

Supplimentary material - A plot is worth a thousand tests: assessing residual diagnostics with visual inference

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Appendix

Effect size derivation

Effect size can be defined as the difference of a parameter for a particular model or distribution, or a statistic derived from a sample. Importantly, it needs to reflect the treatment we try to measure. Centred on a conventional statistical test, we usually can deduce the effect size from the test statistic by substituting the null parameter value. When considering the diagnostics of residual departures, there exist many possibilities of test statistics for a variety of model assumptions. Meanwhile, diagnostic plots such as the residual plot have no general agreement on measuring how strong a model violation pattern is. To build a bridge between various residual-based tests, and the visual test, we focus on the shared information embedded in the testing procedures, which is the distribution of residuals. When comes to comparison of distribution, Kullback-Leibler divergence (@ Kullback and Leibler 1951) is a classical way to represent the information loss or entropy increase caused by the approximation to the true distribution, which in our case, the inefficiency due to the use of false model assumptions.

Following the terminology introduced by Kullback and Leibler (1951), P represents the measured probability distribution, and Q represents the assumed probability distribution. The Kullback-Leibler divergence is defined as $\int_{-\infty}^{\infty} \log(p(x)/q(x))p(x)dx$, where $p(\cdot)$ and $q(\cdot)$ denote probability densities of P and Q .

Let $\mathbf{X}_a = (\mathbf{1}, \mathbf{X})$ denotes the p regressors with n observations, $\mathbf{R}_a = \mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$ denotes the residual operator, and let $\boldsymbol{\varepsilon} \sim N(\mathbf{0}, \sigma^2\mathbf{I})$ denotes the error. Using the Frisch-Waugh-Lovell theorem, residuals $\mathbf{e} = \mathbf{R}_a\boldsymbol{\varepsilon}$. Because $\text{rank}(\mathbf{R}_a) = n - p < n$, \mathbf{e} follows a degenerate multivariate normal distribution and does not have a density. Since the Kullback-Leibler divergence requires a proper density function, we need to simplify the covariance matrix of \mathbf{e} by setting all the off-diagonal elements to 0. Then, the residuals will assumed to follow $N(\mathbf{0}, \text{diag}(\mathbf{R}_a\sigma^2))$ under the null hypothesis that the model is correctly specified. If the model is however misspecified due to omitted variables \mathbf{Z} , or a non-constant variance \mathbf{V} , the distribution of residuals can be derived as $N(\mathbf{R}_a\mathbf{Z}\boldsymbol{\beta}_z, \text{diag}(\mathbf{R}_a\sigma^2))$ and $N(\mathbf{0}, \text{diag}(\mathbf{R}_a\mathbf{V}\mathbf{R}_a'))$ respectively.

By assuming both P and Q are multivariate normal density functions, the Kullback-Leibler divergence can be rewritten as

$$KL = \frac{1}{2} \left(\log \frac{|\Sigma_p|}{|\Sigma_q|} - n + \text{tr}(\Sigma_p^{-1}\Sigma_q) + (\mu_p - \mu_q)' \Sigma_p^{-1} (\mu_p - \mu_q) \right).$$

Then, we can combine the two residual departures into one formula

$$KL = \frac{1}{2} \left(\log \frac{|\text{diag}(\mathbf{R}_a\mathbf{V}\mathbf{R}_a')|}{|\text{diag}(\mathbf{R}_a\sigma^2)|} - n + \text{tr}(\text{diag}(\mathbf{R}_a\mathbf{V}\mathbf{R}_a')^{-1}\text{diag}(\mathbf{R}_a\sigma^2)) + \boldsymbol{\mu}_z^T (\mathbf{R}_a\mathbf{V}\mathbf{R}_a')^{-1} \boldsymbol{\mu}_z \right). \quad (1)$$

When there are omitted variables but constant error variance, the formula can be reduced to

$$KL = \frac{1}{2} (\boldsymbol{\mu}_z^T (\text{diag}(\mathbf{R}_a\sigma^2))^{-1} \boldsymbol{\mu}_z).$$

And when the model equation is correctly specified but the error variance is non-constant, the formula can be reduced to

$$KL = \frac{1}{2} \left(\log \frac{|\text{diag}(\mathbf{R}_a \mathbf{V} \mathbf{R}_a')|}{|\text{diag}(\mathbf{R}_a \sigma^2)|} - n + \text{tr}(\text{diag}(\mathbf{R}_a \mathbf{V} \mathbf{R}_a')^{-1} \text{diag}(\mathbf{R}_a \sigma^2)) \right).$$

Since we assume $\sigma = 1$ for the heteroskedasticity model, the final form of the formula is

$$KL = \frac{1}{2} \left(\log \frac{|\text{diag}(\mathbf{R}_a \mathbf{V} \mathbf{R}_a')|}{|\text{diag}(\mathbf{R}_a)|} - n + \text{tr}(\text{diag}(\mathbf{R}_a \mathbf{V} \mathbf{R}_a')^{-1} \text{diag}(\mathbf{R}_a)) \right).$$

Experiment setup

Mapping of subjects to experimental factors

Mapping of subjects to experimental factors is an important part of experiment design. Essentially, we want to maximum the difference in factors exposed to a subject. For this purpose, we design an algorithm to conduct subject allocation. Let L be a set of available lineups and S be a set of available subjects. According to the experimental design, the availability of a lineup is associated with the number of subjects it can assign to. For lineups with uniform fitted value distribution, this value is 11. And other lineups can be allocated to at most five different subjects. The availability of a subject is associated with the number of lineups that being allocated to this subject. A subject can view at most 18 different lineups.

The algorithm starts from picking a random subject $s \in S$ with the minimum number of allocated lineups. It then tries to find a lineup $l \in L$ that can maximise the distance metric D and allocate it to subject s . Set L and S will be updated and the picking process will be repeated until there is no available lineups or subjects.

Let F_1, \dots, F_q be q experimental factors, and f_1, \dots, f_q be the corresponding factor values. We say f_i exists in L_s if any lineup in L_s has this factor value. Similarly, $f_i f_j$ exists in L_s if any lineup in L_s has this pair of factor values. And $f_i f_j f_k$ exists in L_s if any lineup in L_s has this trio of factor values. The distance metric D is defined between a lineup l and a set of lineups L_s allocated to a subject s if L_s is non-empty:

$$D = C - \sum_{1 \leq i \leq q} I(f_i \text{ exists in } L_s) - \sum_{\substack{1 \leq i \leq q-1 \\ i < j \leq q}} I(f_i f_j \text{ exists in } L_s) - \sum_{\substack{1 \leq i \leq q-2 \\ i < j \leq q-1 \\ j < k \leq q}} I(f_i f_j f_k \text{ exists in } L_s)$$

where C is a sufficiently large constant such that $D > 0$. If L_s is empty, we define $D = 0$.

The distance measures how different a lineup is from the set of lineups allocated to the subject in terms of factor values. Thus, the algorithm will try to allocate the most different lineup to a subject at each step.

Demographics

Along with the responses to lineups, we have collected a series of demographic information including age, pronoun, education background and previous experience in studies involved data visualization. Figure 1 and 2 provide summary of the demographic data.

As shown in Figure 1, most participants have Diploma or Bachelor degrees, followed by High school or below. The survey data is gender balanced and the majority of participants are between 18 to 39 years old.

Figure 2 shows no particular difference between the number of participants who have previous experience and the number of those who haven't. Age distributions are also similar for these two groups.

Data collection interface

The survey data is collected via a self-hosted website designed by us. Once the participant is recruited from Prolific (ref here), it will be redirected to the entry page of our study website. An image of the entry page is provided in Figure 3. Then, the participant needs to submit the online consent form and fill in the

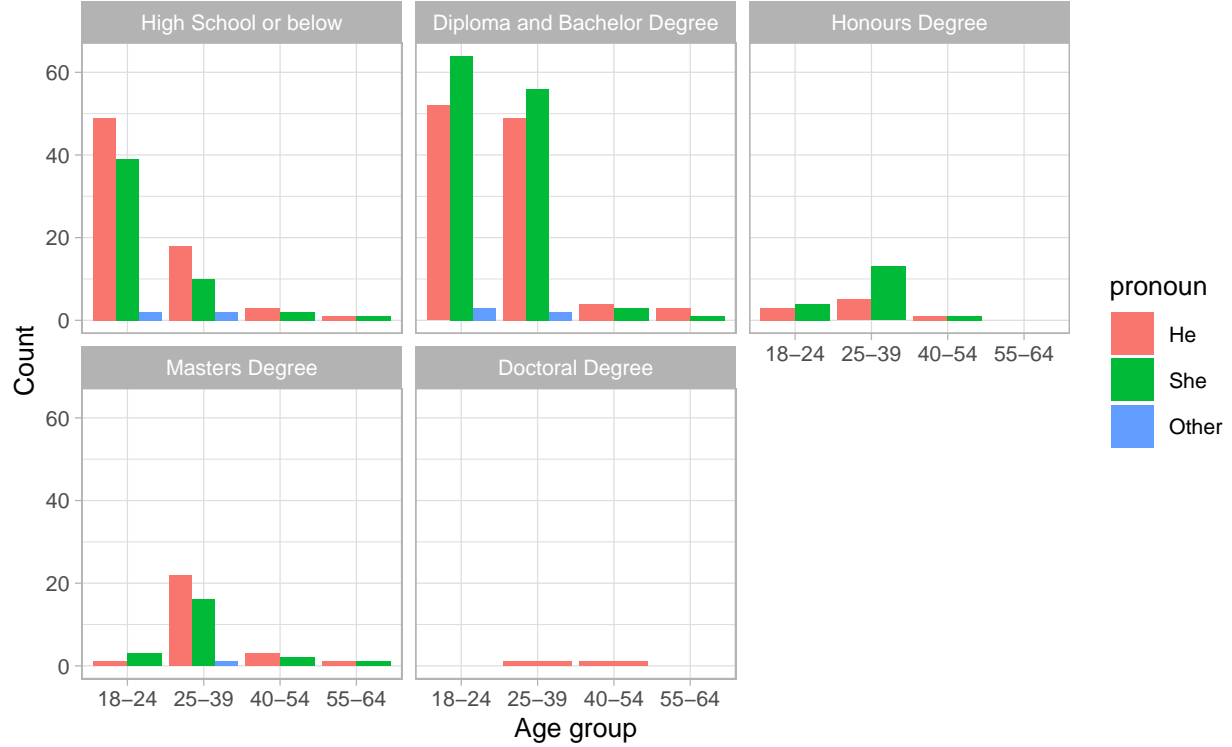


Figure 1: Education distribution of subjects recruited in this study group by age and pronoun.

demographic information as shown in ?? and 5 respectively. Before evaluating lineups, participant also need to read the training page as provide in Figure 6 to understand the process. An example of the lineup page is given in Figure 7. A half of the page is taken by the lineup image to attract participant’s attention. The button to skip the selections for the current lineup is intentionally put in the corner of the bounding box with smaller font size, such that participants will not misuse this functionality.

Batch effect size

We have the same type of model collected over different data collection periods, that may lead to unexpected batch effect. Figure 8 and 9 provide two lineups to examine whether there is an actual difference across data collection periods for non-linearity model and heteroskedasticity model respectively. To emphasize the tail behaviour and display fewer outliers, we use the “letter-value” boxplot (ref here) which is an extension of the number of “letter value” statistics (ref here) to check the weighed proportion of detect over different data collection period. The weighted proportion of detect is calculated by taking the average of c_i of a lineup over a data collection period. Within our research team, we can not identify the data plot from the null plots for these two lineups, result in p -values much greater than 5%.

Figure 10 shows the data plot, where the distribution for the heteroskedasticity patterns are almost identical in period II and III, while the distribution for the non-linearity patterns have a shift in the median. The p -values of the t-test for testing the mean difference across data periods are 0.46 and 0.98 for non-linearity and heteroskedasticity patterns respectively. Both are much greater than 5%. Therefore, both the visual test and the conventional test, there is no clear evidence of batch effect.

Sensitivity analysis for α

The parameter α used for the p -value calculation needs to be estimated from responses to null lineups. However, The way we generate Rorschach lineup is not strictly the same as what suggested in VanderPlas et

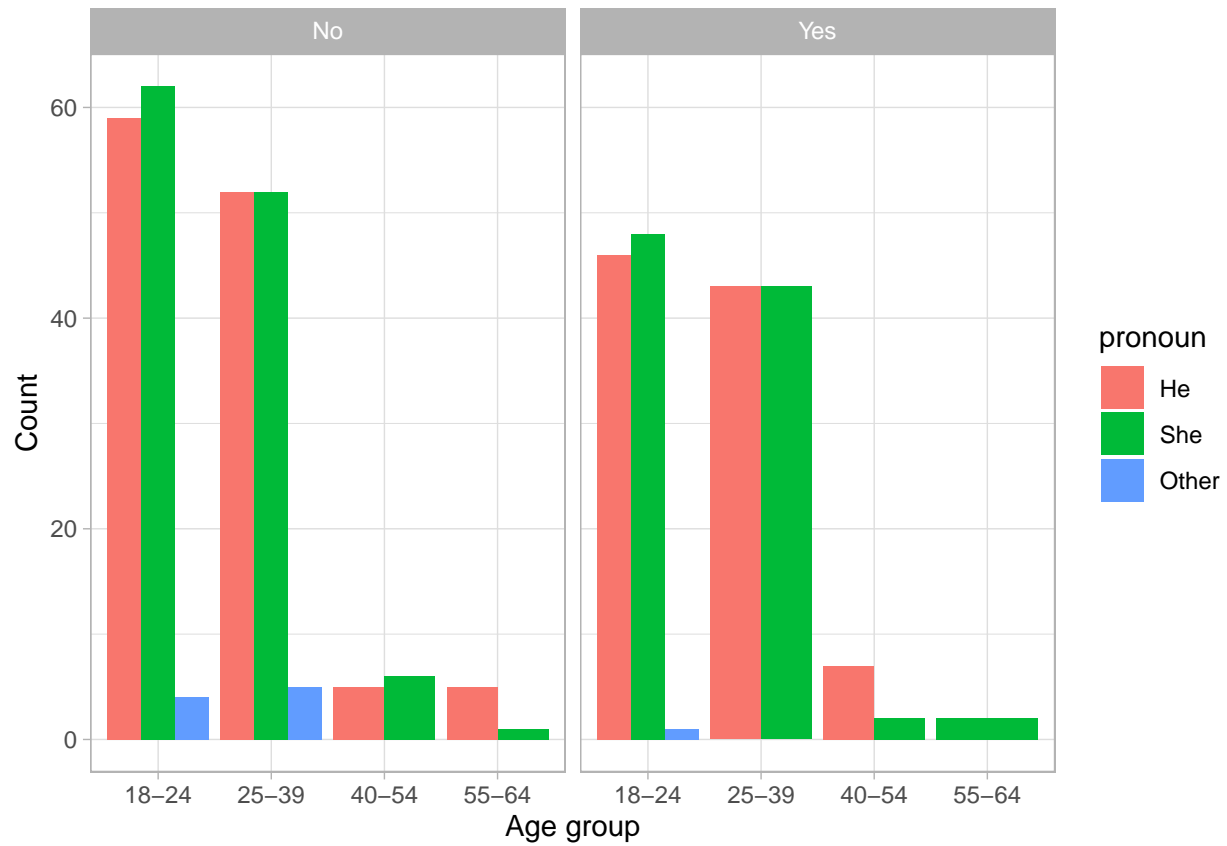


Figure 2: Status of previous experience of subjects recruited in this study group by age and pronoun.

Completion Progress

Visual Inference Please do not refresh the page. If you have any question, please contact the research team via the Prolific messaging system.

Please read the **Explanatory Statement**. To continue, click the checkbox below and hit "Continue".

This study will take you **10-15 minutes**. You must complete the study in **1 hour**.

Please do not refresh the page during the study.

EXPLANATORY STATEMENT
(Prolific users)

Project ID: 29199
Project title: Advances in Artificial Intelligence for Data Visualization: Developing Computer Vision Models to Automate Reading of Data Plots, with Application to Predictive Model Diagnostics

Chief Investigator's name: Emi Tanaka
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Student's name: Weihao Li
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Other investigator's name: Dianne Cook
Department of Econometrics and Business Statistics, Monash University
email: dicook@monash.edu

You are invited to take part in this study. Please read this Explanatory Statement in full before deciding whether or not to participate in this research. If you would like further information regarding any aspect of this project, you are encouraged to contact the researchers via the email addresses listed above.

☐ I have read and understood the Explanatory Statement.

Figure 3: The entry page of the study website.

Completion Progress

Visual Inference Please do not refresh the page. If you have any question, please contact the research team via the Prolific messaging system.

To continue, click the checkbox below and hit "Continue".

Consent Form

Project ID: 29199
Project title: Advances in Artificial Intelligence for Data Visualization: Developing Computer Vision Models to Automate Reading of Data Plots, with Application to Predictive Model Diagnostics
Chief Investigator: Emi Tanaka
Other Investigator's name: Dianne Cook
Student's name: Weihao Li

I consent to the following:

☒ The data that I provide during this research may be used by the research team or other researchers in future research projects.

☒ I have been asked to take part in the Monash University research project specified above. I have read and understood the Explanatory Statement and I hereby consent to participate in this project.

Continue

Figure 4: The consent form provided in the study website.

Completion Progress

Visual Inference Please do not refresh the page. If you have any question, please contact the research team via the Prolific messaging system.

Survey Questions

Please enter your Prolific ID:

Prolific ID

Please select your age category:

☐ 18-24 ☐ 25-39 ☐ 40-54 ☐ 55-64 ☐ 65 or above

Please select your highest level of education:

☐ High school or below ☐ Diploma and Bachelor Degree ☐ Honours Degree ☐ Masters Degree ☐ Doctoral Degree

Please select your preferred pronoun:

☐ He
☐ She
☐ They
☐ Other

Have you participated in any research that requires reading data graphs?

☐ Yes
☐ No

Figure 5: The form to provide demographic information.

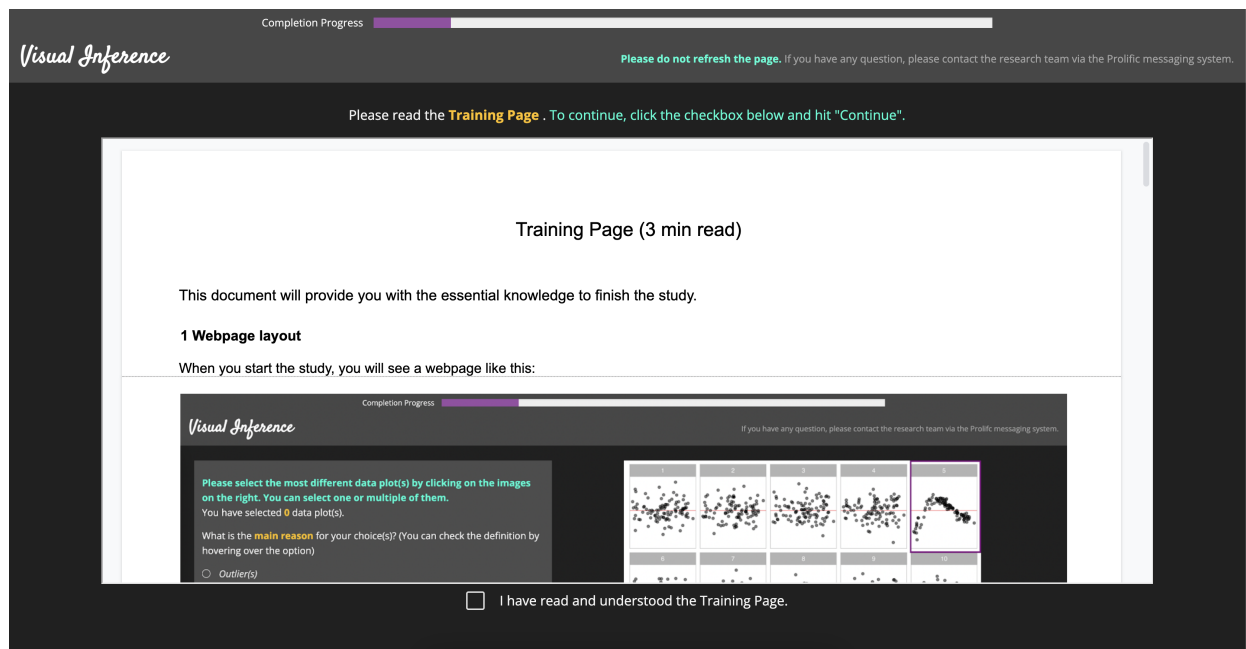


Figure 6: The training page of the study website.

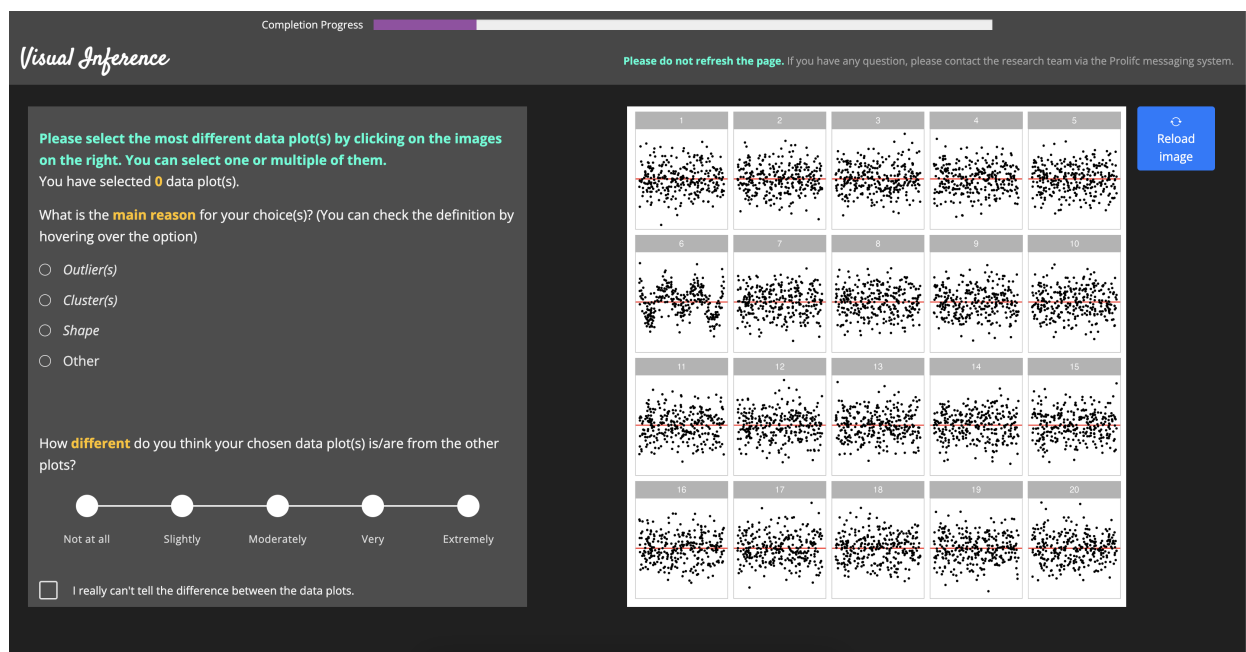


Figure 7: The lineup page of the study website.

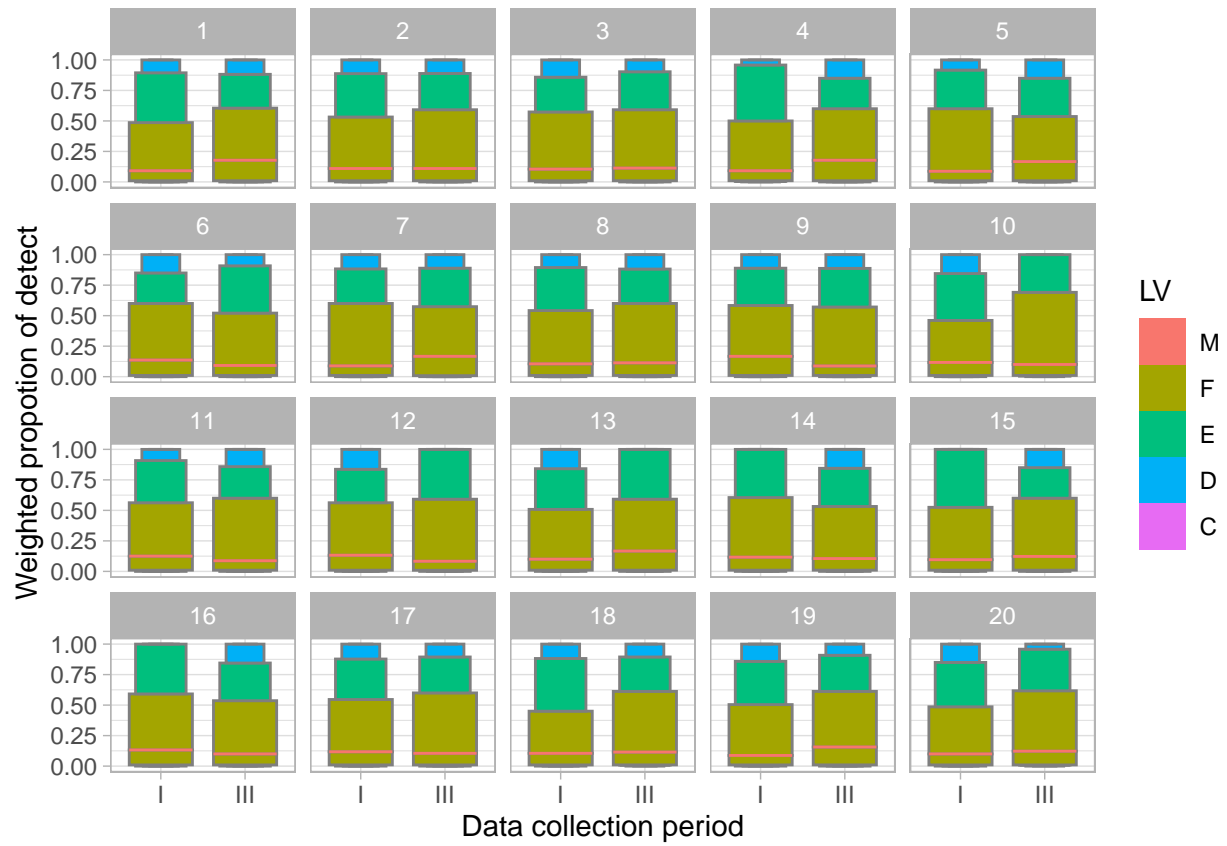


Figure 8: A lineup of “letter-value” boxplots of weighted propotion of detect for lineups over different data collection periods for non-linearity model. Can you find the most different boxplot? The data plot is positioned in panel $2^3 - 1$.

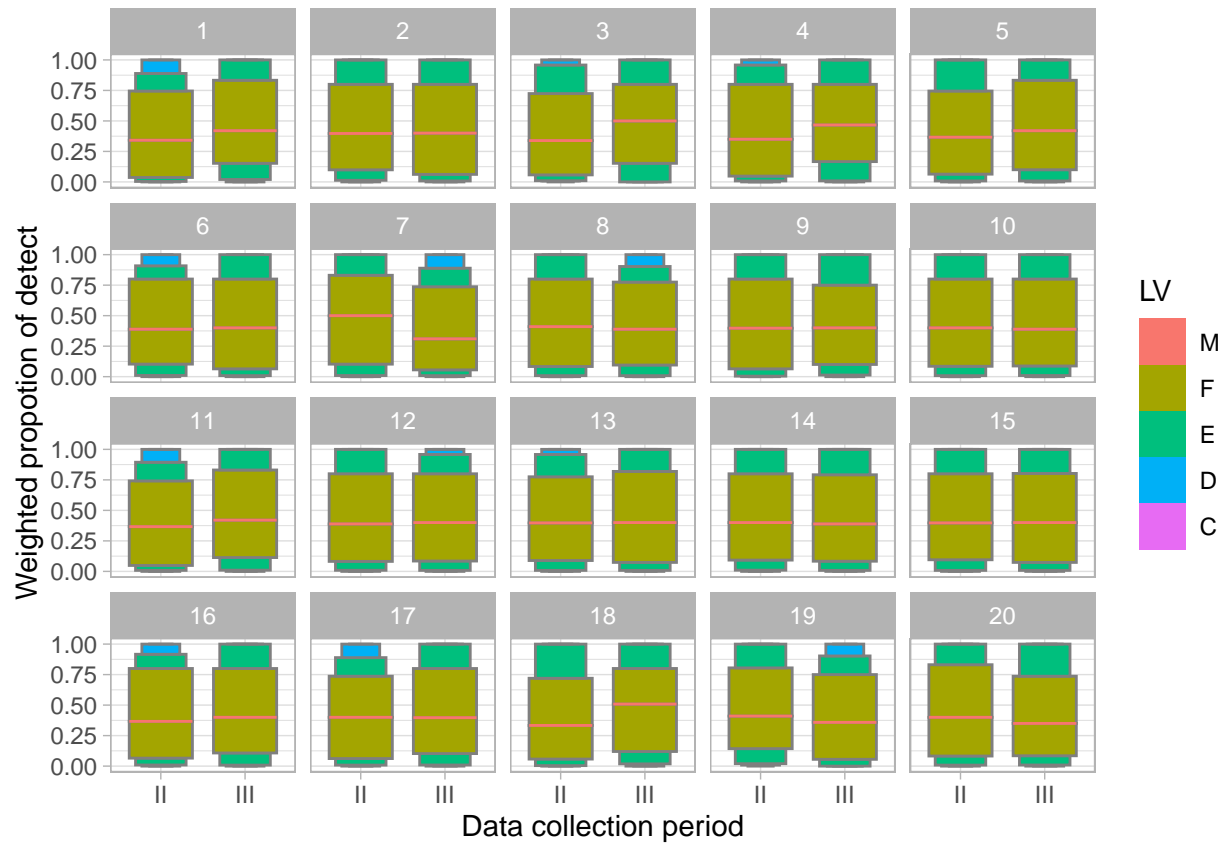


Figure 9: A lineup of “letter-value” boxplots of weighted proportion of detect for lineups over different data collection periods for heteroskedasticity model. Can you find the most different boxplot? The data plot is positioned in panel $2^4 - 2$.

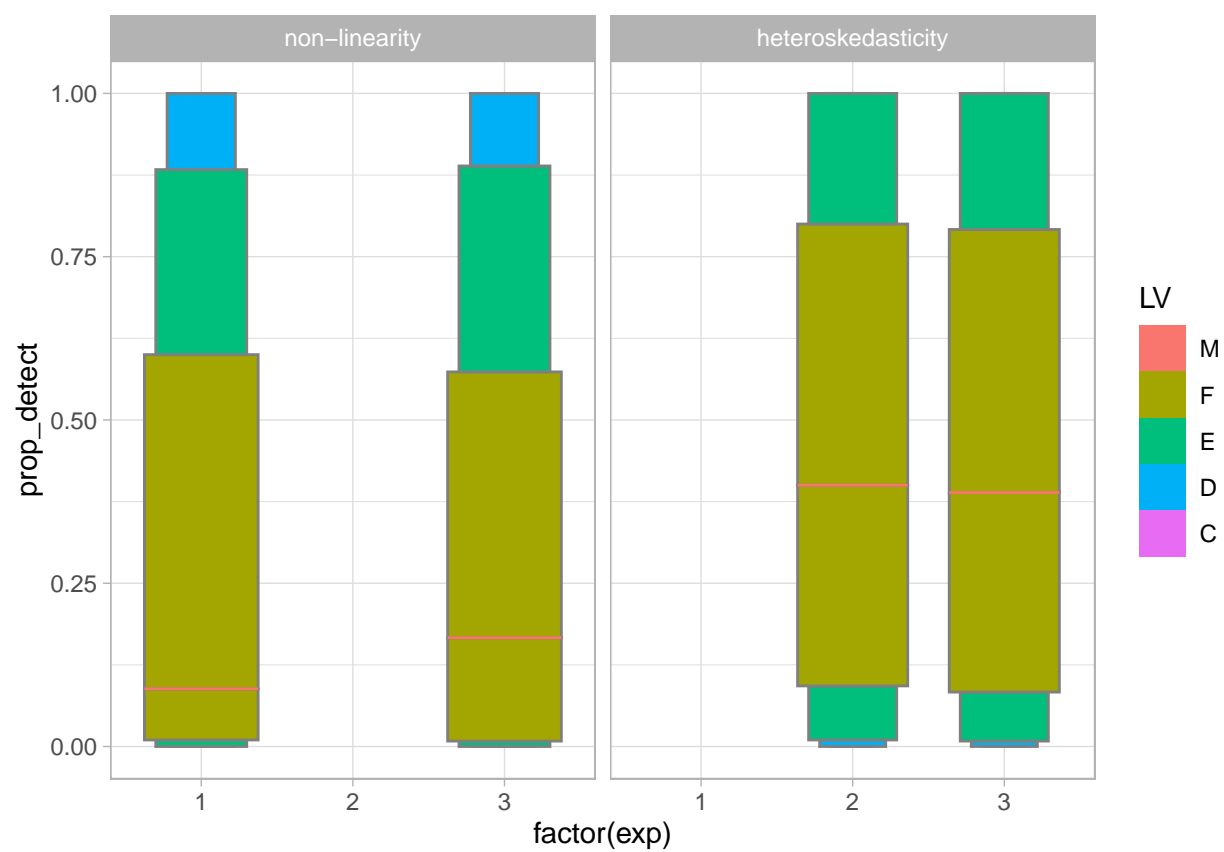


Figure 10: A “letter-value” boxplot of weighted propotion of detect for lineups over different data collection periods.

al. (2021) and Buja et al. (2009). Therefore, we conduct a sensitivity analysis in this section to examine the impact of the variation of the estimator α on our primary findings.

The analysis is conducted by setting up two relatively extreme scenarios, where the α is under or overestimated by 25%. Using the inflated and deflated $\hat{\alpha}$, we recalculate the p -value for every lineup and show the results in Figure 11. It can be observed that p -value changes very little. It is very unlikely the findings will be affected because of the estimate of α .

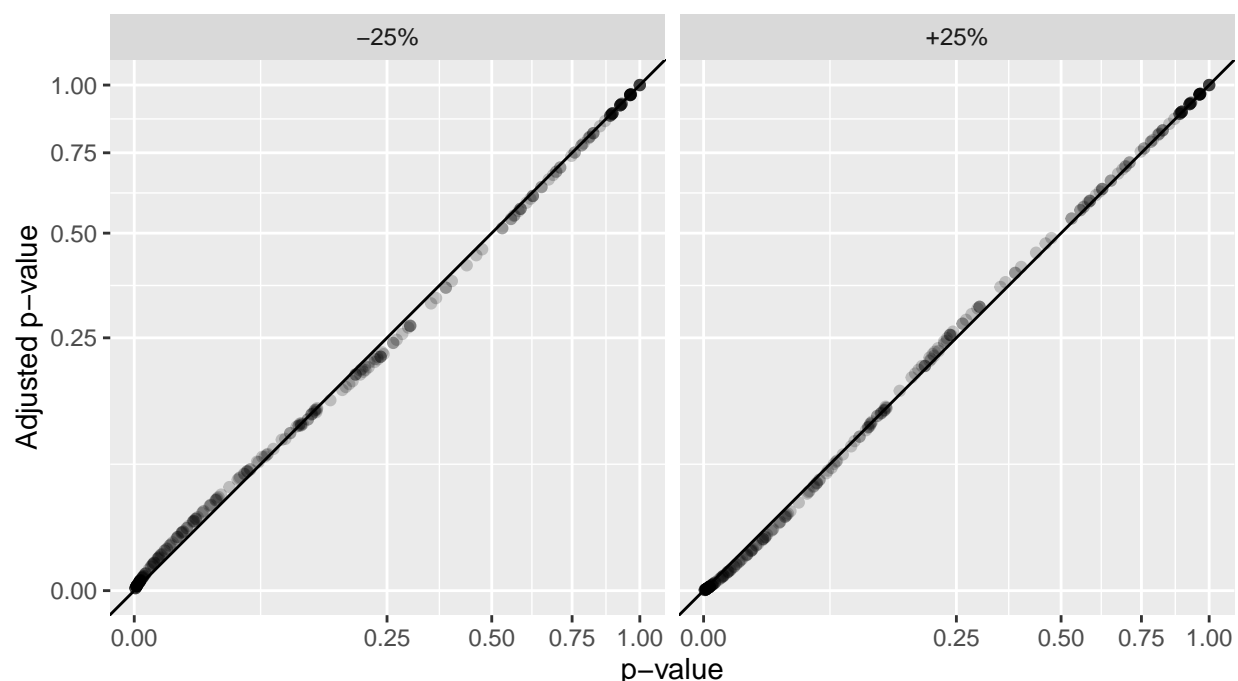


Figure 11: Change of p -values with $\hat{\alpha}$ inflated by 25% and deflated by 25%.

Curious effect of predictor distribution on conventional test power

- Buja, Andreas, Dianne Cook, Heike Hofmann, Michael Lawrence, Eun-Kyung Lee, Deborah F. Swayne, and Hadley Wickham. 2009. "Statistical Inference for Exploratory Data Analysis and Model Diagnostics." *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences* 367 (1906): 4361–83. <https://doi.org/10.1098/rsta.2009.0120>.
- Kullback, Solomon, and Richard A Leibler. 1951. "On Information and Sufficiency." *The Annals of Mathematical Statistics* 22 (1): 79–86.
- VanderPlas, Susan, Christian Röttger, Dianne Cook, and Heike Hofmann. 2021. "Statistical Significance Calculations for Scenarios in Visual Inference." *Stat* 10 (1): e337.