My wonderful paper

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ABSTRACT

In data analysis, unexpected results often prompt researchers to revisit their procedures to identify potential issues. While experienced researchers can often quickly diagnose problems by checking a few key assumptions, others may struggle to identify the root causes. These checked assumptions, or expectations, are typically informal, difficult to trace, and rarely discussed in publications. In this paper, we formalize these informal assumptions by framing them as binary analysis validation checks. We then introduce a procedure to quantify how violations of these checks may lead to unexpected results in the analysis. The procedure relies on simulations of the original data and evaluates both accuracy and redundancy. Accuracy is calculated through a binary classification metric, while redundancy is measured using mutual information. We demonstrate this approach with a toy example based on fitness step count data and a generalized linear model example examining the effect of particulate matter air pollution on daily mortality.

README:

- Check for TODOs, things inside "[...]", other than references, are my comments
- Literature review: Section diagnosing unexpected outcomes in data analysis
- Discussion and Conclusion
- In Section Application: provide more context on the PM10-mortality study and add reference of the [0, 0.005] PM10 coefficient

1. Introduction

In data analysis, experienced researchers often rely on their prior knowledge or domain expertise to quickly assess whether results align with their expectations. When a result falls outside of this interval, it prompts the researchers to investigate backwards on the data quality, the analysis steps, or the assumptions made during the analysis process. This mental process of where to diagnose unexpected outcomes is often difficult to trace and discuss in publications. As a result, readers are typically presented with the final outcomes of the analysis cycle where the results and expectations are aligned, achieved either by refining the analysis or updating the expectations based on statistical evidence [Grolemund and Wickham, 2014]. These missing pieces of information provides little guidance for diagnosing issues in the analysis when the same methodology is applied to a new dataset that produces different outcomes. Similarly, when researchers with different background knowledge view results that they find to be unexpected, it becomes unclear whether discrepancies arise from differing expectations or from the use of statistical techniques.

One might gain insight into analysts' thought processes by speaking with them directly or watching them work via screencast videos they produce, such as, TidyTuesday screencast videos or think-aloud type studies [e.g. Gu et al., 2024]. However, direct observation of analysis is not scalable and may not always be feasible; creating educational screencast videos requires significant effort from the researchers. Ideally, there could be a way to make expectations about data analysis explicit and accessible to others. Even better, if the encoding were machine-readable, we could analyze these expectations and learn from the analysis itself. For example, we could answer questions about whether the checks also apply to other researchers analyzing new data in the same context, whether

they reflect common practices in the field, or whether they are specific to the data or analysis at hand.

The externalization of the data analysis process is a practice that has potential to improve the trustworthiness of analyses in general and the trustworthiness of subsequent products, such as machine learning models, that may be built on such analyses. While publication of analysis code and data is now a common a requirement for the sake of reproducibility [Peng, 2011], the publication code alone is often insufficient for understanding the thought process behind an analysis. Code corresponding to published analyses often reflect the final decisions made about analysis and do not reveal the decisions or assumptions made about the data processing. Thus, a reader looking at published code can often be left with many questions about why certain choices were made. Developing an approach to reveal some of this process without requiring a reader to essentially reconstruct the analysis process from the raw data would provide an improved basis for trusting an analysis result [Peng and Hicks, 2021].

In this paper, we conceptualize these internal expectations and assumptions as analysis validation checks, which allows us to examine the assumptions made during an analysis and to diagnose unexpected outcomes. We then introduce a procedure that provides a quantitative measure of how violations in a tree of analysis checks, derived from individual checks, will lead to an unexpected result. The procedure, based on simulations of the original data, calculates the accuracy and redundancy of the analysis checks. Accuracy is determined using binary classification metrics, precision and recall, from a logic regression fit [Ruczinski et al., 2003], while redundancy is measured using mutual information. The proposed workflow offers a numerical guarantee that the analysis will produce the expected results, assuming the assumptions about the data generating mechanism hold.

The rest of the paper is organized as follows: Section 2 reviews the concepts of diagnosing unexpected outcomes and general data quality checks. Section 3 introduces the concept of analysis validation checks, illustrated with a toy example based on fitness step count data. Section 4 describes the procedure that quantifies how analysis validation checks combined using logical operators can predict unexpected outcomes in an analysis. Section 5 applies this procedure to a larger example that estimates the effect of particulate matter air pollution on daily mortality. Section 6 discusses a few key considerations and Section 7 concludes the paper.

2. Related Work

2.1. Diagnosing unexpected outcomes in data analysis

The concept of framing data analysis as a sense-making process was originally presented by [Grolemund and Wickham, 2014] based on seminal work by [Wild and Pfannkuch, 1999]. Key to any sense-making process is a model for the world (i.e. expectations for what we might observe) and observed data with which we can compare our expectations. If there is a significant deviation between what we observe and our expectations, then a data analysis must determine what is causing that deviation. A naive approach would be to update our model for the world to match the data, under the assumption that the initial expectation was incorrect. However, experienced analysts know that the reality can be more nuanced than that, with errors occurring in data collection or data processing that can have an impact on final results.

The skill of diagnosing unexpected data analysis results is not one that has received significant attention in the statistics literature. While the concept of diagnosis is often embedded in model checking or data visualization techniques, systematic approaches to

identifying the root cause of an unexpected analysis result are typically not presented [Peng and Parker, 2022]. [Peng et al., 2021] proposed a series of exercises for training students in data analysis to diagnose different kinds of analysis problems such as coding errors or outliers. They provide a systematic approach involving working backwards from the analysis result to identify potential causes. There are parallels here to the concept of debugging and testing in software engineering [Donoghue et al., 2021]. For example, [Li et al., 2019] found that experienced engineers were generally able to identify problems in code faster than novices, and that the ability to debug code required knowledge that cut across different domains.

If it is true that the speed with which data analysts can identify problems with an analysis is related to their experience working with a given type of data, then there is perhaps room to improve the analytic process by externalizing the aspects that an analyst learns through experience. That way, inexperienced analysts could examine the thought process of an experienced analyst and learn to identify factors that can cause unexpected results to occur.

2.2. Data analysis checks

A substantial body of literature has addressed the definition of data quality [Cichy and Rass, 2019, more] and has developed frameworks that include dimensions, attributes, and measures to evaluate and improve data quality [Cai and Zhu, 2015, Wang and Strong, 1996, Sidi et al., 2012, Woodall et al., 2014]. These frameworks are often used in information systems and database management and support business decision-making in various industries. For research purposes, high-quality data ensures the credibility of scientific findings and supports reproducibility and re-usability in future studies [ref]. With the growing prevalence of open data in scientific research, the consumers or users

of the data typically are no longer the producers or collectors of the data who would have the full knowledge of data in hand, prompting more interest towards data quality checks in the data analysis process. In R, there are some packages, like skimr [Waring et al., 2022] and dataMaid [Petersen and Ekstrøm, 2019], that provide basic data screening and reporting tools, while another class of packages, e.g. assertr [Fischetti, 2023], validate [van der Loo and de Jonge, 2021], and pointblank [Iannone et al., 2024] focuses on providing data validation tools, allowing users to define customized data quality checks based on the applications.

The literature on data quality typically focuses on the intrinsic or inherent quality of the data themselves, rather than the data's relationship to any specific data analysis. So for example, if a column in a data table is expecting numerical data, but we observe a character value in one of the entries, then that occurrence would trigger some sort of data quality check. This type of quality check can be triggered without any knowledge of what the data will ultimately be used for. However, for a given analysis, we may require specific aspects of the data to be true because they affect the result being computed. Conversely, certain types of poor quality data may have little impact on the ultimate result of an analysis (e.g. data that are missing completely at random). Defining data quality in terms of what may affect a specific analysis outcome or result has the potential to open new avenues for defining data checks and for building algorithms for optimizing the collection of checks defined for a specific analysis.

3. Analysis validation checks

Expectations represent our understanding of certain aspects of the analysis and the data, independent of the results of the analysis itself. When observed outcomes deviate

from these expectations, analysts often revisit the analysis process to identify potential issues, refine methods, or revise assumptions. Experienced analysts can typically identify issues quickly and correct them on the spot, but they often do so without discussing the underlying reasoning, making it harder for less experienced researchers to learn and master these skills.

Here, we introduce the concept of analysis validation checks, which frame these expectations or assumptions as explicit checks that return a TRUE or FALSE result given the data analyzed at hand. Inspired by the concept of data validation checks (van der Loo and de Jonge [2021]), which are designed to ensure that datasets meet expected formats and quality, analysis validation checks reverse the approach: they validate the assumptions about the data necessary for the analysis to produce the *expected results*, as defined by the analyst. The focus on expected results allows the concept of analysis validation checks to encompass a broad range of checks, such as data quality (i.e. missing data, how the data are structured), data distribution and outliers, bivariate and multivariate relationships between variables, and other contextual information.

Our proposed analysis validation checks provide insights into an analyst's thought process and offer the following benefits:

- Serve as clear checkpoints to support the replication or application of methods to (new) data by programmatically communicating the requirements or assumptions made of the data;
- 2. Align assumptions among researchers from different domain backgrounds who may have different expectations about the data;
- 3. Improve analysis transparency, reproducibility, and trustworthiness by externalizing a key part of the analysis process; and

4. Quantify the effectiveness of analysis checks for predicting the expected outcome (see Section 4);

In addition to the above benefits, the development and publication of analysis checks has the potential to help students, inexperienced analysts, and junior researchers develop the skills needed to diagnose unexpected analysis results for a given type of data because the assumptions made about the data are made transparent. The analysis checks can serve as a basis for new analysts to have conversations about the data they are analyzing and to develop a better understanding of the potential data generation process.

3.1. A Toy Example

Consider a 30-day step count experiment in public health. Subjects are instructed to walk at least 8,000 steps each day, with an expected average of 9,000 steps, tracked by a step counter app. After 30 days, we review the data and examine the number of steps taken each day. With data of this nature, we may expect there to be occasional "low" days due to factors such as forgetting to wear their watch or unfavorable weather conditions limiting outdoor activities. We may also expect "high" days recorded after an outdoor hike or intense workout. Given the requirements of the study, we expect that for a given subject there would be no more than five days with step counts falling below the 8,000-step threshold ("invalid days"). If there were more than five invalid days, the data from that subject would not be usable for the study.

In this scenario, the outcome is that the number of days with a step count below 8,000 and the expectation is that this outcome would take a value no more than 5. If the expectation is violated, we can consider the potential configurations of the data that could lead to such an anomaly. To diagnose potential reasons why this outcome

expectation might fail, we can establish a few analysis validation checks in anticipation of seeing the data. For example, if the average step count is too low, this may suggest that the subject is incapable of taking the required number of steps, potentially leading to the unexpected outcome. Similarly, we can also check the quantile of the step count, if more than a third of the days fall below 8,000, this could indicate an excess of low-count days. Additionally, we may may expect the standard deviation of the step count not to be overly large. These considerations yield the following three analysis validation checks:

- $\bullet\,$ test1: the test fails if the mean step count is below 8,200
- test2: the test fails if the 30th percentile of the observed step counts is below 8,200
- test3: the test fails if the standard deviation of the observed step counts exceeds 2,500.

The cutoff values chosen for these tests would presumably be chosen based on prior experience with these kinds of data, but could also be optimized using the method presented in the next section.

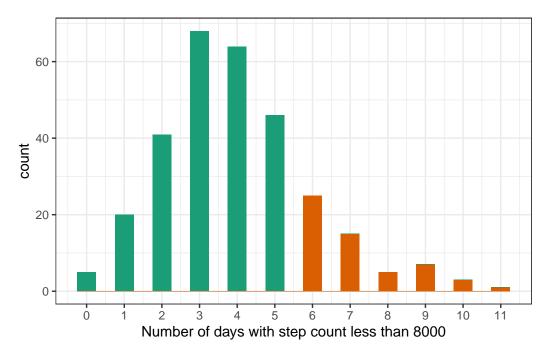


Figure 1. Number of days with fewer than 8,000 steps across 300 simulated 30-day periods. The orange bars indicate instances where the count exceeds five days, representing an unexpected outcome in this scenario.

To simulate this data, three normal distributions are used for the daily step counts: $\mathcal{N}(4000, 200)$ for low days, $\mathcal{N}(12000, 200)$ for high days, and $\mathcal{N}(9000, 300)$ for typical days. The number of low and high days can be simulated from a Poisson distribution with $\lambda = 4$. Figure 1 displays the number of days with fewer than 8,000 steps across 300 simulated 30-day periods.

4. Method

While some checks may be crucial and directly indicate an unexpected outcome, others may be tangential to the problem at hand and not indicate a root cause of an unexpected outcome. In this section, we propose a procedure to measure the effectiveness of checks that, when combined using logical operators, contribute to an unexpected outcome. A small set of independent checks is considered effective if it translates to unexpected

outcomes.

The approach relies on the use of simulated datasets that are generated based on the analyst's knowledge and assumptions about the data generation mechanism. Datasets are simulated to have the same structure and characteristics of the observed data that will be analyzed at some point in the future. For each simulated dataset, we can apply a collection of analysis validation checks to the dataset and record which ones were TRUE and which were FALSE. We can also compute the outcome of the analysis to see whether the outcome is unexpected in a given simulated datasets. We can then generate many datasets, each time applying the analysis validation checks and computing the outcome. After generating many datasets, we can relate the patterns in the analysis validation checks to the likely that the outcome will be unexpected in a given dataset.

Figure 2 provides an overview of the process.

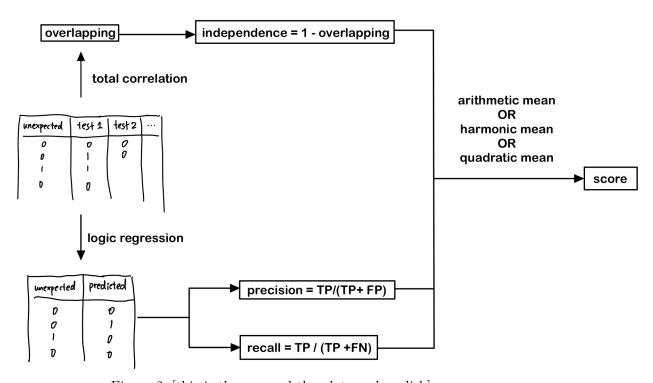


Figure 2. [this is the cap and the plot needs polish]

From the simulated data, the accuracy branch refers to a set of checks' ability to accu-

rately detect unexpected outcomes while minimizing false positives and false negatives. While a false positive can raise caution or skepticism on the data, the presence of both false positives and false negatives suggest that the checks are overly sensitive or lack sensitivity to unexpected outcomes.

To incorporate the effect of multiple checks on the outcome, a logic regression model [Ruczinski et al., 2003] is fitted to the analysis validation checks using the indicator of an unexpected result as the outcome in the model. Originally developed for SNP microarray data, logic regression constructs Boolean combinations of binary variables, in a tree structure, to predict both binary and numerical outcomes. Compared to other tree-based methods for binary-binary prediction, the Boolean combinations from the logic regression model produce a tree structure that can be directly interpreted as the possible combination of checks leading to an unexpected outcome, without the need to invert the tree as required in classic tree-based recursive partitioning methods. The logic regression model is then used to predict the analysis result based on the values of checks, and the prediction is compared to the actual analysis result in order to calculate the precision and recall of the checks.

While tests may score high on accuracy, they may be less effective at explaining the various reasons behind unexpected results. This could happen if, for example, a set of tests are all tangentially related to the cause of the unexpected results, but none addresses the root cause. It may also occur if the tests are highly correlated with one another, leading to redundancy.

To quantify redundancy, the concept of mutual information is used. Mutual information I(x,y) measures the amount of information shared between two random variables and is defined as the KL-distance $D(p \parallel q)$ between the joint distribution of the two variables

and the product of the marginal distributions:

$$I(x,y) = D(p(x,y) \parallel p(x)p(y)) = \sum_{x} \sum_{y} p(x,y) \log \frac{p(x,y)}{p(x)p(y)}$$

This concept extends naturally to multiple variables through total correlation, $C(X_1, X_2, \cdots, X_n)$, which captures redundancy across a set of n variables:

$$C(X_1, X_2, \cdots, X_n) = \sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} p(x_1, x_2, \cdots, x_n) \log \frac{p(x_1, x_2, \cdots, x_n)}{p(x_1) p(x_2) \cdots p(x_n)}$$

A high mutual information value indicates redundancy among the tests, while a low value suggests that the tests are independent and provides unique information to diagnose the unexpected outcome. To standardize this measure, the total correlation *per observation* is calculated, and an independence score, ranging between 0 and 1, is defined as 1 - mutual information.

To combine precision, recall, and independence into a single metric, we can combine the three scores using the arithmetic mean, harmonic mean, or quadratic mean. The differences among these means are minimal when the three metrics are similar. However, as the differences among the metrics increases, the harmonic mean tends to produce the smallest overall score, as it penalizes low values, while the quadratic mean tends to produce the largest score by rewarding higher values more. For simple interpretation of the score, the arithmetic mean is preferred, while in applications where the difference between precision, recall, and independence need to be penalized or rewarded more, the

harmonic and quadratic mean should be considered.

4.1. Toy Example Revisited

Returning to the step count example introduced in Section 3.1, the logic regression model is fitted to the three analysis checks described previously to generate the prediction of the unexpected outcome, which is whether the number of days with fewer than 8,000 steps is greater than 5. The predictions from the logic regression model can be compared with the simulated true outcome for calculating the precision and recall metrics. Figure 3 shows the best-fitting logic regression model, which is a combination of test1 ("mean step count is below 8,200") and test3 ("standard deviation exceeds 2,500") with an OR operator. In other words, if either test1 or test3 is true, then we would predict an unexpected outcome in the analysis (i.e. the number of days with fewer than 8,000 steps is greater than 5).

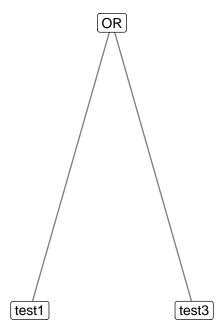


Figure 3. Logic regression model fitted to the three unit tests (test1, test2, test3). The model suggests using an OR rule to combine test1 and test3 to predict the outcome expectation.

Table 1 presents the calculated precision, recall, and independence for the three individual tests and the combined test rule (test1 OR test3) from the logic regression. We also include the metric calculated from fitting a regression tree model to the data to compare the performance of the logic regression model. The harmonic and arithmetic means are included to combine the three measures. The results show that the two tests produced by the logic regression can accurately predict 83.6% cases of all actual unexpected results in the simulation data. Furthermore, 82.1% of all predicted unexpected results were in fact observed to be unexpected.

Table 1. Accuracy (precision and recall) and parsimony (independence) metrics for each individual unit test and for the combined test rule (test1 OR test3) derived from the logic regression model. The harmonic and arithmetic means of the three metrics are included to evaluate the quality of the unit tests in diagnosing unexpected step counts (more than five days with fewer than 8,000 steps).

tests	precision	recall	independence	harmonic	arithmetic
test1	0.482	0.964	1.000	0.730	0.815
test2	0.214	1.000	1.000	0.450	0.738
test3	0.589	0.805	1.000	0.762	0.798
test1 OR test3	0.821	0.836	0.999	0.879	0.886
regression tree	0.821	0.836	1.000	0.879	0.886

For comparison, the regression tree produces a similar prediction to the logic regression, by first splitting on test1 and then splitting on test3, and results in the same accuracy and overall score as the logic regression model. However, we argue that the logic regression tree shown in Figure 3 is more interpretable for our purposes because it provides a direct representation of which combinations of analysis checks lead to unexpected outcomes. The logic regression tree is also directly comparable to other diagnostic tech-

niques, which we discuss further in Section 6.

5. Application

In the study of the health effects of outdoor air pollution, one area of interest is the association between short-term, day-to-day changes in particulate matter air pollution and daily mortality counts. Substantial work has been done to study this question and to date, there appears to be strong evidence of an association between particulate matter less than $10 \ \mu g/m^3$ in aerodynamic diameter (PM10) and daily mortality from all non-accidental causes [Samet et al., 2000]. For our second example, we use the problem of studying PM10 and mortality along with data from the National Morbidity, Mortality, and Air Pollution Study (NMMAPS) to demonstrate how our analysis validation checks described in Section 4 can be applied.

The typical approach to studying the association between PM10 and mortality is to apply a generalized linear model with a Poisson link to relate daily mortality counts to daily measures of PM10. Based on previous work and the range of effect sizes published in the literature, an analyst might expect the coefficient for PM10 in this GLM to lie between [0, 0.005], after adjusting for daily temperature [?Welty and Zeger, 2005]. Observing an estimated coefficient outside of this interval would be highly unusual and would warrant a serious re-examination of the analysis process. Therefore, our unexpected outcome in this analysis will be the binary indicator of whether the estimated coefficient for PM10 in the GLM lies outside of the interval [0, 0.005]. In addition to providing a more substantial problem for our methods, this example also demonstrates how the procedure presented in Section 4 can be used to select cutoff values in the analysis checks to diagnose an unexpected PM10 coefficient from the generalized linear

model.

This PM10 coefficient expectation can be framed as an analysis check that fails, labelled as 1, if the estimate of the PM10 coefficient (adjusted for temperature) is outside the range [0, 0.005], and 0 if it is within. Multiple factors can affect the estimated PM10 coefficient, such as the sample size, the strength of the correlation between mortality and PM10, and the strength of the correlation between mortality and temperature. Analysts may expect a reasonable sample size to ensure the reliability of the coefficient estimate. Outliers in the three variables can also leverage the coefficient. While these are possible factors that could affect the analysis result, it is not clear what the cutoff values for these checks should be to determine a failure. Here we consider a list of checks in Table 2 with varied cutoff values for each:

Table 2. A list of checks considered for the generalized linear model of mortality on PM10 and temperature. The checks are based on the sample size, correlation between mortality and PM10, correlation between mortality and temperature, and univariate outlier detection. Multiple cutoff values are specified for each check to determine a failure.

the check fails if ...

Sample size less than or equal to 200

Sample size less than or equal to 400

Sample size less than or equal to 600

Sample size less than or equal to 800

Mortality-PM10 correlation less than -0.03

Mortality-PM10 correlation less than -0.04

Mortality-PM10 correlation less than -0.05

Mortality-PM10 correlation less than -0.06

Mortality-temperature correlation greater than -0.3

the check fails if ...

Mortality-temperature correlation greater than -0.4

Mortality-temperature correlation greater than -0.45

Mortality-temperature correlation greater than -0.35

Outlier(s) are presented in the variable PM10

Outlier(s) are presented in the variable mortality

5.1. Data Simulation

To generate replicates of the dataset, we first generate the correlation matrix of the three variables (PM10, mortality, and temperature) in a grid and then use a Gaussian copula to generate a multivariate normal distribution based on the specified correlation matrix and sample size. The multivariate normal distribution is transformed using the normal CDF before the inverse CDF of the assumed distributions of the three variables is applied. To determine the appropriate distribution of each variable, various distributions are fitted and compared. This includes poisson and negative binomial for mortality; gamma, log-normal, exponential, weibull, and normal for PM10 and temperature; and beta for PM10 after rescaling the data to [0, 1].

To ensure a reasonable likeness to data that might be used in such an analysis, we use characteristics of the observed dataset to refine our simulations. AIC is used to determine the best distribution fit for each variable with the QQ-plot presented in Figure 4 to evaluate the fit. AIC suggests a negative binomial distribution for mortality, a beta distribution for PM10 (multiple by 100 to recover the original scale), and a Weibull distribution for temperature. To include the potential effect of outliers, we add a single outlier to the data for both the mortality and PM10 variables.

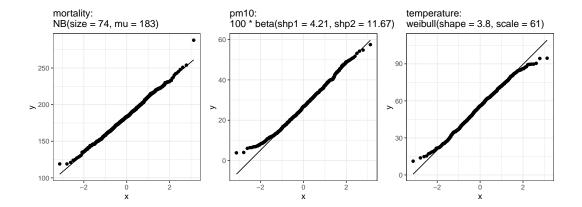


Figure 4. QQ-plot of the distribution fit for mortality, PM10, and temperature based on the fitted distribution from the original data. The fitted distribution is compared to the observed data to assess the distribution fit.

A logic regression is fitted using all variations of the tests in Table 2 to predict whether the PM10 coefficient is unexpected. Figure 5 shows the optimal logic regression tree from the fitted model. Precision, recall, and independence score, along with their harmonic and arithmetic mean are calculated in Table 3.

tree 1 out of 1 total size is 4

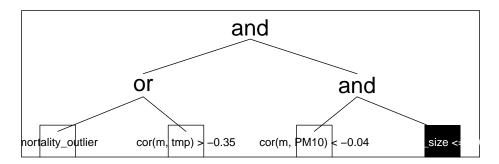


Figure 5. Logic regression model fitted to the fourteen unit tests and the outcome expectation (unexpected) as the response variable. The model suggests the relationship: (sample size greater than 200 AND mortality-PM10 correlation < -0.04) AND (mortality-temperature correlation > -0.35 OR there exist mortality outlier) to predict the unexpected PM10 coefficient. [sorry the proper plot is not ready].

Table 3. Accuracy (precision and recall) and parsimony (independence) metrics derived from the logic regression model, along with harmonic and arithmetic means, for individual unit tests (1: sample size, 2: mortality-PM10 correlation, 3: mortality-temperature correlation, 4: mortality outlier), and the combined test rule 5: (sample size AND mortality-PM10 correlation) AND (mortality-temperature correlation OR mortality outlier).

tests	precision	recall	overlapping	independence	harmonic	arithmetic
1	0.087	0.215	0	1	0.175	0.434
2	0.988	0.610	0	1	0.822	0.866
3	0.392	0.581	0	1	0.569	0.658
4	0.649	0.641	0	1	0.732	0.763
5	0.760	0.880	0	1	0.869	0.880

As indicated in Figure 5, the logic regression model picks up the following cutoff values for each type of check:

- sample size larger than 200
- mortality-temperature correlation greater than -0.35
- mortality-PM10 correlation less than -0.04
- mortality data contains outliers that are detected by the univariate outlier detection

The tree structure suggests checking mortality-PM10 correlation and a sample size larger than 200 with an additional check of either outlier on mortality or correlation between mortality and temperature. This combined check rule generates a precision of 0.76 and a recall of 0.88 for predicting the unexpected PM10 coefficient. The single check, cor(m, PM10) < -0.03, is also powerful with a high precision of 0.988, but the low recall value of 0.61 suggests its high false positive rate, as compared to the combined rule suggested

by the logic regression.

As shown in Figure 5, there is no single analysis check in the tree that predicts an unexpected outcome. rather at least three checks in the tree must be TRUE in order for the model to predict an unexpected outcome. Given the high independence of the tests (Table 3), this suggests that unexpected results are only likely after multiple anomalies are observed in the data.

6. Discussion

In this paper we have developed an approach to using analysis validation checks to externalize the assumptions about the data and analysis tools made during the data analysis process. These checks can serve as a useful summary of the analyst's thought process and can desscribe how characteristics of the data may lead to unexpected outcomes. Using logic regression, we can develop a graphical summary of the analysis validation checks as well as use the logic regression fitting process to choose the optimal set of checks. The logic regression model can also be used to develop summaries of the precision and recall of the collection of analysis validation checks in predicting the likelihood of an unexpected outcome. We demonstrated our method on an example relating daily mortality to outdoor air pollution data.

An interesting connection can be drawn between our logic regression trees and a tool used in systems engineering known as a fault tree. A fault tree is used for conducting a structured risk assessment and has a long history in aviation, aerospace, and nuclear power applications [Vesely et al., 1981]. A fault tree is a graphical tool that describes the possible combinations of causes and effects that lead to an anomaly. At the top of the tree is a description of an anomaly. The subsequent branches of the tree below the top

event indicate possible causes of the event immediately above it in the tree. The tree can then be built recursively until we reach a root cause that cannot be further investigated. Each level of the tree is connected together using logic gates such as AND and OR gates. The leaf nodes of the tree indicate the root causes that may lead to an anomaly. While the logic regression tress are not identical to fault trees, they share many properties, such as the tree-based structure and the indicator of root causes at the leaf nodes. Perhaps more critically, both serve as graphical summaries of the assumptions made in a problem and the specific violations of those assumptions that could lead to an unexpected result. While fault trees are often used to discover the root cause of an anomaly after it occurs, an important use case for fault trees is to develop a comprehensive understanding of a system before an anomaly occurs [Michael et al., 2002].

TODO

- how to systematically simulate data is still unknown
- plotting is a critical way to check data and they can still be frame into checks.
 i.e. the density/ histogram suggests there are outliers. It is a open problem to how to encode the visualization into checks.
- currently no automated way to generate checks. It is interesting to see how check generation can be automated, although it requires the inputs from experts across a wide array of common scenarios.
- checks are also closely related to the concept of unit tests in software engineering.
 While unit tests are designed to isolate and test specific aspects of the code, it is difficult for analysis validation check to do so.
- There are cost and benefit on setting expectation on different granularity. At the lowest level, one may have a plan for each data entry and every data handling

steps. This requires more work from the analysts and may not be practical in practice. For more complex analyses, analysts may divide the analysis into sections and set expectations for each. They can then focus on the specific sections flagged by the tests and sub-divide the sections to set expectation and diagnose the analysis in a hierarchical manner.

7. Conclusion

TODO

8. Acknowledgement

The article is created using Quarto [Allaire et al., 2022] in R [R Core Team, 2023]. The source code for reproducing the work reported in this paper can be found at: https://github.com/huizezhang-sherry/paper-avc.

References

- J.J. Allaire, Charles Teague, Carlos Scheidegger, Yihui Xie, and Christophe Dervieux.

 Quarto, January 2022. URL https://github.com/quarto-dev/quarto-cli.
- Li Cai and Yangyong Zhu. The challenges of data quality and data quality assessment in the big data era. *Data science journal*, 14:2–2, 2015.

Corinna Cichy and Stefan Rass. An overview of data quality frameworks. $IEEE\ Access,$ 7:24634–24648, 2019. .

Thomas Donoghue, Bradley Voytek, and Shannon E Ellis. Teaching creative and practi-

- cal data science at scale. Journal of Statistics and Data Science Education, 29(sup1): S27–S39, 2021.
- Tony Fischetti. assertr: Assertive Programming for R Analysis Pipelines, 2023. URL https://CRAN.R-project.org/package=assertr. R package version 3.0.1.
- Garrett Grolemund and Hadley Wickham. A Cognitive Interpretation of Data Analysis.

 International Statistical Review, 82(2):184–204, 08 2014. URL https://onlinelibrary.

 wiley.com/doi/10.1111/insr.12028.
- Ken Gu, Madeleine Grunde-McLaughlin, Andrew McNutt, Jeffrey Heer, and Tim Althoff. How do data analysts respond to ai assistance? a wizard-of-oz study. In *Proceedings of the CHI Conference on Human Factors in Computing Systems*, pages 1–22, 2024.
- Richard Iannone, Mauricio Vargas, and June Choe. pointblank: Data Validation and Organization of Metadata for Local and Remote Tables, 2024. URL https://CRAN.R-project.org/package=pointblank. R package version 0.12.2.
- Chen Li, Emily Chan, Paul Denny, Andrew Luxton-Reilly, and Ewan Tempero. Towards a framework for teaching debugging. In *Proceedings of the Twenty-First Australasian Computing Education Conference*, pages 79–86, 2019.
- Stamatelatos Michael, D Joane, F Joseph, M Joseph, and R Jan. Fault tree handbook with aerospace applications. NASA Office of Safety and Mission Assurance-NASA Headquarters, Washington, pages 2–8, 2002.
- Roger D Peng. Reproducible research in computational science. *Science*, 334(6060): 1226–1227, 2011.

- Roger D Peng and Stephanie C Hicks. Reproducible research: a retrospective. *Annual review of public health*, 42(1):79–93, 2021.
- Roger D Peng and Hilary S Parker. Perspective on data science. Annual Review of Statistics and Its Application, 9(1):1–20, 2022.
- Roger D. Peng, Athena Chen, Eric Bridgeford, Jeffrey T. Leek, and Stephanie C. Hicks. Diagnosing Data Analytic Problems in the Classroom. *Journal of Statistics and Data Science Education*, 29(3):267–276, September 2021. URL https://doi.org/10.1080/26939169.2021.1971586.
- Anne Helby Petersen and Claus Thorn Ekstrøm. datamaid: Your assistant for documenting supervised data quality screening in r. *Journal of Statistical Software*, 90: 1–38, 2019.
- R Core Team. R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, Vienna, Austria, 2023. URL https://www.R-project.org/.
- Ingo Ruczinski, Charles Kooperberg, and Michael LeBlanc. Logic Regression. Journal of Computational and Graphical Statistics, 12(3), September 2003. ISSN 1061-8600.
 . URL https://doi.org/10.1198/1061860032238. Publisher: ASA Website pages = 475-511,.
- Jonathan M Samet, Francesca Dominici, Frank C Curriero, Ivan Coursac, and Scott L Zeger. Fine particulate air pollution and mortality in 20 us cities, 1987–1994. New England journal of medicine, 343(24):1742–1749, 2000.
- Fatimah Sidi, Payam Hassany Shariat Panahy, Lilly Suriani Affendey, Marzanah A. Jabar, Hamidah Ibrahim, and Aida Mustapha. Data quality: A survey of data quality

- dimensions. In 2012 International Conference on Information Retrieval & Knowledge Management, pages 300–304, 2012.
- Mark PJ van der Loo and Edwin de Jonge. Data validation infrastructure for r. *Journal* of Statistical Software, 97:1–33, 2021. URL https://www.jstatsoft.org/article/view/v097i10.
- William E Vesely, Francine F Goldberg, Norman H Roberts, and David F Haasl. Fault tree handbook. Technical report, Nuclear Regulatory Commission Washington DC, 1981.
- Richard Y Wang and Diane M Strong. Beyond accuracy: What data quality means to data consumers. *Journal of management information systems*, 12(4):5–33, 1996.
- Elin Waring, Michael Quinn, Amelia McNamara, Eduardo Arino de la Rubia, Hao Zhu, and Shannon Ellis. *skimr: Compact and Flexible Summaries of Data*, 2022. URL https://CRAN.R-project.org/package=skimr. R package version 2.1.5.
- Leah J Welty and Scott L Zeger. Are the acute effects of particulate matter on mortality in the national morbidity, mortality, and air pollution study the result of inadequate control for weather and season? a sensitivity analysis using flexible distributed lag models. American journal of epidemiology, 162(1):80–88, 2005.
- Chris J Wild and Maxine Pfannkuch. Statistical thinking in empirical enquiry. *International statistical review*, 67(3):223–248, 1999.
- Philip Woodall, Martin Oberhofer, and Alexander Borek. A classification of data quality assessment and improvement methods. *International Journal of Information Quality* 16, 3(4):298–321, 2014.