

ARTICLE TEMPLATE

Why aren't significance tests commonly used for linear regression diagnostics?

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ARTICLE HISTORY

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ABSTRACT

Abstract to fill.

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data visualization; visual inference; hypothesis testing; residual plots;

1. Introduction

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

Diagnosing a model is the key to determining whether there is anything importantly wrong. For linear regression analysis, it is typical to interrogate the residuals. Residuals summarise what is not captured by the model, and thus provide the capacity to identify what might be wrong. There are many ways that residuals could be assessed.

Residuals might be plotted, as a histogram or quantile-quantile plot to examine the distribution. Using the classical normal linear regression model as an example, if the distribution is symmetric and unimodal, it is well-behaved. But if the distribution is skewed, bimodal, multimodal, or contains outliers, there is cause for concern. The distribution could also be inspected by conducting a goodness of fit test, such as the Shapiro-Wilk Normality test (Shapiro and Wilk 1965).

Plotting the residuals against predicted values and each of the explanatory variables on a scatter plot is a recommend way to scrutinize their relationships. If there is any visually discoverable patterns, the model is potentially misspecified. However, it is a very difficult task for a human judge, though to make a decision that there's nothing there. It is especially common, particularly among new data analysts to report patterns when an experienced data analyst might quickly conclude that there are none. Generally, one looks for departures from nothingness like non-linear dependency or heteroskedasticity. It is also possible to conduct hypothesis tests for non-linear dependence (Ramsey 1969), and use a Breusch-Pagan test (Breusch and Pagan 1979) for heteroskedasticity.

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There is an abundance of literature describing appropriate diagnostic methods for linear regression: Draper and Smith (1998), Montgomery and Peck (1982), Belsley, Kuh, and Welsch (1980), Cook and Weisberg (1999) and Cook and Weisberg (1982). The diligent reader of these sage writings will also notice sentences that express sentiments like *based on their experience, statistical tests are not widely used in regression diagnostics. The same or even larger amount of information can be provided by diagnostic plots than the corresponding tests in most empirical studies*. There is a common guidance by experts that plots are the best for diagnosing model fits.

This is curious, and investigating why this might be common advice is the subject of this paper. The paper is structured as follows. The next background section describes the the types of departures that one expects to detect, and describes a formal process for reading residual plots, called visual inference, that can avoid the concerns about subjectiveness of human readers. Section 3 describes the experimental setup to enable a comparison between decision made by formal hypothesis testing, and how humans would read diagnostic plots. The results are reported in Section ???. We finish with a discussion on future work, in particular how the responsibility for residual plot reading might be passed on to computer vision.

2. Background

2.1. Departures from good residual plots

(This section discusses the visual patterns data analysts expect to see and their implications.)

Graphical summaries in which residuals are plotted against fitted values or other functions of the predictor variables that are approximately orthogonal to residuals are referred to as standard residual plots in Cook and Weisberg (1982). As shown in Figure 1, the top-left panel is a good residual plot with residuals evenly distributed at both sides of the horizontal zero line showing no noticeable patterns. There are various types of departures from a good residual plot. Two most commonly checked departures - non-linearity, heteroskedasticity and non-normality will be discussed in this paper.

Non-linearity is a type of model misspecification caused by failing to include higher order terms of the regressors in the regression equation. Any non-linear functional form of residuals on fitted values presented in the residual plot could be considered as an indicative of non-linearity. An example residual plot containing visual pattern of non-linearity is given at the top-right of Figure [ref here]. One can clearly observe the “S-shape” from the residual plot as the cubic term is not captured by the misspecified model.

Heteroskedasticity refers to the presence of nonconst error variance in a regression model. It is mostly due to the strict but false assumptions on the variance-covariance matrix of the error term. The usual pattern of heteroskedasticity on a residual plot is the inconsistent spread of the residuals at different x values. Visually, it sometimes results in the so-called “butterfly” shape as shown in the bottom-left panel of Figure 1, or the “left-triangle” and “right-triganle” shape where the smallest variance occurs at the edges of the x -axis.

Compared to non-linearity and heteroskedasticity, non-normality is usually harder to be detected from a residual plot since scatter plot is not excel in revealing marginal distribution. A favourable graphical summarise for this task is the quantile-quantile

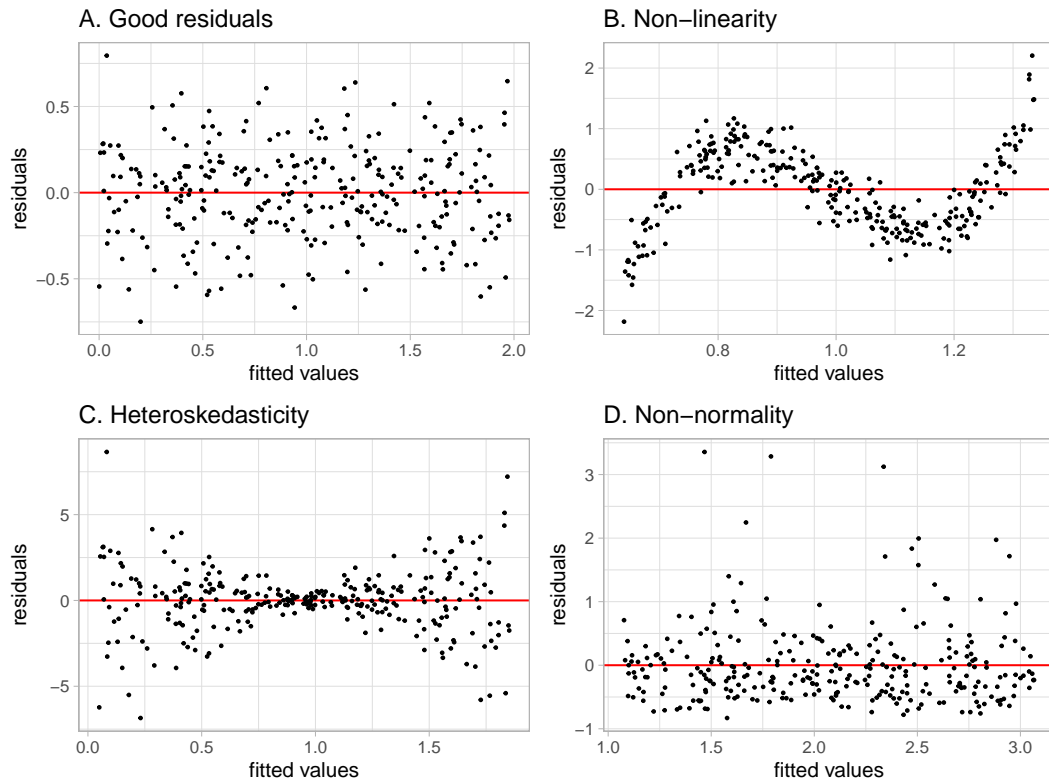


Figure 1. Example fitted vs residual plots: (A) classically good looking residuals, (B) non-linear pattern indicates that the model has not captured a non-linear association, (C) heteroskedasticity indicating that variance around the fitted model is not uniform, and (D) non-normality where the residual 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 plot.

Table 1. Results of example residual plots given in Figure 1 examined by the Model structural test (F-test), the Breusch-Pagan test and the Shapiro-Wilk test. P-values smaller than 0.05 are showed in bold.

Plot	Departures	Model structural	Breusch-Pagan	Shapiro-Wilk
A	None	0.434	0.133	0.728
B	Non-linearity	0.000	0.000	0.039
C	Heteroskedasticity	0.378	0.000	0.000
D	Non-normality	0.667	0.736	0.000

plot. However, for a consistent comparison in the later part of this paper, residual plot will be the focus. Besides, it is important to note that not all regression models assume normality for the error term, but a certain amount do including the classical normal linear regression model. In the case that the normality assumption doesn't hold, it is expected to observe data points that do not centralize around the horizontal zero line and unevenly distribute at both sides of the zero line. For example, given a skewed error distribution, fewer data points and more outliers are on one side of the zero line as shown at the bottom-right of Figure 1.

2.2. Conventionally testing for departures

(This section discusses the tests that will be used in the analysis and shows the results for the residual plots displayed in the previous section.)

Other than checking diagnostic plots, analysts may perform formal hypothesis testing for detecting model defects. Depending on the alternative hypothesis that is focused on, a variety of tests can be applied. For example, the presence of heteroskedasticity can usually be tested by applying the White test (White 1980) or the Breusch-Pagan 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. For testing 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 regressors, or the significance of proxy variables as in the Ramsey Regression Equation Specification Error Test (RESET) (Ramsey 1969). And for testing normality, the Shapiro-Wilk test [ref here] is perhaps the most widely used test included by many of the statistical softwares. Another choice will be the Jarque-Bera test [ref here] which directly checks if the sample skewness and kurtosis match a normal distribution.

Example residual plots given in Figure 1 are examined by the corresponding model structural test, Breusch-Pagan test and Shapiro-Wilk test as shown in Table 1. In the example, both the Breusch-Pagan test and the Shapiro-Wilk test rejects the null hypothesis for departures that they do not intend to examine. As discussed in Cook and Weisberg (1982), most residual-based tests for a particular type of departure from model assumptions are sensitive to other types of departures. It is likely the null hypothesis is correctly rejected but for the wrong reason, which is known as the "Type III error". Additionally, outliers will often incorrectly trigger the rejection of the null hypothesis despite the residuals are well-behaved (Cook and Weisberg 1999). This can be largely avoided in diagnostic plots as experienced analysts can evaluate the acceptability of assumptions flexibly, even in the presence of outliers.

2.3. Visual testing for departures

(This section introduces the lineup protocol, and briefly discusses the method for sampling null data, calculating the p-value and estimating power.)

2.3.1. Lineup protocol

Unlike hypothesis testing built upon rigorous statistical procedures, reading diagnostic plots relies on graphical perception - human’s ability to interpret and decode the information embedded in the graph (Cleveland and McGill 1984), which is to some extent subjective and indecisive. Further, visual discovery suffers from its unsecured and unconfirmed nature where the degree of the presence of the visual features typically can not be measured quantitatively and objectively, which may lead to over or under-interpretations of the data. One such example is finding an over-interpretation of the separation between gene groups in a two-dimensional projection from a linear discriminant analysis when in fact there are no differences in the expression levels between the gene groups and separation is not an uncommon occurrence (Roy Chowdhury et al. 2015).

Visual inference was first introduced in a 1999 Joint Statistical Meetings (JSM) talk with the title “Inference for Data Visualization” by Buja, Cook, and Swayne (1999) as an idea to address the issue of valid inference for visual discoveries of data plots (Gelman 2004). Later, Buja et al. (2009) proposed the lineup protocol as a visual test inspired by the “police lineup” or “identity parade” which is the act of asking the eyewitness to identify criminal suspect from a group of irrelevant people. The protocol consists of m randomly placed plots, where one plot is the actual data plot, and the remaining $m - 1$ plots have the identical graphical production as the data plot except the data has been replaced with data consistent with the null hypothesis. Then, an observer who have not seen the actual data plot will be asked to point out the most different plot from the lineup. Under the null hypothesis, it is expected that the actual data plot would have no distinguishable difference with the null plots, and the probability of the observer correctly picks the actual data plot is $1/m$. If we reject the null hypothesis as the observer correctly picks the actual data plot, then the Type I error of this test is $1/m$.

Figure 2 is an example of a lineup protocol. If the actual data plot at position 11 is identifiable, then it is evidence for the rejection of the null hypothesis that the regression model is correctly specified. In fact, the actual residual plot is obtained from a misspecified regression model with non-linearity issue.

The effectiveness of lineup protocol has already been validated by Majumder, Hofmann, and Cook (2013) under relatively simple classical normal linear regression model settings with only one or two regressors. Their results suggest visual test is capable of testing the significance of a single regressor with a similar power as a t-test, though they expressed that in general it is unnecessary to use visual inference if there exists a conventional test and they didn’t expect the visual test to perform equally well as the conventional test. In their third experiment, where there does not exist a proper conventional test, visual test outperforms the conventional test for a large margin. This is encouraging as it promotes the use of visual inference in border field of data science where there are no existing statistical testing procedures. In fact, lineup protocol has been integrated successfully into diagnostic tools of hierarchical linear models (Loy and Hofmann 2013).

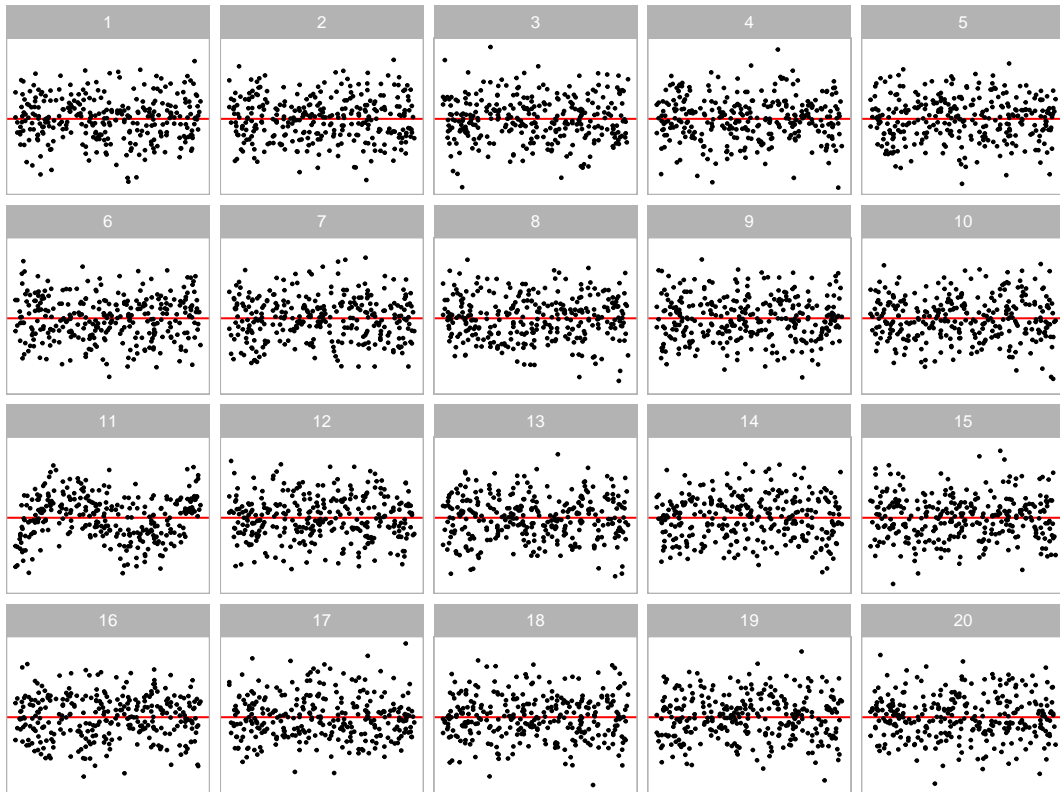


Figure 2. An example lineup consists of 20 randomly placed residual plots, where 19 are null plots with data consistent with the null hypothesis, and one is the actual residual plot. Can you find the most different plot?

2.3.2. Sampling from the null distribution

Data used in the $m - 1$ null plots need to be simulated. In the context of regression diagnostics, sampling data from H_0 is equivalent to sampling data from the assumed model. As Buja et al. (2009) suggested, H_0 is usually composited by a collection of distributions 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 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 regressors, then rescaling it by the ratio of residual sum of square in two regressions.

2.3.3. P-value calculation

Further, a visual test can involve K independent observers. Let $D_i = \{0, 1\}$ be a binomial random variable denoting whether subject i correctly detecting the actual data plot, and $X = \sum_{i=1}^K X_i$ be the number of observers correctly picking the actual data plot. Then, by imposing a relatively strong assumption on the visual test that all K evaluations are fully independent, under the null hypothesis, $X \sim \text{Binom}_{K, 1/m}$. Therefore, the p -value of a lineup of size m evaluated by K observer is given as $P(X \geq x) = 1 - F(x) + f(x)$, where $F(\cdot)$ is the cumulative distribution function, $f(\cdot)$ is the probability mass function and x is the realization of number of observers correctly picking the actual data plot (Majumder, Hofmann, and Cook 2013).

As pointed out by VanderPlas et al. (2021), the binomial model doesn’t take into account the possible dependencies in the visual test due to repeated evaluations of the same lineup. And it is inapplicable to visual test where subjects are asked to select one or more “most different” plots from the lineup. They summarized three common scenarios in visual inference: (1) K different lineups are shown to K subjects, (2) K lineups with different null plots but the same actual data plot are shown to K subjects, and (3) the same lineup is shown to K subjects. Out of these three scenarios, Scenario 3 is the most common in previous studies as it puts the least constraints on the experimental design. For Scenario 3, VanderPlas et al. (2021) modelled the probability of a plot i being selected from a lineup as θ_i , where $\theta_i \sim \text{Dirichlet}(\alpha)$ for $i = 1, \dots, m$ and $\alpha > 0$. And defined c_i to be the number of times plot i being selected in K evaluations. In case subject j makes multiple selections, they decided to add $1/s_j$ to c_i instead of one, where s_j is the number of plots subject j selected for $j = 1, \dots, K$. This ensured $\sum_i c_i = K$. Thus, the visual p -value followed by the above model is given as

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

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

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

The parameter α used in Equation 1 is usually unknown and hence needs to be estimated from the survey data. For low values of α , only a few plots are attractive to the observers and tend to be selected. For higher values of α , the distribution of the probability of each plot being selected is more evenly. VanderPlas et al. (2021) suggested that α can be estimated using maximum likelihood estimation or visual estimation. But if α is small and only a few null plots in a lineup are attractive, MLE could fail to provide accurate estimates.

2.3.4. Power calculation

3. Experimental design

(This section discusses the experimental design including the motivation of the experiment, an overview of the experiment, the simulation setting of the depatures from good residual plots, parameter choices, allocation of the lineups and other technical details.)

3.1. Motivation and overview

With our knowledge, the effectiveness of visual test relative to the equivalent conventional test in regression diagnostics has not been validated. Particularly, its ability to detect non-linearity and heteroskedasticity compared to model structural test and Breusch–Pagan test. Meanwhile, as mentioned in Section 1 section, we keen to understand the differences between conventional hypothesis testing and graphical diagnostics in the application of linear regression diagnostics and why conventional tests are not preferred by data analysts in linear regression diagnostics. Attempting to find the answer to these questions, three experiments were conducted.

The experiment I has ideal scenario for conventional testing, where the visual test is not expected to outperform the conventional test. The experiment II is a scenario where the conventional test is an approximate test, in which the visual test may have a chance to match the performance of the conventional test. The experiment III is designed for collecting human responses to lineup with only good residual plots such that the parameter α in Equation 1 can be estimated.

Subjects for all three experiments were recruited from an crowdsourcing platform called Prolific [ref here]. Prescreening procedure was applied during the recruitment, subjects were required to be fluent in English, with 98% minimum approval rate in other studies and 10 minimum submissions.

During the experiment, every subject was presented with a block of 20 lineups. For each lineup, the actual data plot was drawn as a standard residual plot of the null model with raw residuals on the y-axis and fitted values on the x-axis. An additional horizontal red line was added at $y = 0$ as a helping line. The 19 null datasets were generated by the residual rotation technique, and plotted in the same way. The lineup consisted of 20 residual plots with one randomly placed actual data plot. And for every lineup, the subject was 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 were from others. If there was no noticeable difference between plots in a lineup, subjects were permitted to select zero plots without providing the reason. No subject was shown the same lineup twice. Information about preferred pronoun, age group, education, and previous experience in visual experiment were also collected.

In every block of 20 lineups that presented to a subject, two lineups with obvious visual patterns were included as attention checks. A subject's submission was only accepted if the actual data plot was identified for at least one attention check. Data of rejected submissions were discarded automatically to maintain the overall data quality.

Overall, we planned to collect 7974 evaluations on 1152 unique lineups performed by 443 subjects.

3.2. *Simulating departures*

Two types of departures were considered with the corresponding data generating process being designed for experiment I and II.

3.2.1. *Non-linearity*

Experiment I is designed to study the ability of human subjects to detect the effect of a non-linear term \mathbf{z} which is a probabilist's Hermite polynomial [Hermite ref here] of another random vector \mathbf{x} in a two variable statistical model formulated as:

$$\mathbf{y} = 1 + \mathbf{x} + \mathbf{z} + \boldsymbol{\varepsilon}, \quad (3)$$

$$\mathbf{x} = g(\mathbf{x}_{raw}, 1), \quad (4)$$

$$\mathbf{z} = g(\mathbf{z}_{raw}, 1), \quad (5)$$

$$\mathbf{z}_{raw} = He_j(g(\mathbf{z}, 2)), \quad (6)$$

where \mathbf{y} , \mathbf{x} , $\boldsymbol{\varepsilon}$, \mathbf{x}_{raw} , \mathbf{z}_{raw} are vector 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 $\{-k, k\}$ defined as

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

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 leaves out by the null regression, which will result in model misspecification.

3.2.2. *Heteroskedasticity*

Experiment II is designed to study the ability of human subjects to detect the appearance of a heteroskedasticity pattern under a simple linear regression model setting:

Table 2. Parameter values for n, j, σ, X_{raw}

Sample size (n)	Order of Hermite polynomial (j)	Error SD (σ)	Distribution of X_{raw}
50	2	0.5	$U(-1, 1)$
100	3	1.0	$N(0, 0.3^2)$
300	6	2.0	$lognormal(0, 0.6^2)/3$
	18	4.0	$U\{1, 5\}$

$$\mathbf{y} = 1 + \mathbf{x} + \boldsymbol{\varepsilon}, \quad (9)$$

$$\mathbf{x} = g(\mathbf{x}_{raw}, 1) \quad (10)$$

$$\boldsymbol{\varepsilon} \sim N(\mathbf{0}, 1 + 2 - |a|b(\mathbf{x} - a)^2 \mathbf{I}), \quad (11)$$

$$(12)$$

where $\mathbf{y}, \mathbf{x}, \boldsymbol{\varepsilon}$ are vector of size n and $g(\cdot)$ is the scaling function defined in 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 regressor x , which will lead to the presence of heteroskedasticity.

3.3. Experimental setup

3.3.1. Treatments

Experiment I

- Treatments for nonlinearity experiment (plots summarising levels)

Data of experiment I were simulated using four different order of probabilist's Hermite polynomials ($j = 2, 3, 6, 18$), three different sample sizes ($n = 50, 100, 300$), four different standard deviations of the error ($\sigma = 0.5, 1, 2, 4$) and four different distribution of X_{raw} : (1) $U(-1, 1)$, (2) $N(0, 0.3^2)$, (3) $lognormal(0, 0.6^2)/3$ and (4) $u\{1, 5\}$. A summary of the parameters used in this experiment is given in Table 2.

The values of j was chosen so that different shapes of non-linearity were included in the residual plot. As shown in Figure 3, these include "U" shape, "S" shape, "M" shape and "Triple-U" shape.

The range of σ , which is a factor controlling the strength of the signal, was chosen so that different difficulty levels of lineups were generated, and therefore, the estimated power curve would be smooth and continuous. The example residual plots are given in Figure 4.

Four different distribution were used to generate X_{raw} shown in Figure 5. The uniform and the normal distribution are symmetric and commonly assumed in statistical models. The adjusted log-normal distribution provides skewed density. And the discrete uniform distribution provides discreteness in residual plot, which could enrich the pool of visual patterns.

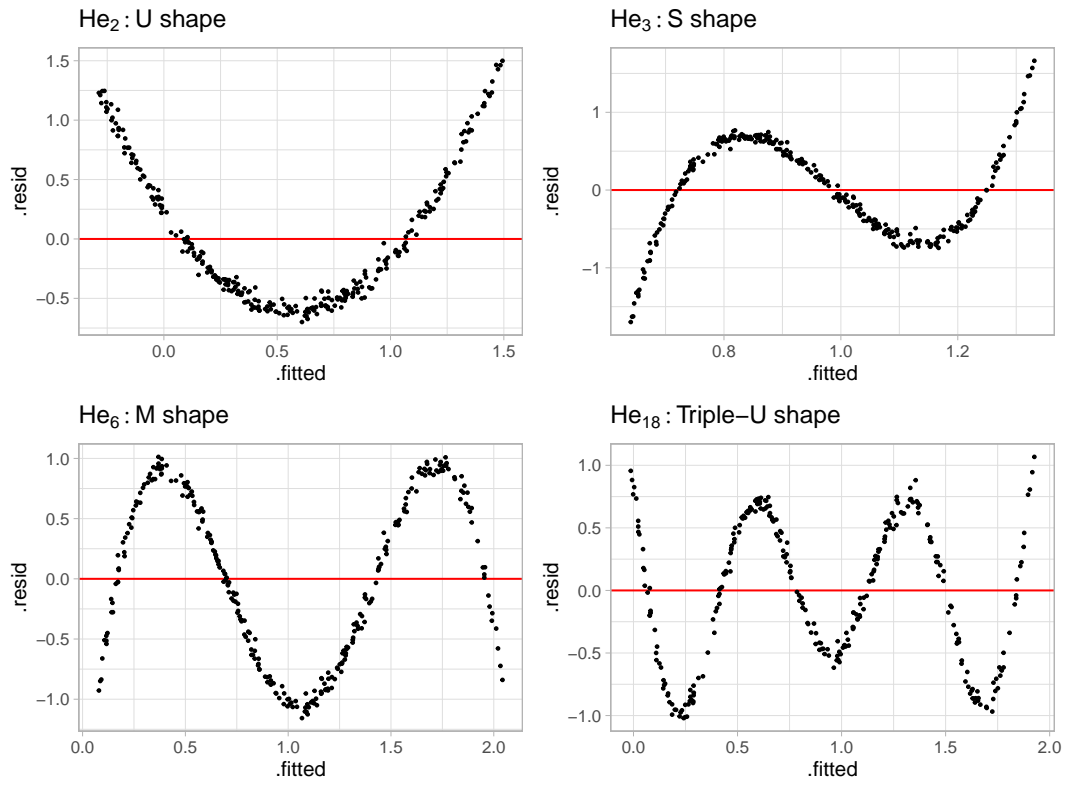


Figure 3. Example residual plots of the linear regression model used in experiment I. Four different values of j are included in the experiment results in four different shapes of residuals.

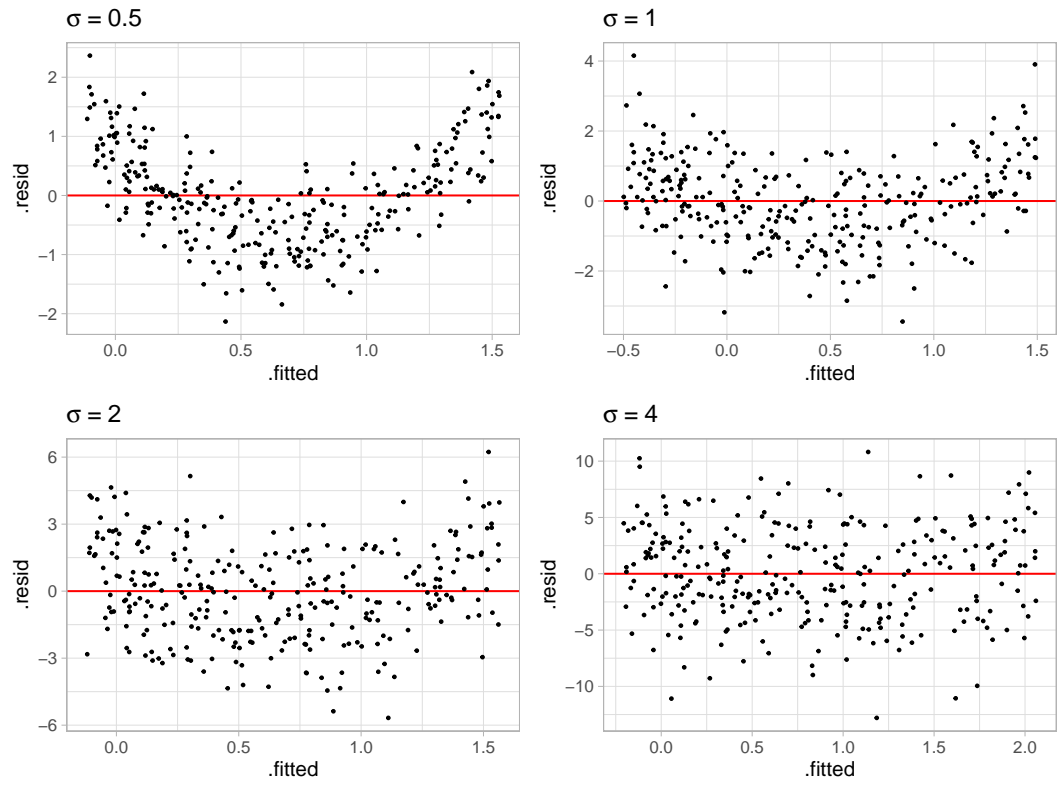


Figure 4. Example residual plots of the linear regression model used in experiment I. Four different values of σ are included in the experiment to control the strength of the signal.

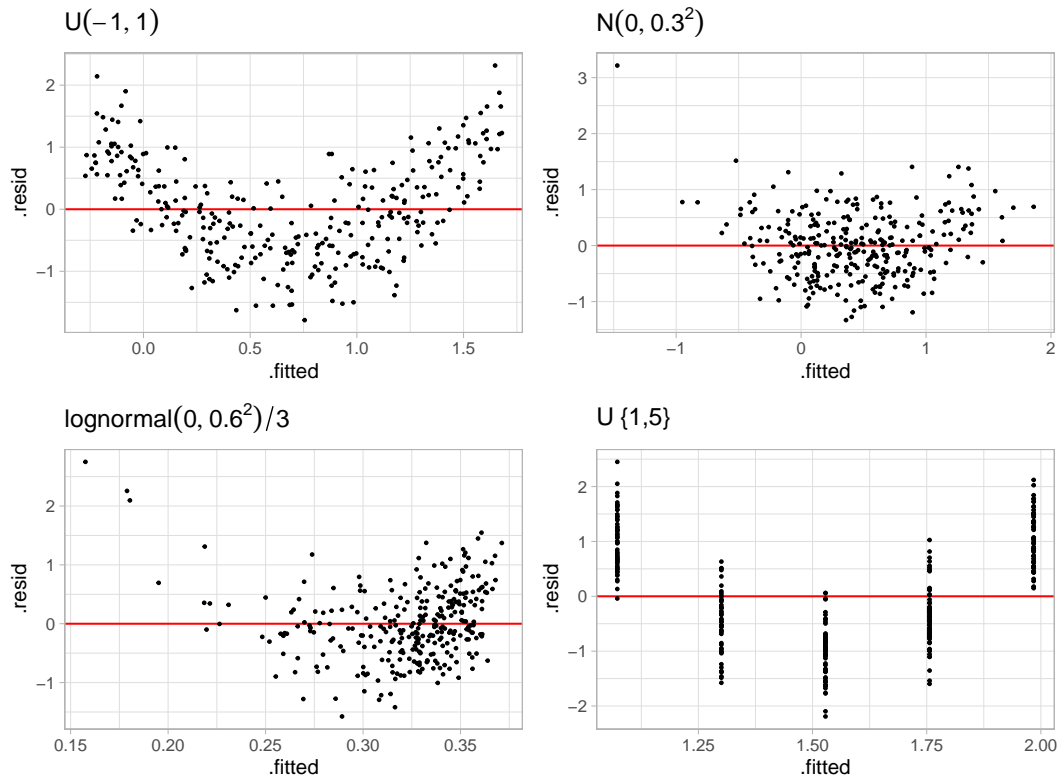


Figure 5. Example residual plots of the linear regression model used in experiment I. Four different distribution of x_{raw} are used in the experiment to provide various visual patterns.

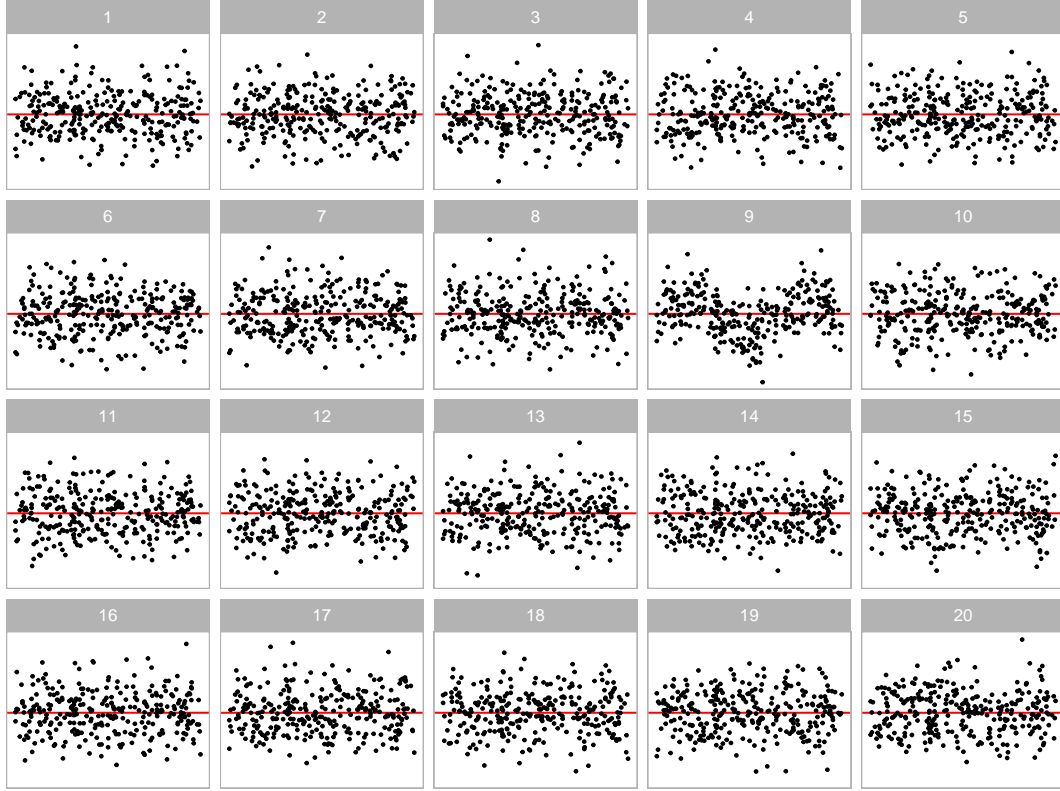


Figure 6. Lineup 24 in experiment I. Can you spot the most different plot?

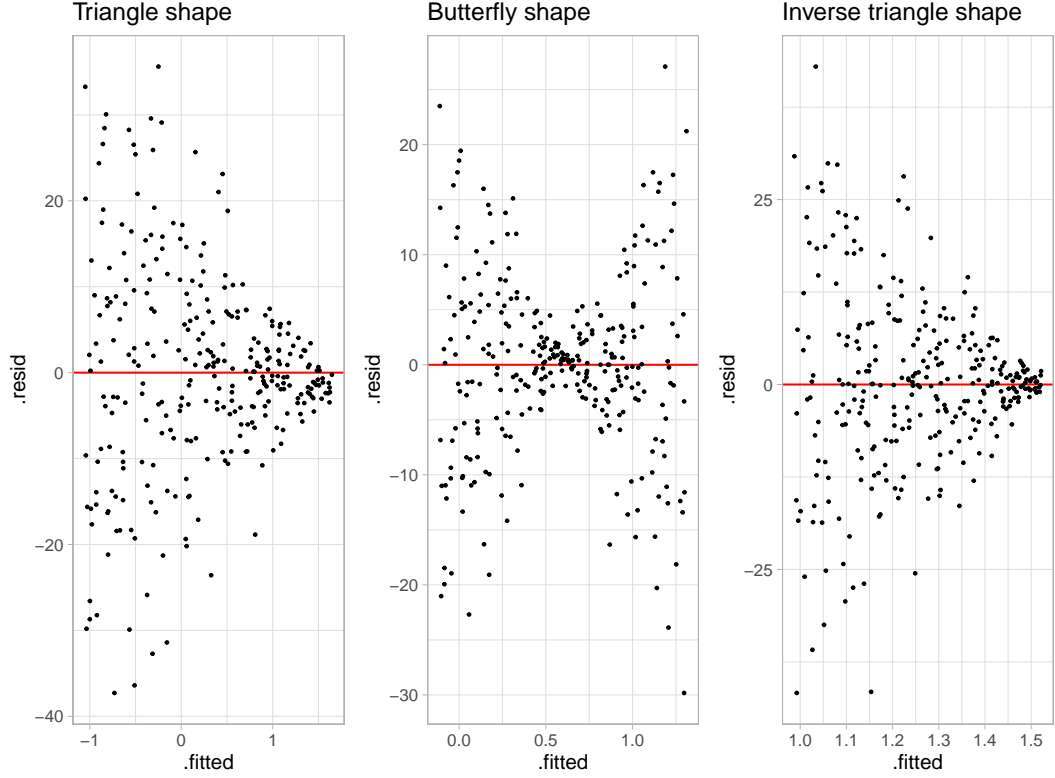
Figure 6 shows one of the lineups used in experiment I. This lineup was produced under $n = 300$, $j = 6$, $\sigma = 1$ and $X_{raw} \sim N(0, 0.3^2)$. The actual data plot location was four. All five subjects correctly identified the actual data plot for this lineup.

Experiment II

- Treatments for heteroskedasticity experiment (plots summarising levels)

Experiment data were simulated using three different shapes ($a = -1, 0, 1$), five different values of b ($b = 0.25, 1, 4, 16, 64$), three different sample sizes ($n = 50, 100, 300$) and four different distribution of X_{raw} : (1) $U(-1, 1)$, (2) $N(0, 0.3^2)$, (3) $\text{lognormal}(0, 0.6^2)/3$ and (4) $u\{1, 5\}$. A summary of the parameters used in this experiment is given in Table 2.

The values of a was chosen so that different shapes of heteroskedasticity were included in the residual plot. These include triangle shape, butterfly shape and inverse triangle shape.



The range of b , which is a factor controlling the strength of the signal, was chosen so that different difficulty levels of lineups were generated, and therefore, the estimated power curve would be smooth and continuous.

3.3.2. Assigning subjects

Three replications are made for each of the parameter values shown in Table 2 resulting in 192 different lineups. For each lineup, the actual data plot was drawn as a standard residual plot of the null model with raw residuals on the y-axis and fitted values on the x-axis. The 19 null datasets were generated by the residual rotation technique, and plotted in the same way. The lineup consisted of 20 residual plots with one randomly placed actual data plot. Figure 6 is an example of one of these lineups. It was produced by using $n = 300$, $j = 6$, $\sigma = 0.5$ and $X_{raw} \sim N(0.0.3^2)$. The actual data plot location was four. All five subjects correctly identified the actual data plot for this lineup.

In addition, each lineup is designed to be evaluated by five different subjects to provide reasonable estimates of the visual p-value. Thus, $192 \times 3 \times 5 / (20 - 2) = 160$ subjects were recruited to satisfy the design of the experiment I.

3.3.3. Collecting results

software/technical

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