding age_group value and propagate these row annotations forward. Subsequent operations like join, selection, and missing value imputation, which may change group proportions in the data, rely on these propagated group membership annotations to compute a histogram of group memberships of all inspected operator outputs, and test them for distribution changes.

We implement additional inspections to compute histograms of intersectional group membership. We also provide a check for calculating the removal probabilities of different demographic groups in the data. This check detects cases where filter-like operations that affect only a small subset of the data disparately impact specific demographic groups.

4.3 Execution of inspections, checks, and DAG extraction

Next, we discuss the detailed execution of inspecting a preprocessing script with mlinspect. The execution proceeds according to the following steps (which we detail in the remainder of this section):

1. **Preparation:** Determination of a minimal required set of inspections based on the inspections and checks specified by the user.
2. **Instrumentation:** Instrumentation of function calls in the AST of the user program.
3. **Execution of the instrumented program:** Delegation of the execution of inspections to library-specific backends; joint execution with pipeline operations; creation of the dataflow DAG.
4. **Results:** Evaluation of checks using the DAG and the inspection results.

4.3.1 Preparation

Determining a minimal required set of inspections The first step consists of determining which inspections to execute. Users have two ways to specify inspections: they can either use the check API or specify inspections they are interested in directly. We collect all of the required inspections from these two sources and build a unified set with them.

Capturing relevant function calls As discussed in Sect. 3.2, we instrument the user code via monkey patching and callback functions. It is crucial to only patch relevant function calls, due to the high amount of additional function calls for the callback functions. Determining whether a given function call is relevant for us (e.g., maps to an operator in our DAG) is difficult without executing the code. Monkey patching allows us to create specific patches for function calls relevant for `mlinspect`, while leaving other function calls unaffected. We leverage the Python package `gorilla`[5], which simplifies monkey patching, while also retaining the original unpatched version of the function. When a user executes source code with `mlinspect`, AST nodes corresponding to the following code before and after the original user code are added. The two added function calls only need to be executed once per user script and patch all functions supported by `mlinspect` from libraries like pandas and scikit-learn.

```
from mlinspect.instrumentation
 import monkey_patch, undo_monkey_patch
monkey_patch()
# ...original user code...
undo_monkey_patch()
```

Handling indirect function calls Monkey patching affects all calls to a patched function, even though we only want to execute inspections for calls relevant to the user pipeline. An example for a problematic case is the constructor `pandas.DataFrame(...)`, which is internally used by Pandas as well. As we are only interested in the invocations by our user program, we detect whether a certain operation is directly called by the user program as follows: In the patched code, we call the Python function `sys._getframe` to determine the source code filename of the stack frame of the call and check whether the source file is the root level file executed by `mlinspect`.

Example We present the code for a simplified example of our instrumentation technique, which adds support for the sklearn function `label_binarize` (which creates a binary vector from a categorical column with two distinct values). We initiate the patching of the method `label_binarize` in the package `sklearn.preprocessing` via gorilla's annotations. Next, we implement a patched version of the function, which creates a new DAG operator and retrieves the corresponding DAG parent node and the input annotations required for our inspections. Afterward, we call both the backend responsible for the operation (the `SklearnBackend` in this case), as well as the original function and insert the newly created operator node to our DAG. We would like to note that adding support for a new API function to `mlinspect` only requires a similar patching implementation, which makes it easy to extend our library with moderate engineering efforts.

```
@gorilla.patches(sklearn.preprocessing)
class SklearnPreprocessingPatching:
 @gorilla.name('label_binarize')
 @gorilla.settings(allow_hit=True)
 def execute_label_binarize(*args, **kwargs):
  original = gorilla.get_original_attribute(
   sklearn.preprocessing, 'label_binarize')
  # Patched function
  def patched(...):
   function_info = FunctionInfo(
    'sklearn.preprocessing._label',
    'label_binarize')
   # Operator mapping for DAG
   op_ctx = OperatorContext(
    OperatorType.PROJECTION_MODIFY,
    function_info)
   parent_info = get_parent_node_info(
    args[0], ...)
   # Initiate inspection execution via
   #  backend
   input_df = SklearnBackend.before_call(
    op_ctx, [parent_info])
   # Execute original function
   result = original(input_df,
    *args[1:], **kwargs)
   # Finalize inspection execution via
   #  backend
   backend_result = SklearnBackend\
    .after_call(op_ctx, input_df, result)
   # Append DAG node with inspection result
   add_new_operator_node_to_dag(
    DagNode(...), [parent_info],
    backend_result)
   # Return original result
   return backend_result.updated_result_df
  return execute(original, patched, *args,
   **kwargs)
```

Indirect data processing ML pipelines often contain several functions calls that only lead to data processing indirectly. Scikit-learn's `ColumnTransformer` pipeline step for specifying a set of feature transformations on a dataframe is an example for this. The user code defines a nested pipeline first and then passes the data to it in a second step by calling `fit` on the final pipeline object. The resulting `fit` calls on the contained transformers such as a `OneHotEncoder` or the projections required by the `ColumnTransformer` are only executed indirectly. Our approach identifies and handles these indirect calls by patching the constructors of the pipeline steps and using the source code location retrieved during the constructor invocation to determine that the fit calls originate from the user pipeline code (and must therefore be handled by the system).

Tracking source code locations of operators Python stack frames only contain the line number of the corre-

[5] https://pypi.org/project/gorilla/.

sponding operations. mlinspect can add extra function calls to the AST to track code locations. The AST of the user program, extracted by the Python parser, contains more detailed information: nodes have the attributes lineno and coloffset that indicate the start of the code location, and one can also determine where the snippet corresponding to an operator ends (the end_lineno and end_coloffset). These two attributes are provided by a recent addition to the parser in Python 3.8. Instrumentation is conducted with an ast.NodeTransformer in Python, where the code locations are directly added as arguments to callback functions. This more detailed tracking is configurable, as the additional function calls introduce a minor overhead. We experimentally evaluate the overheads of different instrumentation techniques in Sect. 5.1.4.

4.3.2 Execution of the instrumented program

After instrumenting the user pipeline code, the instrumented AST is compiled and executed, which triggers the execution of the patched functions and the build up of the DAG as described in Sect. 3.2. The execution of each inspection is delegated to the corresponding backend, e.g., inspections for a merge call on a pandas dataframe will be handled by the pandas backend. The API for the different backends comprises of two functions: before_call and after_call, where the before_call function can modify the input before the original function is called. In case of a pandas merge call, for example, an index column is introduced to later associate output rows with the corresponding input rows. The after_call method then executes the inspections and removes metadata such as the index column.

Handling control flow We discuss the implementation details for handling control flow (Sect. 3.2). In order to be able to work with pipelines containing control flow, a DAG is built from the actual execution of the program, instead of just relying on information in the AST (as in previous versions of mlinspect [17]). This prior approach does not allow for the determination of which branches are executed. The current version directly patches function calls, independently of where they occur. Based on these function calls, the DAG is built up dynamically at runtime. During the execution of a patched function, the current stack frame is investigated to determine whether the function call is relevant for the inspections, as described in Sect. 4.3.1. We carefully implemented the corresponding logic to ensure a low overhead for repeated function calls that are not of interest to mlinspect, and experimentally evaluate this overhead in Sect. 5.1.4.

Efficient execution of our Python-based inspections via scan-sharing We implement inspections to both consume and produce iterators, based on for-comprehensions and the yield keyword in Python.

```
def visit_op(self, op_context, rows) -> Iterable
  for row in rows:
    annotation = annotate_and_update_state(self,row)
    yield annotation
```

The inspections are supplied with an iterator over their input rows. To create the iterator, three different arguments are needed: the output of the operator, the corresponding input, and the annotations for the input. They all have the same order and an equal number of rows, so one can scan over those three list-like elements at the same time to create the row_iterator. However, we only want to do a single scan over this even if we have multiple inspections. The only complication is that each inspection has its own separate annotations for each record. The following listing shows how scan-sharing is done with Python iterators and the itertools library[6]. It starts by creating multiple iterators over the input and output rows, one copy per inspection. For each inspection, an iterator is constructed over the inspection's annotations of the input rows. Finally, the functions zip and map are used to create a single iterator that outputs simple data class objects with the current input row, the input row annotation, and the output row. These data class object iterators are the input for the inspections.

```
# Duplicate iterators for each inspection
duplicated_inputs = itertools.tee(input_rows,
   len(inspections))
duplicated_outputs = itertools.tee(output_rows,
   len(inspections))
# Create the inspection_iterator for each inspection
for inspection_index, _ in enumerate(inspections):
  inputs = duplicated_inputs[inspection_index]
  outputs = duplicated_outputs[inspection_index]
  annotations = iterator_for_annotation(
    input_annotations, inspection_index)
row_it_for_inspection = map(
  lambda input_tuple: RowUnaryOperator(*input_tuple),
   zip(inputs, annotations, outputs))
```

The function itertools.tee internally uses one iterator over the input and one over the output and buffers the values until each duplicated iterator processed the value. All inspections consume the iterator elements at the same pace, so only one pass over the data is being made and itertools.tee only needs to buffer the current input and output row. This approach is based on the *banana split law* [20] for loop fusion. When we have multiple functions that we can express using a fold (e.g., computing the count or the sum for a numerical column), we can build a single fold function that combines them to conduct the same computation with a single pass over the data. Here, the visit_op functions of each inspection work similarly to folds. Therefore, we can apply the fusion from the banana split law, to avoid repeated scans over the data.

Handling different types of data Backends also provide a custom function to create datatype-specific iterators for all datatypes that can currently be passed around in the supported ML pipelines. For example, the following listing shows the code to create iterators for pandas dataframes.

[6] https://docs.python.org/3/library/itertools.html.

Table 2 Overview of the internal operator types

Operator(s)	Operator type
Data Source, Group by Agg	Data Source
Projection (Mod), Transformer, Train Data, Train Labels	Unary map
Concatenation	N-ary map
Selection, Train/Test-Split	Unary resampling
Join	Join
Estimator	Sink

```
def get_df_row_iterator(dataframe):
  column_info = ColumnInfo(list(
    dataframe.columns.values))
  arrays = []
  arrays.extend(dataframe.iloc[:, k] for k in
       range(0, len(dataframe.columns)))
  return column_info, map(tuple, zip(*arrays))
```

We provide corresponding implementations for other datatypes like the `ndarray` in numpy, the `Series` in pandas, the sparse matrix `csr_matrix` in scipy, and plain Python `list` objects. Our support for tensors is currently restricted to two-dimensional cases where it is obvious which dimensions correspond to the rows and columns of a dataframe. A prime example for this is feature matrices built from vectorized input samples. We leave support for operations on higher-dimensional tensors (e.g., to represent images, pixels, and channels in three dimensions) for future work.

Instrumentation for different operator types To execute our inspections, we only need to differentiate between a small set of different types of operators, as listed in Table 2. We base the classification on the number of parent operators, whether the operator produces output data, and whether the operator can change the order or number of elements. A `Data Source`-type operator does not get input data from a parent operator and does produce an arbitrary output. A `Unary map` uses the data from one parent operator as input and outputs one output row per input row without changing the existing order of elements. The `N-ary map` has data from multiple parent operators as input, each of them having the same number of elements, and maps n-tuples of input rows to one output row without changing the existing order of elements. `Unary resampling` receives data from one parent operator as input, and can arbitrarily reorder or drop input elements to produce its output. A `Join`-type operator receives input data from multiple parent operators, and combines and reorders them in arbitrary ways to produce its output. A `Sink`-type operator gets input data from a parent operator but does not produce any output data.

The previous examples assumed the operator type of a unary map. In the following, we describe how to handle the remaining types of operators. Data source operator types are simpler because we do not have input data or input annotations we need to consider. The N-ary map works analogously: we can associate row annotations, input, and the corresponding output based on them having the same order and number of elements. The only difference is that we have multiple input dataframes instead of a single one, each with its own annotations. The sink also works analogously; we can associate input and input annotations based solely on the order and number of elements. Functions for operators of the type unary resampling require more complex logic to associate input rows, input annotations and the corresponding output rows. For them, an index column to the input data using the callback functions like `before_call` needs to be added. After execution, this column is removed during the `after_call` function to hide it from the user code. We then utilize these index columns as follows. We start by concatenating the input and the input annotations. Next, we read the index column and join the annotated input with the output. Subsequently, we create iterators over this join result, giving us the required for input, output, and the different annotations. The remaining execution proceeds analogously to the unary map function. In the case of joins, we need to apply the described indexing techniques for both join inputs. In the majority of cases, we use pandas dataframes as data structure to store the actual annotations. They are convenient because we can then leverage joins and concatenation in pandas for the execution of inspections. Once the data is inside a scikit-learn pipeline, we switch to plain Python lists to store the annotations.

Optimizable inspections based on dataframe operators A drawback of our Python-based inspections is the high runtime overhead inherited from Python and a lack of vectorization, which typically requires calling external C code. Due to this, we design an alternative, less general but more efficient method for executing inspections. As outlined in Sect. 3.2, we also support the implementation of inspections based on dataframe operators. The core idea is to model both the inspections and the user program operations as dataframe operators and execute them jointly. This approach is less general than allowing users to write arbitrary python code for inspections, but has a much lower overhead, as we can leverage optimized operator implementations (which apply vectorization) and common techniques from query optimization.

For this approach, inspections are again expressed via two functions, one for computing output annotations for each row and one for computing the final annotations for the current DAG operator. However, instead of relying on the Python generator abstraction, these functions return a partial query plan comprised of dataframe operators. For the annotation propagation, inspections still operate on output rows of the instrumented user operations and the corresponding annotated input rows, but express the computation of the output annotations for each row with dataflow operators.

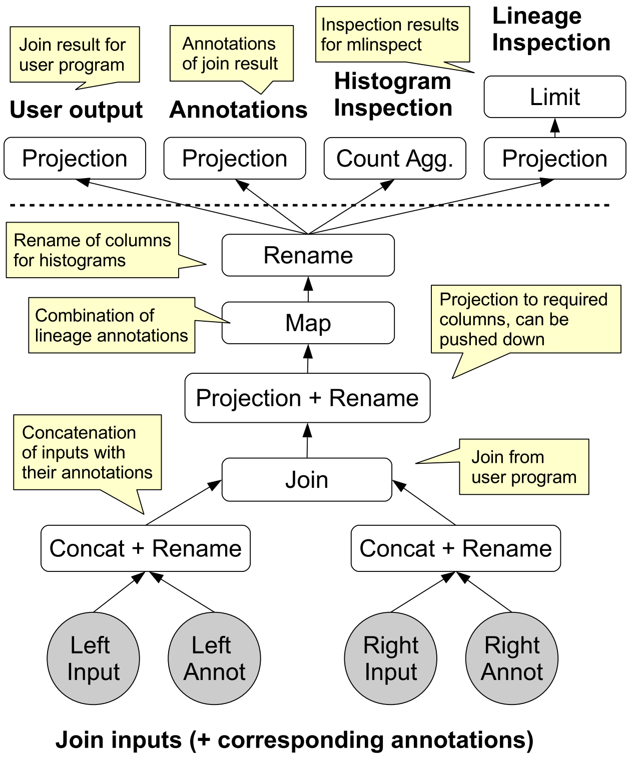

Join result for user program
Annotations of join result
Inspection results for mlinspect
Lineage Inspection
User output
Annotations
Histogram Inspection
Limit
Projection
Projection
Count Agg.
Projection
Rename of columns for histograms
Rename
Combination of lineage annotations
Map
Projection to required columns, can be pushed down
Projection + Rename
Concatenation of inputs with their annotations
Join
Join from user program
Concat + Rename
Concat + Rename
Left Input
Left Annot
Right Input
Right Annot
Join inputs (+ corresponding annotations)

Fig. 5 Example for optimizable inspections: we generate and execute a query plan to apply the histogram and the lineage annotations to a join on two dataframes

Example We discuss how to build up a query plan to apply the histogram and the lineage annotations to a join on two dataframes, illustrated in Fig. 5. As shown in the figure, we start by concatenating each of the two input dataframes with the dataframes holding their input annotations. Next, we apply the original user operation, the join. We use a projection on the joint results to create the result from which the inspections compute the output annotations. This dataframe contains all input columns from both sides and the output columns. This dataframe offers our optimized inspection the same logical view with separated input and output columns as we provide for the Python-based inspections. The histogram inspection forwards the existing annotation column and renames it to follow our naming conventions for inputs and outputs; the lineage inspection combines the two lineage annotation input columns using a map operation. Now, we have a dataframe with the annotated output rows and their corresponding input rows.

In our example, we compute four final outputs from the intermediate dataframe with the annotated output rows and the corresponding inputs. The first output is for the user program: the original result dataframe of the join without annotations and inputs. We use a projection on the intermediate result to remove the annotations and the input columns. Subsequently, we compute the dataframe containing the new output annotations for each row, again using a projection to retrieve only the annotation columns from the intermediate result. The last two outputs correspond to the DAG node annotations from the histogram inspection and the lineage inspection. The histogram inspection uses a groupby operation with a count aggregation, while the lineage inspection applies a limit operation and a projection to materialize the first n output rows and their lineage annotations. Finally, we can optimize and execute the query plan. We experimentally evaluate the performance benefits of this approach in Sect. 5.1.3.

Garbage collecting the annotations Once we obtain the final data structure with the annotations, we need to decide where to store it. One option would be to just save the annotations in the different backends. For example, we could maintain a map from specific function calls to the annotations. However, this would result in unnecessary memory overhead because we do not know when we can free the annotation variables. We only want to remember annotations for a variable as long as that version of the variable exists. For this reason, we store the annotations along with the variables themselves. We achieve this for each data representation relevant to the ML pipelines by either adding the attributes to the original class via monkey patching for pure Python classes, or via a simple wrapper class for classes like numpy arrays that are partially implemented directly in C. These wrapper classes extend the original class and do not change the behavior in any way observable by the original pipeline. Based on this design, the garbage collector of the Python runtime automatically takes care of freeing obsolete annotations.

4.3.3 Extraction of the dataflow graph and evaluation of checks

As discussed in Sect. 3.2, we extract the DAG during the execution of the instrumented user code. As a consequence, the DAG exactly represents the actual dataflow, even if the user code has complex control flow. After obtaining all inspection results and the dataflow graph, we evaluate all user-specified checks on the DAG and the inspection results. Finally, `mlinspect` returns the complete DAG, the inspection results, and the check results.

4.4 Implementation of our example

We provide an executable implementation of our example [7] from Sect. 2, along with a Jupyter Notebook [8] that details

[7] https://github.com/stefan-grafberger/mlinspect/tree/19ca0d6ae8672249891835190c9e2d9d3c14f28f/example_pipelines.

[8] https://github.com/stefan-grafberger/mlinspect/blob/19ca0d6ae8672249891835190c9e2d9d3c14f28f/demo/feature_overview/feature_overview.ipynb.

and visualizes the automatically extracted DAG representation and inspection results for this example. We offer a declarative API for users to state their expectations using the aforementioned checks, which we will then internally convert to constraints on inspection results, e.g.,

```
PipelineInspector
  .on_pipeline_from_py_file('healthcare.py')
  .check(NoBiasIntroducedFor(['age_group',
    'race']))
  .check(NoIllegalFeatures())
  .check(NoMissingEmbeddings())
.execute()
```

The expectation about the lack of the introduction of technical bias refers to the issues ①, ②,③, and ④ from our example and requires the aforementioned change detection inspection from Sect. 4.2 to (i) trace the group membership variables `age_group` and `race` through the DAG, and handle the fact that the former is projected out early (issue ②).

With this in mind, `mlinspect` proceeds as follows: when we visit the projection operator that removes the attribute, we annotate each row with its corresponding `age_group` value and propagate these row annotations forward; (ii) the join, selection, and imputation operators might change the proportions of groups in the data. To handle this, we use the propagated group membership annotations, compute a histogram of group memberships of all inspected operator outputs, and test them for distribution changes afterward. To check whether illegal features have been used (issue ⑤), we simply search the list of projected attributes that are used as features. This information is available as part of our DAG. The check for missing embeddings (issue ⑥) only requires counting the null values in the outputs of the embedding operator.

5 Experimental evaluation

In this section, we present results of an extensive quantitative and qualitative evaluation of `mlinspect`. In Sect. 5.1, we measure the runtime overhead of `mlinspect` for different operators, inspections, and instrumentation techniques. Then, in Sect. 5.2, we present results of an interview-based user study of effectiveness of `mlinspect`. Finally, in Sect. 5.3, we qualitatively compare our library to an experiment tracking and workflow provenance solution.

5.1 Runtime overhead

As `mlinspect` operates on Python scripts and allows for user-defined inspection functions with generic code, it naturally runs in Python, inheriting its overheads. Therefore, our experiments focus on the overhead in terms of the number of input and output rows of the operators. We designed our approach with a constant overhead per tuple and therefore expect the overhead to be linear in the number of input and output rows of an instrumented operator. This is due to the fact that our design requires us to only conduct a single scan over operator inputs and outputs to execute our Python-based inspections and to only materialize intermediate results of interest, which requires a constant overhead per processed row for our discussed inspections. We present a set of experiments to measure the runtime overhead of our `mlinspect` research prototype. We evaluate the overhead of instrumenting operators in Sect. 5.1.1, the overhead of our Python-based inspection execution in Sect. 5.1.2, and we show how we can drastically reduce the inspection overhead with our optimized execution of inspections in Sect. 5.1.3. Additionally, we measure the overhead of instrumenting function calls in the AST in Sect. 5.1.4.

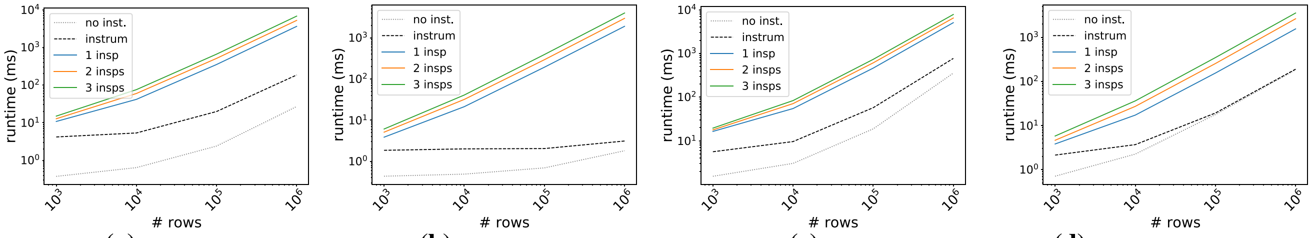
5.1.1 Overhead of python-based operator instrumentation

In our first experiment, we measure the runtime overhead of instrumenting different operators. In particular, we focus on the selection, projection and join operators of pandas, and on an ML-specific operator, the one-hot encoder from scikit-learn, which transforms a categorical string column into a sparse matrix representation. For each operator, we measure the execution time (i) without instrumentation; (ii) with instrumentation without inspections; and (iii) with instrumentation and with one to three empty inspections that read the respective inputs and outputs of operators but do not propagate annotations.

We report the average runtime from 20 repetitions of the experiment for 1000 to 1,000,000 input rows on the logarithmic scale. (For join, we generate the same number of rows for both join inputs.) The results are shown in Fig. 6. We observe the expected increase in the absolute runtime stemming from our usage of Python. However, the overhead per tuple is constant, indicated by the fact that the runtime overhead grows linearly with the number of input and output rows for all operators, as expected. We scale with operator output size for operations like many-to-many joins, where the output is potentially larger than the inputs. This is because inspections need to scan all output rows, along with the corresponding input rows and input annotations. Note that the runtime for projection without instrumentation, and with instrumentation but without inspections, is constant due to the underlying columnar data layout.

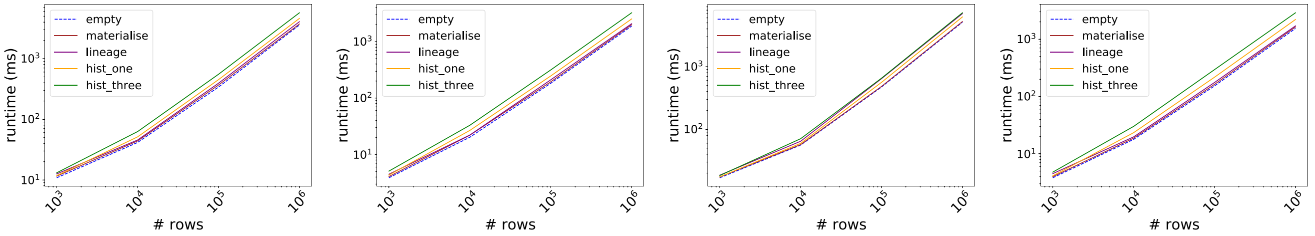
5.1.2 Python-based inspection overhead

We repeat our experiment with the four previously chosen operators and measure the runtime overhead of inspections. For each instrumented operator, we compare the runtime of an empty inspection to the runtime of the following inspections (each of which scans all processed rows): (i) materialize



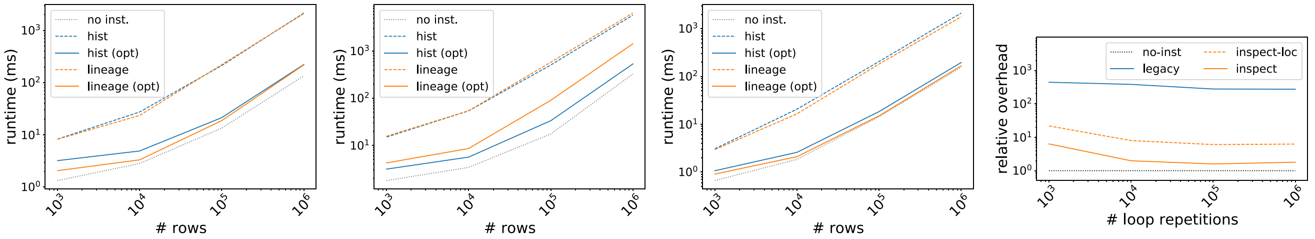
(a) Selection. **(b)** Projection. **(c)** Join. **(d)** One-Hot-Encoder.

Fig. 6 Instrumentation overhead for different operators. We compare the runtime of the execution of a given operator with no instrumentation (`no inst`), instrumentation without inspections (`instrum`), and with one to three empty inspections. We find that the overhead is linear in the number of input and output rows of the operators



(a) Selection. **(b)** Projection. **(c)** Join. **(d)** One-Hot-Encoder.

Fig. 7 Runtime overhead for different inspections in various operators. We compare the runtime of the execution of a given instrumented operator with an "empty" inspection (`empty`) to inspections for materialization (`materialize`), lineage tracking (`lineage`) and histogram computation for one and three columns (`hist_one` and `hist_three`). We find that the overhead is linear in the number of input and output rows of the operators



(a) pandas `dropna`. **(b)** pandas `merge`. **(c)** sklearn `1-hot`. **(d)** AST instrumentation.

Fig. 8 **(a)**–**(c)** Runtime overhead for executing inspections. Our optimized execution with dataframe operators reduces the overhead by an order of magnitude compared to the Python-based execution and exhibits an overhead of less than 8% compared to non-instrumented execution in some cases; **(d)** AST instrumentation overhead for function calls in a loop. Our patched-based instrumentation approach outperforms the previous approach by up to an order of magnitude and its runtime is within a factor of two of the uninstrumented runtime for a large number of repetitions with disabled code location tracking

a sample of output rows for each operator; (ii) track the lineage via annotation propagation for a sample of output rows for each operator; (iii) compute histograms over one or three columns of the outputs for each operator. We report the average runtime from 20 repetitions of the experiment for 1000, 10,000, 100,000, and 1,000,000 input rows.

The results are shown in Fig. 7. We again observe an overhead for all inspections that is linear in the number of input and output rows. We see that the overhead for the actual inspection logic (e.g., lineage tracking via annotation propagation) is low compared to the empty inspection, which indicates that most of the overhead stems from instrumentation and data access. We also see that the overhead of running additional inspections within one execution is a tiny fraction of the overall instrumentation overhead. This is a validation of the benefits of our loop fusion technique from Sect. 4.3.2. Recall that we implement our inspections with generator-like iterators that yield their elements, and execute the inspections in a way that avoids multiple scans over the data by exposing each record to all inspections during a single scan over the data.

5.1.3 Optimized execution of inspections

We introduced an additional approach to execute inspections in Sect. 4.3.2, based on query plans built from dataframe operations. This approach is less general than Python-based inspections from Sect. 5.1.2 that allow for arbitrary Python code, but has a much lower overhead. In the following, we evaluate both approaches on three operators and two inspections. We implement the optimized execution for our lineage and histogram inspections applied to the pandas functions `dropna` and `merge`, as well as for the `OneHotEncoder` from scikit-learn. We vary the number of randomly generated input rows from 1000 to 1,000,000 on the logarithmic scale and compare the runtime of the original operation without instrumentation `no_inst`, the Python-based `mlinspect` execution from Sect. 5.1 (`hist` and `lineage`), and the optimized execution with dataframe operators (`hist-opt` and `lineage-opt`).

Figure 8a–c shows the results of this experiment. We find that the relative overhead of our optimized inspections is an order of magnitude lower than for the Python-based execution. For the highest number of rows in this experiment, the overhead varies between the factors of only 1.08 and 4.3, compared to the runtime of the operation without instrumentation. This is due to the fact that we can optimize data access during the execution of the query plan corresponding to the inspections, that is, the lineage inspection no longer needs to scan all of the data. For the one-hot encoder, for example, it only needs to forward-propagate the existing lineage annotation column. We only materialize a small row sample from the output dataframe with an additional lineage column, and apply selection pushdown to optimize the computation of the final DAG node annotation. In summary, the optimized execution strategy drastically reduces overhead.

5.1.4 AST instrumentation overhead

In Sect. 4.3.1, we introduced an improved patch-based AST instrumentation mechanism. In the following, we measure the overhead of the instrumentation approach in a worst-case scenario, where it is necessary to instrument a cheap function that is invoked an excessive number of times. The following code snippet is used for the experiment, where list access via an index subscript is executed n-times in a loop.

```
n = ...
test_list = list(range(n))
for index in range(0, n):
  test_list[index] = index
```

We execute this code snippet for different values of n with different instrumentation mechanisms: `inspect` refers to the instrumentation mechanism described in Sect. 4.3.1, `inspect-loc` refers to the instrumentation mechanism with detailed source location tracking enabled, `legacy` refers to the instrumentation used in previous versions of `mlinspect` [17], and `no-inst` refers to the execution of the code without any instrumentation. In this experiment, we exclude the time it takes the library `gorilla` to apply the monkey patches and remove them again after execution of the instrumented user code. This constant cost only needs to be paid once per script and it is independent of the user code. In our measurements, this one-time cost was lower than 7ms.

Figure 8d shows the corresponding execution times. We find that the patch-based instrumentation approach is more than an order of magnitude faster than the earlier `legacy` approach. We also find that the instrumentation overhead diminishes for large values of n, where `inspect` exhibits less than twice the runtime of the uninstrumented execution `no-inst` as soon as the number of loop repetitions is 10,000 or higher. Furthermore, we find that `inspect-loc`, which tracks the exact source code locations (e.g., not only the line number but the character offsets in the line), introduces an overhead proportional to the overhead of `inspect`. Note that these experiments show an extreme worst-case scenario and that code location tracking is optional.

In summary, we find that instrumentation based on monkey patching drastically reduces AST instrumentation overhead.

5.2 Exploratory interview study with experts

We conduct an exploratory interview study with six expert users to qualitatively evaluate `mlinspect` in an ML pipeline debugging task. We provide the materials used in the study[9].

Participants Six participants solicited from our professional networks were interviewed. All participants have several years of experience in domains like data science, data engineering, and algorithmic fairness. The group consists of an expert data scientist from a large European retail company, a research engineer who previously worked on data science topics at an NLP-focused startup, three PhD students in machine learning and data management, and a data science Masters student.

Methodology We first give a fifteen-minute presentation about `mlinspect`, focused on data distribution bugs, to the participants. Next, a demonstration of `mlinspect` was given for ten-to-fifteen minutes, showing the detection of a data distribution bug in an example pipeline. Participants were allowed to ask questions. After this introduction, participants were instructed to individually solve two tasks similar to the demonstration. The first task uses a pipeline on a dataset about recidivism [6] with two artificial data distribution bugs caused by filter operations, which participants

[9] https://github.com/stefan-grafberger/mlinspect-exploratory-user-study/tree/b9546a7ff675af95811d3fe0c517093eb184e8d2.

had to identify. In the second task, a synthetic dataset from the healthcare domain and a pipeline with one data distribution bug were used. The goal of this setting was to find out whether `mlinspect` helps participants to quickly discover data distribution bugs and understand their root cause in complex pipelines with multiple operations, all potentially affecting the data distribution. Once participants completed the tasks, we studied their solutions, asked them a predefined set of questions about their experience with the library and about the technical aspects of its application, and also gathered their unstructured verbal feedback.

Results We briefly summarize the results from the tasks and interview questions.

Feasibility of the tasks All participants were successfully able to perform the two tasks within half an hour, despite not having any previous experience with the library. Most participants solved the second task much faster than the first one, after getting more familiar with the library. One participant stated that she spent most of the time on understanding the task pipeline, not on the usage of `mlinspect`.

Effectiveness for debugging All participants stated during the user interview that they could complete the tasks using `mlinspect` effectively. None of the participants were aware of alternative libraries to `mlinspect` for debugging ML pipelines. When asked how they would handle the tasks without `mlinspect`, all participants stated that they would repeatedly adjust the code to compute histograms of intermediate results and analyze the distribution changes manually. Based on their professional experience, all of them estimated that the alternative approach would have been more time-intensive, tedious, and error-prone than using `mlinspect`.

We highlight one quote from a participant: *The tool [...] can detect bias to the precision of which operator. That is quite impressive. [...] The DAG representation is powerful.*

Real-world applicability All participants thought that `mlinspect` is useful for data scientists; one participant commented that PySpark support is required to work with larger datasets. All but one participant stated that they would use `mlinspect` again when encountering an applicable problem. The remaining participant said they would only use our library again if it included additional functionality for model debugging.

Feature requests Participants named features they would like to see added to `mlinspect`, such as support for PySpark and support for detecting intersectional data distribution bugs. Another suggested feature was the detection of bias that is gradually amplified by multiple operators. The current implementation will not detect an issue if all operator changes are under the detection threshold, despite the overall change being over the threshold. Four users stated that they would have liked a final report by `mlinspect` that directly summarizes all potential issues, and includes detailed information about the issues that triggered alerts. One of the participants wanted `mlinspect` to integrate the detection of data quality issues like duplicate rows. Another suggestion was to test the initial input distribution and not just detect whether user code introduces new issues or amplifies existing issues. We note that the modular design of `mlinspect` allows for the implementation of all of the suggested features in future work. Indeed, we were able to already build an inspection for intersectional group memberships in response to a feature request.

In summary, participants confirmed the need to simplify data distribution debugging and found `mlinspect` helpful and usable.

5.3 Qualitative comparison against experiment tracking and workflow provenance tools

We are not aware of any system that offers the functionality `mlinspect` provides. As a consequence, we compare it against two systems from adjacent use cases: MLFlow[10] and noWorkflow [40]. MLFlow is an open-source experiment tracking solution with a rich feature set; noWorkflow is an open-source workflow provenance system that can handle unmodified programs. We qualitatively evaluate these tools for detecting the issues outlined in our example pipeline from Sect. 2.

5.3.1 MLFlow

MLFlow offers two different ways to log experiment data: (i) users can manually add logging statements to their code to track events and parameters of experiments with statements like `create_experiment()`, `start_run()`, `log_param()`, `log_metric()`, and `log_ar-tifact()`; (ii) the tool offers an auto-logging API, which is still in an experimental state, to log certain parameters and metrics for libraries like scikit-learn and Tensorflow. Auto-logging is implemented by patching all `fit` methods of all estimators. To enable auto-logging, users only need to add a single function call to the beginning of the pipeline, `mlflow.sklearn.autolog()`. MLFlow then logs data like sampled input rows from `the train_data` used as input to `pipeline.fit`, the parameters of all nested estimators, the training score, as well as strings describing the applied transformers. During execution, MLFlow saves all of the captured data to a directory. Afterward, a UI can be started with the command `mlflow ui` in the browser. There, users can get an overview of past runs and experiments and see a summary of important information, including certain metrics. There is also a detailed view for runs. Based on the information presented in the UI, it is easy for users to find a particular version of the experiment code, deploy the trained

[10] https://github.com/mlflow/mlflow.

model from that run, and obtain a file containing the initial column names and five example rows.

However, MLFLow does not capture intermediate versions of the data between different transformers in the pipeline. It also does not capture preprocessing operations in pandas. For discovering data distribution bugs like the shown in Fig. 1, users will still have to debug the pipeline on their own; the only help they would get from MLFLow would be artifact logging, to save CSV-versions of dataframes. To add detailed logging to scikit-learn pipelines, users still have to modify the pipeline code, for example, by adding transformers with the sole purpose of logging the data flowing through them[11].

Revisiting our running example in Fig. 1: we could detect issue ① with the help of straightforward artifact logging to the pandas part of the code. However, we would still need to directly load the CSV-files created by MLFlow and manually compute histograms. We could also deal with issue ② and ③ in a similar way, but we would have to build a custom mechanism to track group membership through the selection. For detecting issues ④ and ⑥, we would have to implement scikit-learn debug transformers using CSV logging provided by MLFlow. For issue ⑤, we would have to manually inspect the code to discover columns used as features.

In summary, we find that MLFlow is designed for recording experiment metadata, but it does not provide strong support for debugging data-related issues in the user code. Using MLFlow does not make it significantly more convenient to identify data distribution bugs in our running example. However, for other use cases, the auto-logging approach is very convenient.

5.3.2 noWorkflow

The noWorkflow[12] tool runs unmodified Python files, collects provenance information, and optionally other information such as variable usage and dependencies. It allows users to browse the data of past executions and investigate details such as module dependencies, function activations, and file accesses. Furthermore, it can generate a dataflow graph with fine-grained provenance data for the function call graph. (Figure 9 shows this call graph for our example pipeline.)

How can noWorkflow help us detect the data distribution bugs outlined in Sect. 2? We can list all function activations, including their parameters and return values. For these captured function calls, noworkflow stores and can display all intermediate dataframes and tensors passed around. We could use this to detect issue ①, but we would have to implement custom code to compute histograms of the data before and after the join. Issues ② and ③ are more problematic: once the projection removes important columns, the intermediate results stored by noWorkflow will not help us anymore; we would have to write custom debugging code to trace the group membership attributes. For detecting issues ④ and ⑥, noWorkflow provides no help. Unfortunately, the tool only captures function calls related to user-defined functions. Because of this, noWorkflow cannot capture the intermediate data of nested scikit-learn pipelines: a `pipeline.fit` call lead to many `.fit` calls on child transformers. These indirect calls are not captured. To detect issue ⑤, we would also have to identify it manually, by looking at the code.

In addition to not providing the required support for detecting these issues, noWorkflow also slows down the pipeline's execution: its execution time for our example pipeline is about an order of magnitude longer than `mlinspect`'s execution time. For its detailed tracking, noWorkflow saves all inputs and outputs of captured function calls to disk, leading to a considerable overhead compared to `mlinspect`, which only stores histograms and group membership information in-memory. Overall, modifying the pipeline code directly instead of using noWorkflow would likely be easier for data distribution debugging. This is because working with the original pipeline code is more straightforward in this case than implementing custom code that uses the data captured by noWorkflow.

Internally, noWorkflows captures function calls via the Python profiling API[13], where it registers itself as a listener. During pipeline execution, the Python profiler informs noWorkflow of all function activations. However, even a simple test script provided by the noWorklow authors leads to 156,086 function activations [33]. This is because the profiling API itself also considered function activations that were called indirectly. To avoid overloading users with large volumes of information (and likely to avoid performance problems), the authors decided to let noWorkflow only register function activations related to user-defined functions. This decision, in turn, leads to noWorkflow ignoring indirect scikit-learn calls.

In summary, we find that noWorkflow is designed for provenance tracking at a lower level (function calls) than `mlinspect`, and, as a consequence, it does not appropriately capture the semantics of relational and ML operations in the code, which greatly reduces its utility as a data distribution debugger, the issue of the interest of our work.

[11] https://stackoverflow.com/questions/34802465/sklearn-is-there-any-way-to-debug-pipelines.

[12] https://github.com/gems-uff/noworkflow.

[13] https://github.com/gems-uff/noworkflow/blob/cbb8964eba7d58a5e87f96fb5bb91ac452b80763/capture/noworkflow/now/collection/prov_execution/profiler.py.

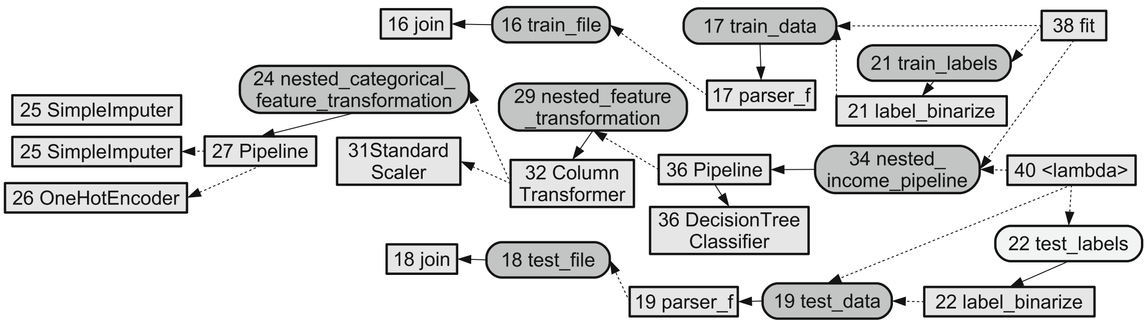


Fig. 9 Simplified illustration of the call graph for our example pipeline produced by noWorkflow. Unfortunately, it is difficult to understand the dataflow of ML pipelines using pandas and scikit-learn. The graph directly reflects each function call in the user code and does not provide an abstract representation of the dataflow of the ML components

6 Related work

The challenges of data management for end-to-end ML pipelines [41] and the Python-based data science ecosystem [44,45] are coming into the focus of the data management community in recent years. Proposed approaches often borrow ideas from provenance for relational workloads, a well-studied subject [13].

6.1 Provenance for relational workloads

There have been different notions of provenance for relational workloads, and there are several surveys of the field [13,19]. In the rest of this section, we will highlight a few important notions and use examples and explanations, mainly taken from the survey by Cheney et al. [13]. For more information, we refer to that survey and other papers cited in this section.

Provenance information is sometimes also called *lineage*. Three forms of provenance we want to discuss here briefly are why-, how-, and where-provenance. However, a lot of existing work does not fall into one of these categories. The idea behind why-provenance is to collect a set of all *witness* tuples that contributed to the existence of a tuple in the output of a query. However, for example, when the *distinct* keyword is used in a query, multiple tuples can result in the same output tuple while not needing to coexist. In contrast, the results of a natural join require multiple tuples to coexist. Why-provenance does not capture these distinctions as precisely as necessary for some purposes. Further, because the number of witnesses for each output tuple can be exponential in the size of the input database, the focus is usually on subsets of witnesses.

The precision issues mentioned just now are addressed by how-provenance, which aims to capture *how* a query output was derived. Important work in this area are provenance semirings [18]. The idea behind this is to use polynomials to capture how a query output was derived. Suppose two identical tuples t_1 and t_2 are present in a dataset, and we use the *distinct* keyword to only get one of the two in the result. In that case, we can represent the provenance information of the output tuple as $t_1 + t_2$: the existence of one of the two is enough to produce that output tuple. If we join t_1 and t_2, we can represent the output's provenance as $t_1 * t_2$, because both tuples need to coexist to produce that output. If a tuple can be the output of joining t_1 with either t_2 or t_3, then we can represent the provenance of the tuple as $t_1 * (t_2 + t_3)$. Extensions of this approach to aggregate queries [4] and linear algebra operators [57] also exist. In practice, however, it is not easy to use this approach due to performance reasons. It requires a lot of metadata to be captured, as the polynomial for one single output tuple can be arbitrarily complex depending on the query and the data.

Where-provenance captures the relationship between source and output locations. In a relation, the location refers to the cell. For example, where-provenance can capture that the *Smith* cell in the tuple t_1: $(123, \mathit{Jane}, \mathit{Smith})$ was copied from the *name* cell of some tuple t_2. However, where-provenance would not capture that t_1 is only present in the output because a join partner t_3 existed at some point during query execution.

There are many applications and implementations of the different notions of provenance. When using provenance in practice, paying attention to performance is crucial. Psallidas et al. [43], for example, present many tricks to implement provenance capturing efficiently. The authors implement core database operators with fine-grained lineage support baked-in. They list many optimization techniques that can be used when considering lineage support from the start.

6.2 Workflow provenance

There exist a large number of approaches for tracking provenance more broadly [31] and specifically in general data processing workflows [3,5,22,24,27,35,40,61]. However, none of these approaches can leverage the semantics of ML-specific operators such as the components of estimator/-transformer pipelines. NoWorkflow [40] is such an approach. It extracts provenance from function calls in Python scripts in three different levels: definition, deployment, and execution. It also uses the AST and extracts a dependency graph of the variables and directly handles unmodified programs. However, it considers functions as black boxes and does not capture fine-grained provenance inside called functions. Their system has many technical similarities with ours. However, their focus is on general Python scripts containing arbitrary functions. Because of that, they do not know of, e.g., the semantics of declarative pipeline operators and cannot track finer-grained lineage. For more information, we refer to Sect. 5.3.2. YesWorkflow [27] is a system that aims to bring the advantages of workflow analysis and modeling features to scripts written in languages like Python and R that define workflows. However, they heavily rely on users annotating their code. StarFlow is similar to YesWorkflow, but offers features like automatic parallelization [5]. It combines dynamic runtime analysis, static code analysis, and user annotations. It enables workflow abstraction, and it was implemented in the cloud. Lipstick [3] is a system that marries database-style and workflow-style provenance. While typical workflow provenance systems treat different modules as black box, they expose the functionality of modules using Pig Latin. This way, they can generate a detailed provenance graph with fine-grained provenance information. They use a provenance formalization that is based on the provenance semiring framework. Further, Inspector Gadget [35] is a framework for custom monitoring and debugging of distributed dataflows. They implemented it in Pig and called the implementation Penny. They exploit forward processing only, do not require dataflow engine modifications, and do not rely on injecting paint columns that may be observed by the operators. They allow users to insert monitoring agents that observe edges in the dataflow graph and propagate annotations through the execution. Their system is technically similar to our system in some aspects but does not consider ML-specific operators or applications. Titian [22] is another system using provenance to support users with debugging. It enables fine-grained data provenance capturing in Apache Spark. When implementing Spark support for our system in future work, the implementation described in their paper will likely be a great reference. Logothetis et al. [24] present Newt, a scalable architecture for capturing and using record-level data lineage to discover and resolve errors in analytics. As case studies, Newt is used to instrument two DISC systems, Hadoop and Hyracks. Zhang et al. [61] propose a system to capture lineage for distributed machine learning pipelines. Their focus is on how to efficiently encode the lineage information, especially in scenarios with image features. It records input and output datasets and cell-level mapping between the two. They do this by defining different mapping types for operators, e.g., a geometric mapping that can map regions of pixels to other regions of pixels. They built their system to support KeystoneML, which runs over Spark and HDFS. They expose this mapping interface to users, who need to decide which information they want to capture with it. Users can then ask provenance queries after executing the pipeline with lineage capturing. Not knowing the types of queries before pipeline execution requires a lot of metadata capturing, so they use these mapping types to reduce this overhead.

6.3 Experiment tracking and model management

Capturing high-level provenance, hyperparameters, and evaluation results is in the focus of model management systems such as ModelDB [53], mlflow [60], and ExperimentTracker [46], where the latter proposed the analysis of declarative abstractions like estimator/transformer pipelines. In contrast to our work, these systems only capture basic metadata and mainly require users to instrument their code with system-specific logging statements manually. ModelDB automatically tracks ML models in their native environment [53]. It tracks metadata about models and allows visual exploration of this metadata. To capture this metadata, it requires users to modify their script and add logging statements. ModelHub [29] focuses on deep neural networks and captures used parameters and hyperparameters like neural network weights across different versions of a model. It also logs information like loss values during the training of the model and performance metrics. Then, it allows users to query this captured information. In 2017, ExperimentTracker was proposed, a system for tracking metadata and provenance of ML experiments [46]. It tracks data provenance for SparkML and scikit-learn pipelines. For this, it also relies on abstractions like transformers and estimators. However, it relies on the user to expose certain data structures and integrate their code with their system's API. To our knowledge, this system was the first to use logical abstractions of SparkML and scikit-learn pipelines. ProvDB [30] stores metadata and some provenance information as well. It focuses on collaborative model development and offers a command-line interface for users to commit their changes. It uses a graph-model internally to store this provenance information. Node types in this graph are agents (e.g., team members or system components), activities (train, git commit, cron), and entities (project artifacts like files, datasets, and scripts). It then allows users to query this information. As a lot of information is being produced, they carefully consider how to store and efficiently query it. Overall, the tool requires users to organize their whole workflow around this system and use their command-line interface tools. Another system from 2018 is MLFlow that also aims to address challenges like experimentation and reproducibility [60]. They offer an API to support experiment tracking, reproducible runs, and model packaging and deployment. They again rely on users to provide additional metadata and integrate their pipelines with MLFlow. They then help in tasks like production deployment and reproducing, e.g., parameter settings of previous experiment runs. As MLFlow is currently one of the most successful tools in this area, we decided to try it out in practice and discovered that they recently added a still experimental option to log certain predefined metadata for libraries like scikit-learn automatically. For this, MLFlow requires users to add an auto-logging statement to their code. For more information, we refer to Sect. 5.3.1.

While systems like MLFlow rely on users to explicitly mark operations in their ML pipeline that should be saved in their metadata store, Ormenisan et al. [36] try to move from explicit provenance capturing to implicit provenance capturing. To achieve this, the authors rely on change capture APIs that capture events such as the usage or creation of files. In addition to this, they rely on file naming conventions and tagging of files. This way, they can capture the relation between different ML artifacts. However, only capturing events like the creation of files is not fine-grained enough for many use-cases. While these experiment-tracking tools mostly focus on particular experiments by particular teams, there also is the need to communicate information like how a particular dataset or model was created across different teams. For datasets, Gebru et al. [16,32] propose manually curated information in the form of *datasheets* and *model cards* to accompany them. The FAIR data principles [56] also propose guidelines to improve the findability, accessibility, interoperability, and reuse of digital assets but emphasize machine-actionability. Stoyanovich et al. [51] go one step further and propose nutritional labels for data and models, analogous to nutritional labels for the food industry. The goal is to provide simple, standard labels to evaluate the "fitness for use" of a model or dataset. The authors discuss these labels' desired properties and describe Ranking Facts [59], a system that can automatically derive labels for rankings.

6.4 Debugging for ML pipelines and data

Dagger [26] is a data-centric debugger that allows users to set data-breakpoints and store and query intermediate results from Python-based data pipelines. It requires users to mark code blocks in their Python pipelines, becoming nodes in their Dagger pipeline. It logs the data and provides its own query language for users to post queries through a command-line interface. Data breakpoints allow users to write assertions for the data between the different user-defined blocks. We see our system, `mlinspect`, as a complementary solution to Dagger: `mlinspect` can point users to hard-to-identify issues in their pipeline; Dagger will then enable them to drill-down and explore the data and identify the root causes of the problems. Vamsa [34] is a provenance-based analysis approach for data science scripts in Python that is technically close to ours. Like, `mlinspect`, Vamsa does not require changes to user code and uses a knowledge base about different ML libraries. However, Vamsa has a much narrower focus, as it only aims to identify which columns of the input contributed to a particular feature used for an ML model. Their system also aims to work for general Python code using various libraries and leverages the AST and intermediate representations. Vizier [9] is a notebook environment integrating Python, SQL, and data debugging and exploration techniques. It requires a tight integration into the user's development process and offers support for fine-grained provenance capture for SQL queries only.

Deequ [48] is another approach for the validation of ML data. It enables users to write "unit tests for data" using a declarative API. Breck et al. propose another data validation system [10]. It was integrated into TensorFlow Extended (TFX) to detect anomalies specifically in data fed into machine learning pipelines. However, these tools mostly focus on detecting data issues, not debugging them. There is also MISTIQUE, a system from 2018 to store and query model intermediates from ML pipelines and hidden representations from deep learning [54]. BugDoc [25] is a framework that implements and combines methods to select pipeline instances to try out to find root causes of problems in pipelines. However, it can only identify the root causes of problems related to the input parameter space, which has to be manually specified by the user.

There has been a large-scale study of the usage of different data science tools [44]. Many of their findings support our research direction, despite our restriction to specific libraries. Besides confirming assumptions that Python is by far the most used language for these types of problems, they also find that most data science code is linear and a mere orchestration of different libraries. This makes projects like ours feasible. They also confirm that most work relies on a handful of core libraries, such as scikit-learn, numpy, matplotlib and pandas. Another important finding is that in the last few years, declarative specification of data science logic is becoming increasingly common. Polyzotis et al. [41] wrote a survey of data lifecycle challenges in production ML. They identify data-related open challenges in areas such as data understanding, data validation and cleaning, and data preparation. An interesting tool inspired by various best practices in ML data preparation is DataLinter [21]. They propose data linting for deep neural networks, based on predefined linting rules applied to the training data and the outputs of the model, but they cannot inspect pipeline code. DeepXplore [38] is a system for automated white-box testing of ML models. It can find corner cases in application areas like self-driving cars.

They measure neuron coverage, which they describe as measuring the part of the neurons that are exercised in test inputs. Then they try to generate test cases that produce errors. Their test inputs can also be used to train the model to improve its performance.

6.5 Fairness-specific analysis of ML pipelines and predictions

In recent years, a set of specialized analysis tools with respect to the fairness and accountability of ML-based decision-making systems has been developed. Examples include SliceFinder [42], Coverage [7], and fairDags [58]. `mlinspect` provide a general runtime for implementing and integrating these and similar approaches into a common inspection platform. In our work on FairDags [58], we initially proposed extracting a DAG from ML pipelines to check for data distribution issues that result in bad model performance for sensitive demographic groups. Asudeh et al. [7] propose techniques to assess the coverage of a dataset over multiple categorical variables. The authors present an efficient strategy for traversing the combinatorial explosion of value combinations to identify problematic regions of the attribute space. Even with their optimized approach, the number of attributes to consider has a high impact on the performance. Slice finder [42] is a system to assist with finding slices of data an ML model performs particularly bad on. AI Fairness 360 (AIF360) [8] is a Python toolkit to calculate many fairness metrics and different algorithms to mitigate bias in datasets and models. Fairlearn [1] is another Python package to assess the fairness of AI systems and mitigate observed unfairness issues. Fairlearn also contains different mitigation algorithms and a Jupyter widget for model assessment.

Fairness issues in software are not just limited to issues specific to ML pipelines. Brun et al. [11] discuss how software engineering as a discipline needs to consider fairness from the start when building software systems (e.g., with fairness annotations like in Fairness-Aware Programming [2]), and Galhotra et al. [15] propose to test software for discrimination issues based on a schema of valid system inputs.

7 Conclusion and future work

We discussed several hard-to-identify data issues in ML pipelines that have the potential to impact correctness, reliability, and fairness. We proposed `mlinspect`, a library that enables lightweight lineage-based inspection of ML preprocessing pipelines. The `mlinspect` library extracts a directed acyclic graph representation of the dataflow from a pipeline and automatically instruments the code with predefined *inspections* based on a lightweight annotation propagation approach. We describe several custom inspections that data scientists can use to detect data distribution bugs in their pipelines. In contrast to existing work, `mlinspect` operates on declarative abstractions of popular data science libraries like estimator/transformer pipelines and does not require manual code instrumentation. We discuss the design and implementation of `mlinspect` and give a comprehensive end-to-end example that illustrates its functionality.

A future challenge is to assist data scientists in the analysis of the outputs of `mlinspect`. Complex pipelines can produce a variety of inspection results, and it may be helpful to explore anomaly detection techniques to point data scientists to potentially problematic cases or to suggest thresholds for checks. We also plan to incorporate additional backends for popular ML libraries into `mlinspect`, including Tensorflow Transform and Apache SparkML [28]. For these libraries, it will be challenging to find efficient ways to include inspections during the distributed execution of Beam and Spark operators. As discussed in Sect. 4.3.2, a future challenge is to support complex ML pipelines on high-dimensional tensors; it is still unclear whether such tensor operations are sufficiently captured by the dataframe algebra (Sect. 3.4) onto which `mlinspect` is built. As also outlined in Sect. 4.3.2, we intend to explore query optimization techniques for more efficient execution of inspections based on dataframe operations as a means to reduce the runtime overhead induced by Python.

Acknowledgements This work was supported in part by Ahold Delhaize, and by NSF Awards No. 1934464, 1916505 and 1922658. All contents represent the opinion of the authors, which is not necessarily shared or endorsed by their respective employers and/or sponsors.

References

1. Agarwal, A., Beygelzimer, A., Dudik, M., Langford, J., Wallach, H.: A reductions approach to fair classification. In: FAT* (2017)
2. Albarghouthi, A., Vinitsky, S: Fairness-aware programming. In: FAT* (2019)
3. Amsterdamer, Y., Davidson, S.B., Deutch, D., Milo, T, Stoyanovich, J. Tannen, V. Enabling database-style workflow provenance. In: PVLDB, Putting Lipstick on Pig (2011)
4. Amsterdamer, Y., Deutch, D., Tannen, V: Provenance for aggregate queries. In: PODS (2011)
5. Angelino, E., Yamins, D., Seltzer, M.: Starflow: a script-centric data analysis environment. In: Provenance and Annotation of Data and Processes (2010)
6. Angwin, J., Larson, J., Mattu, S., Kirchner, L.: Machine bias. (propublica) (2016)
7. Asudeh, A., Jin, Z., Jagadish, H.V.: Assessing and remedying coverage for a given dataset. In: ICDE (2019)
8. Bellamy, R.K.E., Dey, K., Hind, M., Hoffman, S.C., Houde, S., et al.: AI fairness 360: an extensible toolkit for detecting, understanding, and mitigating unwanted algorithmic bias (2018)
9. Brachmann, M., Bautista, C., Castelo, S., Feng, S., Freire, J., et al.: Data debugging and exploration with vizier. In: SIGMOD, Su Feng (2019)

10. Breck, E., Zinkevich, M., Whang, S., Roy, S.: Data validation for machine learning. In: SysML, Neoklis Polyzotis (2019)
11. Brun, Y., Meliou, A.: Software fairness. In: ESEC/FSE (2018)
12. Chen, I., Johansson, F.D., Sontag, D.: Why is my classifier discriminatory? In: NeurIPS (2018)
13. Cheney, J., Chiticariu, L., Tan, W.C: Provenance in Databases: Why, How, and Where. Found. Trends Databases, vol. 1, no. 4 (2009)
14. Chouldechova, A., Roth, A.: A snapshot of the frontiers of fairness in machine learning. In: CACM, vol 63, no. 5 (2020)
15. Galhotra, S., Brun, Y., Meliou, A: Testing software for discrimination. In: ESEC/FSE, Fairness Testing (2017)
16. Gebru, T., Morgenstern, J., Vecchione, B. et al.: Datasheets for datasets (2018)
17. Grafberger, S., Stoyanovich, J., Schelter, S.: Lightweight inspection of data preprocessing in native machine learning pipelines. In: Conference on Innovative Data Systems Research (CIDR) (2021)
18. Green, T.J., Karvounarakis, G., Tannen, V.: Provenance semirings. In: PODS (2007)
19. Herschel, M., Diestelkämper, R., Lahmar, H.B.: A survey on provenance: What for? What form? What from? VLDBJ **26**(6) (2017)
20. Hutton, G.: A tutorial on the universality and expressiveness of fold. J. Funct. Program, 8 (1999)
21. Hynes, N., Sculley, D., Terry, M. The data linter: lightweight, automated sanity checking for ml data sets. In: MLSystems workshop at NeurIPS (2017)
22. Interlandi, M., Shah, K., et al. Titian: data provenance support in spark. In: VLDB (2015)
23. Jindal, A., Emani, K.V., Daum, M., Poppe, O., et al: Magpie: python at speed and scale using cloud backends. In: CIDR (2021)
24. Logothetis, D., De, S., Yocum, K: Scalable lineage capture for debugging disc analytics. In: SoCC (2013)
25. Lourenço, R., Freire, J., Shasha, D.: A system for debugging computational pipelines. In: SIGMOD, Bugdoc (2020)
26. Madden, S., Ouzzani, M., Tang, N., Stonebraker, M.: Dagger: a data (not code) debugger. In: CIDR (2020)
27. McPhillips, T.M., Song, T., Kolisnik, T., et al.: Yesworkflow: a user-oriented, language-independent tool for recovering workflow information from scripts. In: CoRR, abs/1502.02403 (2015)
28. Meng, X., Bradley, J., Yavuz, B., Sparks, E., Venkataraman, S., Liu, D., Freeman, J., Tsai, D.B., Amde, M., Owen, S., et al.: Mllib: machine learning in apache spark. JMLR **17**(1), 1235–1241 (2016)
29. Miao, H., Li, A., Davis, L.S., Deshpande, A.: Towards unified data and lifecycle management for deep learning. In: ICDE, pp. 571–582 (2017)
30. Miao, H., Deshpande, A.: Provdb: provenance-enabled lifecycle management of collaborative data analysis workflows. IEEE Data Eng. Bull **41** (2018)
31. Moreau, L.: The foundations for provenance on the web. Found. Trends Web Sci. **2**(2–3), 29, 99–241 (2010)
32. Mitchell, M., et al.: Model cards for model reporting. In: FAT* (2019)
33. Murta, L., Braganholo, V., Chirigati, F., Koop, D., Freire, J.: noworkflow: capturing and analyzing provenance of scripts. In: VLDB (2017)
34. Namaki, M.H., Floratou, A., Psallidas, F., Krishnan, S., Agrawal, A., Wu, Y.: Tracking provenance in data science scripts. In: KDD, Vamsa (2020)
35. Olston, C., Reed, B.: Inspector gadget: A framework for custom monitoring and debugging of distributed dataflows. In: SIGMOD (2011)
36. Ormenisan, A.A., Meister, M., Buso, F., Andersson, R., Haridi, S., Dowling, J.: Time travel and provenance for machine learning pipelines. In: OpML at USENIX (2020)
37. Pedregosa, F., Varoquaux, G., Gramfort, A. et al.: Scikit-learn: Machine learning in python. In: JMLR, vol. 12 (2011)
38. Pei, K., Cao, Y., Yang, J., Jana, S.: Deepxplore. In: SOSP (2017)
39. Petersohn, D., Macke, S., Xin, D., Ma, W., Lee, D., Mo, X., Gonzalez, J.E., Hellerstein, J.M., Joseph, A.D., Parameswaran, A: Towards scalable dataframe systems. In: VLDB (2020)
40. Pimentel, J.F., Murta, L., Braganholo, V. and Freire, J.: noworkflow: a tool for collecting, analyzing, and managing provenance from python scripts. In: PVLDB (2017)
41. Polyzotis, N., Roy, S., Whang, S.E., Zinkevich, M.: Data lifecycle challenges in production machine learning: a survey. In: SIGMOD Record (2018)
42. Polyzotis, N., Whang, S., Kraska, T.K. and Chung, Y.: Automated data slicing for model validation. In: ICDE, Slice finder (2019)
43. Psallidas, F., Wu, E.: Smoke: Fine-grained lineage at interactive speed. In: VLDB (2018)
44. Psallidas, F., Zhu, Y., Karlas, B., et al: Data science through the looking glass and what we found there (2019)
45. Raasveldt, M., Mühleisen, H.: Data management for data science-towards embedded analytics. In: CIDR (2020)
46. Schelter, S., Boese, J.H., Kirschnick, J., Klein, T., Seufert, S.: Automatically tracking metadata and provenance of machine learning experiments. In: ML Systems Workshop at NeurIPS (2017)
47. Schelter, S., He, Y., Khilnani, J. and Stoyanovich, J.: Fairprep: Promoting data to a first-class citizen in studies on fairness-enhancing interventions. In: EDBT (2019)
48. Schelter, S., Lange, D., Schmidt, P., Celikel, M., Biessmann, F., Grafberger, A: Automating large-scale data quality verification. In: PVLDB, Meltem Celikel (2018)
49. Sebastian, S.: Stoyanovich, J: Taming technical bias in machine learning pipelines. IEEE Data Eng. Bull. **43**, 39–50 (2020)
50. Sparks, E.R., Venkataraman, S., Kaftan, T., Franklin, M.J., Recht, B.: Keystoneml: Optimizing pipelines for large-scale advanced analytics. In: ICDE (2017)
51. Stoyanovich, J., Howe, B.: Nutritional labels for data and models. IEEE Data Eng. Bull. **42**(3), 13–23 (2019)
52. Stoyanovich, J., Howe, B., Jagadish, H.V.: Responsible data management. In: VLDB (2020)
53. Vartak, M., Madden, S.: Modeldb: opportunities and challenges in managing machine learning models. IEEE Data Eng. Bull. **41**(4), 16–25 (2018)
54. Vartak, M., Joana, Trindade, J.M., Madden, S., Zaharia, M: A system to store and query model intermediates for model diagnosis. In: SIGMOD (2018)
55. Wikipedia. Monkey patch. https://en.wikipedia.org/wiki/Monkey_patch (2021). Accessed 9 Sept 2021
56. Wilkinson, M.D., Dumontier, M., Aalbersberg, I.J.J., Appleton, G., Axton, M., Baak, A., Blomberg, N., et al.: The fair guiding principles for scientific data management and stewardship. Sci. Data **3**(1), 1–9 (2016)
57. Yan, Z., Tannen, V., Ives, Z.G.: Fine-grained provenance for linear algebra operators. In: TaPP (2016)
58. Yang, K., Huang, B., Stoyanovich, J., Schelter, S.: Fairness-aware instrumentation of preprocessing pipelines for machine learning. In: HILDA Workshop at SIGMOD (2020)
59. Yang, K., Stoyanovich, J., Asudeh, A., Howe, B., Jagadish, H.V., Miklau, G.: A nutritional label for rankings. In: SIGMOD (2018)
60. Zaharia, M., Chen, A., Davidson, A., Ghodsi, A., Hong, S.A., Konwinski, A., Murching, S., et al.: Accelerating the machine learning lifecycle with MLflow. IEEE Data Eng. Bull. **41**(4), 39–45 (2018)
61. Zhang, Z., Sparks, E.R., Franklin, M.J.: Diagnosing machine learning pipelines with fine-grained lineage. In: HPDC (2017)