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Automated Residual Plot Assessment with the R Package autovi and the Shiny App autovi.web

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Summary

Visually assessing residual plots is a common advice for linear model diagnostics, however this approach requires manual human evaluation and thereby is not scalable for assessing many models. Human evaluation also has the potential to produce inconsistent decisions from different analysts. Using a lineup protocol, where the residual plot is embedded among null plots, can help to alleviate inconsistency, but requires even more human effort. This is the type of task that in today's world we might employ a robot to do the tedious work for a human. Here we describe a new R package that includes a computer vision model for automated assessment of residual plots, and an accompanying Shiny app for ease of use. For a user-provided sample of residuals, it predicts a measure of visual signal strength (VSS) and provides a suite of supporting information to assist the analyst decide on the appropriateness their model fit.

Key words: initial data analysis; statistical graphics; data visualization; visual inference; computer vision; machine learning; hypothesis testing; regression analysis; model diagnostics

1. Introduction

Regression analysis is a widely used statistical modeling technique for data in many fields. There is a vast array of software for conducting regression modeling and generating diagnostics. The package `lmtest` (Zeileis & Hothorn 2002) provides a suite of conventional tests. The `stats` package (R Core Team 2022) offers standard

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diagnostic plots such as residuals vs. fitted values, quantile-quantile (Q-Q) plots, and residuals vs. leverage plots. Packages like `jtools` (Long 2022), `olsrr` (Hebbali 2024), `rockchalk` (Johnson 2022), and `ggResidpanel` (Goode & Rey 2019) provide similar graphical diagnostics, often with alternative aesthetics or interactive features. All of these tools deliver the types of diagnostic plots outlined in the classical text by Cook & Weisberg (1982). The `ecostats` package (Warton 2023) incorporates simulation envelopes into residual plots, while `DHARMa` (Hartig 2022) compares empirical quantiles (0.25, 0.5, and 0.75) of scaled residuals to their theoretical counterparts. `DHARMa` is particularly focused on detecting model violations such as heteroscedasticity, incorrect functional forms, and issues specific to generalized linear and mixed-effect models, like over/under-dispersion. It also includes conventional test annotations to help avoid misinterpretation.

However, relying solely on subjective assessments of these plots can lead to issues such as over-interpreting random patterns as model violations. Li et al. (2024a) demonstrated that visual methods using the lineup protocol (Buja et al. 2009) for assessing residuals are more useful, and also perform more practically than conventional tests due to their reduced sensitivity to minor departures. Packages such as `nullabor` (Wickham et al. 2020), `HLMdiag` (Loy & Hofmann 2014), and `regressinator` (Reinhart 2024), enable users to compare observed residual plots with plots of samples from null distributions, helping to quantify the significance of any detected patterns.

However, as discussed in Li et al. (2024b), the lineup protocol has significant limitations in large-scale applications due to dependence on human labor. Thus, a computer vision model was developed with an associated statistical testing procedure to automate the assessment of residual plots. This model takes a residual plot and a vector of auxiliary variables (such as the number of observations) as inputs and outputs the predicted visual signal strength (VSS). This strength estimates the distance between the residual distribution of the fitted regression model and the reference distribution assumed under correct model specification.

To make the statistical testing procedure and trained computer vision model widely accessible, we developed the R package `autovi`, and a web interface, `autovi.web` to make it easy for users to automatically read their residual plots with the trained computer vision model.

The remainder of this paper is structured as follows: Section 2 introduces the definition and computation of visual signal strength. Section 3 provides a detailed documentation of the `autovi` package, including its usage and infrastructure. Section 4 focuses on the

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`autovi.web` interface, describing its design and usage, along with illustrative examples. Finally, Section 5 presents the main conclusions of this work.

2. Definition and computation of visual signal strength

To train a computer vision model, a measure of the visible pattern in a plot is needed. We call this the **visual signal strength** (VSS), which measures how prominently a specific set of visual patterns appears in an image. This can be computed for a training set of data, and plots, where the generating distributions are specified.

In the context of regression model diagnostics, VSS describes the clarity of visual patterns on a diagnostic plot that may indicate model violations. Violations can be categorized as weak, moderate, or strong, but here we treat it as a continuous positive real variable. Importantly, its interpretation depends on how it is linked to a function of the data or the underlying data generating process. Consequently, the calculation of VSS can be vary across different model classes or within the same model, depending on the generating function.

VSS is an estimate of the distance between the residual distribution of a fitted classical normal linear regression model and a reference distribution; more details can be found in Li et al. (2024b). The distance measure is based on the Kullback-Leibler (KL) divergence:

$$D = \log\left(1 + D_{KL}\right),$$

where D_{KL} is given by:

$$D_{KL} = \int_{\mathbb{R}^n} \log \frac{p(\boldsymbol{e})}{q(\boldsymbol{e})} p(\boldsymbol{e}) d\boldsymbol{e},$$

here, $p(.)$ and $q(.)$ are the probability density functions of the reference residual distribution P and the true residual distribution Q, respectively.

This distance measure depends on knowledge of the true residual distribution, which is often unknown. However, it can be estimated by identifying or approximating a mapping from a set of residuals to its corresponding distance measure. The computer vision model presented in Li et al. (2024b) approximates this mapping. It is trained on a large number of synthetic regression models, where the data-generating process

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is known, allowing the distance measure to be explicitly calculated. The model takes a residual plot as input and outputs the corresponding distance measure. Additional details are provided in Li et al. (2024b).

3. R package: autovi

The main purpose of `autovi` is to provide rejection decisions and p-values for testing the null hypothesis (H_0) that the regression model is correctly specified. The package provides automated interpretation of residual plots using computer vision. The name `autovi` stands for **auto**mated **v**isual **i**nference. This functionality can be accessed through the R package `autovi`, or through a web interface, `autovi.web`, which allows use without the full installation of R, Python, and package dependencies on the user's system. locally.

3.1. Motivation

Figure 1 shows three sets of plots of residuals against fitted values. The simulated example in (a) might be interpreted as a heteroscedastic pattern, however the automated reading would predict this to have a visual signal strength (VSS) of 1.53, with a corresponding p-value of 0.25. This means it would be interpreted as a good residual plot, that there is nothing in the data to indicate a violation of model assumptions. Skewness in the predictor variables is generating the apparent heteroscedasticity, where the smaller variance in residuals at larger fitted values is due to smaller sample size only. The Breusch-Pagan test (Breusch & Pagan 1979) for heteroscedasticity would also not reject this as good residual plot.

The data in (b) is generated by fitting a linear model predicting `mpg` based on `hp` using the `datasets::mtcars`. It is a small data set, and there is a hint of nonlinear structure not captured by the model. The automated plot reading would predict a VSS of 3.57, which has a p-value less than 0.05. That is, the nonlinear structure is most likely real, and indicates a problem with the model. The conventional test, a Ramsey Regression Equation Specification Error Test (RESET) (Ramsey 1969) would also strongly detect the nonlinearity.

The third example is generated using the `surreal` package (Balamuta 2024) where structured residuals are hidden in data, to be revealed if the correct model is specified. Here a quote based on Tukey is used as the residual structure "visual summaries focus on unexpected values". The automated plot reading predicts the VSS to be 5.87, with a p-value less than 0.05. This structure is blindingly obvious visually, but a RESET

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test for nonlinear structure would not report a problem. (It would be detected by a Breusch-Pagan for heteroscedasticity and also Shapiro-Wilk test (Shapiro & Wilk 1965) for non-normality.)

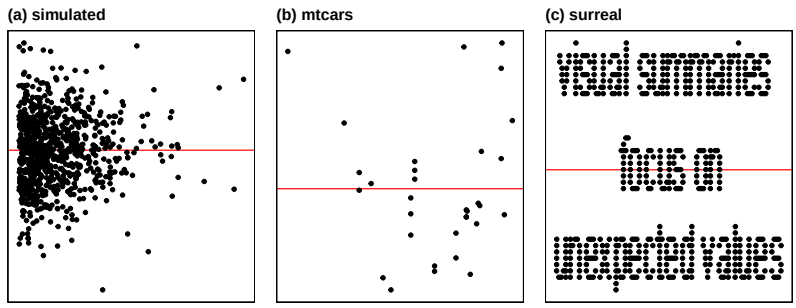

Figure 1. Reading residual plots can be a difficult task, particularly for students new to statistical modeling. The `autovi` package makes it easier. Here are three examples of residual plots, which may appear to have structure. According to autovi, the visual signal strengths (VSS) of these three examples are approximately (a) 1.53, (b) 3.57, (c) 5.87, resulting in (b), (c) being significant violations of good residuals, but (a) is consistent with a good residual plot.

3.2. Implementation

The `autovi` package is built on the `bandicoot` object-oriented programming (OOP) system (Li 2024), marking a departure from R's traditional S3 generic system. This OOP architecture enhances flexibility and modularity, allowing users to redefine key functions through method overriding XXX I think the technical term is overloading? XXX. While similar functionality could be achieved using R's S3 system with generic functions, the OOP framework offers a more structured and extensible foundation for the package. XXX Not sure if this last sentence is necessary XXX

The `autovi` infrastructure effectively integrates multiple programming languages and libraries into a comprehensive analytical tool. It relies on five core libraries from Python and R, each playing a critical role in the analysis pipeline. In Python, `pillow` (Clark et al. 2015) handles image processing tasks such as reading and resizing PNG files of residual plots, then converting them into input tensors for further analysis. `TensorFlow` (Abadi et al. 2016), a key component of modern machine learning, is used to predict the VSS of these plots using a pre-trained convolutional neural network.

In the R environment, `autovi` utilizes several libraries. `ggplot2` (Wickham 2016) generates the initial residual plots, saved as PNG files for visual input. `cassowaryr` (Mason et al. 2022) computes scagnostics (scatter plot diagnostics), providing numerical

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features that capture statistical properties of the plots. These scagnostics complement the visual analysis by offering quantitative metrics as secondary input to the computer vision model. `reticulate` (Ushey, Allaire & Tang 2024) enables seamless communication between R and Python.

3.3. Installation

The `autovi` package is available on CRAN. It is actively developed and maintained, with the latest updates accessible on GitHub. This paper uses `autovi` version 0.4.1. The package includes internal functions to check the current Python environment used by the `reticulate` package. If the necessary Python packages are not installed in the Python interpreter, an error will be raised. If you want to select a specific Python environment, you can do so by calling the `reticulate::use_python()` function before using the `autovi` package.

We recommend using the Shiny app `autovi.web` if users encounter installation problems.

3.4. Usage

3.4.1. Numerical summary

Three steps are needed to get an automated assessment of a set of residuals and fitted values:

1. Load the `autovi` package using the `library()` function.
2. Create a checker object with a linear regression model.
3. Call the `check()` method of the checker, which, by default, predicts the VSS for the true residual plot, 100 null plots, and 100 bootstrapped plots. The method stores the predictions internally and prints a concise results report.

The code to do this is:

```
library(autovi)
checker <- residual_checker(lm(dist ~ speed, data = cars))
checker$check()
```

It produces the following summary:

```
-- <AUTO_VI object>
```

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```
Status:
 - Fitted model: lm
 - Keras model: UNKNOWN
    - Output node index: 1
 - Result:
    - Observed visual signal strength: 3.162 (p-value = 0.0396)
    - Null visual signal strength: [100 draws]
       - Mean: 1.274
       - Quantiles:

    25%    50%    75%    80%    90%    95%    99%
0.8021 1.1109 1.5751 1.6656 1.9199 2.6564 3.3491

    - Bootstrapped visual signal strength: [100 draws]
       - Mean: 2.786 (p-value = 0.05941)
       - Quantiles:

  25%   50%   75%   80%   90%   95%   99%
2.452 2.925 3.173 3.285 3.463 3.505 3.652

    - Likelihood ratio: 0.7275 (boot) / 0.06298 (null) = 11.55
```

The summary includes observed VSS of the true residual plot and associated p-value of the automated visual test. The p-value is the proportion of null plots (out of the total 100) that have VSS greater than or equal to that of the true residual plot. The report also provides sample quantiles of VSS for null samples and bootstrapped data plots, providing more information about the sampling variability and a likelihood of model violations. The likelihood is computed from the proportion of values greater than the observed VSS in both the bootstrapped data values and the simulated null values.

3.4.2. Visual summary

Users can visually inspect the original residual plot alongside a sample null plot using `plot_pair()` or a lineup of null plot `plot_lineup()`. This visual comparison can clarify why H_0 is either rejected or not, and help identify potential remedies.

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```
checker$plot_pair()
```

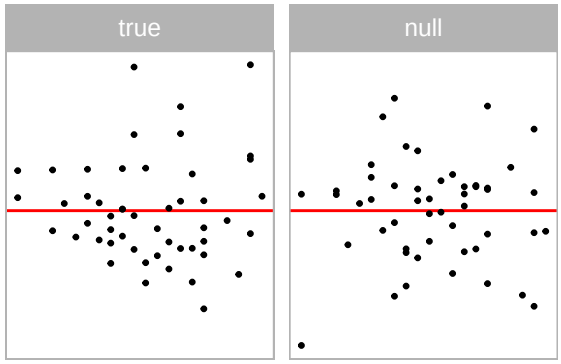

Figure 2. True plot alongside one null plot, for quick comparison.

The `plot_pair()` method (Figure 2) displays the true residual plot on the left and a single null plot on the right. If a full lineup was shown, the true residual plot would be embedded in a page of null plots. Users should look for any distinct visual patterns in the true residual plot that are absent in the null plot. Running these functions multiple times can help any visual suspicions, as each execution generates new random null plots for comparison.

The package offers a straightforward visualization of the assessment result through the `summary_plot()` function.

```
checker$summary_plot()
```

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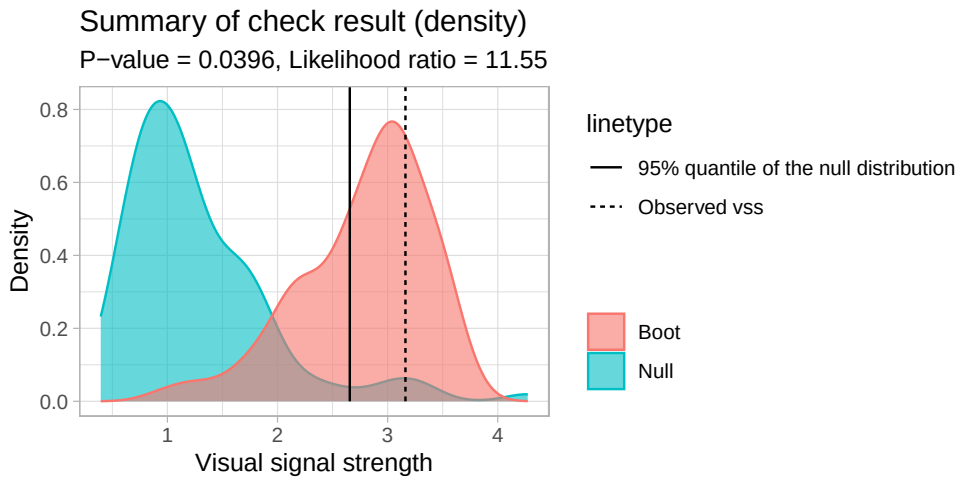

Figure 3. Summary plot comparing the densities of VSS for bootstrapped residual samples (red) relative to VSS for null plots (blue).

In the result, shown in Figure 3, the blue area represents the density of VSS for null residual plots, while the red area shows the density for bootstrapped residual plots. The dashed line indicates the VSS of the true residual plot, and the solid line marks the critical value at a 95% significance level. The p-value and the likelihood ratio are displayed in the subtitle. The likelihood ratio represents the ratio of the likelihood of observing the VSS of the true residual plot from the bootstrapped distribution compared to the null distribution.

Interpreting the plot involves several key aspects. If the dashed line falls to the right of the solid line, it suggests rejecting the null hypothesis. The degree of overlap between the red and blue areas indicates similarity between the true residual plot and null plots; greater overlap suggests more similarity. Lastly, the portion of the red area to the right of the solid line represents the percentage of bootstrapped models considered to have model violations.

This visual summary provides an intuitive way to assess the model's fit and potential violations, allowing users to quickly grasp the results of the automated analysis. XXX It might be a good idea to include a basic message explaining the plot and how it's used when it is generated, because a lot of non-statisticians aren't going to be used to interpreting these plots XXX

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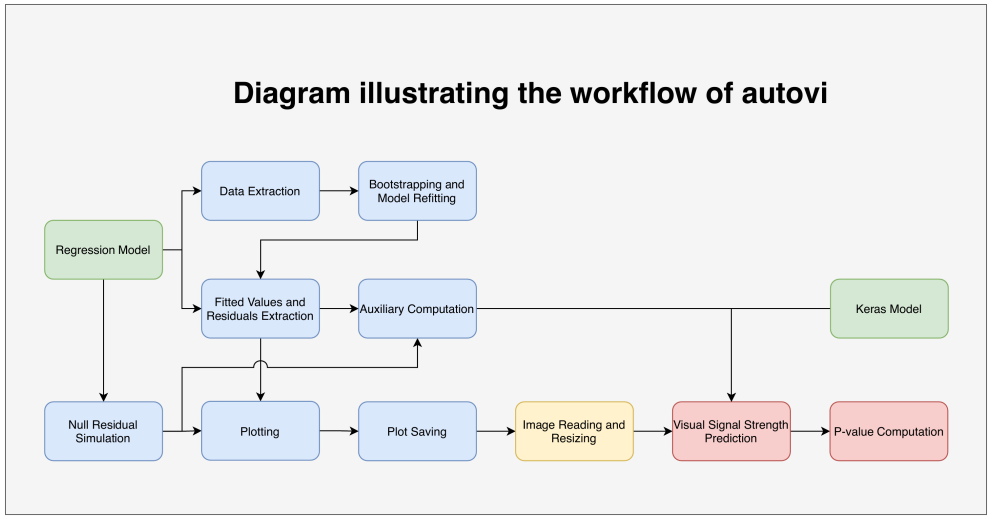

Figure 4. Diagram illustrating the infrastructure of the R package `autovi`. The modules in green are primary inputs provided by users. Modules in blue are overridable methods that can be modified to accommodate users' specific needs. The module in yellow is a pre-defined non-overridable method. The modules in red are primary outputs of the package.

3.5. Modularized infrastructure

The initial motivation for developing `autovi` was to create a convenient interface for sharing the models described and trained in Li et al. (2024b). However, recognizing that the classical normal linear regression model represents a restricted class of models, we sought to avoid limiting the potential for future extensions, whether by the original developers or other developers. As a result, the package was designed to function seamlessly with linear regression models with minimal modification and few required arguments, while also accommodating other classes of models through partial infrastructure substitution. This modular and customizable design allows `autovi` to handle a wide range of residual diagnostics tasks.

The infrastructure of `autovi` consists of ten core modules: data extraction, bootstrapping and model refitting, fitted values and residuals extraction, auxiliary computation, null residual simulation, plotting, plot saving, image reading and resizing, VSS prediction, and p-value computation. Each module is designed with minimal dependency on the preceding modules, allowing users to customize parts of the infrastructure without affecting its overall integrity. An overview of this infrastructure is illustrated in Figure 4.

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The modules for VSS prediction and p-value computation are predefined and cannot be overridden, although users can interact with them directly through function arguments. Similarly, the image reading and resizing module is fixed but will adapt to different Keras models by checking their input shapes. The remaining seven modules are designed to be overridable, enabling users to tailor the infrastructure to their specific needs. These modules are discussed in detail in the package documentation.

4. Web interface: autovi.web

The `autovi.web` shiny application extends the functionality of `autovi` by offering a user-friendly web interface for automated residual plot assessment. This eliminates the common challenges associated with software installation, so users can avoid managing Python environments or handling version requirements for R libraries. The platform is cross-platform and accessible on various devices and operating systems, making it suitable even for users without R programming experience. Additionally, updates are managed centrally, ensuring that users always have access to the latest features. This section discusses the implementation based on `autovi.web` version 0.1.0.

4.1. Implementation

The interface `autovi.web` is built using the `shiny` (Chang et al. 2022) and `shinydashboard` (Chang & Borges Ribeiro 2021) R packages. Hosted on the shinyapps.io domain, the application is accessible through any modern web browser. The R packages `htmltools` (Cheng et al. 2024) and `shinycssloaders` (Sali & Attali 2020) are used to render markdown documentation in shiny application, and for loading animations for shiny widgets, respectively.

Determining the best way to implement the backend was difficult. In our initial planning for `autovi.web`, we considered implementing the entire web application using the `webr` framework (Moon 2020), which would have allowed the entire application to run directly in the user's browser. However, `webr` does not support packages which use compiled fortran code, which is required by `splancs` (Rowlingson & Diggle 2023), a dependency of `autovi`. In the future, it is possible that a working Emscripten (Zakai 2011) version of this package may allow full `webr` support.

We also explored the possibility of implementing the web interface using frameworks built on other languages, such as Python. However, server hosting domains that natively support Python servers typically do not have the latest version of R installed. Additionally, calling R from Python is typically done using the `rpy2` Python library

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(Gautier 2024), but this approach can be awkward when dealing with language syntax related to non-standard evaluation. Another option we considered was renting a server where we could have full control, such as those provided by cloud platforms like Google Cloud Platform (GCP) or Amazon Web Services (AWS). However, deploying and maintaining the server securely requires some expertise. Ultimately, the most practical solution was to use the `shiny` and `shinydashboard` frameworks, which are well-established in the R community and offer a solid foundation for web application development.

The server-side configuration of `autovi.web` is carefully designed to support its functionality. Most required Python libraries, including `pillow` and `numpy`, are pre-installed on the server. These libraries are integrated into the Shiny application using the `reticulate` package, which provides an interface between R and Python.

Due to the resource allocation policy of shinyapps.io, the server enters a sleep mode during periods of inactivity, resulting in the clearing of the local Python virtual environment. Consequently, when the application "wakes up" for a new user session, these libraries need to be reinstalled. While this ensures a clean environment for each session, it may lead to slightly longer loading times for the first user after a period of inactivity.

In contrast to `autovi`, `autovi.web` leverages `TensorFlow.js`, a JavaScript library that allows the execution of machine learning models directly in the browser. This choice enables native browser execution, enhancing compatibility across different user environments, and shifts the computational load from the server to the client-side. `TensorFlow.js` also offers better scalability and performance, especially when dealing with resource-intensive computer vision models on the web.

While `autovi` requires downloading the pre-trained computer vision models from GitHub, these models in ".keras" file format are incompatible with `TensorFlow.js`. Therefore, we extract and store the model weights in JSON files and include them as extra resources in the Shiny application. When the application initializes, `TensorFlow.js` rebuilds the computer vision model using these pre-stored weights.

To allow communication between `TensorFlow.js` and other components of the Shiny application, the `shinyjs` R package (Attali 2021) is used. This package allows calling custom JavaScript code within the Shiny framework. The specialized JavaScript code for initializing `TensorFlow.js` and calling `TensorFlow.js` for VSS prediction is deployed alongside the Shiny application as additional resources.

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4.2. Usage

The workflow of `autovi.web` is designed to be straightforward, with numbered steps displayed in each panel. There are two example datasets provided by the web application. The single residual plot example uses the `dino` dataset from the R package `datasauRus` (Davies, Locke & D'Agostino McGowan 2022). The lineup example uses residuals from a simulated regression model that has a non-linearity issue. We walk through the lineup example to further demonstrate the workflow of the web application.

4.2.1. Reading data and setting parameters

The user can select to upload data as either a single set of residuals and fitted values in a two (or more) column CSV file or a pre-computed lineup of residuals and null datasets in a three (or more) column CSV file (i.e. multiple sets of residuals and fitted values with a column indicating the set label). Here we illustrate use with lineup example data sets (Figure 5). To use the lineup example data, click the "Use Lineup Example" button. The data status will then update to show the number of rows and columns in the dataset, and the CSV type will automatically be selected to the correct option. Since the example dataset follows the variable naming conventions assumed by the web application, the columns for fitted values, residuals, and labels of residual plots are automatically mapped such that the column named as `.fitted` is mapped to fitted values, `.resid` is mapped to residuals and if applicable, `.sample` to labels of the residual set (middle image). If the user is working with a custom dataset, these options must be set accordingly. Whenever a data containing a lineup, the user must manually select the label for the true residual plot, otherwise the web application does not provide all the results. The last step is to click the play button (right image) to start the assessment.

4.2.2. Results provided

Results are provided in multiple panels. The first row of the table Figure 6 is the most crucial to check, as it provides the VSS and the rank of the true residual plot among the other plots. The summary text beneath the table provides the p-value, which can be used for quick decision-making. The lineup is for manual inspection, and the user should see if the true residual plot is visually distinguishable from the other plots, to confirm if the model violation is serious.

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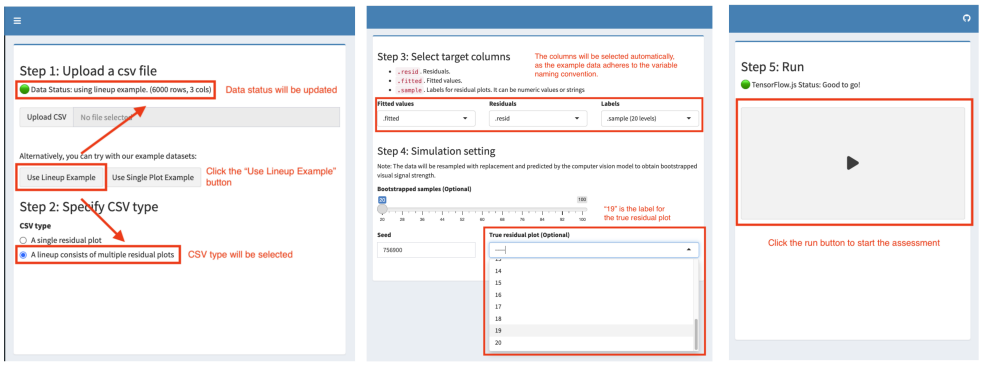

Figure 5. To begin the workflow for `autovi` using the lineup example dataset, the user clicks the "Use Lineup Example" button (left) to load the example dataset, during which the data status and CSV type will be automatically updated. The user must manually select the label for the true residual plot (middle) to compute further results. The user initiates the assessment of the lineup example data by clicking the run button (right).

The density plot in Figure 7 offers a more robust result, allowing the user to compare the distribution of bootstrapped VSS with the distribution of null VSS. Finally, the grayscale attention map (right image) can be used to check if the target visual features, like the non-linearity present in the lineup example, are captured by the computer vision model, ensuring the quality of the assessment.

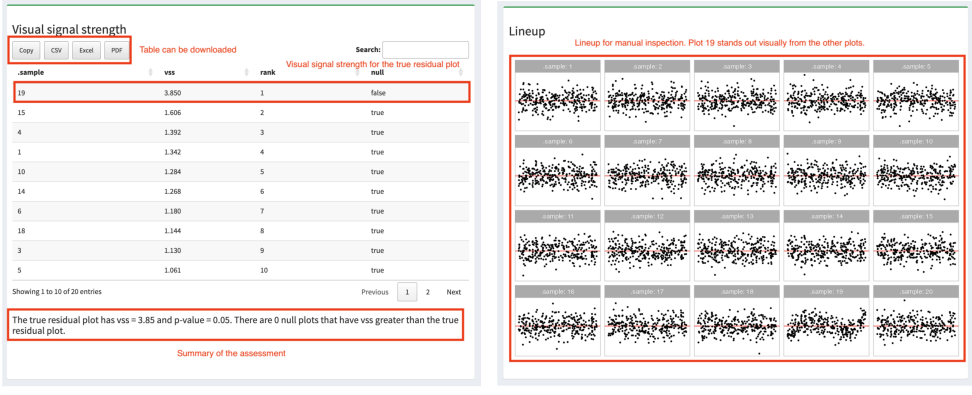

Figure 6. Results for the lineup. The VSS of the true residual plot is displayed in the first row of the table of VSS values for all the null plots (left image), with a summary text beneath the table providing the p-value to aid in decision-making. A lineup of residual plots allows for manual inspection (right image).

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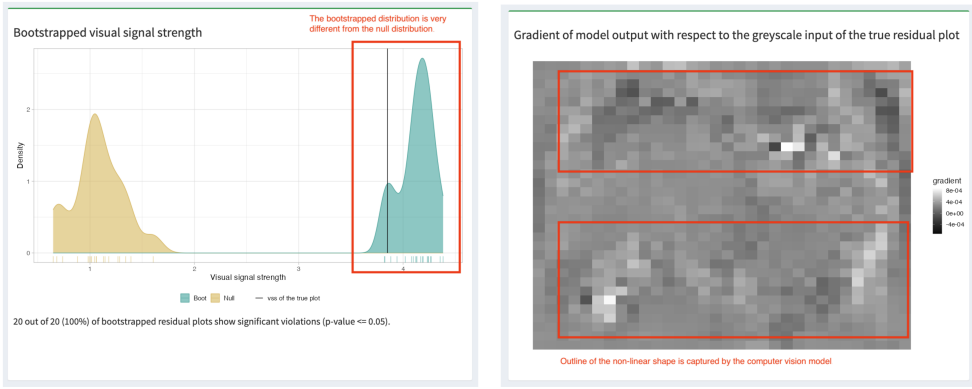

Figure 7. Summaries assessing the strength of the pattern and which elements of the plot contribute. The density plot helps verify if the bootstrapped distribution differs from the null distribution (left image). The attention map (right image) offers insights into whether the computer vision model has captured the intended visual features of the true residual plot.

5. Conclusions

This paper presents new regression diagnostics software, the R package `autovi` and its accompanying web interface, `autovi.web`. It addresses a critical gap in the current landscape of statistical software. While regression tools are widely available, effective and efficient diagnostic methods have lagged behind, particularly in the field of residual plot interpretation.

The `autovi` R package, introduced in this paper, automates the assessment of residual plots by incorporating a computer vision model, eliminating the need for time-consuming and potentially inconsistent human interpretation. This automation improves the efficiency of the diagnostic process and promotes consistency in model evaluation across different users and studies.

The development of the accompanying Shiny app, `autovi.web`, expands access to these advanced diagnostic tools, by providing a user-friendly interface. It makes automated residual plot assessment accessible to a broader audience, including those who may not have extensive programming experience. This web-based solution effectively addresses the potential barriers to adoption, such as complex dependencies and installation requirements, that are often associated with advanced statistical software.

The combination of `autovi` and `autovi.web` offers a comprehensive solution to the challenges of residual plot interpretation in regression analysis. These tools have the potential to significantly improve the quality and consistency of model diagnostics

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across various fields, from academic research to industry applications. By automating a critical aspect of model evaluation, they allow researchers and analysts to focus more on interpreting results and refining models, rather than grappling with the intricacies of plot assessment.

The framework established by `autovi` and `autovi.web` opens up exciting possibilities for further research and development. Future work could explore the extension of these automated assessment techniques to other types of diagnostic plots and statistical models, potentially revolutionizing how we approach statistical inference using visual displays more broadly.

6. Resources and supplementary material

The current version of `autovi` can be installed from CRAN, and source code for both packages are available at `github.com/TengMCing/autovi` and `github.com/TengMCing/autovi_web` respectively. The web interface is available from `autoviweb.netlify.app`.

This paper is reproducibly written using Quarto (Allaire et al. 2024) powered by Pandoc (MacFarlane, Krewinkel & Rosenthal 2024) and pdfTeX. The full source code to reproduce this paper is available at `github.com/TengMCing/autovi_paper`.

These `R` packages were used for the work: `tidyverse` (Wickham et al. 2019), `lmtest` (Zeileis & Hothorn 2002), `kableExtra` (Zhu 2021), `patchwork` (Pedersen 2022), `rcartocolor` (Nowosad 2018), `glue` (Hester & Bryan 2022), `here` (Müller 2020), `magick` (Ooms 2023), `yardstick` (Kuhn, Vaughan & Hvitfeldt 2024) and `reticulate` (Ushey, Allaire & Tang 2024).

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