

## ARTICLE TEMPLATE

# A Plot is Worth a Thousand Tests: Assessing Residual Diagnostics with the Lineup Protocol

Weihao Li<sup>a</sup>, Dianne Cook<sup>a</sup>, Emi Tanaka<sup>a,b,c</sup>, Susan VanderPlas<sup>d</sup>

<sup>a</sup>Department of Econometrics and Business Statistics, Monash University, Clayton, VIC, Australia; <sup>b</sup>Biological Data Science Institute, Australian National University, Acton, ACT, Australia; <sup>c</sup>Research School of Finance, Actuarial Studies and Statistics, Australian National University, Acton, ACT, Australia; <sup>d</sup>Department of Statistics, University of Nebraska, Lincoln, Nebraska, USA

## ARTICLE HISTORY

Compiled April 23, 2023

## ABSTRACT

Regression experts consistently recommend plotting residuals for model diagnosis, despite the existence of numerous hypothesis test procedures. This paper provides evidence for why this is good advice, using data from a visual inference experiment. We show how conventional tests are too sensitive to be practically useful, and how the lineup protocol can be used to yield reliable and consistent reading of residual plots for better model diagnosis.

## KEYWORDS

statistical graphics; data visualization; visual inference; hypothesis testing; regression analysis; cognitive perception; simulation; practical significance; effect size

## 1. Introduction

*“Since all models are wrong the scientist must be alert to what is importantly wrong.”*  
(Box 1976)

Diagnosing a model is an important part of analysing data. In linear regression analysis, studying the residuals from a model fit is a common diagnostic activity. Residuals summarise what is not captured by the model, and thus provide the capacity to identify what might be wrong.

We can assess residuals in multiple ways. To examine the their univariate distribution, residuals may be plotted as a histogram or normal probability plot. Using the classical normal linear regression model as an example, if the distribution is symmetric and unimodal, we would consider it to be well-behaved. However, if the distribution is skewed, bimodal, multimodal, or contains outliers, there would be cause for concern. We can also inspect the distribution by conducting a goodness-of-fit test, such as the Shapiro-Wilk normality test (Shapiro and Wilk 1965).

In addition, scatterplots of residuals plotted against the fitted values and each of the explanatory variables, can be used to scrutinize their relationships. If there are

---

CONTACT Weihao Li. Email: [weihao.li@monash.edu](mailto:weihao.li@monash.edu), Dianne Cook. Email: [dicook@monash.edu](mailto:dicook@monash.edu), Emi Tanaka. Email: [emi.tanaka@anu.edu.au](mailto:emi.tanaka@anu.edu.au), Susan VanderPlas. Email: [susan.vanderplas@unl.edu](mailto:susan.vanderplas@unl.edu)

any visually discoverable patterns, the model is potentially inadequate or incorrectly specified. In general, one looks for noticeable departures from the model such as non-linear pattern or heteroskedasticity. A non-linear pattern would suggest that the model needs to have some additional non-linear terms. Heteroskedasticity suggests that the error is dependent on the predictors, and hence violates the independence assumption. However, correctly judging whether NO pattern exists in a residual plot is a difficult task for humans. Humans will almost always will see a pattern (see Kahneman (2011)), so the question that really needs answering is whether any pattern perceived is consistent with randomness, purely sampling variability, or noise. It is especially difficult to teach this to new analysts and students (Loy 2021). To address this, statistical tests are available to check for non-linear patterns (e.g. Ramsey 1969), and heteroskedasticity (e.g. Breusch and Pagan 1979).

Linear regression is a well-established procedure, and there is considerable literature describing diagnostic procedures, e.g. Draper and Smith (1998), Montgomery and Peck (1982), Belsley, Kuh, and Welsch (1980), Cook and Weisberg (1999) and Cook and Weisberg (1982). Interestingly, despite the abundance of conventional tests, ALL of these writings advise that plotting residuals is an essential tool for diagnosing regression model problems:

*Some most useful checks allowed by data plots should be done on a routine basis for every regression.* (Draper and Smith 1998)

*Such formal and informal procedures are complementary, and both have a place in residual analysis.* (Cook and Weisberg 1982)

*In our experience, statistical tests on regression model residuals are not widely used. In most practical situations the residual plots are more informative than the corresponding tests. However, since residual plots do require skill and experience to interpret, the statistical tests may occasionally prove useful.* (Montgomery and Peck 1982)

The common wisdom of experts is that plotting the residuals is indispensable for diagnosing model fits. The ubiquity of this advice is *curious*: investigating why, is the subject of this paper.

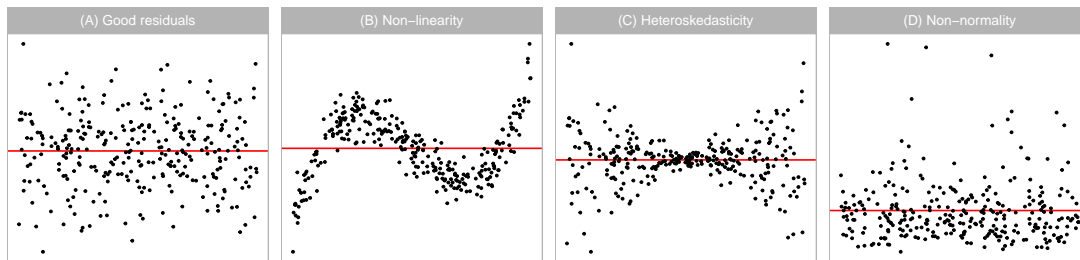
The paper is structured as follows. The next section describes the background on the types of departures that one expects to detect, and outlines a formal statistical process for reading residual plots, called visual inference. Section 4 details the experimental design to compare the decisions made by formal hypothesis testing, and how humans would read diagnostic plots. The results are reported in Section 5. We conclude with a discussion of the presented work, and ideas for future directions.

## 2. Background

### 2.1. Departures from good residual plots

Graphical summaries where residuals are plotted against fitted values, or other functions of the predictors (expected to be approximately orthogonal to the residuals) are considered to be the most important residual plots by Cook and Weisberg (1999). Figure 1A shows an example of an ideal residual plot where points are symmetrically distributed around the horizontal zero line (red), with no discernible patterns. There can be various types of departures from this ideal pattern. Non-linearity, heteroskedasticity and non-normality, shown in Figure 1B,C,D are three commonly checked departures.

Model misspecification occurs if functions of predictors that needed to accurately



**Figure 1.** Example residual vs fitted value plots (red line indicates 0): (A) classically good looking residuals, (B) non-linear pattern indicates that the model has not captured a non-linear association, (C) heteroskedasticity indicating that variance around the fitted model is not uniform, and (D) non-normality where the residual distribution is not symmetric around 0. The latter pattern might best be assessed using a univariate plot of the residuals, but patterns B and C need to be assessed using a residual vs fitted value plot.

describe the relationship between response and predictors are omitted. Any non-linear pattern visible in the residual plot could be indicative of this problem. An example residual plot containing visual pattern of non-linearity is shown in Figure 1B. One can clearly observe the “S-shape” from the residual plot, which corresponds to cubic term that should have been included in the model.

Heteroskedasticity refers to the presence of non-constant error variance in a regression model. It indicates that the distribution of residuals depends on the predictors, violating the independence assumption. This can be seen in a residual plot as an inconsistent spread of the residuals relative to the fitted values or predictors. An example is the “butterfly” shape shown in Figure 1C, or a “left-triangle” and “right-triangle” shape where the smallest variance occurs at one side of the horizontal axis.

Figure 1D shows a scatterplot where the residuals have a skewed distribution, as seen by the uneven vertical spread. Unlike non-linearity and heteroskedasticity, non-normality is usually detected with a different type of residual plot: a histogram or normal probability plot. Because we focus on scatterplots, non-normality is not one of the departures examined in depth in this paper. (loy\_variations\_2016 discuss related work on non-normality checking.)

## 2.2. Conventionally testing for departures

Many different hypothesis tests are available to detect specific model defects. For example, the presence of heteroskedasticity can usually be tested by applying the White test (White 1980) or the Breusch-Pagan (BP) test (Breusch and Pagan 1979), which are both derived from the Lagrange multiplier test (Silvey 1959) principle that relies on the asymptotic properties of the null distribution. To test specific forms of non-linearity, one may apply the F-test as a model structural test to examine the significance of specific polynomial and non-linear forms of the predictors, or the significance of proxy variables as in the Ramsey Regression Equation Specification Error Test (RESET) (Ramsey 1969). The Shapiro-Wilk (SW) normality test (Shapiro and Wilk 1965) is the most widely used test of non-normality included by many of the statistical software programs. The Jarque-Bera test (Jarque and Bera 1980) is also used to directly check whether the sample skewness and kurtosis match a normal distribution.

Table 1 displays the  $p$ -values from the RESET, BP and SW tests applied to the residual plots in Figure 1. The RESET test and BP test were computed using the `resettest` and `bptest` functions from the R package `lmtest`, respectively. The SW test was computed using the `shapiro.test` from the core R package `stats`. (Although

**Table 1.** Statistical significance testing for departures from good residuals for plots in Figure 1. Shown are the  $p$ -values calculated for the RESET, the BP and the SW tests. The good residual plot (A) is judged a good residual plot, as expected, by all tests. The non-linearity (B) is detected by all tests, as might be expected given the extreme structure.

Plot	Departures	RESET	BP	SW
A	None	0.779	0.133	0.728
B	Non-linearity	0.000	0.000	0.039
C	Heteroskedasticity	0.658	0.000	0.000
D	Non-normality	0.863	0.736	0.000

we didn’t use it, it’s useful to know that the R package `skedastic` (Farrar 2020) also contains a large collection of functions to test for heteroskedasticity.) Although, the RESET test is exact, it requires the selection of a power parameter. Ramsey (1969) recommends a power of four, which we adopted in our analysis. The BP and SW tests are approximate.

We would expect the RESET test for non-linearity to reject residual plot B, the BP test for heteroskedasticity to reject the residual plot C, and the SW test for non-normality to reject residual plot D, which they all do and all tests also correctly fail to reject residual plot A. Interestingly, the BP and SW tests also reject the residual plots exhibiting structure that they weren’t designed for. Cook and Weisberg (1982) explain that most residual-based tests for particular types of departure from model assumptions are also sensitive to other types of departures. This could be considered a Type III error (XXXREF), where the null hypothesis of good residuals is correctly rejected but for the wrong reason. Also, some types of departure can have elements of other types of departure, for example, non-linearity could be viewed as heteroskedasticity. Additionally, other data problems such as outliers can trigger rejection (or not) of the null hypothesis (Cook and Weisberg 1999).

With large sample sizes, hypothesis tests may reject the null hypothesis when there is only a small effect. (A good discussion can be found in Kirk (1996).) While such rejections may be statistically correct, their sensitivity may render the results impractical. A key goal of residual plot diagnostics is to identify potential issues that could lead to incorrect conclusions or errors in subsequent analyses, but minor defects in the model are unlikely to have a significant impact and may be best disregarded for practical purposes. The experiment discussed in this paper specifically addresses this tension between statistical and practical statistics.

### 2.3. Visual test procedure based on lineups

The examination of data plots to infer signal or patterns (or lack thereof) is fraught with variation in the human ability to interpret and decode the information embedded in a graph (Cleveland and McGill 1984). Human examination of diagnostic plots can feel subjective. Ideally we would expect visual evaluation to be done objectively with small amounts of human-to-human variation in reading data plots, but we cannot assume this is the case.

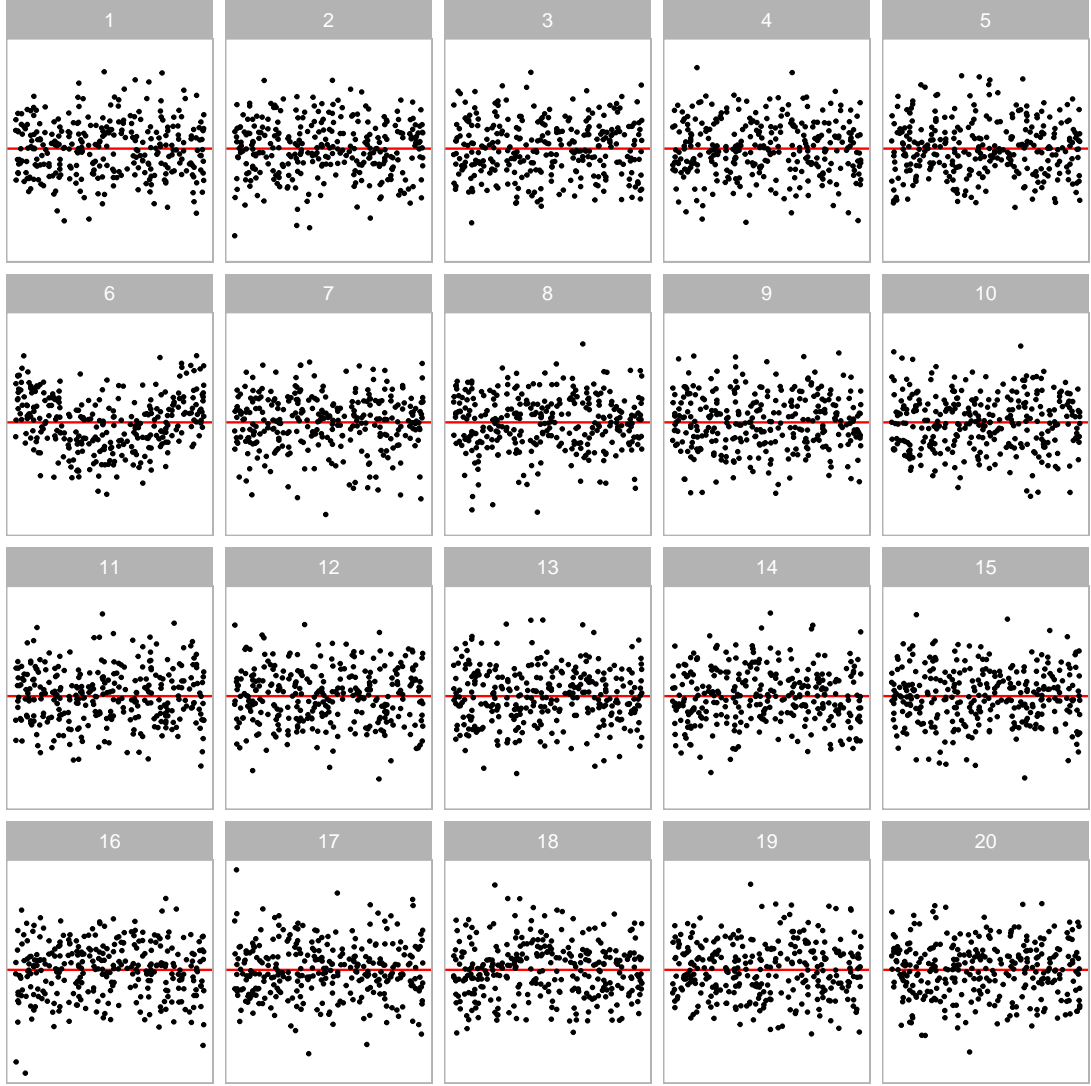
In practice, over-interpretation of a single plot is common. For instance, Roy Chowdhury et al. (2015) described a published example where authors over-interpreted separation between gene groups from a two-dimensional projection of a linear discriminant

analysis. Roy Chowdhury et al. (2015) showed that there were no differences in the expression levels between the gene groups. One solution to over-interpretation is to examine the plot in the context of natural sampling variability assumed by the model, called the lineup protocol, as proposed in Buja et al. (2009). Majumder, Hofmann, and Cook (2013) showed that the lineup protocol is analogous to the null hypothesis significance testing framework. The protocol consists of  $m$  randomly placed plots, where one plot is the data plot, and the remaining  $m - 1$  plots, referred to as the *null plots*, are constructed using the same graphical procedure as the data plot but the data is replaced with null data that is generated in a manner consistent with the null hypothesis,  $H_0$ . Then, an observer who has not seen the data plot is asked to point out the most different plot from the lineup. Under  $H_0$ , it is expected that the data plot would have no distinguishable difference from the null plots, and the probability that the observer correctly picks the data plot is  $1/m$ . If one rejects  $H_0$  as the observer correctly picks the data plot, then the Type I error of this test is  $1/m$ . This protocol requires a priori specification of  $H_0$  (or at least a null data generating mechanism), much like the requirement of knowing the sampling distribution of the test statistic in null hypothesis significance testing framework.

Figure 2 is an example of a lineup protocol. If the data plot at position  $2^2 + 2$  is identifiable, then it is evidence for the rejection of  $H_0$ . In fact, the actual residual plot is obtained from a misspecified regression model with missing non-linear terms.

Data used in the  $m - 1$  null plots is typically simulated. In regression diagnostics, sampling data consistent with  $H_0$  is equivalent to sampling data from the assumed model. As Buja et al. (2009) suggested,  $H_0$  is usually a composite hypothesis controlled by nuisance parameters. Since regression models can have various forms, there is no general solution to this problem, but it sometimes can be reduced to a so called “reference distribution” by applying one of the three methods: (i) sampling from a conditional distribution given a minimal sufficient statistic under  $H_0$ , (ii) parametric bootstrap sampling with nuisance parameters estimated under  $H_0$ , and (iii) Bayesian posterior predictive sampling. The conditional distribution given a minimal sufficient statistic is the best justified reference distribution among the three (Buja et al. 2009). Essentially, null residuals can be simulated by regressing  $N$  i.i.d standard normal random draws on the predictors, then rescaling it by the ratio of residual sum of square in two regressions.

The effectiveness of lineup protocol for regression analysis has been validated by Majumder, Hofmann, and Cook (2013) under relatively simple settings with up to two predictors. Their results suggest that visual tests are capable of testing the significance of a single predictor with a similar power to a t-test, though they express that in general it is unnecessary to use visual inference if there exists a conventional test, and they do not expect the visual test to perform equally well as the conventional test. In their third experiment, where there is not a conventional test, visual test outperforms the conventional test by a large margin. This is encouraging, as it supports the use of visual inference in situations where there are no existing statistical testing procedures. Visual inference has also been integrated into diagnostics for hierarchical linear models where the lineup protocol is used to judge the assumptions of linearity, normality and constant error variance for both the level-1 and level-2 residuals (Loy and Hofmann 2013, Loy and Hofmann (2014) and Loy and Hofmann (2015)).



**Figure 2.** Visual testing is conducted using a lineup, as in the example here. The residual plot computed from the observed data (plot  $2^2 + 2$ , exhibiting non-linearity) is embedded among 19 null plots, where the residuals are simulated from a standard error model. Computing the  $p$ -value requires that the lineup be examined by a number of human judges, each asked to select the most different plot. A small  $p$ -value would result from a substantial number selecting plot  $2^2 + 2$ .

### 3. Calculation of statistical significance and test power

#### 3.1. What is being tested?

In diagnosing a model fit using the residuals, we are generally interested in testing whether “the regression model is correctly specified” ( $H_0$ ) against the broad alternative “the regression model is misspecified” ( $H_a$ ).

However, it is practically impossible to test this broad  $H_0$  with conventional tests, because they need specific structure causing the departure to be quantifiable in order to be computable. For example, the RESET test for detecting non-linear departures is formulated by fitting  $y = \tau_0 + \sum_{i=1}^p \tau_i x_i + \gamma_1 \hat{y}^2 + \gamma_2 \hat{y}^3 + \gamma_3 \hat{y}^4 + u$ ,  $u \sim N(0, \sigma_u^2)$  in order to test  $H_0 : \gamma_1 = \gamma_2 = \gamma_3 = 0$  against  $H_a : \gamma_1 \neq 0$  or  $\gamma_2 \neq 0$  or  $\gamma_3 \neq 0$ . Similarly, the BP test is designed to specifically test  $H_0 : \text{error variances are all}$

equal ( $\zeta_i = 0$  for  $i = 1, \dots, p$ ) versus the alternative  $H_a$  : that the error variances are a multiplicative function of one or more variables (at least one  $\zeta_i \neq 0$ ) from  $e^2 = \zeta_0 + \sum_{i=1}^p \zeta_i x_i + u$ ,  $u \sim N(0, \sigma_u^2)$ .

While a battery of conventional tests for different types of departures could be applied, this is intrinsic to the lineup protocol. The lineup protocol operates as an omnibus test, able to detect a range of departures from good residuals in a single application.

### 3.2. Statistical significance

In hypothesis testing, a  $p$ -value is defined as the probability of observing test results at least as extreme as the observed result assuming  $H_0$  is true. Conventional hypothesis tests usually have an existing method to derive or compute the  $p$ -value based on the null distribution. Here we establish the method to estimate a  $p$ -value for a visual test.

Within the context of visual inference, with  $K$  independent observers, the visual  $p$ -value can be seen as the probability of having as many or more participants detect the data plot than the observed result.

The approach used in Majumder, Hofmann, and Cook (2013) is as follows. Define  $X_j = \{0, 1\}$  to be a Bernoulli random variable measuring whether participant  $j$  detected the data plot, and  $X = \sum_{j=1}^K X_j$  be the total number of observers who detected the data plot. Then, by imposing a relatively strong assumption that all  $K$  evaluations are fully independent, under  $H_0$   $X \sim \text{Binom}_{K, 1/m}$ . Therefore, the  $p$ -value of a lineup of size  $m$  evaluated by  $K$  observer is estimated with  $P(X \geq x) = 1 - F(x) + f(x)$ , where  $F(\cdot)$  is the binomial cumulative distribution function,  $f(\cdot)$  is the binomial probability mass function and  $x$  is the realization of number of observers choosing the data plot.

As pointed out by VanderPlas et al. (2021), this basic binomial model is deficient. It does not take into account the possible dependencies in the visual test due to repeated evaluations of the same lineup, or account for when participants are offered the option to select one or more “most different” plots, or none, from a lineup. They suggest three common lineup scenarios: (1)  $K$  different lineups are shown to  $K$  participants, (2)  $K$  lineups with different null plots but the same data plot are shown to  $K$  participants, and (3) the same lineup is shown to  $K$  participants. Scenario 3 is the most feasible to apply, but has the most dependencies to accommodate for the  $p$ -value calculation. For Scenario 3, VanderPlas et al propose modeling the probability of plot  $i$  being selected from a lineup as  $\theta_i$ , where  $\theta_i \sim \text{Dirichlet}(\alpha)$  for  $i = 1, \dots, m$  and  $\alpha > 0$ . The number of times plot  $i$  being selected in  $K$  evaluations is denoted as  $c_i$ . In case participant  $j$  makes multiple selections,  $1/s_j$  will be added to  $c_i$  instead of one, where  $s_j$  is the number of plots participant  $j$  selected for  $j = 1, \dots, K$ . This ensures  $\sum_i c_i = K$ . Since we are only interested in the selections of the data plot  $i$ , the marginal model can be simplified to a beta-binomial model and thus the visual  $p$ -value is given as

$$P(C \geq c_i) = \sum_{x=c_i}^K \binom{K}{x} \frac{B(x + \alpha, K - x + (m - 1)\alpha)}{B(\alpha, (m - 1)\alpha)}, \quad \text{for } c_i \in \mathbb{Z}_0^+ \quad (1)$$

where  $B(\cdot)$  is the beta function defined as

$$B(a, b) = \int_0^1 t^{a-1} (1-t)^{b-1} dt, \quad \text{where } a, b > 0. \quad (2)$$

We extend the equation to non-negative real number  $c_i$  by applying a linear approximation

$$P(C \geq c_i) = P(C \geq \lceil c_i \rceil) + (\lceil c_i \rceil - c_i)P(C = \lceil c_i \rceil), \quad \text{for } c_i \in \mathbb{R}_0^+, \quad (3)$$

where  $P(C \geq \lceil c_i \rceil)$  is calculated using Equation 1 and  $P(C = \lceil c_i \rceil)$  is calculated by

$$P(C = c_i) = \binom{K}{c_i} \frac{B(c_i + \alpha, K - c_i + (m-1)\alpha)}{B(\alpha, (m-1)\alpha)}, \quad \text{for } c_i \in \mathbb{Z}_0^+. \quad (4)$$

The parameter  $\alpha$  used in Equation 1 and 4 is usually unknown and will need to be estimated from the survey data. An interpretation of  $\alpha$  is that when it is low only a few plots are attractive to the observers and tend to be selected, and when high, most plots are equally likely to be chosen. VanderPlas et al define  $c$ -interesting plot to be if  $c$  or more participants select the plot as the most different. The expected number of plots selected at least  $c$  times,  $E[Z_c]$ , is then calculated as

$$E[Z_c(\alpha)] = \frac{m}{B(\alpha, (m-1)\alpha)} \sum_{\lceil c \rceil}^K \binom{K}{x} B(x + \alpha, K - x + (m-1)\alpha). \quad (5)$$

With Equation 5,  $\alpha$  can be estimated using maximum likelihood estimation. Precise estimation of  $\alpha$ , is aided by evaluation of Rorschach lineups, where all plots are null plots. In a Rorschach, in theory all plots should be equally likely, but in practice some (irrelevant) visual elements may be more eye-catching than others. This is what *alpha* captures, the capacity for extraneous features to distract the observer for a particular type of plot display.

### 3.3. Power of the tests

The power of a model misspecification test is the probability that  $H_0$  is rejected given the regression model is misspecified in a specific way. It is an important indicator when one is concerned about whether model assumptions have been violated. In practice, one might be more interested in knowing how much the residuals deviate from the model assumptions, and whether this deviation is of practical significance.

The power of a conventional hypothesis test is affected by both the true parameter  $\theta$  and the sample size  $n$ . These two can be quantified in terms of effect size  $E$  to measure the strength of the residual departures from the model assumptions. Details about the calculation of effect size are provided in Section 4.2.1 after the introduction of the simulation model used in our experiment. The theoretical power of a test is sometimes not a trivial solution, but it can be estimated if the data generating process is known. We use a predefined model to generate a large set of simulated data under



different effect sizes, and record if the conventional test rejects  $H_0$ . The probability of the conventional test rejects  $H_0$  is then fitted by a logistic regression formulated as

$$Pr(\text{reject } H_0|H_1, E) = \Lambda \left( \log \left( \frac{0.05}{0.95} \right) + \beta_1 E \right), \quad (6)$$

where  $\Lambda(\cdot)$  is the standard logistic function given as  $\Lambda(z) = \exp(z)/(1 + \exp(z))$ . The effect size  $E$  is the only predictor and the intercept is fixed to  $\log(0.05/0.95)$  so that  $\hat{Pr}(\text{reject } H_0|H_1, E = 0) = 0.05$ , the desired significance level.

The power of a visual test on the other hand, may additionally depend on the ability of the particular participant, as the skill of each individual may affect the number of observers who identify the data plot from the lineup (Majumder, Hofmann, and Cook 2013). To address this issue, Majumder, Hofmann, and Cook (2013) models the probability of participant  $j$  correctly picking the data plot from lineup  $l$  using a mixed-effect logistic regression, with participants treated as random effect. Then, the estimated power of a visual test evaluated by a single participant is the predicted value obtained from the mixed effects model. However, this mixed effects model does not work with scenario where participants are asked to select one or more most different plots. In this scenario, having the probability of a participant  $j$  correctly picking the data plot from a lineup  $l$  is insufficient to determine the power of a visual test because it does not provide information about the number of selections made by the participant for the calculation of the  $p$ -value (See Equation 3). Therefore, we directly estimate the probability of a lineup being rejected by assuming that individual skill has negligible effect on the variation of the power. This assumption is not necessary true, but it helps to simplify the model structure, thereby obviating a costly large-scale experiment to estimate complex covariance matrices. The same model given in Equation 6 is applied to model the power of a visual test.

To study various factors contributing to the power of both tests, the same logistic regression model is fit on different subsets of the collated data grouped by levels of factors. These include the distribution of the fitted values, type of the simulation model and the shape of the residual departures.

#### 4. Experimental design

Our experiment was conducted over three data collection periods to investigate the difference between conventional hypothesis testing and visual inference in the application of linear regression diagnostics. Two types of departures, non-linearity and heteroskedasticity, were collected during data collection periods I and II. The data collection period III was designed primarily to measure human responses to null lineups so that the parameter  $\alpha$  in Equation 1 can be estimated. Additional lineups for both non-linearity and heteroskedasticity, using uniform fitted value distributions, were included for additional data, and to avoid participant frustration of too many difficult tasks. Overall, we collected 7974 evaluations on 1152 unique lineups performed by 443 participants throughout three data collection periods.

A summary of the factors used in the experiment can be found in Table 2. There were four levels of the non-linear structure, and three levels of heteroskedastic structure. The signal strength was controlled by error variance ( $\sigma$ ) for the non-linear pattern, and by a ratio ( $b$ ) parameter for the heteroskedasticity. Additionally, three levels of

**Table 2.** Levels of the factors used in data collection periods I, II, III.

Non-linearity		Heteroskedasticity		Common	
Poly Order ( $j$ )	SD ( $\sigma$ )	Shape ( $a$ )	Ratio ( $b$ )	Size ( $n$ )	Distribution of fitted values
2	0.25	-1	0.25	50	Uniform
3	1.00	0	1.00	100	Normal
6	2.00	1	4.00	300	Skewed
18	4.00		16.00		Discrete
			64.00		

sample size ( $n$ ) and four different fitted value distributions were incorporated.

#### 4.1. *Simulating departures from good residuals*

##### 4.1.1. *Non-linearity*

Data collection period I was designed to study the ability of participants to detect the effect of a non-linear term  $\mathbf{z}$  constructed using Hermite polynomials on random vector  $\mathbf{x}$  formulated as

$$\begin{aligned}
\mathbf{y} &= 1 + \mathbf{x} + \mathbf{z} + \boldsymbol{\varepsilon}, \\
\mathbf{x} &= g(\mathbf{x}_{raw}, 1), \\
\mathbf{z} &= g(\mathbf{z}_{raw}, 1), \\
\mathbf{z}_{raw} &= He_j(g(\mathbf{x}, 2)),
\end{aligned}$$

where  $\mathbf{y}$ ,  $\mathbf{x}$ ,  $\boldsymbol{\varepsilon}$ ,  $\mathbf{x}_{raw}$ ,  $\mathbf{z}_{raw}$  are vectors of size  $n$ ,  $He_j(\cdot)$  is the  $j$ th-order probabilist's Hermite polynomials,  $\boldsymbol{\varepsilon} \sim N(\mathbf{0}, \sigma^2 \mathbf{I}_n)$ , and  $g(\mathbf{x}, k)$  is a scaling function to enforce the support of the random vector to be  $[-k, k]^n$  defined as

$$g(\mathbf{x}, k) = (\mathbf{x} - \min(\mathbf{x})) / \max(\mathbf{x} - \min(\mathbf{x})) 2k - k, \quad \text{for } k > 0. \quad (7)$$

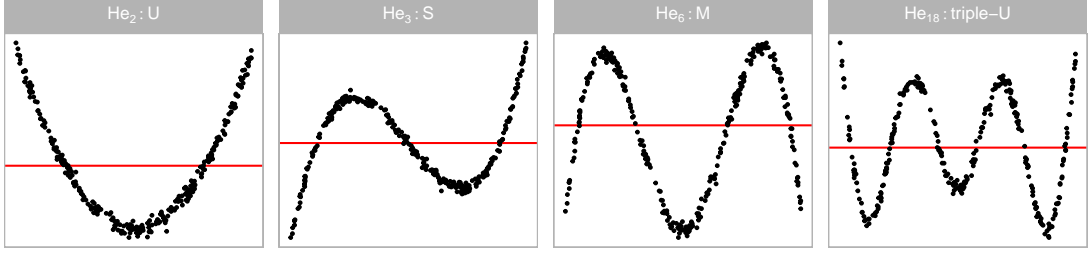
According to Abramowitz and Stegun (1964), Hermite polynomials were initially defined by Laplace (1820), but named after Hermite (1864) because of the unrecognisable form of Laplace's work. The function `hermite` from the R package `mpoly` (Kahle 2013) is used to simulate  $\mathbf{z}_{raw}$  to generate Hermite polynomials.

The null regression model used to fit the realizations generated by the above model is formulated as

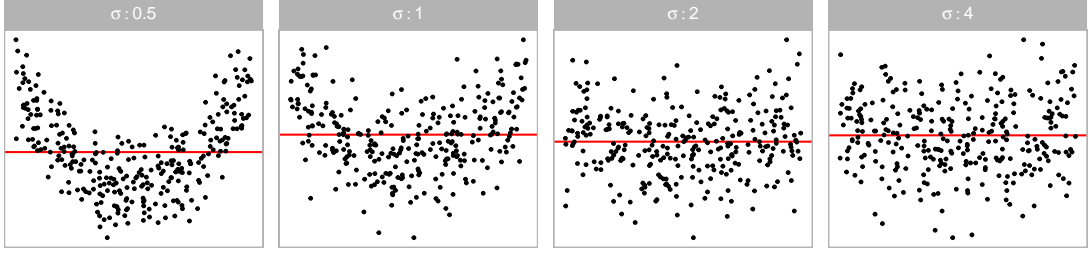
$$\mathbf{y} = \beta_0 + \beta_1 \mathbf{x} + \mathbf{u}, \quad (8)$$

where  $\mathbf{u} \sim N(\mathbf{0}, \sigma^2 \mathbf{I}_n)$ . Since  $z = O(x^j)$ , for  $j > 1$ ,  $z$  is a higher order term left out of the null regression, which will lead to model misspecification.

Visual patterns of non-linearity are simulated using four different orders of probabilist's Hermite polynomials ( $j = 2, 3, 6, 18$ ). The values of  $j$  were chosen so that distinct shapes of non-linearity were included in the residual plot. These include "U",



**Figure 3.** Polynomial forms generated for the residual plots used to assess detecting non-linearity. The four shapes are generated by varying the order of polynomial given by  $j$  in  $He_j(\cdot)$ .



**Figure 4.** Examining the effect of  $\sigma$  on the signal strength in the non-linearity detection, for  $n = 300$ , uniform fitted value distribution and the "U" shape. As  $\sigma$  increases the signal strength decreases, to the point that the "U" is almost unrecognisable when  $\sigma = 4$ .

"S", "M" and "triple-U" shape as shown in Figure 3. A greater value of  $j$  will result in a curve with more turning points. It is expected that the "U" shape will be the easiest detect, as the shape gets more complex it will be harder to perceive in a scatterplot, particularly when there is noise. Figure 4 shows the "U" shape for different amounts of noise ( $\sigma$ ).

Figure 5 is one of the non-linearity lineups used in experiment. This data plot is produced by the non-linearity model with  $j = 6$ , and is in location  $2^3 + 1$ . All five participants who viewed the lineup chose this plot as most different, thus all detected the data plot.

#### 4.1.2. Heteroskedasticity

Data collection period II was designed to study the ability of participants to detect the heteroskedasticity under a simple linear regression model setting:

$$\begin{aligned} \mathbf{y} &= \mathbf{1} + \mathbf{x} + \boldsymbol{\varepsilon}, \\ \mathbf{x} &= g(\mathbf{x}_{raw}, \mathbf{1}), \\ \boldsymbol{\varepsilon} &\sim N(\mathbf{0}, \mathbf{1} + (2 - |a|)(\mathbf{x} - a)^2 b \mathbf{I}), \end{aligned}$$

where  $\mathbf{y}$ ,  $\mathbf{x}$ ,  $\boldsymbol{\varepsilon}$  are vectors of size  $n$  and  $g(\cdot)$  is the scaling function defined in Equation 7. The null regression model used to fit the realizations generated by the above model is formulated exactly the same as Equation 8.

For  $b \neq 0$ , the variance-covariance matrix of the error term  $\boldsymbol{\varepsilon}$  is correlated with the predictor  $\mathbf{x}$ , which will lead to the presence of heteroskedasticity. Visual patterns of heteroskedasticity are simulated using three different shapes ( $a = -1, 0, 1$ ).

Since  $\text{supp}(X) = [-1, 1]$ , choosing  $a$  to be  $-1, 0$  and  $1$  can generate "left-triangle",



**Figure 5.** One of the lineups containing non-linearity patterns used in data collection period I. Can you spot the most different plot? The data plot is positioned at  $2^3 + 1$ .

“butterfly” and “right-triangle” shapes as displayed in Figure 6. The term  $(2 - |a|)$  maintains the magnitude of residuals across different values of  $a$ . Figure 7 shows the butterfly shape as the ratio parameter ( $b$ ) is changed.

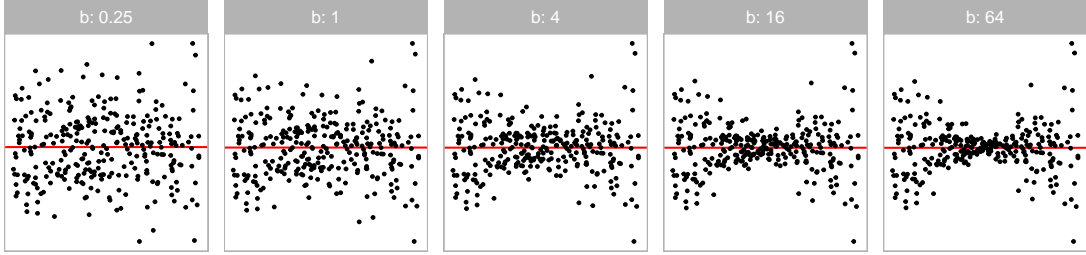
An example lineup of this model used in data collection period II is shown in Figure 8 with  $a = -1$ . The data plot location is in position  $2^4 + 2$ . Nine out of 11 participants chose this plot from the lineup.

#### 4.1.3. Factors common to both data collection periods

Fitted values are a function of the independent variables, and the distribution of the observed values affects the distribution of the fitted values. In the best case scenario the fitted values will have a uniform distribution, which means that there is even coverage of possible observed values across all of the predictors. This is not always present in the collected data. Sometimes the fitted values are discrete because one or more predictors were measured discretely. The distribution may be relatively Gaussian, reflecting a



**Figure 6.** Heteroskedasticity forms used in the experiment. Three different shapes ( $a = -1, 0, 1$ ) are used in the experiment to create left-triangle, "butterfly" and "right-triangle" shapes, respectively.



**Figure 7.** Five different values of  $b$  are used in heteroskedasticity simulation to control the strength of the signal. Larger values of  $b$  yield a bigger difference in variation, and thus stronger heteroskedasticity signal.

linear combination of many predictors, adhering to the Central Limit Theorem. It is also common to see a skewed distribution of fitted values if one or more of the predictors has a skewed distribution. This latter problem is usually corrected before modelling, using a variable transformation. Our simulation assesses this by using four different distributions to represent fitted values, constructed by different sampling of the raw predictor  $X_{raw}$ :

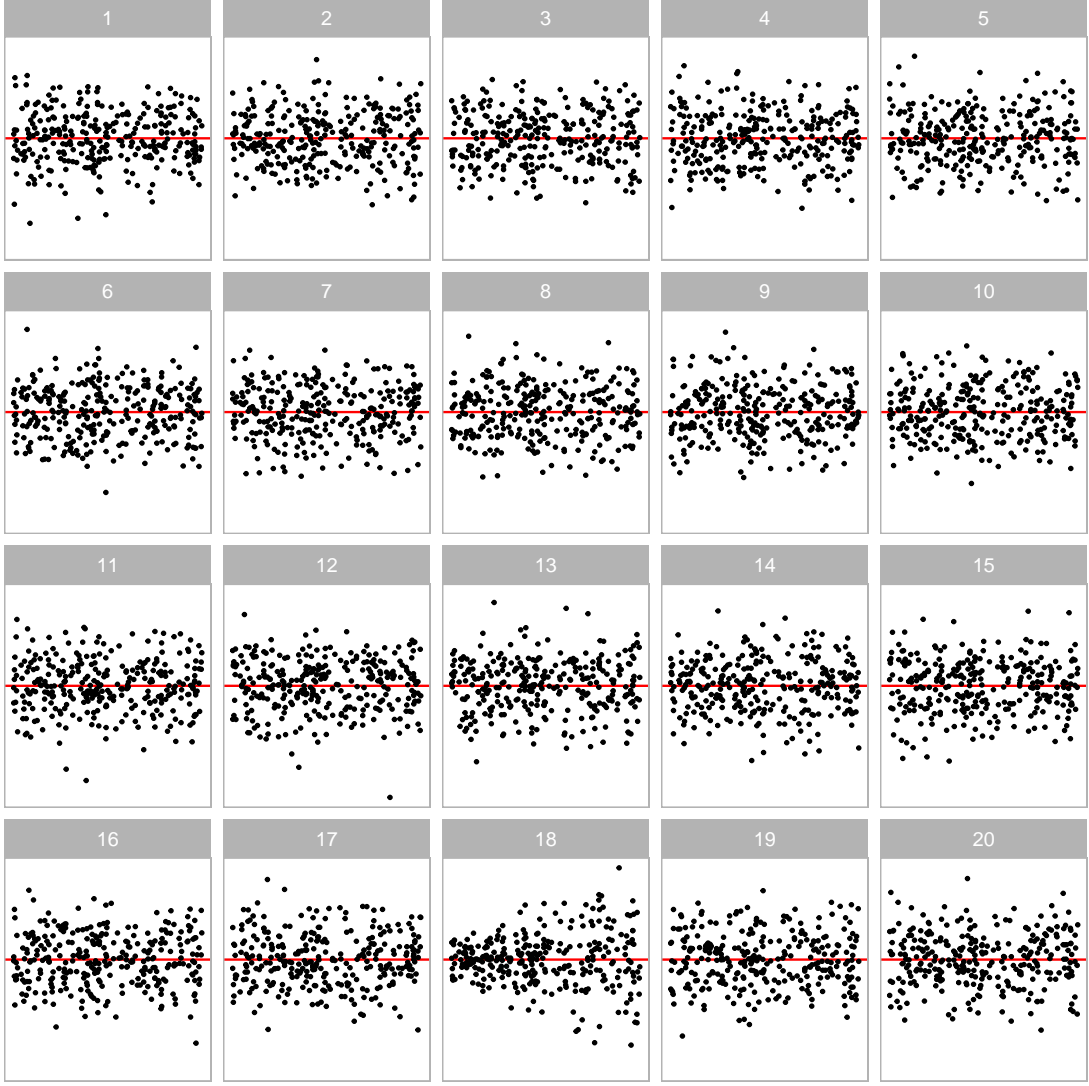
- uniform,  $U(-1, 1)$ ,
- normal,  $N(0, 0.3^2)$ ,
- skewed,  $lognormal(0, 0.6^2)/3$ , and
- discrete,  $U\{1, 5\}$ .

Figure 9 shows the non-linear pattern, a "U" shape, with the different fitted value distributions. We would expect that structure in residual plots would be easier to perceive when the fitted values are uniformly distributed.

Three different sample sizes were used in our experiment:  $n = 50, 100, 300$ . Figure 10 shows the non-linear "S" shape for different sample sizes. We expect signal strength to decline in the simulated data plots with smaller  $n$ . A sample size of 300 is typically enough for structure to be visible in a scatter plot reliably. Beyond 300, structure can be obscured by over-plotting, and a different type of display that included transparency, binning or density mapping, might be needed.

#### 4.1.4. Controlling the signal strength

The three parameters  $n$ ,  $\sigma$  and  $b$  are important for controlling the strength of the signal to generate lineups with a variety of difficulty levels. This will ensure that estimated power curves will be smooth and continuous, and that participants are allocated a set



**Figure 8.** One of the lineups containing heteroskedasticity pattern used in data collection period II. Can you spot the most different plot? The data plot is positioned at  $3^3 - 3^2$ .

of lineups with a range of difficulty.

Parameter  $\sigma \in \{0.5, 1, 2, 4\}$  and  $b \in \{0.25, 1, 4, 16, 64\}$  are used in data collection periods I and II respectively. A large value of  $\sigma$  will increase the variation of the error of the non-linearity model and decrease the visibility of the visual pattern. The parameter  $b$  controls the variation in the standard deviation of the error across the support of the predictor. A larger value of  $b$  generates a larger ratio between its smallest and highest values, making the visual pattern more obvious. The sample size  $n$  sharpens (or blurs) a pattern when it is larger (or smaller). Figures 4, 7 and 10 demonstrate the impact of these parameters on signal strength.

#### 4.2. *Experimental setup*

The lineups are allocated to participants in a manner that covers the experimental design and is relatively uniform. To manage this, we use effect size to measure the



**Figure 9.** Variations in fitted values, that might affect perception of residual plots. Four different distributions are used.



**Figure 10.** Examining the effect of signal strength for the three different values of  $n$  used in the experiment, for non-linear structure with fixed  $\sigma = 1.5$ , uniform fitted value distribution, and "S" shape. For these factor levels, only when  $n = 300$  is the "S" shape clearly visible.

signal strength, which helps in assigning a set of lineups with a range of difficulties to each participant.

#### 4.2.1. Effect size

Effect size in statistics measures the strength of the signal relative to the noise. It is surprisingly difficult to quantify, even for simulated data as used in this experiment.

For the non-linearity model, the key items defining effect size are sample size ( $n$ ) and variance of the error term ( $\sigma^2$ ), and so effect size would be roughly calculated as  $\sqrt{n}/\sigma$ . As sample size increases the effect size would increase, but as variance increases the effect size decreases. However, it is not clear how the additional parameter for the model polynomial order,  $k$ , should be incorporated. Intuitively, the large  $k$  means more complex pattern, which likely means effect size would decrease. For the purposes of our calculations we have chosen to use an approach based on Kullback-Leibler divergence (Kullback and Leibler 1951), coupled with simulation. This formulation defines effect size to be:

$$E = \frac{1}{2} (\boldsymbol{\mu}'_z (\text{diag}(\mathbf{R}\sigma^2))^{-1} \boldsymbol{\mu}_z) \quad (9)$$

where  $\text{diag}(\cdot)$  is the diagonal matrix constructed from the diagonal elements of a matrix,  $\mathbf{R} = \mathbf{I}_n - \mathbf{H}$  is the residual operator,  $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$  is the hat matrix,  $\boldsymbol{\mu}_z = \mathbf{R}\mathbf{Z}\boldsymbol{\beta}_z$  is the expected values of residuals where  $\mathbf{Z}$  contain any higher order terms of  $\mathbf{X}$  left out of the regression equation,  $\boldsymbol{\beta}_z$  contains the corresponding coefficients, and  $\sigma^2\mathbf{I}$  is the assumed covariance matrix of the error term when  $H_0$  is true.

In the heteroskedasticity model, the key elements for measuring effect size are sample size,  $n$ , and the ratio of the biggest variance to smallest variance,  $b$ . Larger values of both would produce higher effect size. However, it is not clear how to incorporate the additional shape parameter,  $a$ . Thus the same approach is used here, where the formula can be written as:

$$E = \frac{1}{2} \left( \log \frac{|\text{diag}(\mathbf{R}\mathbf{V}\mathbf{R}')|}{|\text{diag}(\mathbf{R})|} - n + \text{tr}(\text{diag}(\mathbf{R}\mathbf{V}\mathbf{R}')^{-1} \text{diag}(\mathbf{R})) \right) \quad (10)$$

where  $\mathbf{V}$  is the actual covariance matrix of the error term. Derivations for these equations are provided in the Appendix.

To compute the effect size for each lineup we simulate a sufficient large number of samples from the same model, in each sample, the number of observations  $n$  is fixed. We then compute the effect size for each sample and take the average as the final value. This ensures lineups constructed with the same experimental factors will share the same effect size.

#### 4.2.2. Lineup allocation to participants

From Table 2 it can be computed that there are a total of  $4 \times 4 \times 3 \times 4 = 192$  and  $3 \times 5 \times 3 \times 4 = 180$  combinations of parameter values for the non-linearity model and heteroskedasticity models respectively. Three replications for each combination results in  $192 \times 3 = 576$  and  $180 \times 3 = 540$  lineups, respectively.

Each lineup needs to be evaluated by at least five participants. From previous work, and additional pilot studies for this experiment, we decided to record evaluations from 20 lineups for each participant. Two of the 20 lineups with clear visual patterns were used as attention checks, to ensure quality data. Thus,  $576 \times 5 / (20 - 2) = 160$  and  $540 \times 5 / (20 - 2) = 150$  participants were needed to cover the experimental design for the data collection periods I and II, respectively. The factor levels and range of difficulty was assigned relatively equally among participants. The Appendix contains graphical summaries of these assignments for each subject.

Data collection period III was primarily to obtain Rorschach lineup evaluations to estimate  $\alpha$  from Equation 1, and also to obtain additional evaluations of lineups made with uniform fitted value distribution to ensure consistency in the results. To construct a Rorschach lineup, the data is generated from a model with zero effect size, while the null data are generated using the same simulation method discussed in Section 2.3. This procedure differs from that of the canonical Rorschach lineup, where all 20 plots are generated directly from the null model, so the method suggested in VanderPlas et al. (2021) for typical lineups containing a data plot is used to estimate  $\alpha$ . (The Appendix contains a sensitivity analysis on the effect of uncertainty in the estimation of  $\alpha$ .) The  $3 \times 4 = 12$  treatment levels of the common factors, replicated three times results in 36 lineups. And 6 more evaluations on the 279 lineups with uniform fitted value distribution, results in at least  $(36 \times 20 + 279 \times 3 \times 6) / (20 - 2) = 133$  participants needed.

#### 4.2.3. Collecting results

Participants for all three data collection periods are recruited from an crowdsourcing platform called Prolific (Palan and Schitter 2018). Prescreening procedure is applied



during the recruitment, participants are required to be fluent in English, with 98% minimum approval rate and 10 minimum submissions in other studies.

During the experiment, every participant is presented with a block of 20 lineups. A lineup consists of a randomly placed data plot and 19 null plots, which are all residual plots drawn with raw residuals on the y-axis and fitted values on the x-axis. An additional horizontal red line is added at  $y = 0$  as a helping line.

The data of the data plot is simulated from one of two models described in Section 4.1, while the data of the remaining 19 null plots are generated by the residual rotation technique discussed in Section 2.3.

In every lineup evaluation, the participant is asked to select one or more plots that are most different from others, provide a reason for their selections, and evaluate how different they think the selected plots are from others. If there is no noticeable difference between plots in a lineup, participants are permitted to select zero plots without providing the reason. No participant are shown the same lineup twice. Information about preferred pronoun, age group, education, and previous experience in visual experiments are also collected. A participant's submission is only accepted if the data plot is identified for at least one attention check. Data of rejected submissions are discarded automatically to maintain the overall data quality.

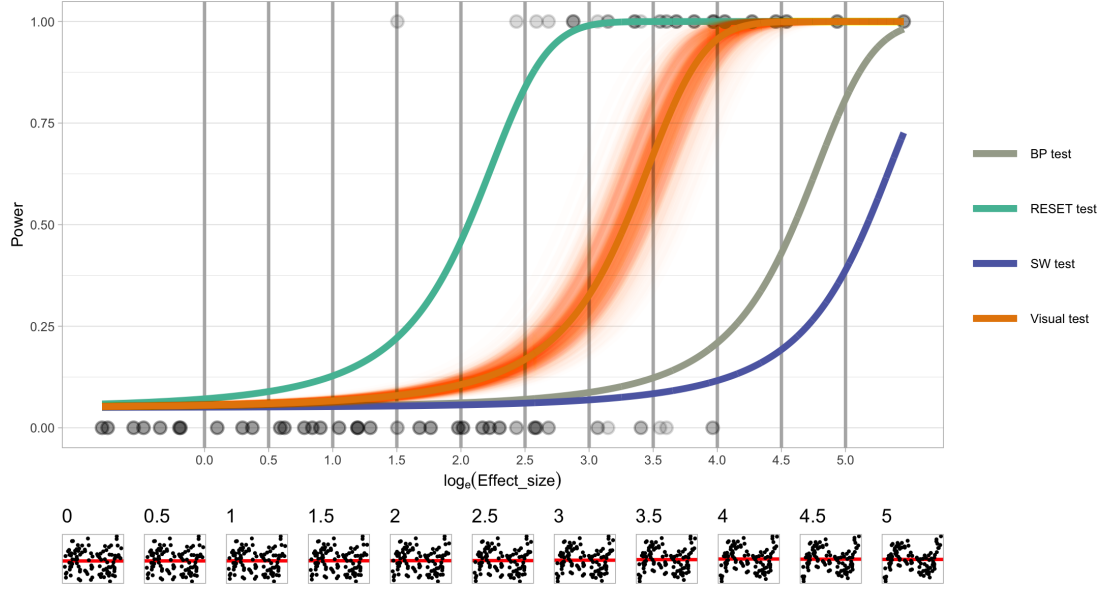
## 5. Results

Data collection used a total of 1152 lineups, and resulted in a total of 7974 evaluations from 443 participants. Roughly half corresponded to the two models, non-linearity and heteroskedasticity, and the three collection periods had similar numbers in each. Each participant received two of the 24 attention check lineups which were used to filter results of participants who were clearly not making an honest effort (only 11 of 454). To estimate  $\alpha$  for calculating statistical significance (see Section 3.2) there were 720 evaluations of 36 null lineups. Neither the attention checks nor null lineups were used for the subsequent analysis. The de-identified data, `vi_survey`, is made available in the R package, `visage`.

The data was collected on lineups constructed from four different fitted value distributions: uniform, normal, skewed and discrete. More data was collected on the uniform (each evaluated by 11 participants) than the others (each evaluated by 5 participants). The analysis in Sections 5.1-5.4, uses only results from lineups generated with uniform fitted values, a total 3069 lineup evaluations. This was decided in order to compare the conventional and visual test performance for an optimal scenario. Section 5.5 examines how the results may be affected if the fitted value distribution was different.

### 5.1. *Power comparison of the tests*

Figures 11 and 12 present the power curves of various tests plotted against the effect size in the residuals, for non-linearity and heteroskedasticity, respectively. In each case the power of visual test is calculated for multiple bootstrap samples leading to the many (orange) curves. The effect size was computed at a 5% significance level and plotted on a natural logarithmic scale. To facilitate visual calibration of effect size values with the corresponding diagnostic plots, a sequence of example residual plots with increasing effect sizes is provided at the bottom of these figures. These plots serve as a visual aid to help readers understand how different effect size values translate to changes in the diagnostic plots. The horizontal lines of dots at 0 and 1 represent the



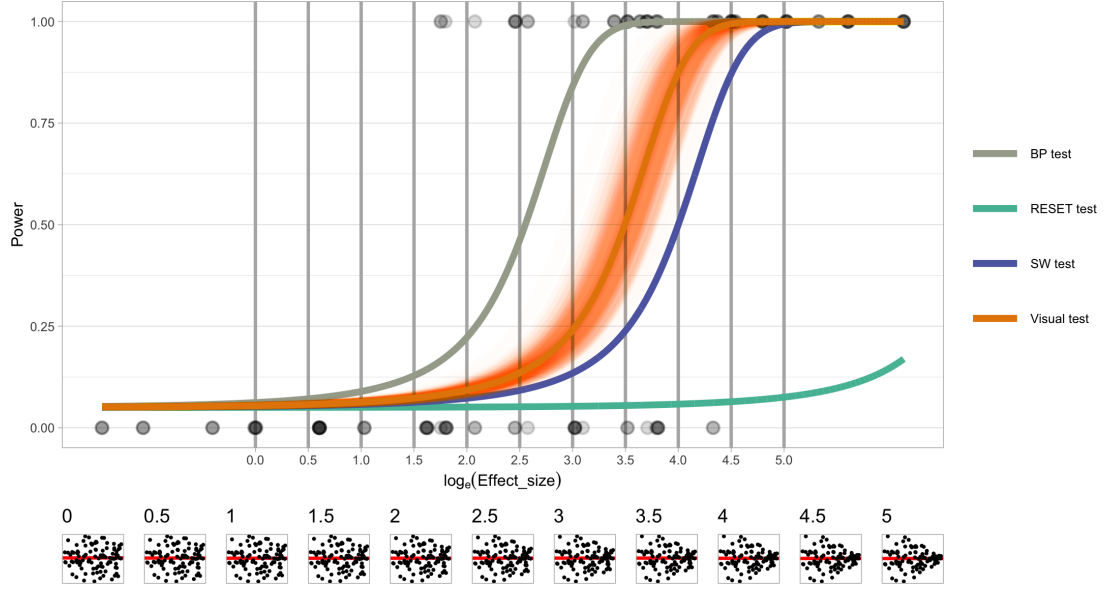
**Figure 11.** Comparison of power between different tests for non-linear patterns (uniform fitted values only). The power curves are estimated using logistic regression, and the horizontal lines of dots represent non-reject and reject results from visual tests for each lineup. The visual test has multiple power curves estimated from bootstrap samples. The row of scatterplots at the bottom are examples of residual plots corresponding to the specific effect sizes marked by vertical lines in the main plot.

non-reject or reject made by visual tests for each lineup.

Figure 11 compares the power for the different tests for non-linear structure in the residuals. The test with the uniformly higher power is the RESET test, one that specifically tests for non-linearity. (Note that the BP and SW tests have much lower power, which is expected because they are not designed to detect non-linearity.) The bootstrapped power curves for the visual test are effectively a shift right from that of the RESET test. This means that the RESET test will reject at a lower effect size (less structure) than the visual test, but otherwise the performance will be similar. In other words, the RESET test is more sensitive than the visual test. This is not necessarily a good feature for the purposes of diagnosing model defects. If one scans the residual plot examples at the bottom, we might argue that the non-linearity is not sufficiently problematic until an effect size of around 3 or 3.5. The RESET test would reject closer to an effect size of 2, but the visual test would reject closer 3.25, for a significance level of 0.05.

For the heteroskedasticity pattern, the power of BP test, designed for detecting heteroskedasticity, is uniformly higher than the other tests. The visual test power curve is a right shift. This shows a similar story to the power curves for non-linearity pattern - the conventional test is more sensitive than the visual test. From the example residual plots at the bottom we might argue that the heteroskedasticity becomes noticeably visible around an effect size of 3 or 3.5. However the BP test would reject at around effect size 2.5. Interestingly, the power curve for the SW test (for non-normality) is only slightly different to that of the visual test, suggesting that it performs reasonably for detecting heteroskedasticity, too. The power curve for the BP test suggests it is not useful for detecting heteroskedasticity, as expected.

Overall, the results show that the conventional tests are more sensitive than the visual test. The conventional tests do have higher power for the patterns they are designed to detect, and are generally unable to detect other patterns. The visual



**Figure 12.** Comparison of power between different tests for heteroskedasticity patterns (uniform fitted values only). Main plot shows the power curves, with dots indicating non-reject and reject in visual testing of lineups. The multiple lines for the visual test arise from estimating the power on many bootstrap samples. The row of scatterplots at the bottom are examples of residual plots corresponding to the specific effect sizes marked by vertical lines in the main plot.

test doesn't require specifying the pattern ahead of time, relying purely on whether the observed residual plot is detectably different from "good" residual plots. They will perform equally well regardless of the type of model defect. This aligns with the advice of experts on residual analysis, who consider residual plot analysis to be an indispensable tool for diagnosing model problems. What we gain from using a visual test for this purpose is the removal of any subjective arguments about whether a pattern is visible or not. The lineup protocol provides the calibration for detecting patterns: that if the pattern in the data plot cannot be distinguished from patterns in good residual plots, then no discernible problem with the model exists.

## 5.2. Comparison of test decisions based on $p$ -values

The power comparison demonstrated that the appropriate conventional tests will reject more aggressively than visual tests, but we don't know how the decisions for each lineup would agree or disagree. Here we compare the reject or fail to reject decisions of these tests, across all the lineups. Figure 13 shows the agreement of the conventional and visual tests using a mosaic plot for both non-linearity patterns and heteroskedasticity patterns.

For both patterns the lineups resulting in a rejection by the visual test are *all* also rejected by the conventional test, except for one from the heteroskedasticity model. This reflects exactly the story from the previous section, that the conventional tests reject more aggressively than the visual test.

For lineups containing non-linearity patterns, conventional tests reject 69% and visual tests reject 32% of the time. Of the lineups rejected by the conventional test, 46% are rejected by the visual test, that is, approximately half as many as the conventional test. There are no lineups that are rejected by the visual test but not by the conventional test.



**Figure 13.** Rejection rate ( $p\text{-value} \leq 0.05$ ) of visual test conditional on the conventional test decision on non-linearity (left) and heteroskedasticity (right) lineups (uniform fitted values only) displayed using a mosaic plot. The visual test rejects less frequently than the conventional test, and (almost) only rejects when the conventional test does. Surprisingly, one lineup in the heteroskedasticity group is rejected by the visual test but NOT the conventional test.

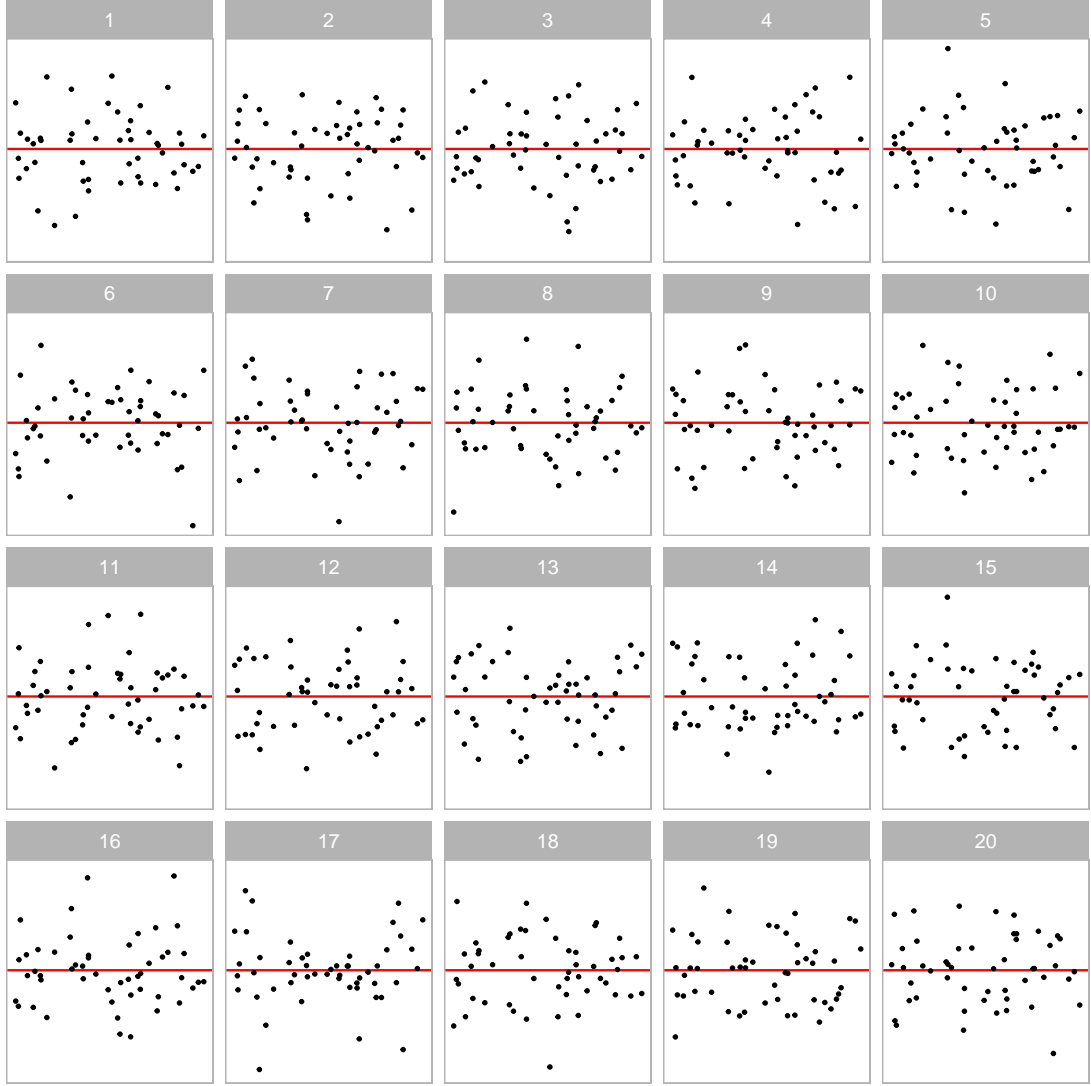
In terms of lineups containing heteroskedasticity patterns, 76% are rejected by conventional tests, while 56% are rejected by visual tests. The visual test rejects 73% of the lineups that the conventional visual test reject.

Surprisingly, the visual test rejects 1 of the 33 (3%) of lineups where the conventional test does not reject. Figure 14 shows this lineup. The data plot in position seventeen displays a relatively strong heteroskedasticity pattern, and has a strong effect size ( $\log_e(E) = 4.02$ ). This is reflected by the visual test  $p\text{-value} = 0.026$ . But the BP test  $p\text{-value} = 0.056$ , is slightly above the significance cutoff of 0.05. This lineup was evaluated by 11 participants, it has experimental factors  $a = 0$  (“butterfly” shape),  $b = 64$  (large variance ratio),  $n = 50$  (small sample size), and a uniform distribution for the fitted values. It may have been the small sample size and the presence of a few outliers that may have resulted in the lack of detection by the conventional test.

Because the power curve of the visual tests are a shift to the right of the conventional test (Figures 11 and 14) it would be curious to know whether adjusting the significance level (to .001, .0001, .00001, ...) of the conventional test would generate similar decisions to that of the visual test. Interestingly, it doesn’t. Despite resulting less rejections, neither the RESET or BP tests come to complete agreement with the visual test (See Appendix).

### 5.3. *Effect of amount of non-linearity*

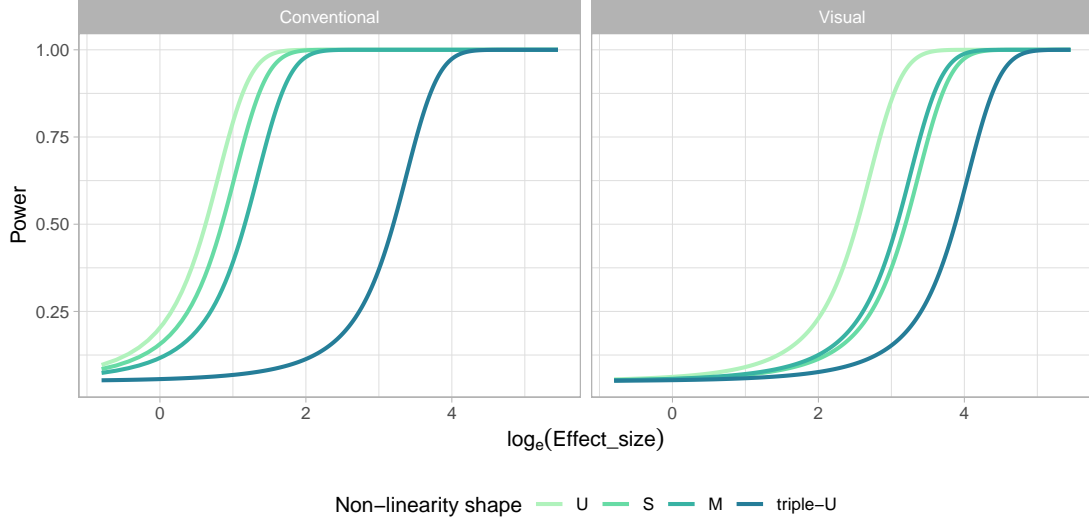
The order of the polynomial is a primary factor contributing to the pattern produced by the non-linearity model. Figure 15 explores the relationship between polynomial order and power of the tests. The conventional tests have higher power for lower orders of Hermite polynomials, and it drops substantially for the “triple-U” shape. To understand why this is, one needs to return to the way the RESET test is applied. It requires a parameter indicating degree of fitted values to test for, and the recom-



**Figure 14.** The single heteroskedasticity lineup that is rejected by the visual test but not by the BP test. The data plot (position 17) contains a “butterfly” shape. It has a log effect size of 3.76, and visibly displays heteroskedasticity, making it somewhat surprising that it is not detected by the BP test.

mendation is to generically use four (Ramsey 1969). However, the “triple-U” shape is constructed from the Hermite polynomials using power up to 18. If the RESET test had been applied using a higher power no less than six, the power curve of “triple-U” shape will be closer to other power curves. This illustrates the sensitivity of the conventional test to the parameter choice, and highlights a limitation that it helps to know the data generating process to set the parameters for the test, which is unrealistic. However, we examined this in more detail (see Appendix) and found that there is no harm for setting the parameter higher than four on the tests’ operation for lower order polynomial shapes. Using a parameter value of six, instead of four, yields higher power regardless of generating process, and would be recommended.

For visual tests, we expect the “U” shape to be detected more readily, followed by the “S”, “M” and “triple-U” shape. From Figure 15, it can be observed that the power curves mostly align with these expectations, except for the “M” shape, which is as easy to be detected as the “S” shape. This suggests a benefit of the visual test:



**Figure 15.** The effect of the order of the polynomial on the power of conventional and visual tests. Deeper colour indicates higher order. The default RESET tests under-performs significantly in detecting the “triple-U” shape. To achieve a similar power as other shapes, a higher order polynomial parameter needs to be used for the RESET test, but this higher than the recommended value.

knowing the shape ahead of time is *not* needed for its application.

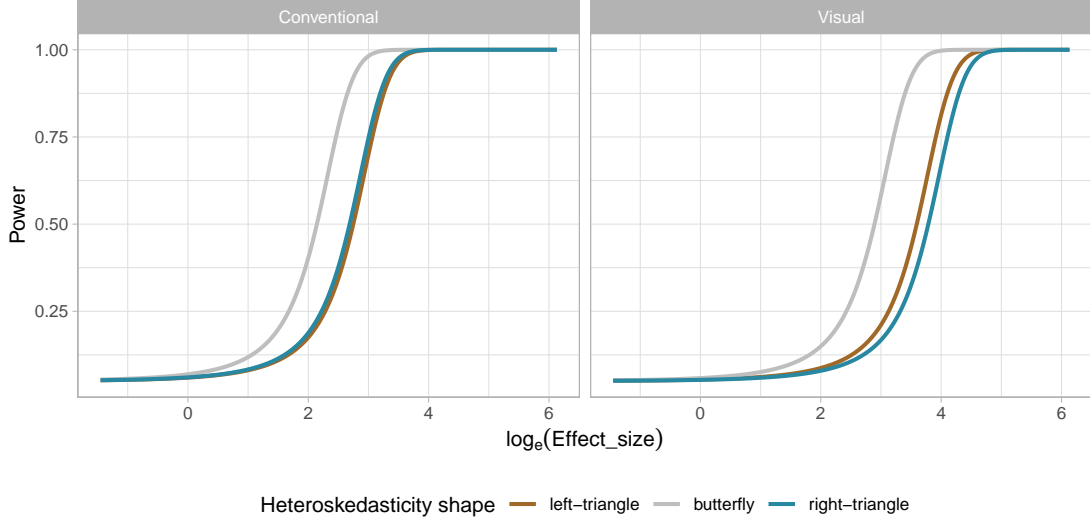
#### 5.4. *Effect of shape of heteroskedasticity*

Figure 16 examines the impact of the shape of the heteroskedasticity on the power of both tests. The butterfly shape has higher power on both types of tests. The “left-triangle” and the “right-triangle” shapes are functionally identical, and this is observed for the conventional test, where the power curves are identical. Interestingly there is a difference for the visual test, where the power curve of the “left-triangle” shape is slightly higher than that of the “right-triangle” shape. This indicates a bias in perceiving heteroskedasticity depending on the direction. This would be worth investigating further.

#### 5.5. *Effect of fitted value distributions*

In regression analysis, predictions are conditional on the observed values of the predictors, that is, the conditional mean of the dependent variable  $Y$  given the value of the independent variable  $X$ ,  $E(Y|X)$ . This is an often forgotten element of regression analysis but it is important. Where  $X$  is observed, particularly the distribution of the  $X$  values in the sample, or consequently  $\hat{Y}$ , may affect the ability to read any patterns in the residual plots. This experiment was constructed to assess this, based on four different distributions of fitted values: uniform, normal, discrete and lognormal (skewed). We would expect that if  $\hat{Y}$  has a uniform distribution, this would make it easier to read the relationship with the residuals.

Figure 17 examines the impact of the fitted value distribution on the power of conventional (left) and visual (right) tests for both the non-linearity (top) and heteroskedasticity (bottom) patterns. For conventional tests, only the power curves of appropriate tests which are RESET tests and BP tests for non-linearity pattern and heteroskedasticity pattern respectively are shown. For visual tests, note that, more



**Figure 16.** The effect of heteroskedasticity shape (parameter  $a$ ) on the power of conventional and visual tests. The butterfly has higher power in both tests. Curiously, the visual test has slightly higher power for the "left-triangle" than the "right-triangle" shape, when it would be expected that they should be identical, which is observed in conventional testing.

evaluations on lineup with uniform fitted value distribution were collected, so to have a fair comparison, we randomly sample five from the total eleven evaluations to estimate the power curves. Re-sampling produces the multiple curves for the uniform, and provides an indication of the variation of the power.

Perhaps surprisingly, the visual tests have more consistent power across the different fitted value distributions. For the non-linear pattern, there is almost no power difference. For the heteroskedastic pattern, uniform and discrete have higher power than normal and lognormal. The likely reason is that these latter two have less observations in the tails where the heteroskedastic pattern needs to be detected.

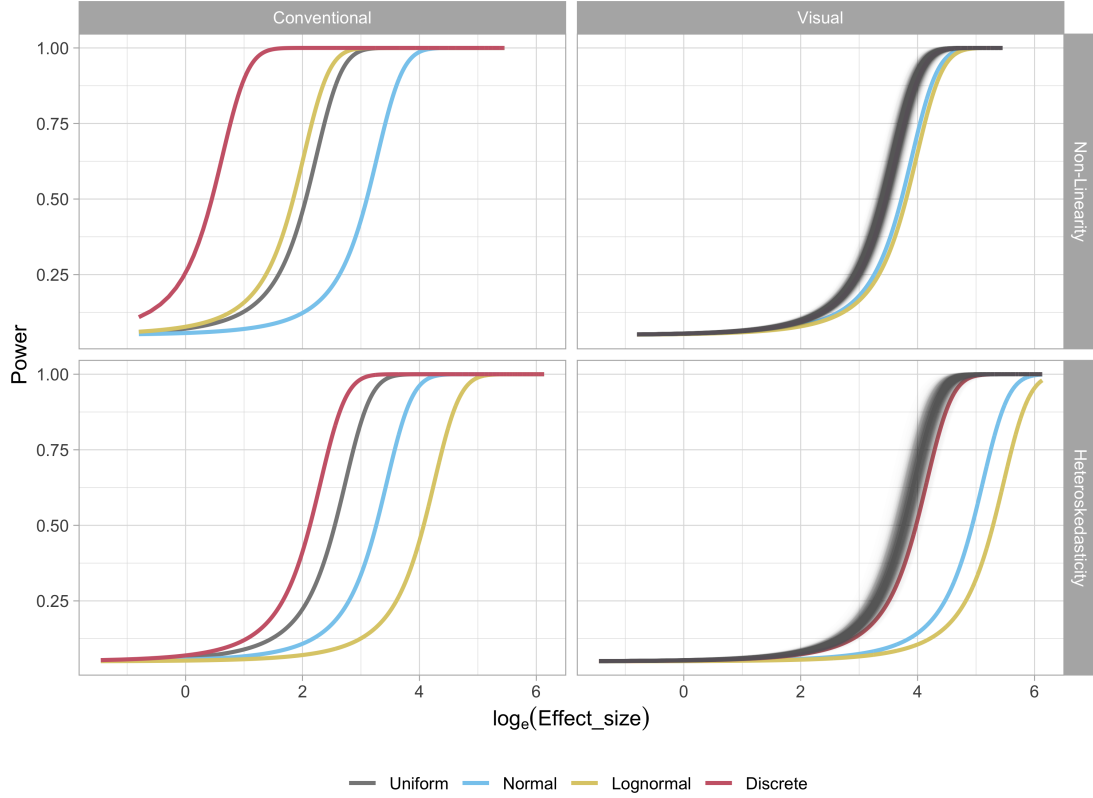
The variation in power in the conventional tests is at first sight, shocking. However, it is discussed, albeit rarely, in the testing literature. See, for example, Jamshidian, Jennrich, and Liu (2007), Olvera Astivia, Gadermann, and Guhn (2019) and Zhang and Yuan (2018) which show derivations and use simulation to assess the effect of the observed distribution of the predictors on test power. The big differences in power curves that are seen in Figure 17 is echoed in the results reported in these articles.

## 6. Conclusions

Motivated by the advice of regression analysis experts, that residual plots as opposed to conventional tests are indispensable methods for assessing model fit, a human subjects experiment was conducted using visual inference. The experiment tested two primary departures from good residuals: non-linearity and heteroskedasticity.

The experiment found that conventional residual-based statistical tests are more sensitive to weak departures from model assumptions than visual tests as would be evaluated by humans. That is, a conventional test concludes there are problems with the model fit almost twice as often as a human would. They often reject when departures in the form of non-linearity and heteroskedasticity are not visibly different from null residual plots.

While it might be argued that the conventional tests are correctly detecting the small



**Figure 17.** Comparison of power on lineups with different fitted value distributions for conventional and visual tests (columns) for non-linearity and heteroskedasticity patterns (rows). The power curves of conventional tests for non-linearity and heteroskedasticity patterns are produced by RESET tests and BP tests, respectively. Power curves of visual tests are estimated using five evaluations on each lineup. For lineups with a uniform fitted value distribution, the five evaluations are repeatedly sampled from the total eleven evaluations to give multiple power curves (grey). Surprisingly, the fitted value distribution has produces more variability in the power of conventional tests than visual tests. Uneven distributions, normal and lognormal distributions, tend to yield lower power.

but real effects, it can also be considered that the conventional tests are rejecting when it is not necessary. Many of these rejections happen even when downstream analysis and results would not be significantly affected by the small departures from a good fit. The results from human evaluations provide a more practical solution, which reinforces the statements from regression experts that residual plots are an indispensable method for model diagnostics.

Now it is important to note that residual plots need to be delivered as a lineup, where it is embedded in a field of null plots. A residual plot may contain many visual features, but some are caused by the characteristics of the predictors and the randomness of the error, not by the violation of the model assumptions. These irrelevant visual features have a chance to be filtered out by participants with a comparison to null plots, resulting in more accurate reading. The lineup enables a careful calibration for reading structure in residual plots.

Human evaluation of residuals is expensive, though. It is time-consuming and laborious. This is possibly why residual plot analysis is often not done, in practice. However, with the emergence of effective computer vision this work could form the basis to provide automated residual plot reading.

The experiment also revealed some interesting results. For the most part, the visual



test performed very similarly to the appropriate conventional test except that it has a power curve shifted in the less sensitive direction. Unlike the conventional tests, where one needs to specifically test for non-linearity or heteroskedasticity the visual test operated effectively across the range of departures from good residuals. If the fitted value distribution is not uniform, there is a small loss of power in the visual test. But quite a surprise to us was the big difference in power of the conventional test, which appear to be quite sensitive to how the predictors are sampled. Another surprising finding was that the direction of heteroskedasticity appears to affect the ability to visually detect it: both triangles being more difficult to detect than the butterfly, and a small difference in detection between left- and right-triangle.

## Acknowledgements

These R packages are used for the work: `cli` (Csárdi 2022), `curl` (Ooms 2022), `dplyr` (Wickham et al. 2023), `ggplot2` (Wickham 2016), `jsonlite` (Ooms 2014), `lmtest` (Zeileis and Hothorn 2002), `mpoly` (Kahle 2013), `progress` (Csárdi and FitzJohn 2019), `tibble` (Müller and Wickham 2022), `ggmosaic` (Jeppson, Hofmann, and Cook 2021), `purrr` (Henry and Wickham 2022), `tidyr` (Wickham and Girlich 2022), `readr` (Wickham, Hester, and Bryan 2022), `stringr` (Wickham 2022), `here` (Müller 2020), `kableExtra` (Zhu 2021), `patchwork` (Pedersen 2022), `rcartocolor` (Nowosad 2018). The study website is powered by PythonAnywhere (PythonAnywhere LLP 2023) and the Flask web framework (Grinberg 2018). The jsPsych framework (De Leeuw 2015) is used to create behavioral experiments that run in our study website.

The article was created with R packages `rticles` (Allaire et al. 2022), `knitr` (Xie 2014) and `rmarkdown` (Xie, Dervieux, and Riederer 2020). The project’s Github repository ([https://github.com/TengMcing/lineup\\_residual\\_diagnostics](https://github.com/TengMcing/lineup_residual_diagnostics)) contains all materials required to reproduce this article.

## Supplementary material

The supplementary material is available at [https://github.com/TengMcing/lineup\\_residual\\_diagnostics/blob/master/appendix.pdf](https://github.com/TengMcing/lineup_residual_diagnostics/blob/master/appendix.pdf). It includes more details about the experimental setup, the derivation of the effect size, the effect of data collection period, and the estimate of  $\alpha$ .

## References

- Abramowitz, Milton, and Irene A Stegun. 1964. *Handbook of mathematical functions with formulas, graphs, and mathematical tables*. Vol. 55. US Government printing office.
- Allaire, JJ, Yihui Xie, Christophe Dervieux, R Foundation, Hadley Wickham, Journal of Statistical Software, Ramnath Vaidyanathan, et al. 2022. *rticles: Article Formats for R Markdown*. R package version 0.24, <https://CRAN.R-project.org/package=rticles>.
- Belsley, David A, Edwin Kuh, and Roy E Welsch. 1980. *Regression diagnostics: Identifying influential data and sources of collinearity*. John Wiley & Sons.
- Box, George EP. 1976. “Science and statistics.” *Journal of the American Statistical Association* 71 (356): 791–799.
- Breusch, T. S., and A. R. Pagan. 1979. “A Simple Test for Heteroscedasticity and Random Coefficient Variation.” *Econometrica* 47 (5): 1287–1294.

- 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): 4361–4383.
- Cleveland, William S., and Robert McGill. 1984. "Graphical Perception: Theory, Experimentation, and Application to the Development of Graphical Methods." *Journal of the American Statistical Association* 79 (387): 531–554.
- Cook, R Dennis, and Sanford Weisberg. 1982. *Residuals and influence in regression*. New York: Chapman and Hall.
- Cook, R Dennis, and Sanford Weisberg. 1999. *Applied regression including computing and graphics*. John Wiley & Sons.
- Csárdi, Gábor. 2022. *cli: Helpers for Developing Command Line Interfaces*. R package version 3.4.1, <https://CRAN.R-project.org/package=cli>.
- Csárdi, Gábor, and Rich FitzJohn. 2019. *progress: Terminal Progress Bars*. R package version 1.2.2, <https://CRAN.R-project.org/package=progress>.
- De Leeuw, Joshua R. 2015. "jsPsych: A JavaScript library for creating behavioral experiments in a Web browser." *Behavior research methods* 47: 1–12.
- Draper, Norman R, and Harry Smith. 1998. *Applied regression analysis*. Vol. 326. John Wiley & Sons.
- Farrar, Thomas J. 2020. *skedastic: Heteroskedasticity Diagnostics for Linear Regression Models*. Bellville, South Africa. R Package Version 1.0.0.
- Grinberg, Miguel. 2018. *Flask web development: developing web applications with python*. "O'Reilly Media, Inc."
- Henry, Lionel, and Hadley Wickham. 2022. *purrr: Functional Programming Tools*. R package version 0.3.5, <https://CRAN.R-project.org/package=purrr>.
- Hermite, M. 1864. *Sur un nouveau développement en série des fonctions*. Imprimerie de Gauthier-Villars.
- Jamshidian, Mortaza, Robert I Jennrich, and Wei Liu. 2007. "A study of partial F tests for multiple linear regression models." *Computational statistics & data analysis* 51 (12): 6269–6284.
- Jarque, Carlos M, and Anil K Bera. 1980. "Efficient tests for normality, homoscedasticity and serial independence of regression residuals." *Economics letters* 6 (3): 255–259.
- Jeppson, Haley, Heike Hofmann, and Di Cook. 2021. *ggmosaic: Mosaic Plots in the 'ggplot2' Framework*. R package version 0.3.3, <https://CRAN.R-project.org/package=ggmosaic>.
- Kahle, David. 2013. "mpoly: Multivariate Polynomials in R." *The R Journal* 5 (1): 162–170.
- Kahneman, Daniel. 2011. *Thinking, Fast and Slow*. New York: Farrar, Straus and Giroux.
- Kirk, Roger E. 1996. "Practical Significance: A Concept Whose Time Has Come." *Educational and Psychological Measurement* 56 (5): 746–759.
- Kullback, Solomon, and Richard A Leibler. 1951. "On information and sufficiency." *The annals of mathematical statistics* 22 (1): 79–86.
- Laplace, Pierre-Simon. 1820. *Théorie analytique des probabilités*. Vol. 7. Courcier.
- Loy, Adam. 2021. "Bringing visual inference to the classroom." *Journal of Statistics and Data Science Education* 29 (2): 171–182.
- Loy, Adam, and Heike Hofmann. 2013. "Diagnostic tools for hierarchical linear models." *Wiley Interdisciplinary Reviews: Computational Statistics* 5 (1): 48–61.
- Loy, Adam, and Heike Hofmann. 2014. "HLMdiag: A suite of diagnostics for hierarchical linear models in R." *Journal of Statistical Software* 56: 1–28.
- Loy, Adam, and Heike Hofmann. 2015. "Are you normal? the problem of confounded residual structures in hierarchical linear models." *Journal of Computational and Graphical Statistics* 24 (4): 1191–1209.
- Majumder, Mahbubul, Heike Hofmann, and Dianne Cook. 2013. "Validation of Visual Statistical Inference, Applied to Linear Models." *Journal of the American Statistical Association* 108 (503): 942–956.
- Montgomery, DC, and EA Peck. 1982. *Introduction to linear regression analysis*. John Wiley

- & Sons.
- Müller, Kirill. 2020. *here: A Simpler Way to Find Your Files*. R package version 1.0.1, <https://CRAN.R-project.org/package=here>.
- Müller, Kirill, and Hadley Wickham. 2022. *tibble: Simple Data Frames*. R package version 3.1.8, <https://CRAN.R-project.org/package=tibble>.
- Nowosad, Jakub. 2018. *'CARTOCOLORS' Palettes*. R package version 1.0, <https://nowosad.github.io/rcartocolor>.
- Olvera Astivia, Oscar L, Anne Gadermann, and Martin Guhn. 2019. "The relationship between statistical power and predictor distribution in multilevel logistic regression: a simulation-based approach." *BMC medical research methodology* 19 (1): 1–20.
- Ooms, Jeroen. 2014. "The jsonlite Package: A Practical and Consistent Mapping Between JSON Data and R Objects." *arXiv:1403.2805 [stat.CO]* <https://arxiv.org/abs/1403.2805>.
- Ooms, Jeroen. 2022. *curl: A Modern and Flexible Web Client for R*. R package version 4.3.3, <https://CRAN.R-project.org/package=curl>.
- Palan, Stefan, and Christian Schitter. 2018. "Prolific. ac—A subject pool for online experiments." *Journal of Behavioral and Experimental Finance* 17: 22–27.
- Pedersen, Thomas Lin. 2022. *patchwork: The Composer of Plots*. R package version 1.1.2, <https://CRAN.R-project.org/package=patchwork>.
- PythonAnywhere LLP. 2023. "PythonAnywhere." <https://www.pythonanywhere.com>.
- Ramsey, J. B. 1969. "Tests for Specification Errors in Classical Linear Least-Squares Regression Analysis." *Journal of the Royal Statistical Society. Series B (Methodological)* 31 (2): 350–371.
- Roy Chowdhury, Niladri, Dianne Cook, Heike Hofmann, Mahbubul Majumder, Eun-Kyung Lee, and Amy L. Toth. 2015. "Using visual statistical inference to better understand random class separations in high dimension, low sample size data." *Computational Statistics* 30 (2): 293–316.
- Shapiro, Samuel Sanford, and Martin B Wilk. 1965. "An analysis of variance test for normality (complete samples)." *Biometrika* 52 (3/4): 591–611.
- Silvey, Samuel D. 1959. "The Lagrangian multiplier test." *The Annals of Mathematical Statistics* 30 (2): 389–407.
- VanderPlas, Susan, Christian Röttger, Dianne Cook, and Heike Hofmann. 2021. "Statistical significance calculations for scenarios in visual inference." *Stat* 10 (1): e337.
- White, Halbert. 1980. "A Heteroskedasticity-Consistent Covariance Matrix Estimator and a Direct Test for Heteroskedasticity." *Econometrica* 48 (4): 817–838.
- Wickham, Hadley. 2016. *ggplot2: Elegant Graphics for Data Analysis*. Springer-Verlag New York. <https://ggplot2.tidyverse.org>.
- Wickham, Hadley. 2022. *stringr: Simple, Consistent Wrappers for Common String Operations*. R package version 1.4.1, <https://CRAN.R-project.org/package=stringr>.
- Wickham, Hadley, Romain François, Lionel Henry, Kirill Müller, and Davis Vaughan. 2023. *dplyr: A Grammar of Data Manipulation*. R package version 1.1.0, <https://CRAN.R-project.org/package=dplyr>.
- Wickham, Hadley, and Maximilian Girlich. 2022. *tidyr: Tidy Messy Data*. R package version 1.2.1, <https://CRAN.R-project.org/package=tidyr>.
- Wickham, Hadley, Jim Hester, and Jennifer Bryan. 2022. *readr: Read Rectangular Text Data*. R package version 2.1.3, <https://CRAN.R-project.org/package=readr>.
- Xie, Yihui. 2014. "knitr: A Comprehensive Tool for Reproducible Research in R." In *Implementing Reproducible Computational Research*, edited by Victoria Stodden, Friedrich Leisch, and Roger D. Peng. Chapman and Hall/CRC. ISBN 978-1466561595, <http://www.crcpress.com/product/isbn/9781466561595>.
- Xie, Yihui, Christophe Dervieux, and Emily Riederer. 2020. *R Markdown Cookbook*. Boca Raton, Florida: Chapman and Hall/CRC. ISBN 9780367563837, <https://bookdown.org/yihui/rmarkdown-cookbook>.
- Zeileis, Achim, and Torsten Hothorn. 2002. "Diagnostic Checking in Regression Relationships."

- R News* 2 (3): 7–10.
- Zhang, Zhiyong, and Ke-Hai Yuan. 2018. *Practical statistical power analysis using Webpower and R*. Isdsa Press.
- Zhu, Hao. 2021. *kableExtra: Construct Complex Table with 'kable' and Pipe Syntax*. R package version 1.3.4, <https://CRAN.R-project.org/package=kableExtra>.