

My wonderful paper

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ARTICLE HISTORY

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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 typically 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 check*. 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 binary classification metric, while redundancy is measured using mutual information. We demonstrate this approach with a toy example on the fitness step count data and a generalized linear model example examining the effect of PM10 on 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

- TODO: emphasize trustworthy data science since it is the theme of the special issue

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 it becomes unclear whether discrepancies arise from differing expectations or from the use of statistical techniques.

One might gain insight into analysts' thought process by speaking with them directly or watching screencast videos they produce, such as, TidyTuesday screencast videos. However, direct conversation are not scalable and may not be feasible while creating educational videos requires significant effort from the researchers. Ideally, there could be a way to make these expectations explicit and accessible to others. Even better, if the encoding is machine-readable, we could analyze these expectations and learn from the analysis – 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.

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

The rest of the paper is organized as follows: Section 2 reviews the concept of diagnosing unexpected outcomes and data quality checks. Section 3 introduces the concept of analysis validation check, illustrated with a toy example on fitness step count. Section 4 describes the procedure that quantify how checks combined in logical operators can predict unexpected outcomes. Section 5 applies this procedure to examine the effect of PM10 on mortality in public health in a generalized linear model. Section 6 discusses a few key considerations and Section 7 concludes the paper.

2. Literature review

2.1. *Diagnosing unexpected outcomes in data analysis*

- They shape how we interpret the results and assess whether they are consistent with existing knowledge or indicate the need for updates. [Grolemund and Wickham, 2014]

- [Peng et al., 2021] describes three pedagogical exercises of introducing diagnosing unexpected outcome into a classroom setting.
- what if the expectation is “wrong”

2.2. *Data analysis checks*

A substantial body of literature has addressed the definition of data quality [Cichy and Rass, 2019, more] and developed frameworks, that includes 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 system and database management and support business decision-making in the industry. For research purposes, high-quality data ensures the credibility of scientific findings and supports reproducibility and reusability 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 data producers or collectors who have the full knowledge of data in hand, prompting more interest towards the 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], provides basic data screening and reporting, 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.

3. Analysis validation checks

3.1. *Framing expectations as checks*

Expectations represent our beliefs about certain aspects of the analysis, independent of the analysis itself. When outcomes deviate from these expectations, analysts often revisit the analysis cycle 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 frames these expectations or assumptions as explicit checks that returns a TRUE or FALSE output given the data analyzed at hand. Inspired by data validation checks [[van der Loo and de Jonge, 2021](#)], where ensure datasets meet expected format and quality, analysis validation checks reverse the approach: they validate the assumptions about the data necessary for the analysis to produce the reported results. This allows the concept to encompass a broad range of checks, such as data quality (i.e. missing data, how the data is structured), data distribution and outliers, bivariate and multivariate relationships between variables, and contextual information. These externalized checks provide insights into analysts' thoughts process process and offer several benefits:

- 1) help students and junior researchers develop skills to diagnose unexpected analysis results,
- 2) serve as clear checkpoints to support replication or application of methods to (new) data,
- 3) align assumptions among researchers from different domain backgrounds, and
- 4) improve analysis transparency, reproducibility, and trustworthiness.

3.2. A toy example

Consider a 30-day step count experiment in public health. Testers 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. While there may be occasional “low” days due to factors such as forgetting to wear their watch or unfavorable weather condition limiting outdoor activities, there are also “high” days after an outdoor hike or intense workout. After 30 days, you review the data and expect no more than five days with step counts falling below the 8,000-step threshold [I think we need a bit more scenario to justify we expect no more than 5 days, say it needs to have at least 25 days for it to be valid for the next stage research??].

To simulation 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.

In this scenario, the outcome is that the number of days with a step count below 8,000 being no more than five. To diagnose potential reasons why this outcome expectation might fail, we can establish a few analysis validation checks. For example, if the average step count is too low, this may suggest there are too many low days, potentially lead 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 unit tests as plan expectations:

- test1: the test fails if the mean step count is below 8,200

- test2: the test fails if the 30th percentile of the step counts is below 8,200
- test3: the test fails if the standard deviation of the step counts exceeds 2,500.

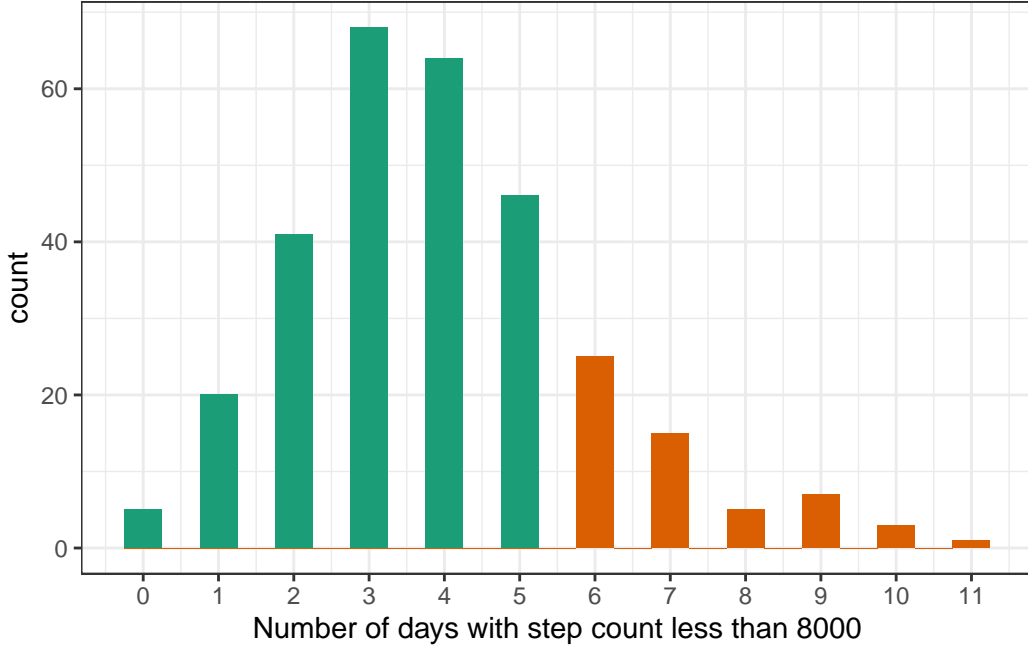


Figure 1. Number of days with fewer than 8,000 steps across 300 simulated 30-day periods. The orange bars indicate instances where the count exceeds five days, representing an unexpected outcome in this scenario.

4. Method

4.1. *A workflow to assess the quality of unit tests*

While some checks are crucial and can lead to unexpected outcomes, others may be tangential to the root cause. In this section, we propose a procedure to measure the violation of checks, combined using logical operators, contribute to an unexpected outcome. A small set of independent checks is considered effective if it translates to unexpected outcomes and Figure 2 provides an overview of the calculation.

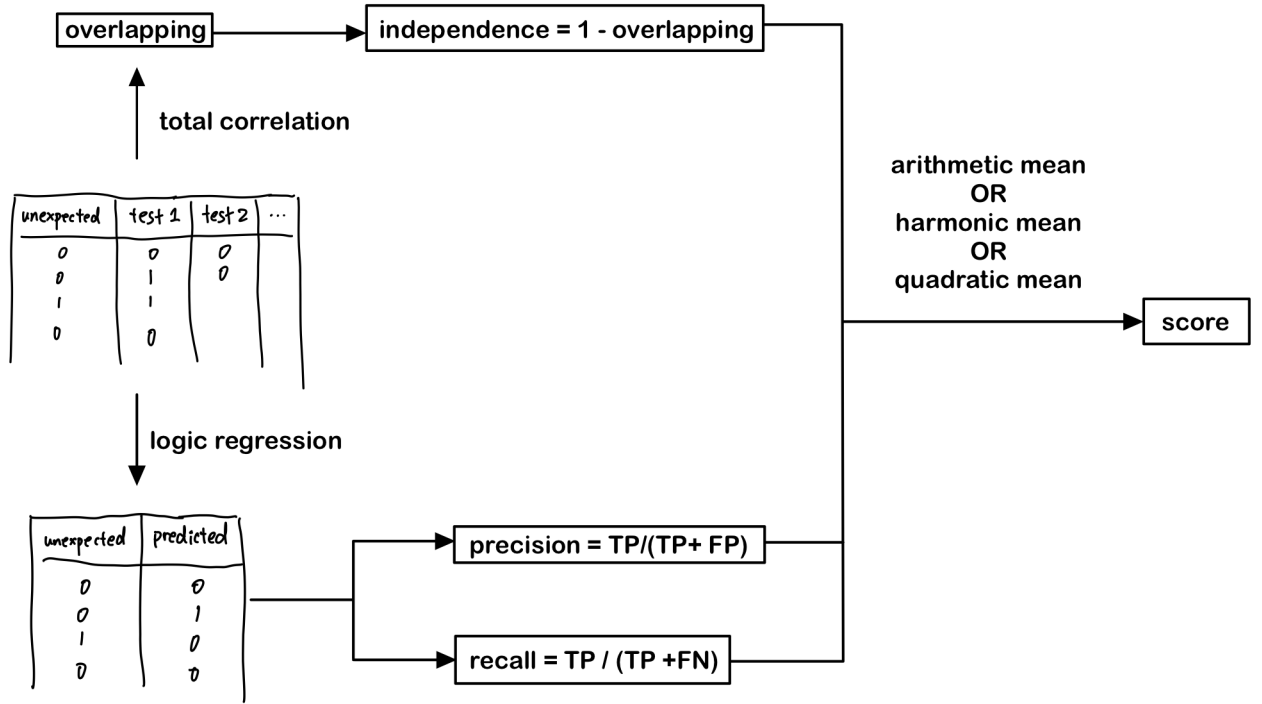


Figure 2. [this is the cap and the plot needs polish]

From the simulated data, the accuracy branch refers to a set of checks' ability to accurately detect unexpected outcomes while minimizing false positives and false negatives. While a false positive can raise caution or skepticism on the data, both false positive and false negative suggest the checks are over 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 checks and whether the outcome is unexpected. 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 methods. The model is then used to predict the outcome expectation based on the checks, and

the prediction is compared to the actual outcome expectation to calculate the precision and recall of the checks.

While tests may score high on accuracy, they may be less effective at explaining the reasons behind unexpected results. This could happen if a set of tests are all tangentially related to the cause of the unexpected results, but none addressing the root cause. It may also occur if the tests are 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, $C(X_1, X_2, \dots, X_n)$, which captures redundancy across a set of n variables:

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

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 $1 - \text{mutual information}$.

To combine precision, recall, and independence into a single metric, mathematical means, such as arithmetic mean, harmonic mean, and quadratic mean can be used. 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.

4.2. *Toy example revisited*

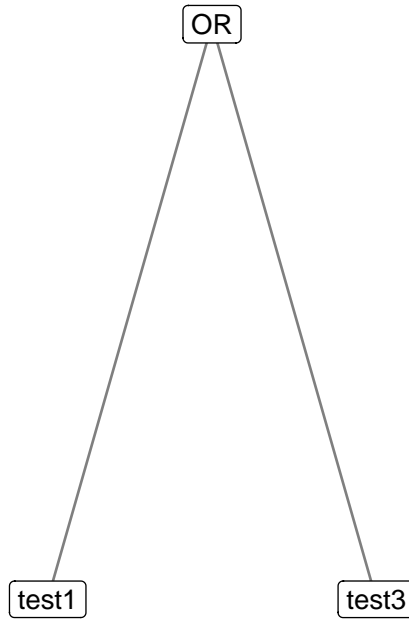


Figure 3. Logic regression model fitted to the three unit tests (test1, test2, test3). The model suggests using an OR rule to combine test1 and test3 to predict the outcome expectation.

Table 1. 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

In the step count example, the logic regression model is fitted to the three unit tests to generate the prediction for calculating precision and recall. Figure 3 shows the chosen logic regression model: a combination of test 1 and test 3 with an OR operator and 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 82.1% of all *predicted unexpected cases*, and 83.6% cases of all *actual unexpected results* in the simulation data. The regression tree produces a similar model of first split on test1 and then split on test3, and results in the same accuracy and overall score as the logic regression model.

5. Application

Consider a generalized linear model (GLM) to study the effect of PM10 on mortality [TODO: provide more context of the mortality-PM10 study]. Analysts may expect a PM10 coefficient between $[0, 0.005]$ after considering the temperature confounding [TODO: reference]. The example demonstrates how the procedure presented in Section 4 can be used to select cutoff values in the checks to diagnose an unexpected PM10 coefficient from the generalized linear model.

This PM10 coefficient expectation can be framed into a check that fails, labelled as 1, if the PM10 coefficient is outside the range $[0, 0.005]$ and 0 if it is within. Multiple factors can affect the 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 the cutoff values for these checks to determine a failure. Here we create 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

the check fails if ...

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

Mortality-temperature correlation greater than -0.35

Mortality-temperature correlation greater than -0.4

Mortality-temperature correlation greater than -0.45

Outlier(s) are presented in the variable PM10

Outlier(s) are presented in the variable mortality

To generate replicate of the data, we first simulate the correlation matrix of the three variables 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 $[0 - 1]$. AIC is used to determine the best distribution fit for each variable with 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 obtain the original scale), and a Weibull distribution for temperature. To include the effect of outlier, we add a

single outlier to the data for both variable mortality and PM10.

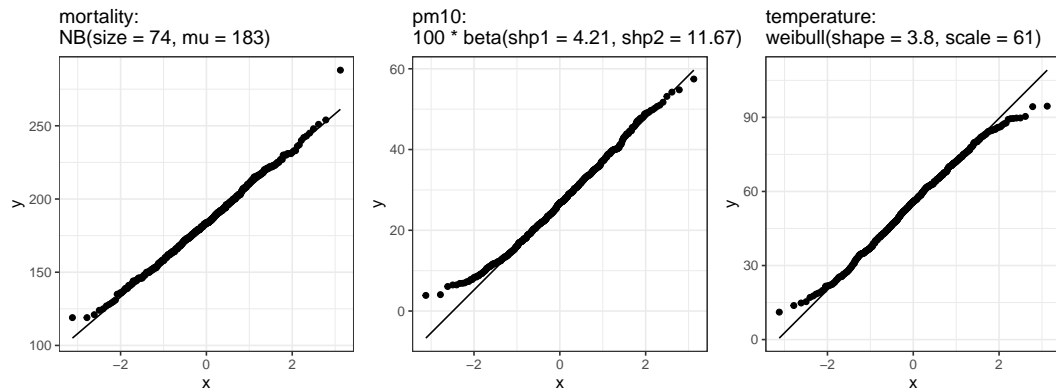


Figure 4. QQ-plot of the distribution fit for mortality, PM10, and temperature based on the fitted distribution from the original data. The fitted distribution is compared to the observed data to assess the distribution fit.

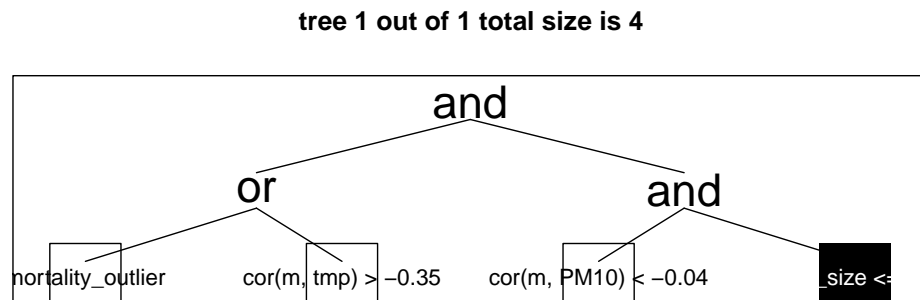


Figure 5. Logic regression model fitted to the fourteen unit tests and the outcome expectation (unexpected) as the response variable. The model suggests the relationship: (sample size *greater than* 200 AND mortality-PM10 correlation < -0.04) AND (mortality-temperature correlation > -0.35 OR there exist 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

A logic regression is fitted to predict whether the PM10 coefficient is unexpected using the checks listed in Table 2 and Figure 5 shows the logic regression tree from the fitted model. Precision, recall, and independence score, along with their harmonic and arithmetic mean are calculated in Table 3. The logic regression model picks up the following cutoff value 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 contain 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.

6. Discussion

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>.

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