Responsible Data Science

The data science lifecycle

February 24 2025 **Prof. Emily Black**

Center for Data Science & Computer Science and Engineering New York University





Center for Data Science



https://docs.google.com/forms/d/e/1FAIpQLSe4f3DYVp uyz78SIqBY271EYx6RII7G0-79w_IaVCH_oCHhIQ/viewform

Julia Stoyanovich



Outline

- Problem formulation: IRS
- Data collection: gender shades
- Data cleaning: shades of null
- Data bias: word embeddings, predict and serve
- Statistical modeling: bias amplification
- Testing and validation: d-hacking/GenAI stuff
- Model integration & deployment: something on the huma—AI paper (I'll have to make that later)



This week's reading

contributed articles

DOI:10.1145/3488717

Example: Automated hiring sys

crete, consider the use of predictive analytics in hiring. Automated hiring

systems are seeing ever broader use and are as varied as the hiring practic-

es themselves, ranging from resume screeners that claim to identify prom-

ising applicants^a to video and voice

ments that promise to surface person-

ality traits indicative of future success.^c Bogen and Rieke⁵ describe the hiring

process from the employer's point of view as a series of decisions that forms

a funnel, with stages corresponding to

https://www.crystalknows.com https://www.hirevue.com

https://www.pymetrics.ai

analysis tools that facilitate the interview process^b and game-based assess-

tems. To make our discussion

Perspectives on the role and responsibility of the data-management research community in designing, developing, using, and overseeing automated decision systems.

BY JULIA STOYANOVICH, SERGE ABITEBOUL, BILL HOWE, H.V. JAGADISH, AND SEBASTIAN SCHELTER

Responsible Data Management

INCORPORATING ETHICS AND legal compliance into data-driven algorithmic systems has been attracting significant attention from the computing research community, most notably under the umbrella of fair8 and interpretable¹⁶ machine learning. While important, much of this work has been limited in scope to the "last mile" of data analysis and has disregarded both the system's design, development, and use life cycle (What are we automating and why? Is the system working as intended? Are there any unforeseen consequences post-deployment?) and the data life cycle (Where did the data come from? How long is it valid and appropriate?). In this article, we argue two points. First, the decisions we make during data collection and preparation profoundly impact the robustness, fairness, and interpretability of the systems we build. Second, our responsibility for the operation of these systems does not stop when they are deployed.

64 COMMUNICATIONS OF THE ACM | JUNE 2022 | VOL. 65 | NO. 6

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 Willam Isaac consider the evidence – and the social consequences



Toward Operationalizing Pipeline-aware ML Fairness: A Research Agenda for Developing Practical Guidelines and Tools

EMILY BLACK, Barnard College, Columbia University, USA RAKSHIT NAIDU, Georgia Institute of Technology, USA RAYID GHANI, Carnegie Mellon University, USA KIT T. RODOLFA, Stanford University, USA DANIEL E. HO, Stanford University, USA HODA HEIDARI, Carnegie Mellon University, USA

While algorithmic fairness is a thriving area of research, in practice, mitigating issues of bias often gets reduced to enforcing an arbitrarily chosen fairness metric, either by enforcing fairness constraints during the optimization step, post-processing model outputs, or by manipulating the training data. Recent work has called on the ML community to take a more holistic approach to tackle fairness issues by systematically investigating the many design choices made through the ML pipeline, and identifying interventions that target the issue's root cause, as opposed to its symptoms. While we share the conviction that this pipeline-based approach is the most appropriate for combating algorithmic unfairness on the ground, we believe there are currently very few methods of *operationalizing* this approach in practice. Drawing on our experience as educators and practitioners, we first demonstrate that without clear guidelines and toolkits, even individuals with specialized ML knowledge find it challenging to hypothesize how various design choices influence model behavior. We then consult the fair-ML literature to understand the progress to date toward operationalizing the pipeline-ware approach: we systematically collect and organize the prior work that attempts to detect, measure, and mitigate various sources of unfairness through the ML pipeline. We utilize this extensive categorization of previous contributions to sketch a research agenda for the community. We hope this work serves as the stepping stone toward a more comprehensive set of resources for ML researchers, practitioners, and students interested in exploring, designing, and testing pipeline-oriented approaches to algorithmic fairness.

ACM Reference Format:

Emily Black, Rakshit Naidu, Rayid Ghani, Kit T. Rodolfa, Daniel E. Ho, and Hoda Heidari. 2023. Toward Operationalizing Pipeline-aware ML Fairness: A Research Agenda for Developing Practical Guidelines and Tools. In *ACM Conference on Equity and Access in Algorithms, Mechanisms, and Optimization 2023.* ACM, New York, NY, USA, 34 pages. https://doi.org/10.1145/3617694.3623259

......



Recall: Bias in computer systems

Pre-existing is independent of an algorithm and has origins in society

Technical is introduced or exacerbated by the technical properties of an ADS

Emergent arises due to context of use

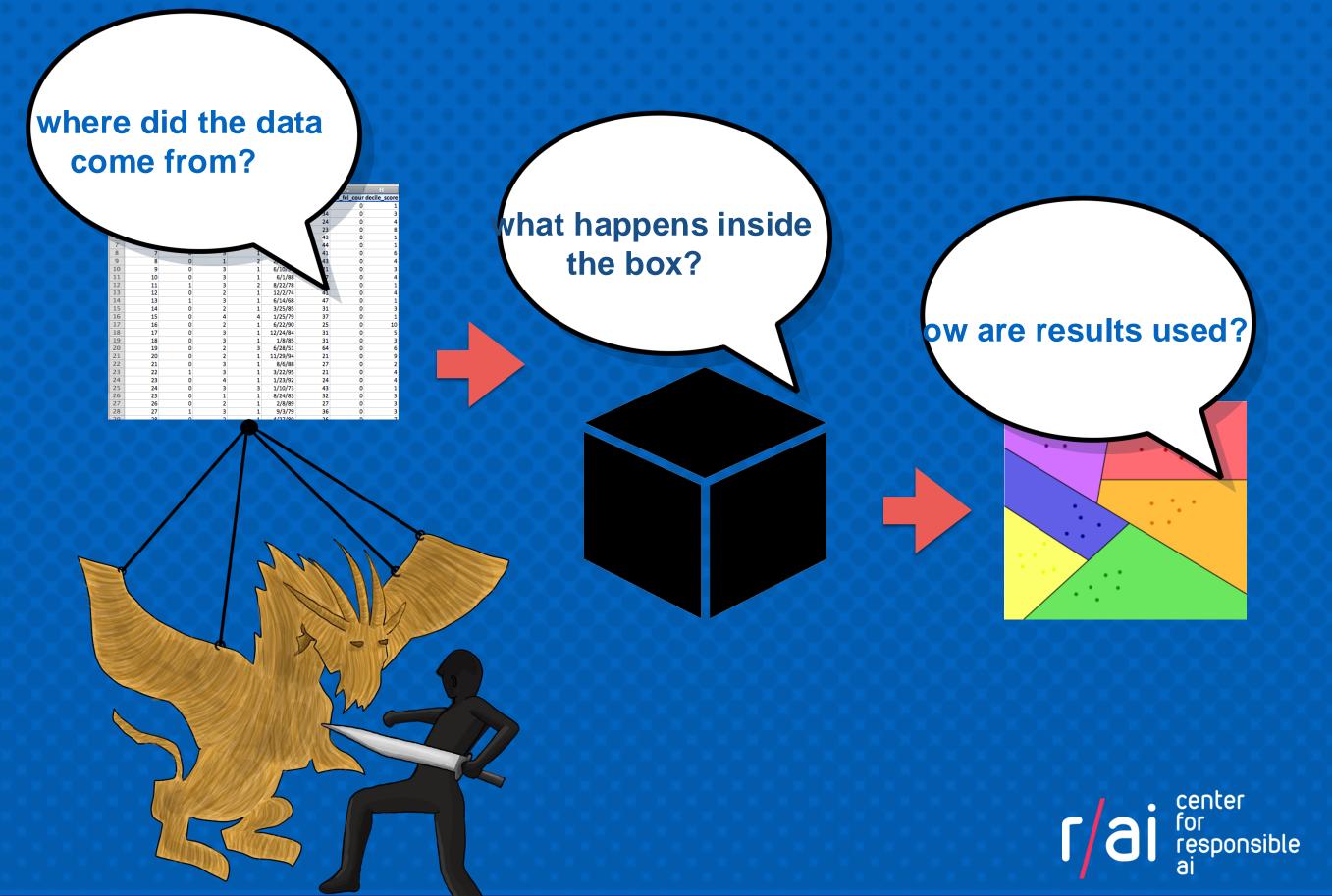
to fight bias, state beliefs and assumptions explicitly

center

sponsible

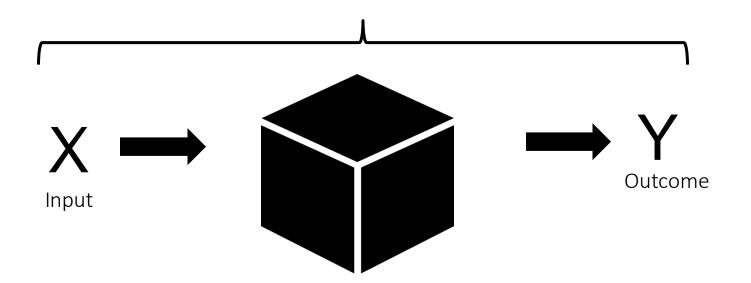


The "last-mile" view of responsible Al



Common approaches to ML fairness

Constrain to satisfy fairness definition



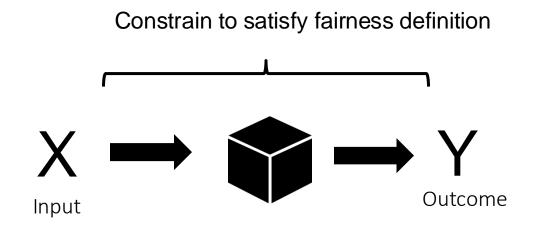
Fairness Definitions

 \hat{Y} : model prediction Y: ground truth Z: protected class (e.g. race)

- Demographic Parity \longrightarrow $P(\hat{Y} = 1 | Z = z) = P(\hat{Y} = 1 | Z = z')$
- Equal False Positive Rates $P(\hat{Y} = 1 | Y = 0, Z = z) = P(\hat{Y} = 1 | Y = 0, Z = z')$
 - Equal Accuracy $P(\hat{Y} = Y | Z = z) = P(\hat{Y} = Y | Z = z')$

e.g. Dwork et al. 2012, Hardt et al. 2016, Chouldechova 2016, Berk et al 2017

A common approach to AI fairness



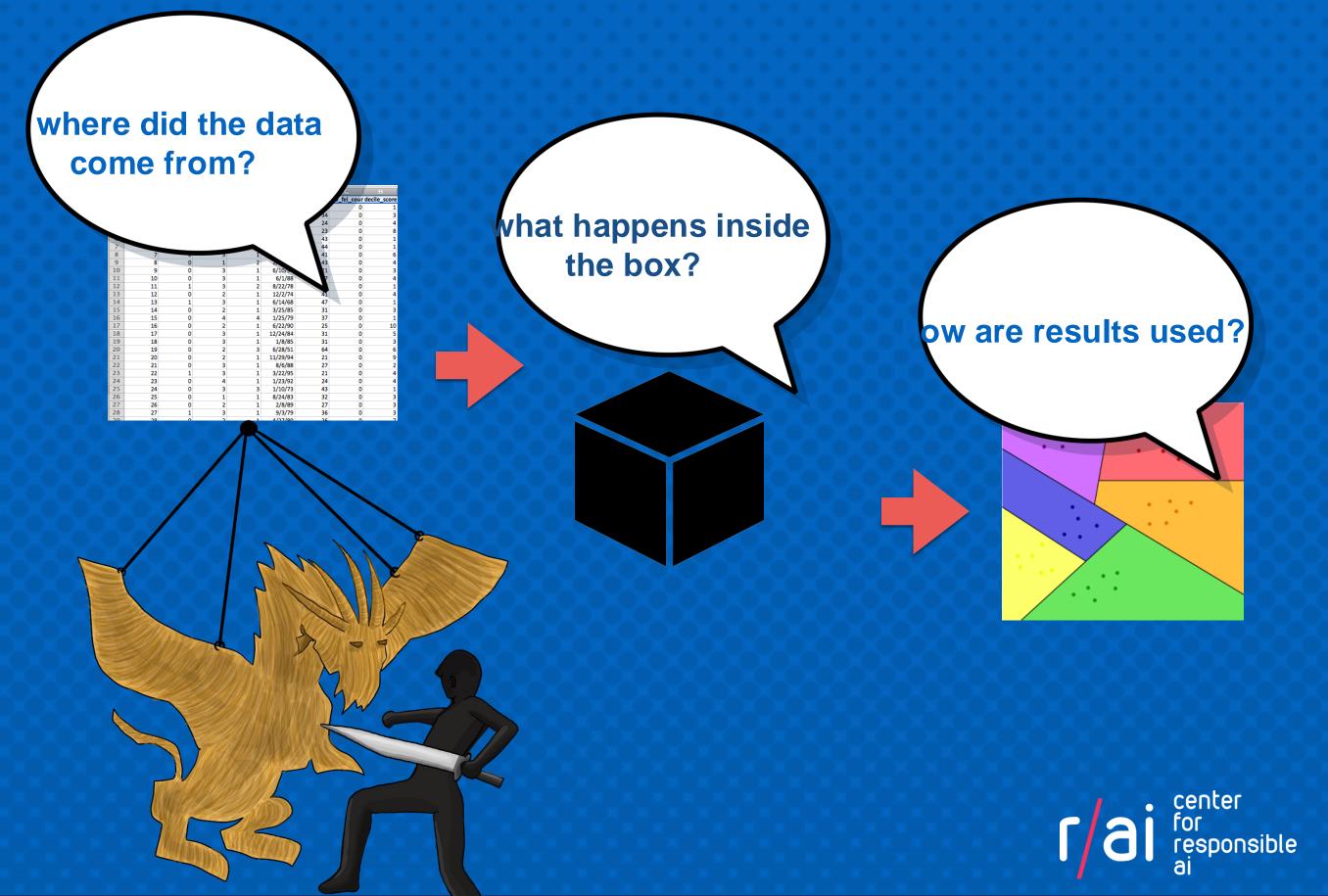
Pros:

- Generalizable across contexts
- Because of this, often easily deployable

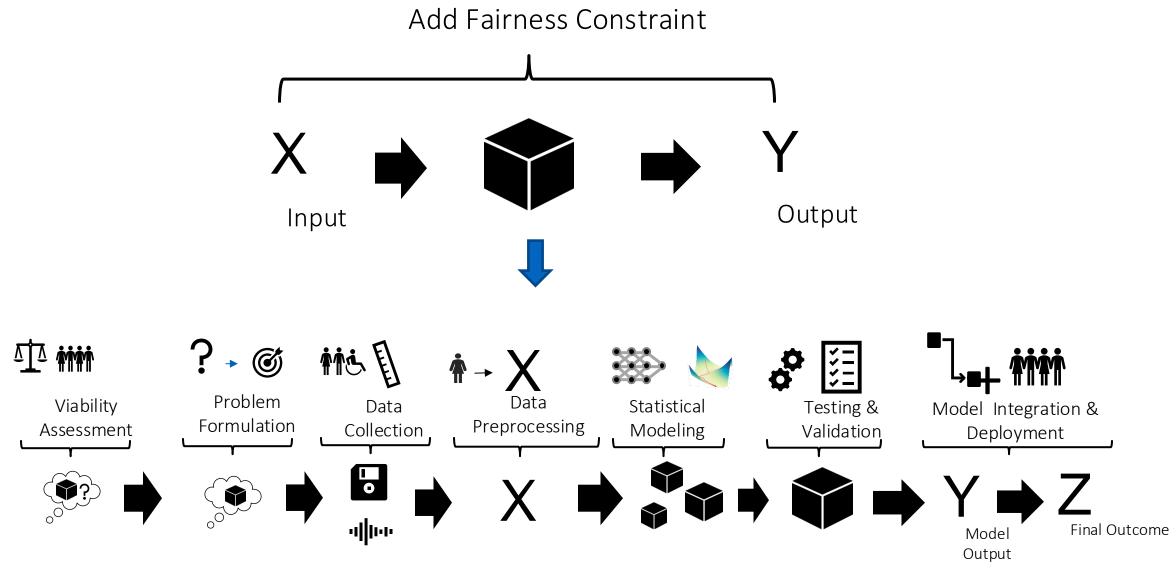
Cons:

- May not address certain unfair behaviors
- Often does not target *core* issue
- Often not legally viable in regulated contexts

The "last-mile" view of responsible Al



There's a lot more going on under the hood



Examples of Pipeline Steps

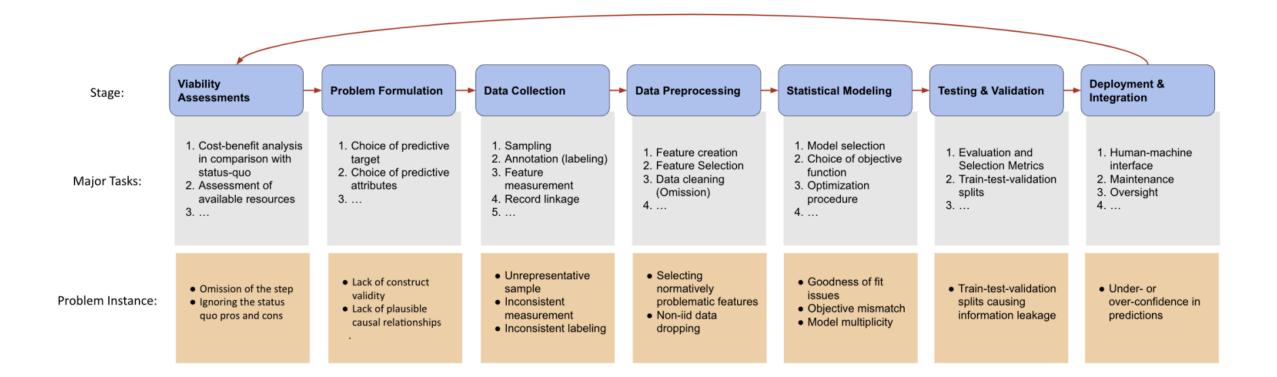
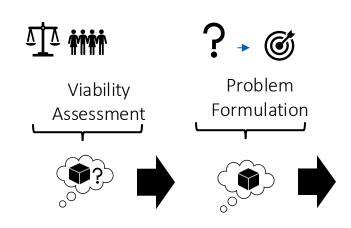


Fig. 1. A simplified view of the ML pipeline, its key stages, and instances of design choices made at each stage.

Viability Assessment, Problem Formulation

- Viability assessment: is making an AI decisionmaking system a good idea? Do we have the resources to do so?
- Problem formulation: How can we use the data we have available to predict what we want to predict-- like "creditworthiness" or "employability"?



Viability Assessment, Problem Formulation

The Fallacy of AI Functionality

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AARON HOROWITZ, American Civil Liberties Union, USA

ANDREW D. SELBST, University of California, Los Angeles, USA

SIDNEY FUSSELL BUSINESS JUN 24, 2020 7:00 AM

An Algorithm That 'Predicts' Criminality Based on a Face Sparks a Furor

Its creators said they could use facial analysis to determine if someone would become a criminal. Critics said the work recalled debunked "race science."

Deployed AI systems often do not work. They can be constructed haphazardly, deployed indiscriminately, and promoted deceptively. However, despite this reality, scholars, the press, and policymakers pay too little attention to functionality. This leads to technical and policy solutions focused on "ethical" or value-aligned deployments, often skipping over the prior question of whether a given system functions, or provides any benefits at all. To describe the harms of various types of functionality failures, we analyze a set of case studies to create a taxonomy of known AI functionality issues. We then point to policy and organizational responses that are often overlooked and become more readily available once functionality is drawn into focus. We argue that functionality is a meaningful AI policy challenge, operating as a necessary first step towards protecting affected communities from algorithmic harm.

CCS Concepts: • Computing methodologies \rightarrow Machine learning; • Applied computing \rightarrow Law, social and behavioral sciences.

A Validity Perspective on Evaluating the Justified Use of Data-driven Decision-making Algorithms

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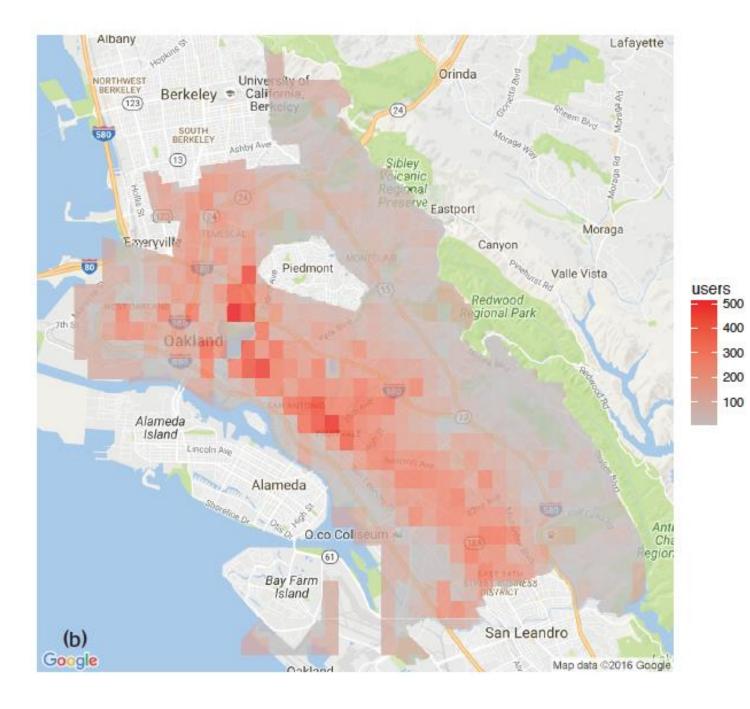
Anna Kawakami Carnegie Mellon University Pittsburgh, USA akawakam@andrew.cmu.edu

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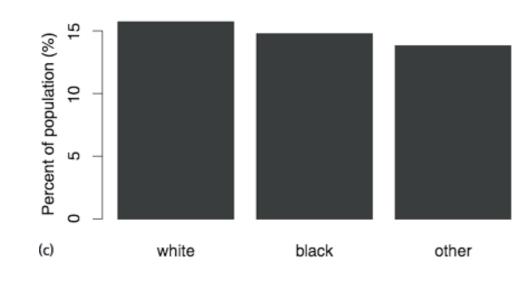
> Hoda Heidari Machine Learning Dept. Carnegie Mellon University Pittsburgh, USA hheidari@cs.cmu.edu

Ken Holstein Human-Computer Interaction Institute Carnegie Mellon University Pittsburgh, USA kjholste@cs.cmu.edu

Is my data biased? (histograms + geo)



Estimated number of drug users, based on 2011 National Survey on Drug Use and Health, in Oakland, CA



Estimated drug use by race

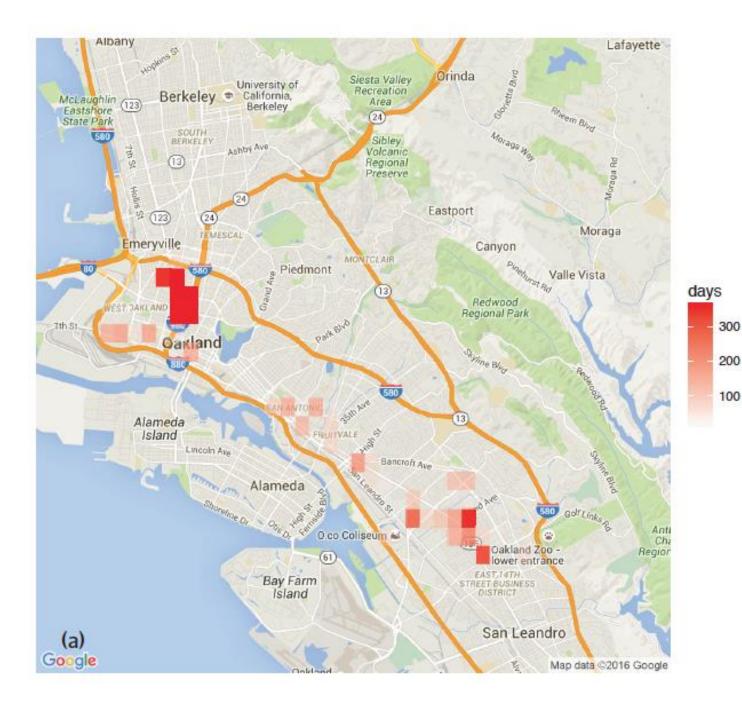
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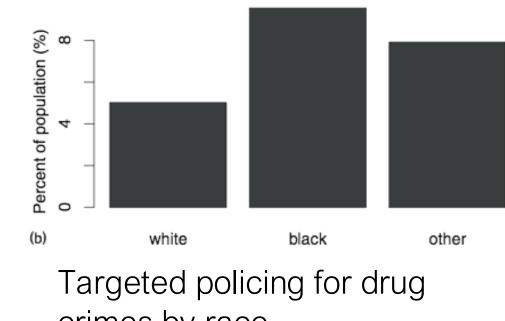
for

[Lum & Isaac (2016)]

Is my data biased? (histograms + geo)



Number of days with targeted policing for drug crimes in areas flagged by PredPol analysis of Oakland, CA, police data for 2011



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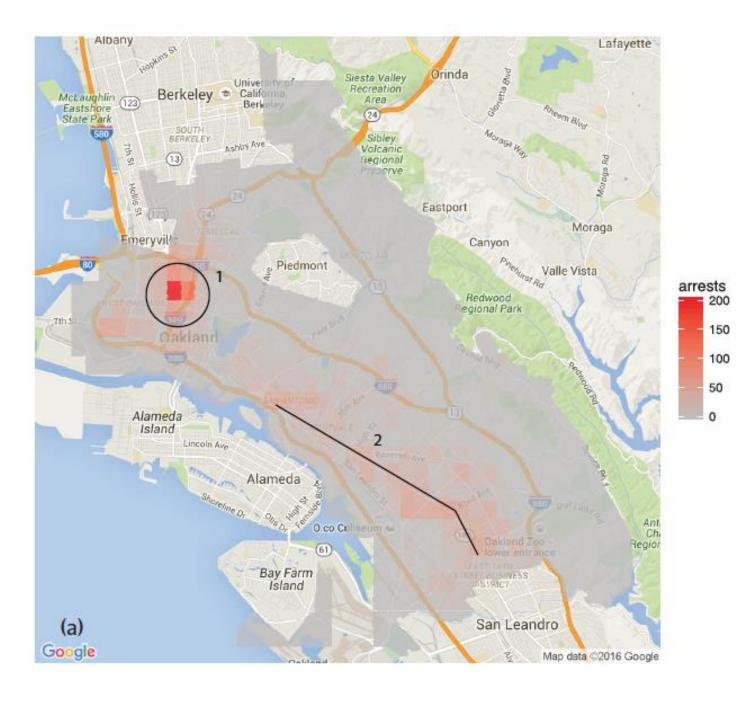
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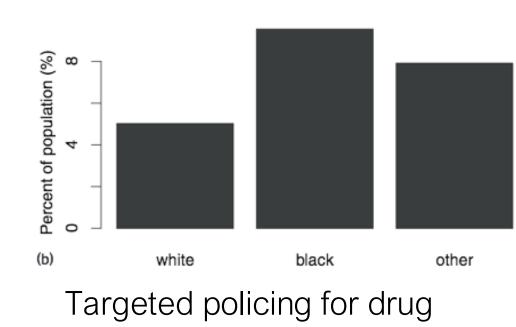
crimes by race

[Lum & Isaac (2016)]

Is my data biased? (histograms + geo)



Number of drug arrests made by the Oakland, CA, police department in 2010



center

responsible

for

crimes by race

[Lum & Isaac (2016)]

Data Collection

 Data collection: collecting or compiling data to train the model



- What population will we sample to build our model?
- How will we collect this data?

Unfairness in Data Collection

• Facial Recognition technologies are notoriously bad at recognizing darker faces



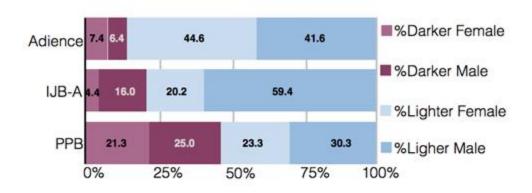


Figure 3: The percentage of darker female, lighter female, darker male, and lighter male subjects in PPB, IJB-A and Adience. Only 4.4% of subjects in Adience are darker-skinned and female in comparison to 21.3% in PPB.

Complications: Should we fix that?

 What are the implications of accurate facial recognition technology?



Wrongfully Accused by an Algorithm

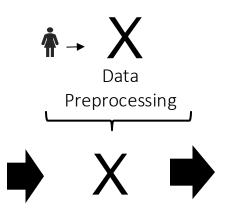
In what may be the first known case of its kind, a faulty facial recognition match led to a Michigan man's arrest for a crime he did not commit.

"I guess the computer got it wrong."

Mr. Williams asked if he was free to go. "Unfortunately not," one detective said.

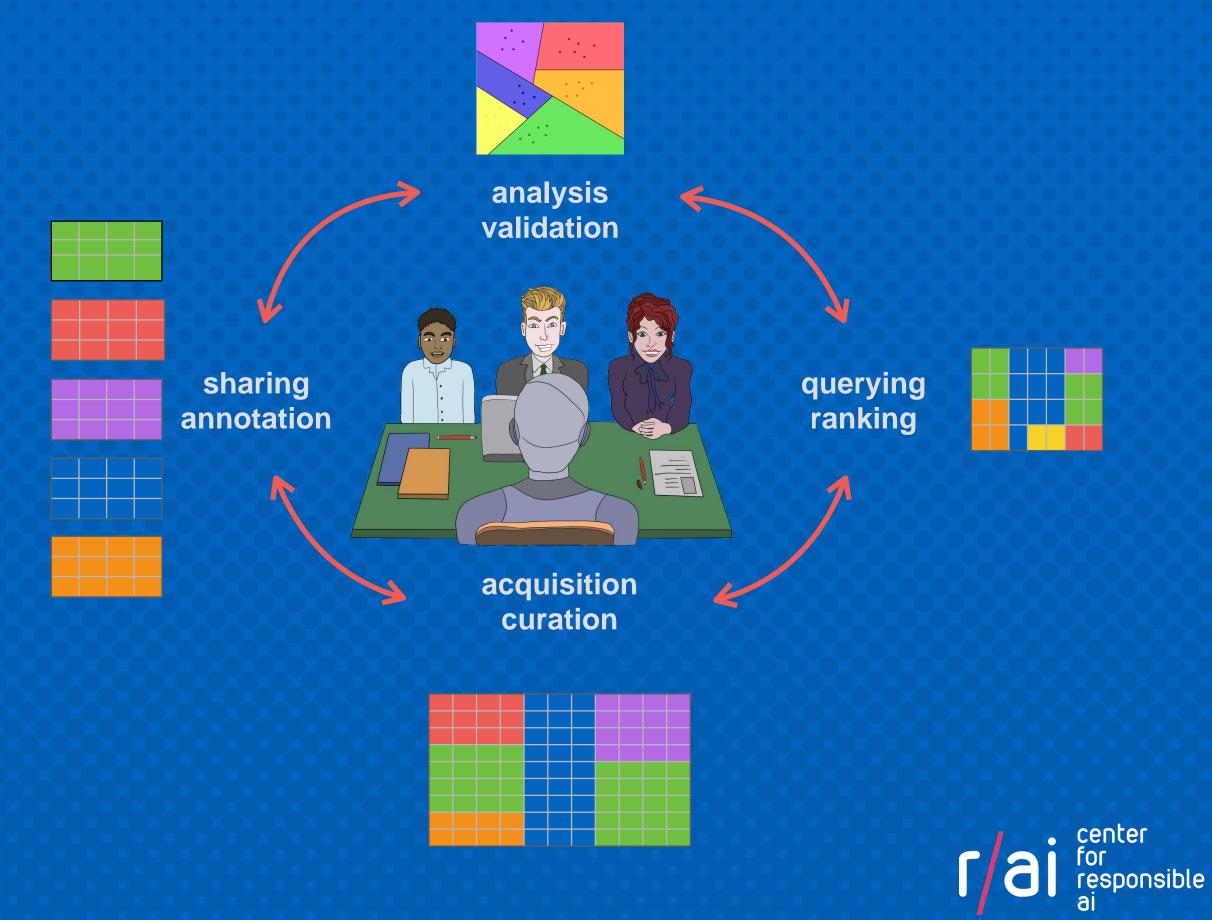
Data Pre-processing

Data preprocessing: steps taken to make data usable by the AI model



- How do we construct features from our data?
- What do we do with missing or incomplete data?

Zooming out to the lifecycle view



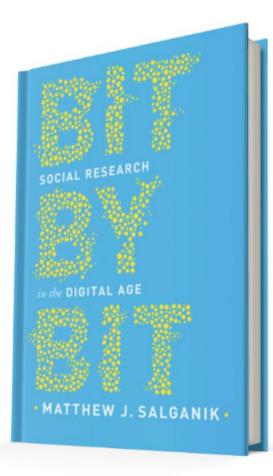




"Given the heterogeneity of the flood of data, it is **not enough merely to record it and throw it into a repository**. Consider, for example, data from a range of scientific experiments. If we just have a bunch of data sets in a repository, it is **unlikely anyone will ever be able to find, let alone reuse**, any of this data. With adequate **metadata**, there is some hope, but even so, challenges will remain due to differences in experimental details and in data record structure."

https://cra.org/ccc/wpcontent/uploads/sites/2/2015/05/bigdatawhitepaper.pdf

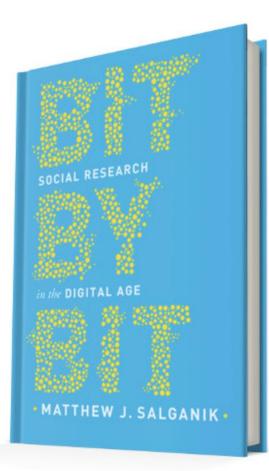




In the analog age, most of the data that were used for social research was created for the purpose of doing research. In the digital age, however, a huge amount of data is being created by companies and governments for purposes other than research, such as providing services, generating profit, and administering laws. Creative people, however, have realized that you can **repurpose** this corporate and government data for research.



2.2 Big data



2.2 Big data

... from the perspective of researchers, big data sources are "found," they don't just fall from the sky. Instead, data sources that are "found" by researchers are **designed by someone for some purpose**. Because "found" data are designed by someone, I always recommend that you **try to understand as much as possible about the people and processes that created your data**.



Need **metadata** to:

- enable data **re-use** (have to be able to find it!)
- determine **fitness for use** of a dataset in a task
- help establish trust in the data analysis process and its outcomes

Data is considered to be of high quality if it's "**fit for intended uses** in operations, decision making and planning"

[Thomas C. Redman, "Data Driven: Profiting from Your Most Important Business Asset." 2013]



Common metadata example

😣 Hugging Face	Q Searc 📦	Models 📄 Datase	ets 📲 Spaces 📖 D	ocs 🔳 Ente	rprise Pricing ~≡ Log In Sign Up
Datasets: G ge Tasks: × _A Translatio		♡like 29 Follow ext Formats: ↔ js	G Google 8.14k	ar 🌐 Abkhaz	z ④ Achinese + 208 Size: 100K - 1M
ArXiv: arxiv:2502.12	2301 arxiv:2303.15	265 Libraries: 🙁	Datasets 🕴 pandas	🥐 Croissant	+1 License: 1 cc-by-4.0
Dataset card	🖽 Data Studio	Files 🏉 Comm	unity 2		
Dataset Viewer	G <u>Au</u> t	to-converted to Parquet	API Embed 🖽 D	ata Studio	Downloads last month 525
Subset (362) gatitosen_aa · 3.99	k rows	Split (1) ✓ train · 3.99k r	ows	~	Use this dataset ~
Q Search this datase	et				:
<pre>src \$ string · lengths</pre>	trgs sequence · lengths	sl string • <i>classes</i>	<pre>tl string · classes</pre>	is_sourc bool	
1 108	1 3	1 value	1 value	1 class	Size of downloaded dataset files: 229 MB
good morning	["maacissee", "Meqe Maaca"]	en	aa		Size of the auto-converted Parquet files: 68.7 MB
what	["maca"]	en	aa		Number of rows: 810,660
why	["macah", "maca sabbatah"]	en	aa		
good	["meqeh", "nagay"	en	aa		

SMOL

SMOL (Set for Maximal Overall Leverage) is a collection professional translations into 221 Low-Resource Languages, for the purpose of training translation models, and otherwise increasing the representations of said languages in NLP and technology.

Please read the <u>SMOL Paper</u> and the <u>GATITOS Paper</u> for a much more thorough description!

There are four resources in this directory:

- SmolDoc: document-level translations into 100 languages
- SmolSent: sentence-level translations into 81 languages
- GATITOS: token-level translations into 172 languages
- SmolDoc-factuality-annotations: factuality annotations and rationales for 661 documents from SmolDoc

Data schemata

The schemata are pretty straightforward. Source and Target languge are provided in sl and tl fields. The is_src_orig field has a value of true if the source text was the original text, and the target field was translated, and avalue of false if the data is b

Known issues

There are several known issues of this dataset:

- The translations of SmolDoc to Ho (Warang Citi script) (hoc) contain some instances of transliterated English, rather than actual Ho text. This is currently being corrected.
- The translations to Mooré (mos) contain a mix of orthographies.
- The translations into Kituba (ktu), Tulu (tcy), Nepali (ne), and Tibetan (bo) caused notable regressions in ChrF, suggesting that they are low-quality, though this could also be an issue with training or evaluation.
- The Manx (gv) split of GATITOS that was originally released was spurious. It has been removed.

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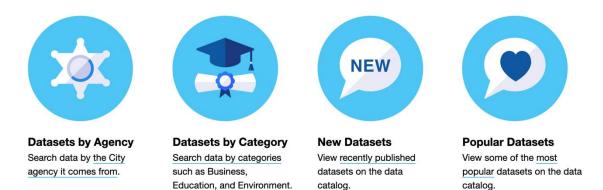
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Get in Touch Ask a question, leave a comment, or suggest a dataset to the NYC Open Data team

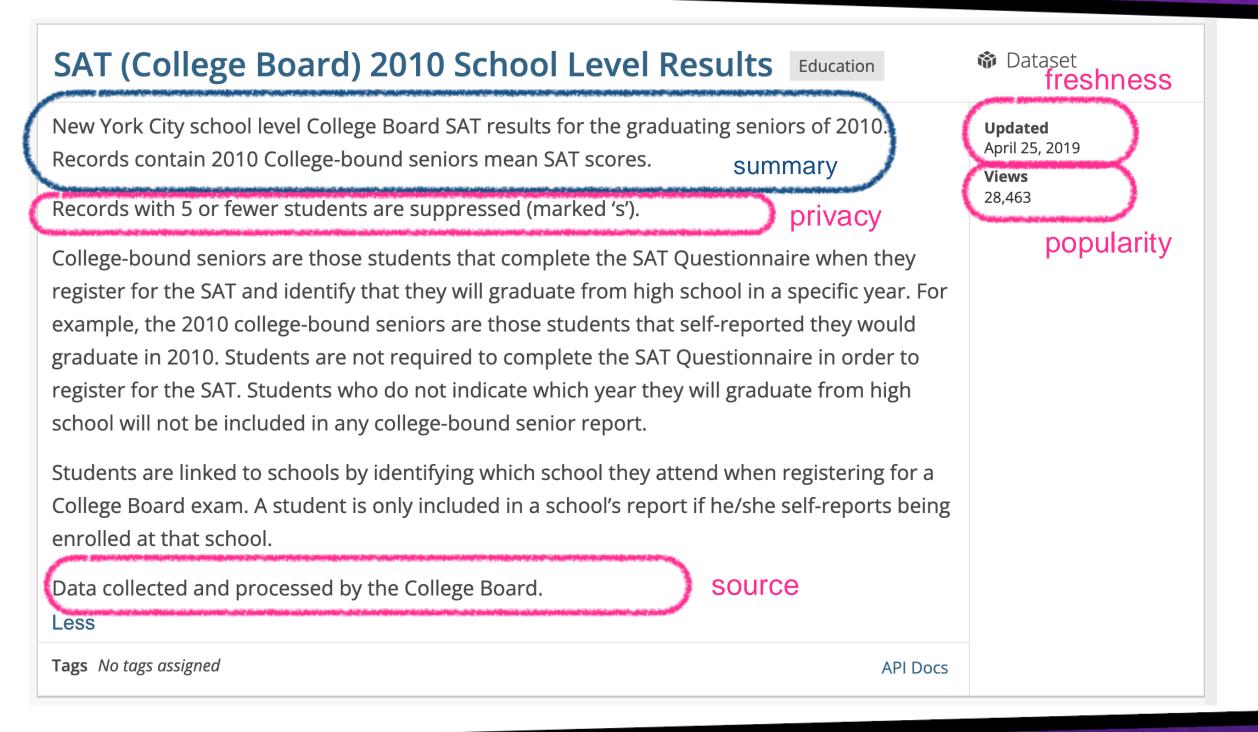


Dive into the Data Already know what you're looking for? Browse the data catalog now.

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About this Dataset

Updated April 25, 2019		Update				
Data Last UpdatedMetadata Last UpdatedFebruary 29, 2012April 25, 2019			Update Frequency	Historical Data		
			Automation	No		
			Date Made Public	10/11/2011		
Date Created October 6, 2011		Dataset Information				
Views Downloa		s	Agency	Department of Education (DOE)		
28.5K	48.4K		Attachments			
Department of Education Own		Dataset	SAT Data Dictionary.xlsx			
		NYC OpenData	Topics			
			Category	Education		
			Tags	This dataset does not have any tags		



https://opendata.cityofnewyork.us/

What's in this Dataset?

Columns in this Dataset

oendata.citvofnewvork.us/

Column Name	Description	Туре		
DBN		Plain Text	Т	\sim
School Name		Plain Text	Т	\sim
Number of Test Takers		Number	#	\sim
Critical Reading Mean		Number	#	\sim
Mathematics Mean		Number	#	\sim
Writing Mean		Number	#	\checkmark



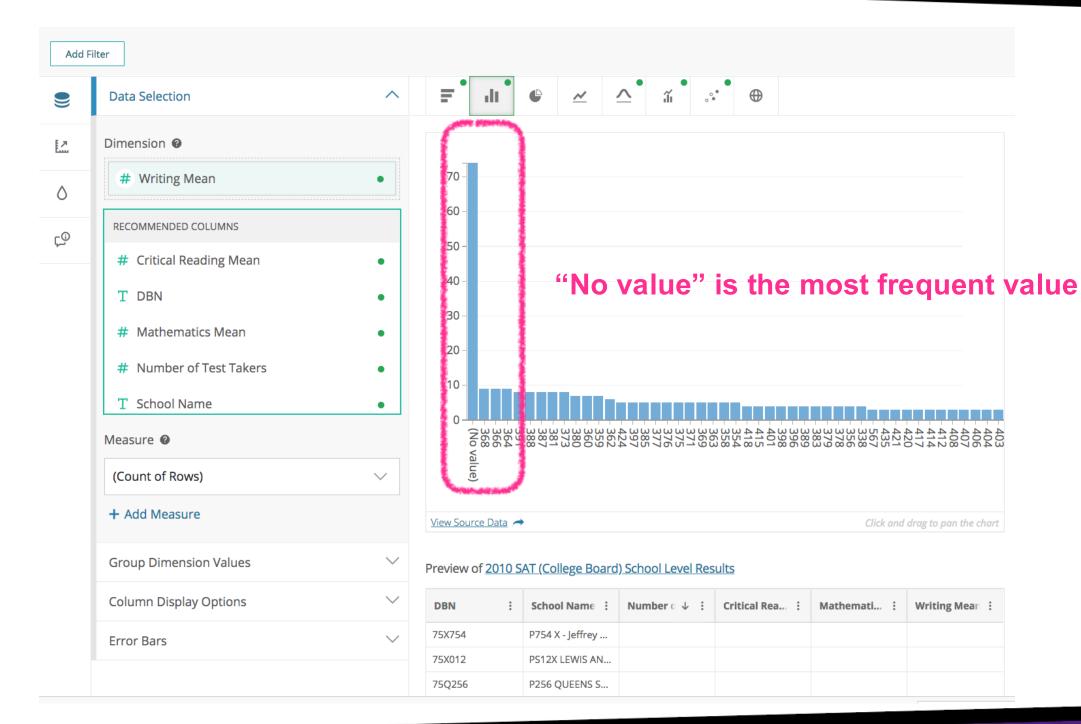
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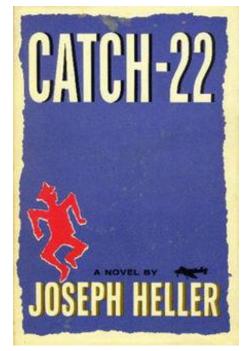
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Data profiling

- Data profiling refers to the activity of creating small but informative summaries of a database
- What is informative depends on the task, or set of tasks, we have in mind

should profiling be task-agnostic or task-specific?



A related activity is data cleaning



Data cleaning







Data cleansing or **data cleaning** is the process of detecting and repairing corrupt or inaccurate records from a data set in order to improve the **quality of data**.

Erhard Rahm, Hong Hai Do: Data Cleaning: Problems and Current Approaches, IEEE Data Engineering Bulletin, 2000.

... data is generally considered high quality if it is "fit for [its] intended uses in operations, decision making and planning"

Thomas C. Redman, Data Driven: Profiting from Your Most Important Business Asset. 2013

Even though quality cannot be defined, you know what it is. Robert M. Prisig, Zen and the Art of Motorcycle Maintenance, 1975

center

slide by Heiko Mueller

Data cleaning

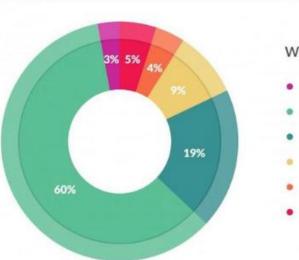
Forbes

52,423 views | Mar 23, 2016, 09:33am

Cleaning Big Data: Most Time-Consuming, Least Enjoyable Data Science Task, Survey Says



Gil Press Contributor ⁽³⁾ I write about technology, entrepreneurs and innovation.



What data scientists spend the most time doing

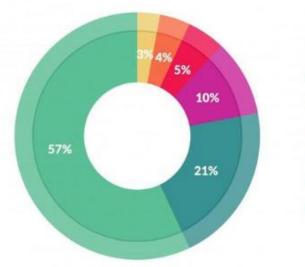
- Building training sets: 3%
- Cleaning and organizing data: 60%
- Collecting data sets; 19%
- Mining data for patterns: 9%
- Refining algorithms: 4%
- Other: 5%

Spend most time doing

Collecting data (19%) Cleaning and organizing data (60%)

Find least enjoyable

Collecting data (21%) Cleaning and organizing data (57%)



What's the least enjoyable part of data science?

- Building training sets: 10%
- Cleaning and organizing data: 57%
- Collecting data sets: 21%
- Mining data for patterns: 3%
- Refining algorithms: 4%
- Other: 5%

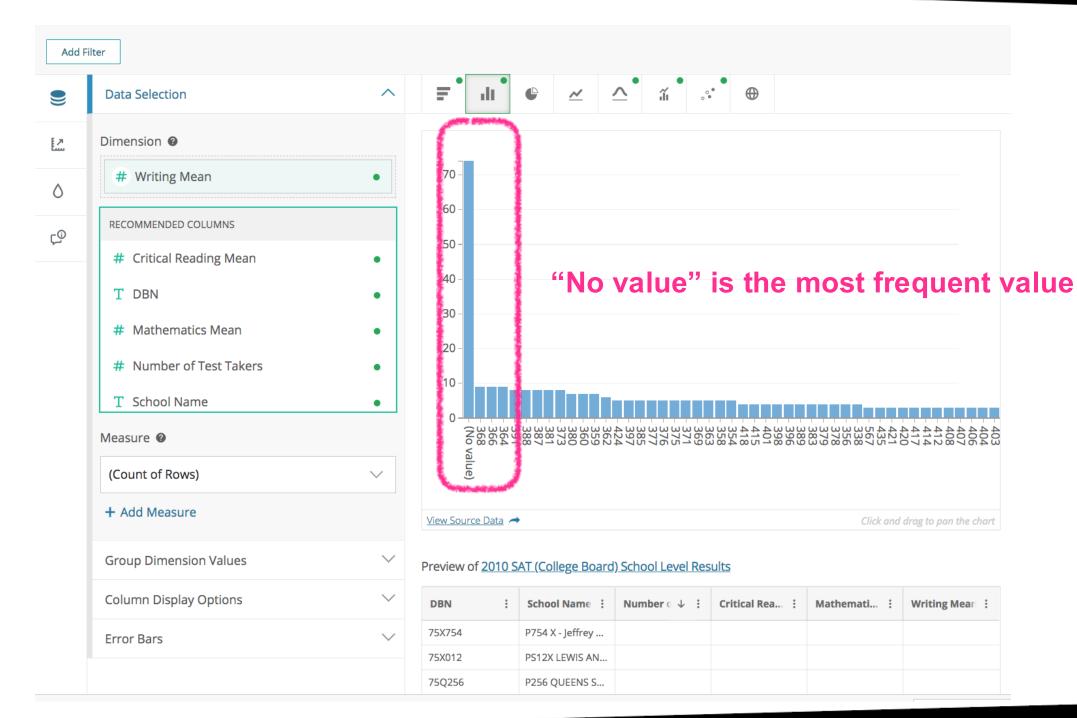
slide by Heiko Mueller



data profiling



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The trouble with null values

THE SQL DATABASE LANGUAGE

0 F

CRITIQUE

Α

C.J.Date

PO Box 2647, Saratoga California 95070, USA

* Null values

December 1983

I have argued against null values at length elsewhere [6], and I will not repeat those arguments here. In my opinion the null value concept is far more trouble than it is worth. Certainly it never been properly thought through in the existing SQL has implementations (see the discussion under "Lack of Urthogonality: Miscellaneous Items", earlier). For example, the fact that functions such as AVG simply ignore null values in their argument violates what should surely be a fundamental principle, viz: The system should never produce a (spuriously) precise answer to a query when the data involved in that query is itself imprecise. At least the system should offer the user the explicit option either to ignore nulls or to treat their presence as an exception.

> enter for responsible ai

50 shades of null

- **Unknown** some value definitely belongs here, but I don't know what it is (e.g., unknown birthdate)
- **Inapplicable** no value makes sense here (e.g., if marital status = single then spouse name should not have a value)
- Unintentionally omitted values is left unspecified unintentionally, by mistake
- **Optional** a value may legitimately be left unspecified (e.g., middle name)
- Intentionally withheld (e.g., an unlisted phone number)

•

(this selection is mine, see reference below for a slightly different list) https://www.vertabelo.com/blog/technical-articles/50-shades-of-null-or-how-a-billion-

dollar-mistake-has-been-stalking-a-whole-industry-for-decades

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50 shades of null... and it gets worse

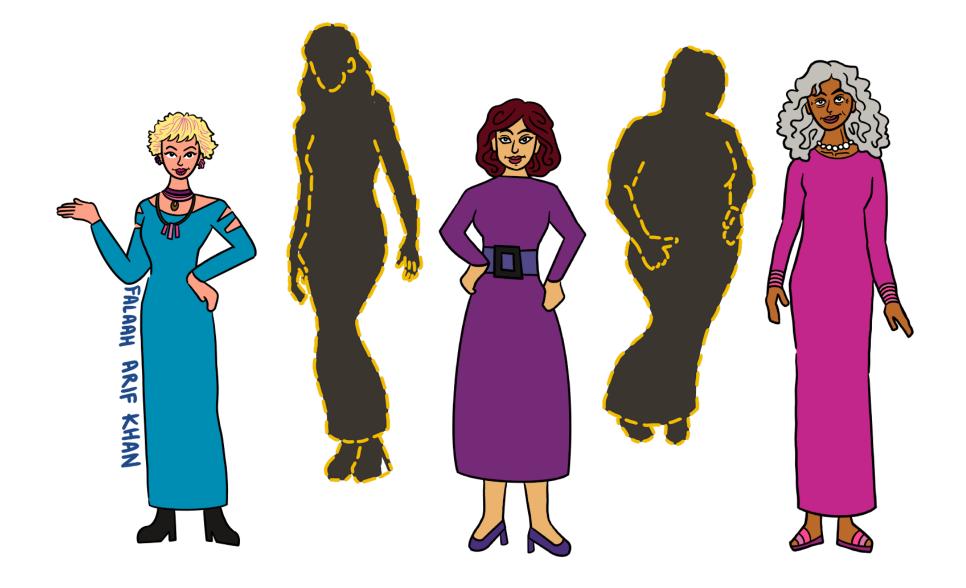
Hidden missing values -

- 99999 for zip code, Alabama for state
- need data cleaning....
- lots of houses in Philadelphia, PA were built in 1934 (or 1936?) - not really!

how do we detect hidden missing values?

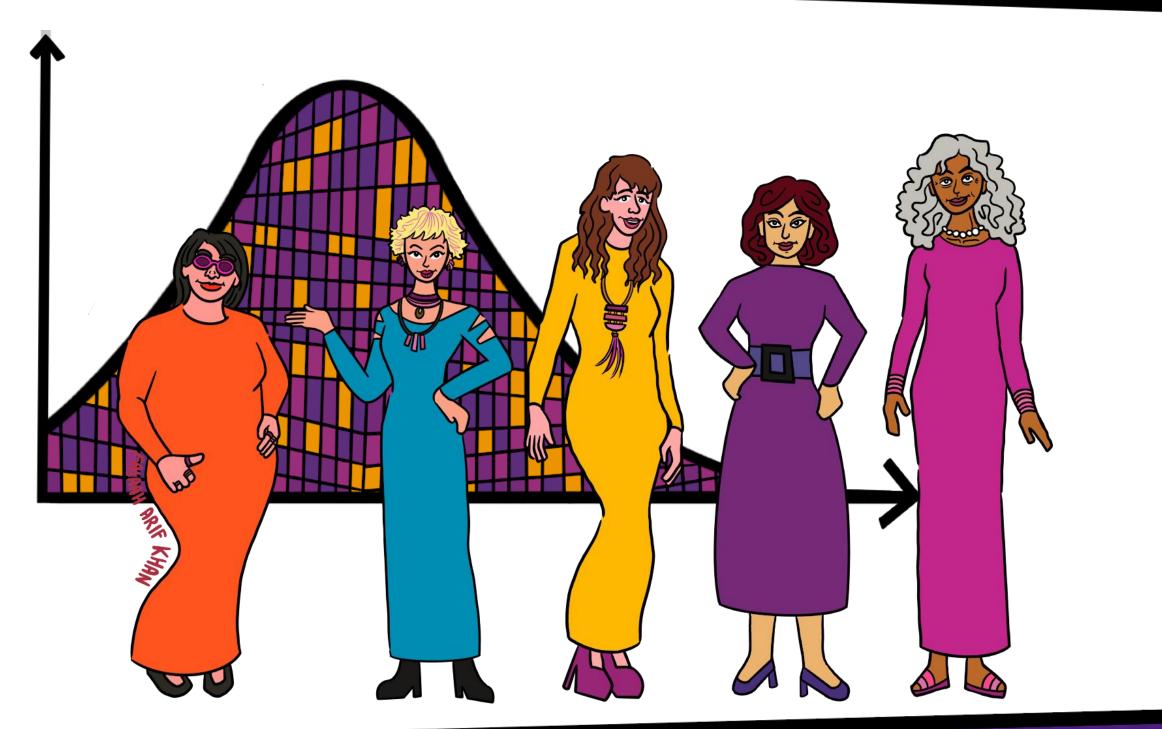


Missing values: Observed data





Missing values: Imputed distribution





Missing values: True distribution



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Missing value imputation

are values **missing at random** (e.g., gender, age, disability on job applications)?

are we ever interpolating **rare categories** (e.g., Native American)

are **all categories** represented (e.g., non-binary gender)?





Data filtering

"filtering" operations (like selection and join), can arbitrarily change demographic roup proportions

select by zip code, country, years of C++ experience, others?

age_group	county
60	CountyA
60	CountyA
20	CountyA
	-
60	CountyB
20	CountyB
20	CountyB

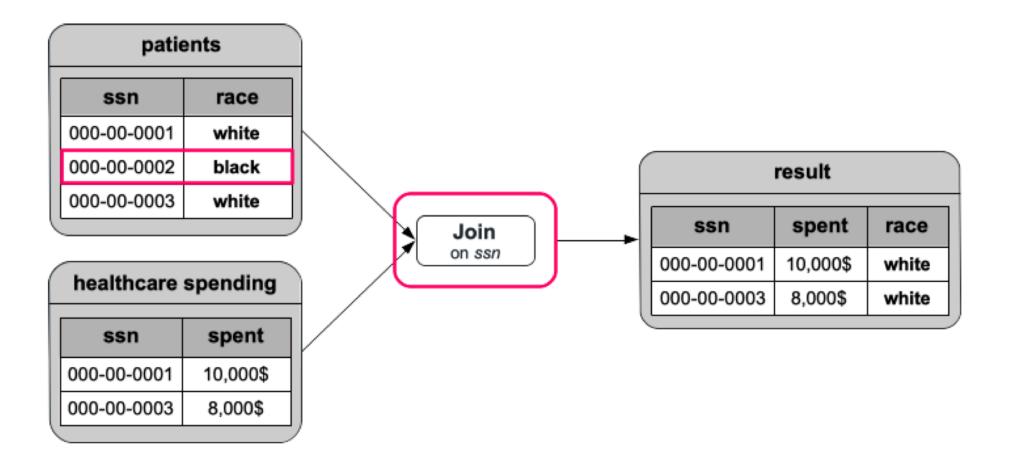
50% vs 50%



Data filtering

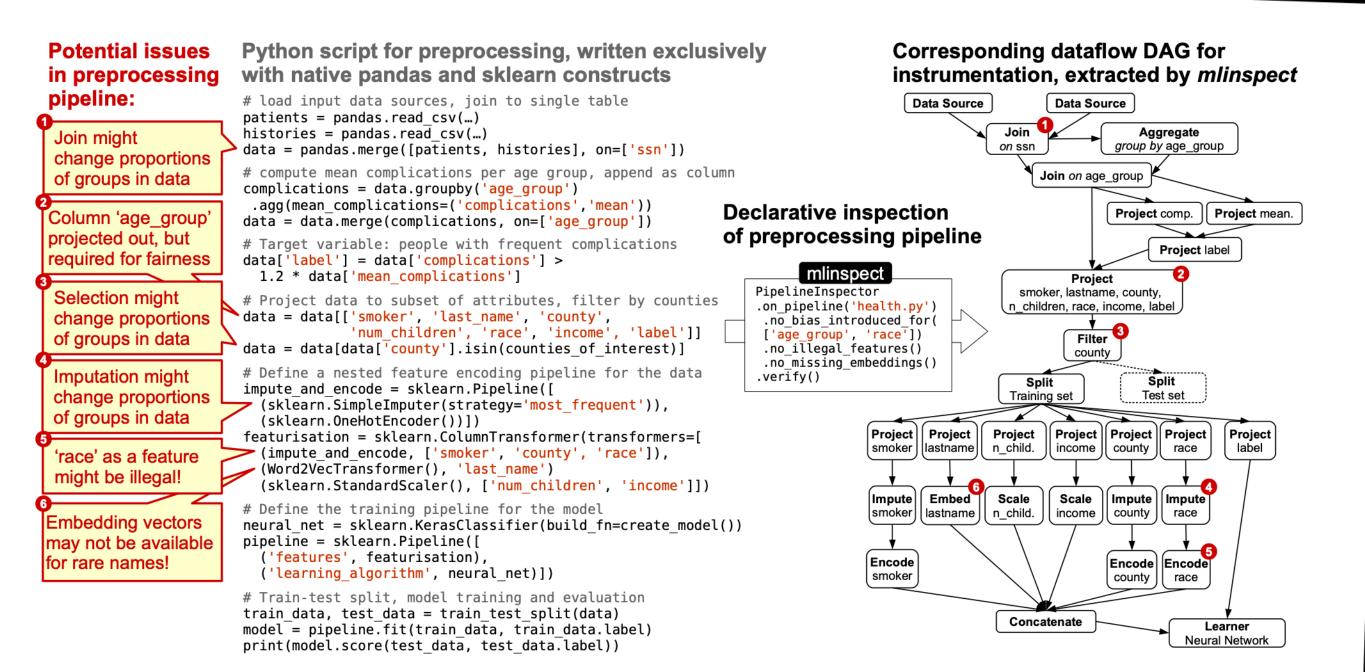
"filtering" operations (like selection and join), can arbitrarily change demographic roup proportions

select by zip code, country, years of C++ experience, others?





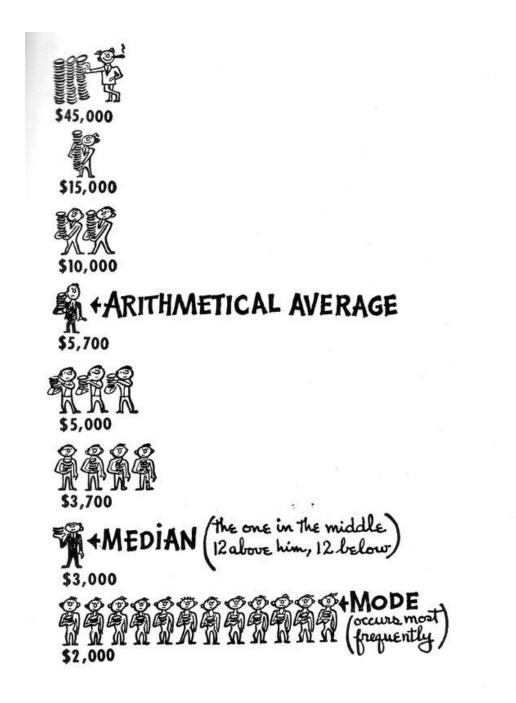
Data distribution debugging: mlinspect

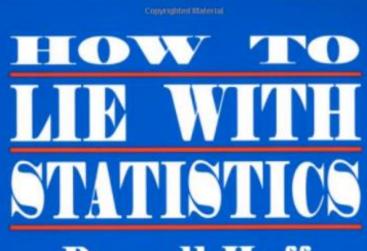


a center for responsible ai

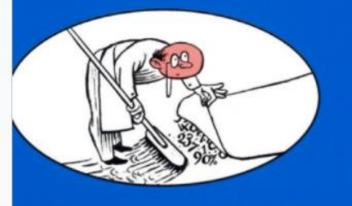
[Grafberger, Stoyanovich, Schelter (2022)]

The well-chosen average





Darrell Huff Hustrated by Irving Geis

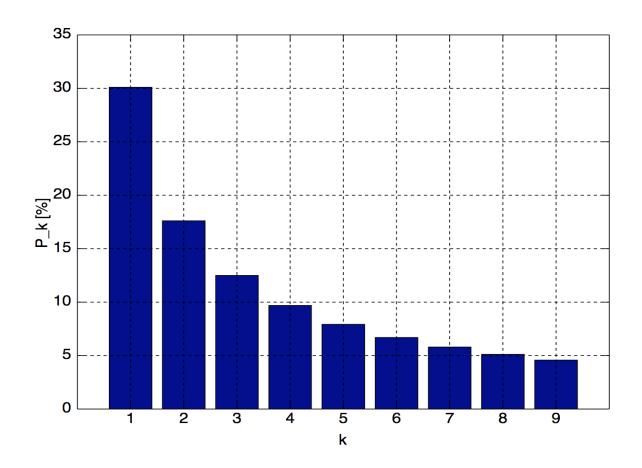


Over Half a Million Copies Sold— An Honest-to-Goodness Bestseller



Benford Law

The distribution of **the first digit d** of a number, in many naturally occurring domains, approximately follows



$$P(d) = \log_{10} \left(1 + \frac{1}{d} \right)$$

center

responsible

for

1 is the most frequent leading digit, followed by 2, etc.

., 1938]

https://en.wikipedia.org/wiki/Benford%27s_law

[Benford: "The law of anomalous numbers"

Benford Law

The distribution of **the first digit d** of a number, in many naturally occurring domains, approximately follows

$$P(d) = \log_{10} \left(1 + \frac{1}{d} \right)$$

., 1938[.]

center

esponsible

Holds if **log(x)** is uniformly distributed. Most accurate when values are distributed across multiple orders of magnitude, especially if the process generating the numbers is described by a power law (common in nature)



A logarithmic scale bar. Picking a random x position uniformly on this number line,

roughly 30% of the time the first digit of the number will be 1.

https://en.wikipedia.org/wiki/Benford%27s_law

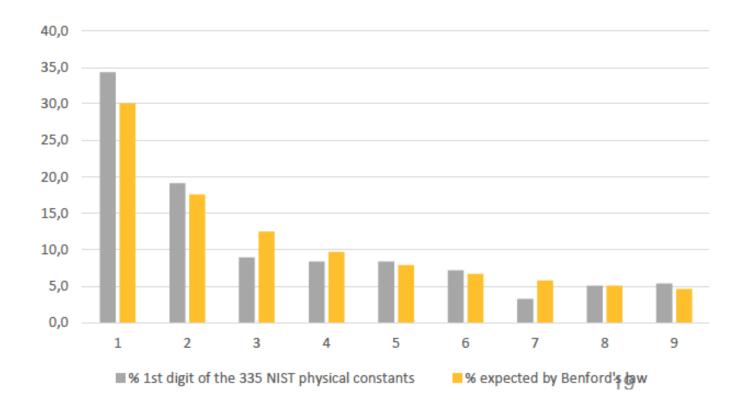
[Benford: "The law of anomalous numbers"

Examples of Benford Law

- surface area of 355 rivers
- sizes of 3,259 US populations
- 104 physical constants
- 1,800 molecular weights

. . . .

- 308 numbers contained in an issue of Reader's Digest
- Street addresses of the first 342 persons listed in American Men of Science



physical constants

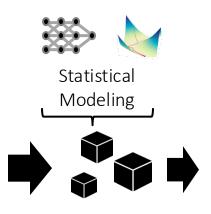
used in fraud detection!

[Abedjan, Golab & Naumann (2015)]



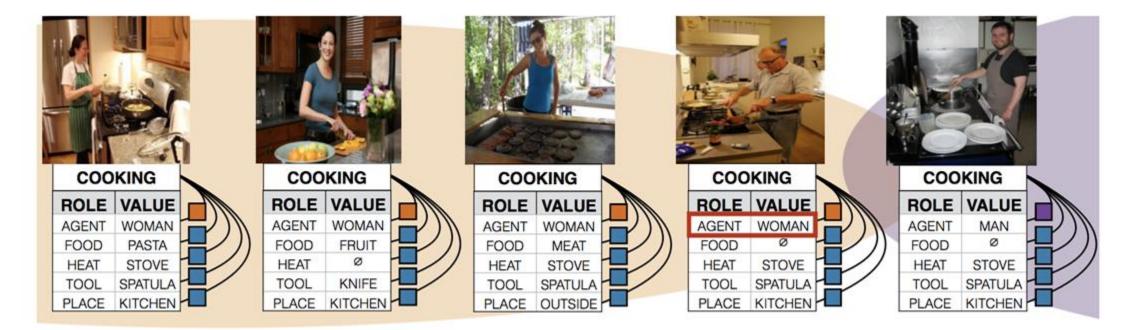
Statistical Modeling

 Statistical modeling: deciding how to crate a model for data and how it will be trained



• What model do we use? What training algorithm?

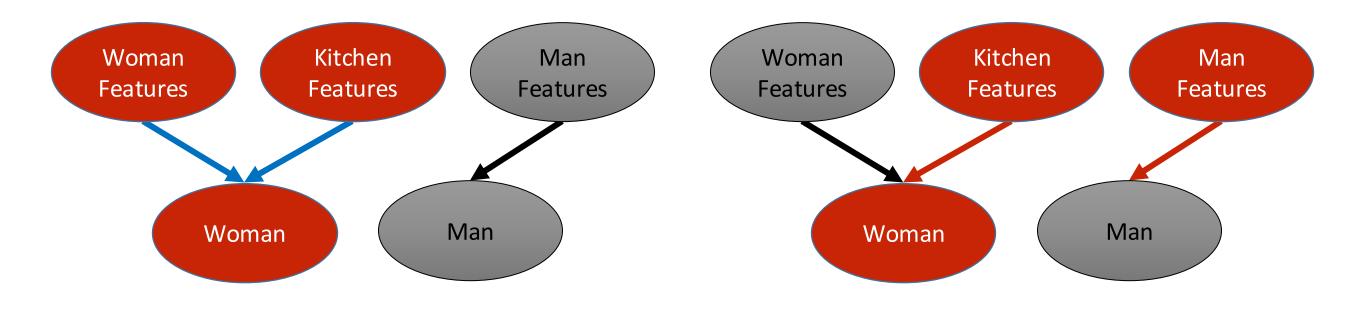
Unfairness in Model: Bias Amplification



Class	Man	Woman
Data prior	33%	67%
Pred. prior	16%	84%

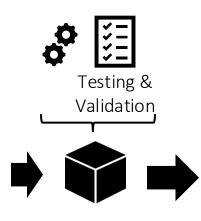
Unfairness in Model: Bias Amplification

We say a model exhibits *bias amplification* if the prior distribution of the model's predictions does not match that of the data: in particular, we don't want the model to *create* or *exaggerate disparities* in the training data.



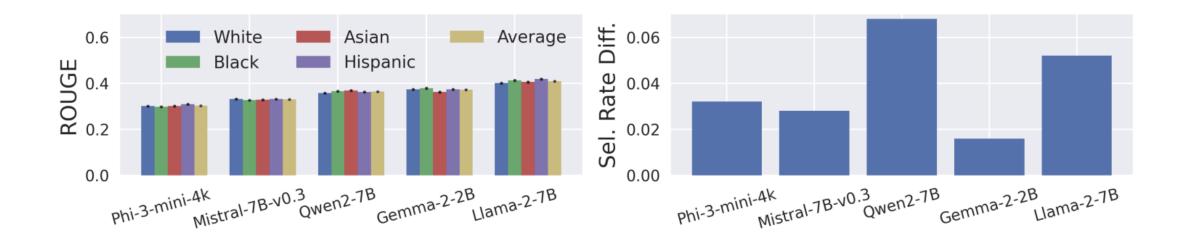
Testing and Validation

 Testing and validation: the processes by which a model is determined to be performing well, both in relation to other models in the training set, but also on unseen data.



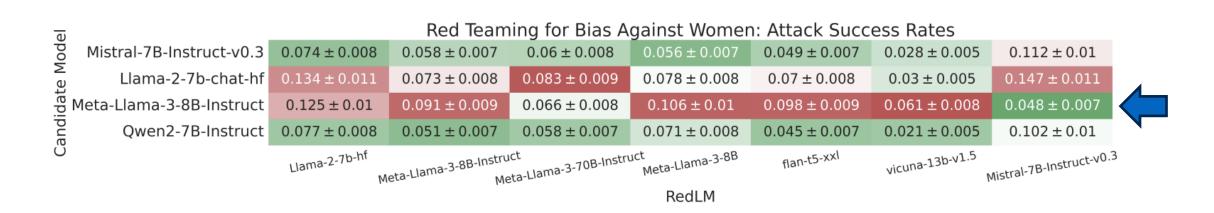
• What data will we test our model with? What metrics will we use?

Equalizing "Generation Quality" Metrics May not Capture Discriminatory Impacts



Rouge score for resume summaries across different demographic groups Selection rate (hiring) differences based on those summaries

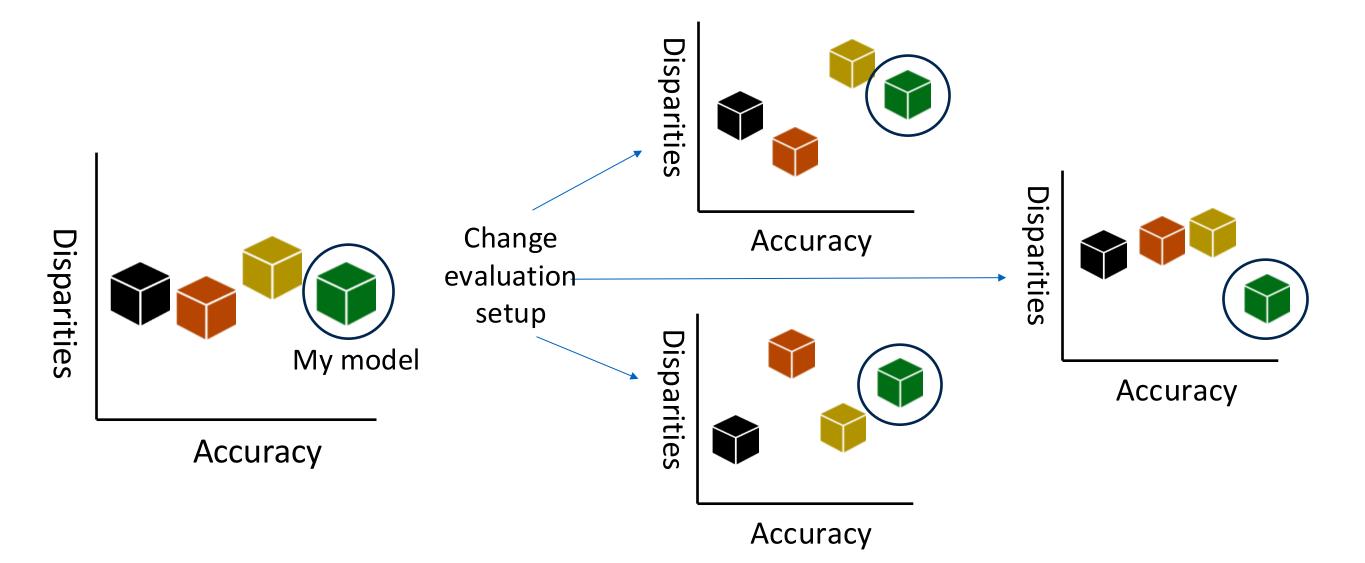
Evaluation schema that do exist are incredibly unstable

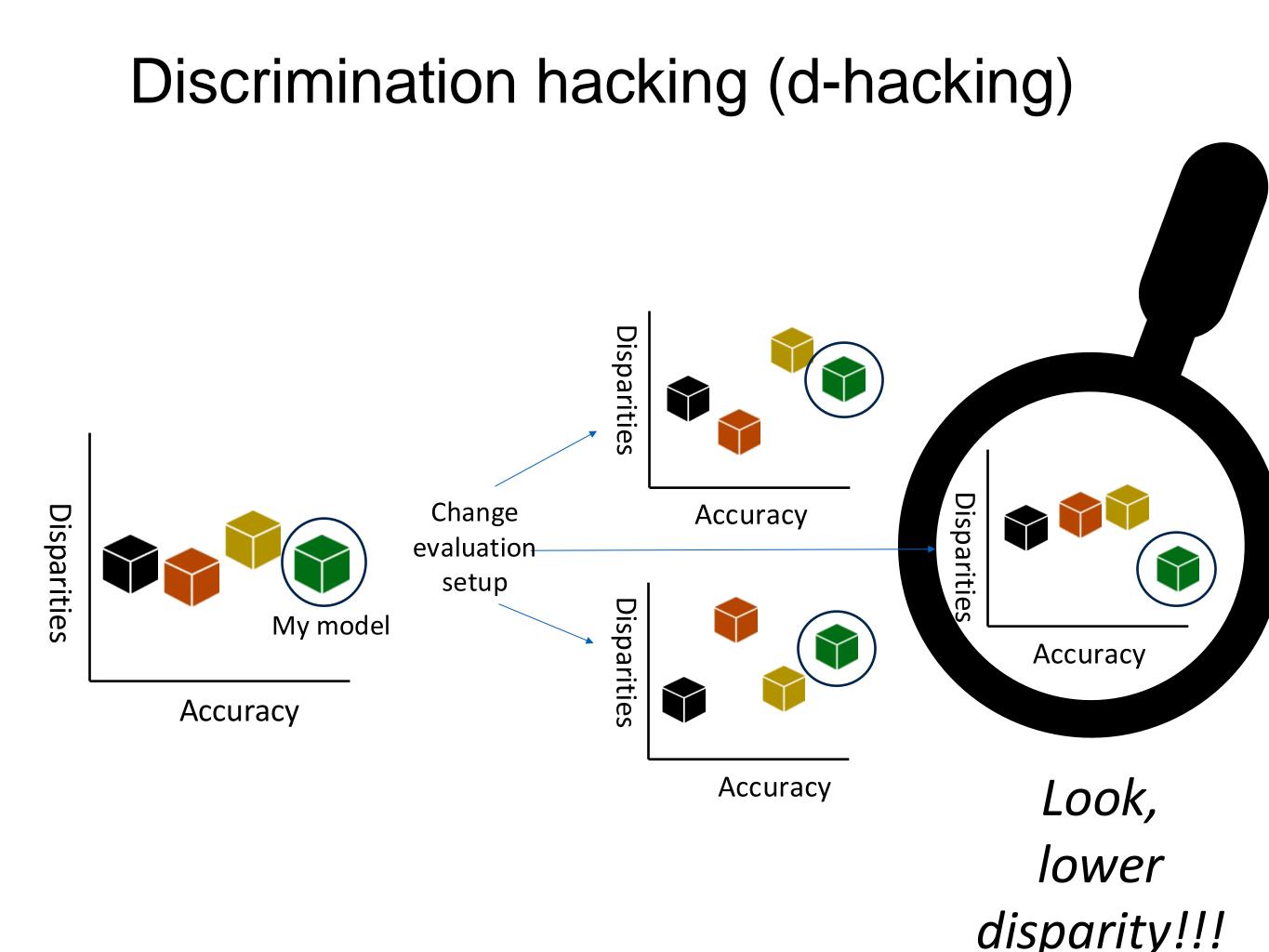


Instability of toxicity scores based on red-teaming with various base RedLM models

Towards Effective Discrimination Testing for Generative AI. Zollo, Rajaneesh, Zemel, Gillis, Black

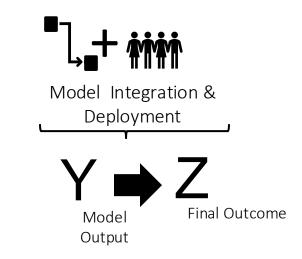
Discrimination hacking (d-hacking)





Model Integration and Deployment

 Model Integration/ Deployment: collecting or compiling data to train the model



- How do we communicate model output to a human decision-maker?
- How do we ensure good performance over time?

Model Integration and Deployment

The Principles and Limits of Algorithm-in-the-Loop Decision Making

BEN GREEN, Harvard University, USA YILING CHEN, Harvard University, USA



- How do humans deviate from AI predictions? Do they do so in a biased way?
- How consistent are human + AI decisions versus just human/just AI?
- How well do humans understand the information coming from the model? Overreliance, under-reliance, etc...

What do we do about all of this?

- Be a data detective!
- Design your evaluations carefully!
- Data science is also an art: But be explicit about your choices an assumptions
- Document your code, your data—so that the next person understands your choices and assumptions
- We're still working on it---join the fun!

Responsible Data Science

The data science lifecycle

Thank you!





Center for Data Science **Cal** center for responsible ai

association rule mining



The early days of data mining

- Problem formulation due to Agrawal, Imielinski, Swami, SIGMOD 1993
- Solution: the Apriori algorithm by Agrawal & Srikant, VLDB 1994
- Initially for market-basket data analysis, has many other applications, we'll see one today
- We wish to answer two related questions:
 - Frequent itemsets: Which items are often purchased together, e.g., milk and cookies are often bought together
 - Association rules: Which items will likely be purchased, based on other purchased items, e.g., if diapers are bought in a transaction, beer is also likely bought in the same transaction



Market-basket data

- $I = \{i_1, i_2, \dots, i_m\}$ is the set of available items, e.g., a product catalog of a store
- **X C** *I* is an **itemset**, e.g., {milk, bread, cereal}
- Transaction t is a set of items purchased together, t ⊆ I, has a transaction id (TID)
 - t1: {bread, cheese, milk}
 - t₂: {apple, eggs, salt, yogurt}
 - t₃: {biscuit, cheese, eggs, milk}
- Database T is a set of transactions $\{t_1, t_2, ..., t_n\}$
- A transaction *t* supports an itemset *X* if *X* ⊆ *t*
- Itemsets supported by at least *minSupp* transactions are called frequent itemsets

minSupp, which can be a number or a percentage, is specified by the user



Itemsets

TID	Items		
1	A		
2	AC		
3	ABD		
4	AC		
5	ABC		
6	ABC		

minSupp = 2 transactions

How many possible itemsets are there (excluding the empty itemset)?

itemset	support	
A	6	
В	3	
С	4	
D	1	
★ AB	3	
AC	4	
AD	1	
<u> </u>	2	
★ BD	1	
CD	0	
ABC	2	
ABD	1	
BCD	0	
ACD	0	er
ABCD	0	onsible

Association rules

An **association rule** is an implication $X \rightarrow Y$, where $X, Y \subset I$, and $X \cap Y = \emptyset$

example: {milk, bread} \rightarrow {cereal}

"A customer who purchased X is also likely to have purchased Y in the same transaction"

we are interested in rules with a single item in Y

can we represent {milk, bread} \rightarrow {cereal, cheese}?

Rule $X \rightarrow Y$ holds with **support** supp in T if supp of transactions contain $X \cup Y$

Rule $X \rightarrow Y$ holds with confidence conf in T if conf % of transactions that contain X also contain Y

 $conf \approx \Pr(Y \mid X)$ $conf(X \rightarrow Y) = supp(X \cup Y) / supp(X)$



Association rules

—	p = 2 transactions f = 0.75	*	itemset A	support 6	
	supp = 3 conf = $3 / 6 = 0.5$ conf = $3 / 3 = 1.0$	*	B C	3	
$B \to C$ $C \to B$	supp = 2 conf = 2 / 3 = 0.67 conf = 2 / 4 = 0.5	\times	D A B A C	1 3 4	
$A \to C$ $C \to A$	supp = 4 conf = 4 / 6 = 0.67 conf = 4 / 4 = 1.0	\star	A D B C B D	1 <u>2</u> 1	
$AB \to X$ $AC \to B$	supp = 2 conf = $2/3 = 0.67$ conf = $2/4 = 0.5$		CD ABC ABD	0 2 J Y) / supp (X)	
$BC \rightarrow A$	$\operatorname{conf} = 2/2 = 1.0 + \operatorname{conf} (X \to Y)$		BCD ACD ABCD	0	er onsible

Association rule mining

- Goal: find all association rules that satisfy the userspecified minimum support and minimum confidence
- Algorithm outline
 - Step 1: find all frequent itemsets
 - Step 2: find association rules
- Take 1: naïve algorithm for frequent itemset mining
 - Enumerate all subsets of **I**, check their support in **T**
 - What is the complexity?



Key idea: downward closure

			All subsets of a frequent itemset X are
	temset	support	themselves frequent
X	А	6	Themselves nequent
\mathbf{A}	В	3	So, if some subset of X is infrequent, then X
	С	4	cannot be frequent, we know this apriori
*	D	1	ABCD
\star	ΑB	3	
\star	AC	4	ABC ABD BCD ACD
	ΑD	1	
	BC	2	
\star	ΒD	1	AB AC BC BD CD AD
	CD	0	
	ABC	2	
	ABD	1 	A B C D
	BCD	⁰ X is n	converse is not true! If all subsets of X are frequer of guaranteed to be frequent
	ACD	0	
/	ABCD	0	for responsible

The Apriori algorithm

Algorithm Apriori(T, minSupp)
F ₁ = {frequent 1-itemsets};
for (<i>k</i> = 2; <i>F</i> _{k-1} ≠ Ø; <i>k</i> ++) do
$C_k \leftarrow candidate-gen(F_{k-1});$
for each transaction <i>t</i> ∈ <i>T</i> do
for each candidate $c \in C_k$ do
if c is contained in t then
c.count++;
end
end
$F_k \leftarrow \{c \in C_k \mid c.count \ge minSupp\}$
end
return $F \leftarrow \bigcup_k F_k$;

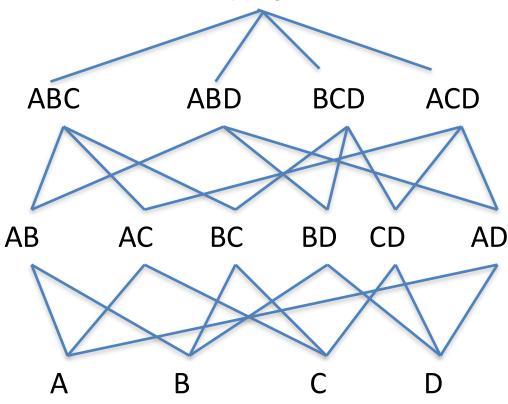
itemset	support
A	6
🍒 в	3
С	4
D	1
📩 AB	3
AC	4
AD	1
BC	2
★ BD	1
CD	0
ABC	2
ABD	1
BCD	0
ACD	0
ABCD	0
ADUU	al

Candidate generation

The **candidate-gen** function takes F_{k-1} and returns a superset (called the candidates) of the set of all frequent k-itemsets. It has two steps:

Join: generate all possible candidate itemsets C_k of length k

Prune: optionally remove those candidates in C_k that have infrequent subsets $$_{\mbox{ABCD}}$$





Candidate generation: join

F ₁ as p	F ₁ as q	C ₂	
Α	А	Α	В
В	В	Α	С
С	С	В	С

itemset	support
A	6
🍝 в	3
С	4
★ D	1
🗡 A B	3
🛧 AC	4
AD	1
BC	2
🗡 B D	1
CD	0
A B C	2
ABD	1
BCD	0
ACD	0
ABCD	0
	ai

Candidate generation: join

					itemset	support
Insert into C _k (A	6
select p.item ₁ , p.item ₂ ,	., p.item _{k-1} , q	.item _{k-1}			🍝 в	3
from $F_{k-1}p, F_{k-1}q$ where pitem, = qitem.					С	4
where $p.item_1 = q.item_1$ and $p.item_2 = q.item_2$					D D	1
and					🗡 A B	3
and $p.item_{k-1} < q.item_{k-1}$)					AC	4
	AD	1				
					B.C.	2
F_2 as p F_2 as q				ЖBD	1	
			I		CD	0
A B	A	В	C ₃		<u> </u>	2
A C	Α	С	<u> </u>		ABD	1
ВС	В	С	Α	В	C 3 C D	0
					ACD	0
					ABCD	0
						ai

Candidate generation

Assume a lexicographic ordering of the items

Join

why not p.item_{k-1} \neq q.item_{k-1}?

Prune

```
for each c in C_k do
for each (k-1) subset s of c do
if (s not in F_{k-1}) then
delete c from C_k
```



Generating association rules

```
Rules = \emptyset
for each frequent k-itemset X do
          for each 1-itemset A \subset X do
            compute conf (X / A \rightarrow A) = supp(X) / sup (X / A)
            if conf (X / A \rightarrow A) \geq minConf then
              Rules \leftarrow \Box X / A \rightarrow A''
          end
     end
end
return Rules
```



Performance of Apriori

- The possible number of frequent itemsets is exponential, O(2^m), where *m* is the number of items
- Apriori exploits sparseness and locality of data
 - Still, it may produce a large number of rules: thousands, tens of thousands,
 - So, thresholds should be set carefully. What are some good heuristics?



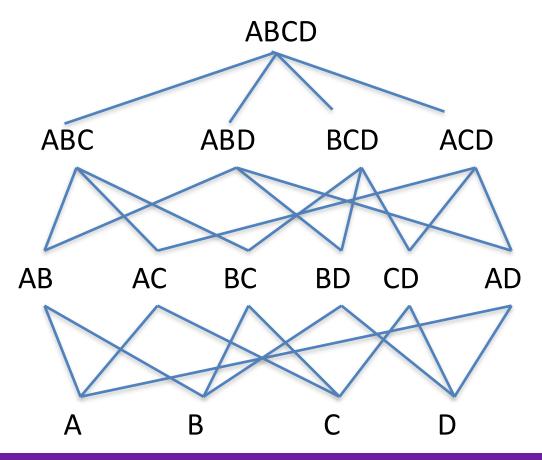
Discovering uniques

Given a relation schema *R* (*A*, *B*, *C*, *D*) and a relation instance *r*, a **unique column combination** (or a **"unique"** for short) is a set of attributes *X* whose **projection** contains no duplicates in *r*

Given a relation schema *R* (*A*, *B*, *C*, *D*) and a relation instance *r*, a set of attributes *Y* is **non-unique** if its projection contains duplicates in *r*

X is **minimal unique** if every subset **Y** of **X** is non-unique

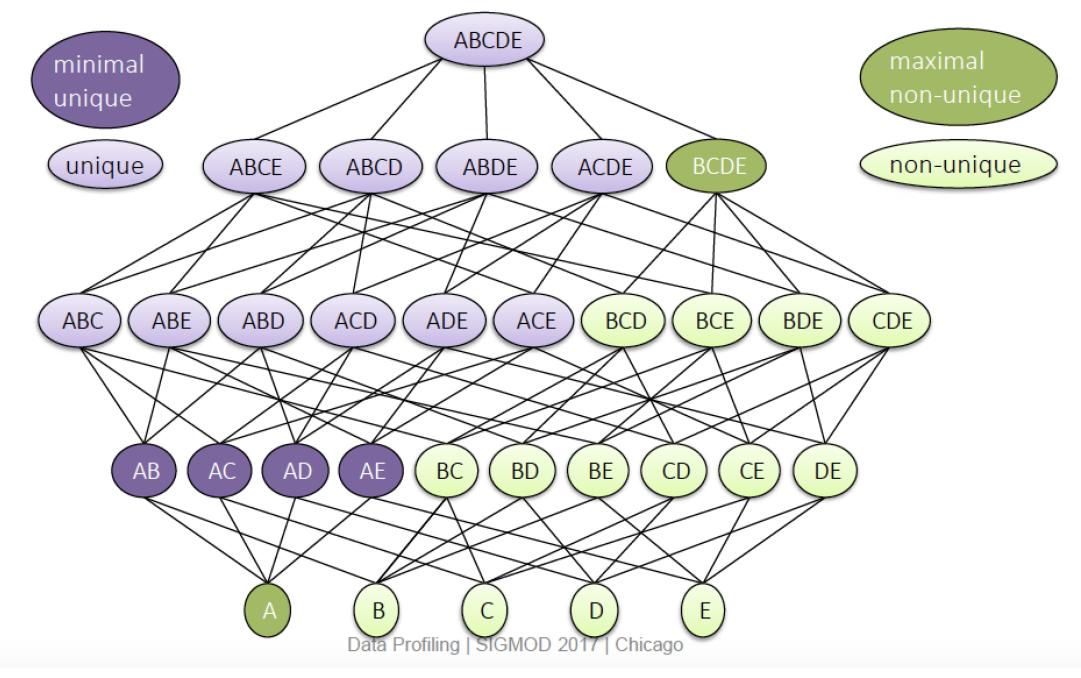
Y is maximal non-unique if every superset **X** of **Y** is unique





[Abedjan, Golab, Naumann; SIGMOD 2017]

Output





From uniques to candidate keys

Given a relation schema *R* (*A*, *B*, *C*, *D*) and a relation instance *r*, a **unique column combination** is a set of attributes *X* whose **projection** contains no duplicates in *r*

Episodes(season,num,title,viewers)

season	num	title	viewers
1	1	Winter is Coming	2.2 M
1	2	The Kingsroad	2.2 M
2	1	The North Remembers	3.9 M

A set of attributes is a **candidate key** for a relation if:

(1) no two distinct tuples can have the value values for all key attributes (candidate key **uniquely identifies** a tuple), *and*

(2) this is not true for any subset of the key attributes (candidate key **is minimal**)

A minimal unique of a relation instance is a (possible) candidate key of the relation schema. To find such possible candidate keys, find all minimal uniques in a given relation instance.



Apriori-style uniques discovery

[Abedjan, Golab, Naumann; SIGMOD 2017]

A minimal unique of a relation instance is a (possible) candidate key of the relation schema.

Algorithm Uniques // sketch, similar to HCA

 $U_1 = \{1 \text{-uniques}\}$ $N_1 = \{1 \text{-non-uniques}\}$

for $(k = 2; N_{k-1} \neq \emptyset; k++)$ **do**

 $C_k \leftarrow \text{candidate-gen}(N_{k-1})$

 $U_k \leftarrow \text{prune-then-check} (C_k)$

// prune candidates with unique sub-sets, and with value distributions that cannot be unique

// check each candidate in pruned set for uniqueness

$$N_k \leftarrow C_k \setminus U_k$$

end

return $U \leftarrow \bigcup_k U_k$;

breadth-first bottom-up strategy for attribute lattice traversal

