maars: Tidy Inference under the ‘Models as Approximations’ Framework in \( R \)

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Abstract

Linear regression using ordinary least squares (OLS) is a critical part of every statistician's toolkit. In R, this is elegantly implemented via \( \texttt{lm()} \) and its related functions. However, the statistical inference output from this suite of functions is based on the assumption that the model is well specified. This assumption is often unrealistic and at best satisfied approximately. In the statistics and econometrics literature, this has long been recognized and a large body of work provides inference for OLS under more practical assumptions. This can be seen as model-free inference. In this paper, we introduce our package \texttt{maars} ("models as approximations") that aims at bringing research on model-free inference to \( R \) via a comprehensive workflow. The \texttt{maars} package differs from other packages that also implement variance estimation, such as \texttt{sandwich}, in three key ways. First, all functions in \texttt{maars} follow a consistent grammar and return output in tidy format, with minimal deviation from the typical \( \texttt{lm()} \) workflow. Second, \texttt{maars} contains several tools for inference including empirical, multiplier, residual bootstrap, and subsampling, for easy comparison. Third, \texttt{maars} is developed with pedagogy in mind. For this, most of its functions explicitly return the assumptions under which the output is valid. This key innovation makes \texttt{maars} useful in teaching inference under misspecification and also a powerful tool for applied researchers. We hope our default feature of explicitly presenting assumptions will become a de facto standard for most statistical modeling in \( R \).

1 Introduction

Multiple linear regression is one of the most commonly used data analytic tools. Although the general notion of "all models are approximations" is well received in terms of inference under model misspecification, most statistical software (including \( R \)) does not yet have a comprehensive implementation of all such aspects. In detail, the elegant implementation of the ordinary least squares estimator through the \( \texttt{lm()} \) function is based on the classical and unrealistic assumptions of a linear model, i.e., linearity, homoscedasticity, and normality. The \( \texttt{lm()} \) implementation does provide methods for diagnosing these assumptions. However, it has long been recognized that inference should be performed under more general assumptions, even if the estimator is constructed based on likelihood principles [Huber, 1967, Buja et al., 2019a].

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Over the years, several R packages such as car [Fox and Weisberg, 2019], clubSandwich [Pustejovsky, 2021], lmtest [Zeileis and Hothorn, 2002], and sandwich [Zeileis, 2004, Zeileis et al., 2020] have been developed to implement heteroscedasticity and non-linearity consistent estimators of the asymptotic variance. In this misspecified setting, a tidy workflow is currently unavailable in R. By a tidy workflow, we mean a suite of functions for variance estimation, confidence interval computation, hypothesis testing, and diagnostics that follow a consistent naming convention, whose outputs are tailored for further exploration, e.g., using the tidyverse set of packages [Wickham et al., 2019]. In this paper, we introduce the maars package that provides such a tidy workflow for data analysis with ordinary least squares (OLS) linear regression. Our package is motivated, in large part, by the discussion of Buja et al. [2019a,b]. Part of our motivation is also pedagogical, in making applied researchers more explicitly aware of the underlying assumptions and the consequences of model-based variance estimators for inference.

In this paper, we introduce the key functionality in the maars package. For illustrative purposes only, we use the LA Homeless data from Buja et al. [2019a] as a running example to demonstrate the maars package functionality.¹ As noted in Buja et al. [2019a], this dataset has 505 observations, each representing a sampled metropolitan LA County Census tract. It also has 7 numeric variables measuring different quantities of interest in each tract. For linear modeling purposes, the response variable (StreetTotal) is a count of the homeless people in each tract. There are six covariates for regression purposes. These include the Median Income of Households (MedianInc ($1000)), and the share of non-Caucasian residents (PercMinority). The remaining four covariates measure the proportion of the different types of lots in each tract (PercCommercial, PercVacant, PercResidential and PercIndustrial).

The rest of the paper is organized as follows. In Section 2, we detail the theoretical properties of the OLS estimator in both the well-specified and misspecified model settings. In Section 3, we describe the key design principles upon which maars is based. Section 4 and Section 5 focus on the variance estimation and graphical model diagnostic functionalities present in the package respectively. In Section 6, we give an overview of the pedagogical vignettes and and guided lesson-plans in the package. In Section 7, we discuss the open-source best practices that we adopted to help build an inclusive community for new users and contributors. Finally, in Section 8 we conclude by outlining future development plans.

2 Theoretical properties of OLS

2.1 OLS under well-specification

Suppose we have regression data \((X_i, Y_i) \in \mathbb{R}^d \times \mathbb{R}, 1 \leq i \leq n\). The well-specified (classical) linear model stipulates that \((X_i, Y_i), 1 \leq i \leq n\) are independent and satisfy

\[
Y_i = X_i^\top \beta_0 + \varepsilon_i,
\]

where \(\varepsilon_i|X_i \sim \text{i.i.d. } N(0, \sigma^2)\). This implies that \(\mathbb{E}[Y_i|X_i] = X_i^\top \beta_0\) (linearity) and \(\text{Var}(Y_i|X_i) = \sigma^2\) (homoscedasticity). Usually one also assumes covariates to be non-stochastic. Under these

¹The package is available at: https://github.com/shamindras/maars.
assumptions, we get that the OLS estimator

\[ \hat{\beta} = \arg \min_{\theta \in \mathbb{R}^d} \sum_{i=1}^{n} (Y_i - X_i^\top \theta)^2, \]

has a normal distribution (conditional on \( X_i, i \leq n \)):

\[ \hat{\beta} - \beta_0 \sim \mathcal{N} \left( 0, \sigma^2 \frac{\hat{J}^{-1}}{n} \right) \quad \text{where} \quad \hat{J} := \frac{1}{n} \sum_{i=1}^{n} X_i X_i^\top. \]  

(2)

This distribution yields confidence intervals, hypothesis tests, and \( p \)-values for \( \beta_0 \). The \( R \) function `lm()` provides inference based on (2). For the LA Homeless data, the implementation of OLS along with its inference (in Figure 1) are as follows:

```r
# load LA county homeless data into dataframe
la_county <- get(data("la_county", package = "maars"))

# fit OLS on LA county data
mod_fit <- lm(formula = StreetTotal ~ ., data = la_county)

# summary of fitted model
summary(mod_fit)
```

Figure 1: Output of `summary(mod_fit)`.

As mentioned, the standard errors, \( t \)-scores, and the \( p \)-values reported in the summary above are most likely invalid because the linear model for LA Homeless data is not well-specified [Buja et al., 2019a]. We will now discuss the properties of OLS under misspecification of the linear model. It should be mentioned here that we will only discuss misspecification of the linear model but require independence of the observations. Dependence will be part of our future work (see Section 8).
2.2 OLS under misspecification

If \((X_i, Y_i) \in \mathbb{R}^d \times \mathbb{R}, 1 \leq i \leq n\) are independent and identically distributed (i.i.d.), then the least squares estimator \(\hat{\beta}\) converges (in probability) to

\[
\beta^\infty := \arg \min_{\theta \in \mathbb{R}^d} \mathbb{E} \left( (Y - X^T \theta)^2 \right),
\]

where \((X, Y) \in \mathbb{R}^d \times \mathbb{R}\) is an independent copy of \((X_i, Y_i)\) and \(\beta^\infty (\hat{\beta} \text{ at } n = \infty)\) is the population projection parameter. If the linear model \((1)\) holds true, then \(\beta^\infty = \beta_0\). Assuming only i.i.d. observations with finite moments, it is easy to obtain the normal limiting distribution:

\[
\sqrt{n}(\hat{\beta} - \beta^\infty) \xrightarrow{d} N(0, J^{-1}VJ^{-1}),
\]

where \(J = \mathbb{E}(XX^T)\), and \(V = \mathbb{E}(XX^T(Y - X^T \beta^\infty)^2)\); see Buja et al. [2019a] for details. A similar limit theorem also holds when the observations are independent but not identically distributed (i.n.i.d.).

The matrices \(J\) and \(V\) can be readily estimated by replacing the expectations by averages and \(\beta^\infty\) by \(\hat{\beta}\) leading to the sandwich estimator \(\hat{J}^{-1}\hat{V}\hat{J}^{-1}\); see Kuchibhotla et al. [2018] for details. Here

\[
\hat{J} = \frac{1}{n} \sum_{i=1}^{n} X_iX_i^T \quad \text{and} \quad \hat{V} = \frac{1}{n} \sum_{i=1}^{n} X_iX_i^T(Y_i - X_i^T \hat{\beta})^2.
\]

It can be shown that \(\hat{J}^{-1}\hat{V}\hat{J}^{-1}\) consistently estimates the asymptotic variance under i.i.d. data and over-estimates the asymptotic variance under i.n.i.d. data [Kuchibhotla et al., 2018]. It is noteworthy that the estimator \(\hat{J}^{-1}\hat{V}\hat{J}^{-1}\) converges to the model-based variance if the linear model \((1)\) holds true. With a model-free estimator of the asymptotic variance, one can perform inference for \(\beta^\infty\) using asymptotic normality. The asymptotic \((1 - \alpha)\) confidence interval for the \(j^{th}\) coefficient \(\beta^\infty(j)\) is then given by

\[
\hat{CI}_j = \left[ \hat{\beta}(j) - z_{\alpha/2} \sqrt{\frac{(\hat{J}^{-1}\hat{V}\hat{J}^{-1})_{jj}}{n}}, \hat{\beta}(j) + z_{\alpha/2} \sqrt{\frac{(\hat{J}^{-1}\hat{V}\hat{J}^{-1})_{jj}}{n}} \right],
\]

where \(z_{\alpha/2}\) is the quantile of the standard normal. The Wald test for \(k\) linear restrictions of the coefficients of the form \(R\beta = r\), where \(R\) and \(r\) are a \(k \times d\) matrix and a \(k\) dimensional vector respectively, is still valid under only the assumption of independence. Under the null hypothesis, the Wald test statistic \((R\hat{\beta} - r)^T(R\hat{J}^{-1}\hat{V}\hat{J}^{-1}R^T)^{-1}(R\hat{\beta} - r)\) asymptotically follows a \(\chi^2\) distribution with \(k\) degrees of freedom; see, e.g., White [1982, Theorem 3.4].

3 maars: Designed for research and pedagogy

Our goal is for the maars package to be a natural research workflow for model-free OLS inference in \(\mathbb{R}\). Equally importantly, we also intend for maars to be a useful pedagogical tool to help convey these rich inferential concepts. In order to satisfy this dual research and pedagogical purpose, maars is built according to the following five design principles (DP.1–DP.5):

DP.1 Build a flexible API to enable easy user access to a diverse set of inferential tools.

4
DP.2 Ensure that the assumptions for all modeling techniques explicit to the user.

DP.3 Develop a consistent tidy grammar for OLS inference under model misspecification to enhance communication of code with other users and developers.

DP.4 Emphasize teaching these inferential techniques and concepts through instructive examples.

DP.5 Utilize modern open-source best practices to create an inclusive package development environment.

We provide brief details on the design principles DP.1–DP.5 and details of how they are applied in maars. First, by DP.1, we intend for maars to provide a user-friendly way to access the rich set of OLS inferential techniques under model misspecification. This is primarily achieved through the comp_var() function, which provides a common API for the user for OLS modeling purposes. By DP.2 we want to ensure that the assumptions behind the modeling techniques are made explicit to the user. By DP.3 we have adopted in maars a consistent function naming convention that follows a tidy grammar and where tidy tibble outputs are returned whenever feasible. This is to better facilitate downstream analysis and communication of results. Details of DP.1–DP.3 are emphasized with examples in Sections 4 and 5.

In DP.4 we emphasize the use of detailed instructive vignettes to teach the inferential techniques for OLS using a tidy maars workflow. See Section 6 for more details. Finally, in DP.5 our aim is for maars to be a long-term part of a applied researcher’s OLS toolkit in R. We achieve this by following and adapting to the best open-source package development practices, and thus building an inclusive environment around maars. For example, we ensure that the maars functions are rigorously benchmarked and unit tested. A well defined benchmarking framework demonstrates how our code is optimized for computational efficiency. A detailed unit testing framework allows us to effectively perform statistical validation and error handling. See Section 7 for details. Finally, we note that the maars package is developed in an open-source manner that is inclusive towards new users and contributors.

4 Variance estimation and inference in maars

Under model misspecification, one of the main inferential tools is accurate and efficient estimation of variance. The maars modeling framework offers a variety of OLS inferential tools that are readily usable as part of a tidy pipe-friendly (%>%*) workflow [Bache and Wickham, 2020].

These tools fall into three categories. First, we have closed-form variance estimators that are computed by default, i.e., lm() and the sandwich standard errors. Second, we have resampling-based variance estimators. These include the empirical bootstrap, multiplier bootstrap, residual bootstrap, and the subsampling-based methods. Third, we provide by default valid hypothesis testing under OLS model misspecification via \( \chi^2 \) tests. The workhorse that enables the simultaneous computations of the several types of variance estimates is the comp_var() function, which provides a common API for the user to access these estimators. For the sake of brevity, in Section 4.1 and Section 4.2 we show how the variance estimators can be run by the user, without displaying individual code outputs. In Section 4.3 we present how the consolidated output summary of all computed variance estimators can be used for downstream inference. We now review the functionality behind each estimation method in turn in this section, starting with the closed-form variance estimators.
4.1 Closed-form variance estimation

In *maars*, we provide two closed form variance estimators: one based on the assumption of a well-specified linear model and another based on the asymptotic normality under potential misspecification of the linear model.

Under the “models as approximations” framework, using only the independence of observations and finite moment assumptions, the asymptotic variance of the OLS estimates can be estimated by the sandwich estimator [Buja et al., 2019a,b]: \[ \hat{\text{Var}}(\hat{\beta}) = n^{-1} \hat{J}^{-1} \hat{V} \hat{J}^{-1} \], with \( \hat{J} \) and \( \hat{V} \) defined in (5). Then the standard error for the \( j \)th coefficient is given by \[ \hat{\text{SE}}_j(\hat{\beta}) = \left( n^{-1} \hat{J}^{-1} \hat{V} \hat{J}^{-1} \right)^{1/2} \].

The classical estimator of asymptotic variance under a well-specified linear model is \( n^{-1} \hat{\sigma}^2 \hat{J}^{-1} \), for the residual sum of squares based estimator \( \hat{\sigma}^2 \). In the *maars* package, this and other inferential summary statistics can be readily computed by calling the `comp_var()` function as follows.

```r
# obtain maars with obj. w/ sandwich variance
maars_var_sand <- mod_fit %>% comp_var()
```

The sandwich estimator is always computed by default, even when no arguments are passed in `comp_var()`. In the above code, `maars_var_sand` is an object of class `maars_lm`. This new object represents an modified version of the `mod_fit` object of class `lm` augmented with the newly computed sandwich variance estimates. As a result, `comp_var()` also returns by default the well-specified OLS standard error output.

4.2 Resampling-based variance estimation

In this subsection, we discuss the resampling-based variance estimation tools in *maars*. These resampling-based variance estimators are not computed by default in `comp_var()` and instead require a list of parameter inputs to be passed in by the user. We now describe the details each of the methods in turn.

4.2.1 Empirical bootstrap

Under the independence and finite moment assumptions, another method for the estimation of variance is the empirical bootstrap. The \( m \)-out-of-\( n \) empirical bootstrap consists of two steps. In the first step, for \( 1 \leq b \leq B \), we resample with replacement \( m \) observations from the original data set and obtain the OLS estimate \( \hat{\beta}_b^* \) on the bootstrapped data set. In the second step, we compute \( B \) times the sample covariance of \( \hat{\beta}_b^* \), \( 1 \leq b \leq B \) as an estimate of \( \hat{J}^{-1} \hat{V} \hat{J}^{-1} \), the asymptotic variance of \( \sqrt{n}(\hat{\beta} - \beta^\infty) \). The justification for this method follows from the fact that, conditional on the original data \( \{(X_i, Y_i)\}_{i=1}^n \), we have

\[
\sqrt{m} (\hat{\beta}_b^* - \hat{\beta}) \xrightarrow{d} N(0, \hat{J}^{-1} \hat{V} \hat{J}^{-1}) \text{ as } m \to \infty
\]  

and thus we can show that

\[
\frac{m}{B-1} \sum_{b=1}^B (\hat{\beta}_b^* - \overline{\hat{\beta}}^*) (\hat{\beta}_b^* - \overline{\hat{\beta}}^*)^T \xrightarrow{p} \hat{J}^{-1} \hat{V} \hat{J}^{-1} \text{ as } B \to \infty.
\]  

Here \( \overline{\hat{\beta}}^* = B^{-1} \sum_{b=1}^B \hat{\beta}_b^* \). Therefore, as \( B \) increases, the covariance of the OLS estimates on the bootstrapped data sets converges in probability to \( \hat{J}^{-1} \hat{V} \hat{J}^{-1} \). We refer the reader to Bickel et al.
for more details. In maars, the \( n \)-out-of-\( n \) empirical bootstrap estimates for the LA Homeless data can be obtained as follows. In this dataset, there are \( n = 505 \) observations and hence setting \( m = 505 \) is the same as running the \( n \)-out-of-\( n \) empirical bootstrap.

\[
\text{# obtain maars obj. w/ emp. boot. variance}
\text{maars_var_emp <- mod_fit %>% comp_var(boot_emp = list(B = 1e3, m = 505))}
\]

### 4.2.2 Multiplier bootstrap

The main disadvantage of the empirical bootstrap is that it requires the computation of the OLS estimate \( B \) times. Furthermore, the bootstrapped design matrix might be singular. The multiplier bootstrap is an alternative method that helps overcome these difficulties. The method consists of estimating \( B \) times

\[
\tilde{\beta}_b^* = \hat{\beta} + \frac{1}{n} \sum_{i=1}^{n} w_{i,b} \hat{J}^{-1} X_i (Y_i - X_i^\top \hat{\beta}), \quad 1 \leq b \leq B.
\]

The weights \( \{w_{i,b}\}_{i=1}^{n} \) are independent with \( \mathbb{E}(w_{i,b}) = 0 \) and \( \text{Var}(w_{i,b}) = 1 \), for each \( 1 \leq i \leq n \), \( 1 \leq b \leq B \). These can be computed as follows:

\[
\text{# obtain maars obj. w/ mul. boot. variance}
\text{maars_var_mul <- mod_fit %>% comp_var(boot_mul = list(B = 1e3, weights_type = "rademacher"))}
\]

The distribution of the weights in (9) is specified through the \texttt{weights_type} parameter. Following the \texttt{boottest} package [Roodman et al., 2019] in Stata, we provide the user with four prespecified options: \texttt{rademacher}, \texttt{mammen}, \texttt{webb}, \texttt{gaussian}. The \texttt{rademacher} weights are sampled from the two point Rademacher distribution which has takes values \( \{-1, 1\} \), with equal probability. The \texttt{mammen} weights are sampled from the two point Mammen distribution which takes values \( (\pm \sqrt{5}/2) \), with probabilities \( (\sqrt{5}/2 \pm 1)/2 \), respectively. The \texttt{webb} weights are sampled from the six point Webb distribution which takes values \( \{\pm \sqrt{3}/2, \pm \sqrt{1}/2, \pm 1\} \), with equal probability. Finally, the \texttt{gaussian} weights are sampled from the standard Gaussian distribution.

### 4.2.3 Residual bootstrap

One of the classical resampling methods for linear regression is residual bootstrap. In this method, one resamples the residuals instead of the pairs \((X_i, Y_i)\) as in empirical bootstrap. With \( \hat{\beta} \) representing the OLS estimator, let the residuals be denoted by \( e_i = Y_i - X_i^\top \hat{\beta} \). Residual bootstrap consists of estimating \( B \) times

\[
\tilde{\beta}_b^* := \arg \min_{\theta \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} (Y_{i,b}^* - X_i^\top \theta)^2,
\]

where \( Y_{i,b}^* = X_i^\top \hat{\beta} + e_{i,b}^* \), \( 1 \leq i \leq n \) for \( e_{i,b}^* \), \( 1 \leq i \leq n \) are drawn i.i.d. from the empirical distribution of \( e_1, \ldots, e_n \). From the closed form expression of \( \tilde{\beta}_b^* \), it readily follows that conditionally on the original data \((X_i, Y_i), 1 \leq i \leq n, \) as \( n \to \infty \), \( \sqrt{n}(\tilde{\beta}_b^* - \hat{\beta}) \overset{d}{\to} N(0, \hat{\sigma}^2 \hat{J}^{-1}) \), where \( \hat{\sigma}^2 = n^{-1} \sum_{i=1}^{n} e_i^2 \). This convergence in distribution does not require any of the linear model assumptions. However, the
asymptotic variance of the residual bootstrap estimator matches the linear model based closed-form variance estimator and is not valid under model misspecification. In \texttt{maars}, residual bootstrap variance estimator can be obtained as follows:

```r
# obtain maars obj. w/ res. boot. variance
maars_var_res <- mod_fit %>%
comp_var(boot_res = list(B = 1e3))
```

### 4.2.4 Subsampling

An alternative to bootstrap is subsampling [Politis and Romano, 1994]. Given our discussion on empirical \((m\text{-out-of-}n)\) bootstrap, subsampling can be described as the \(m\text{-out-of-}n\) bootstrap where samples are drawn without replacement from the original data. Recall that the \(m\text{-out-of-}n\) bootstrap draws samples with replacement. Unlike the \(m\text{-out-of-}n\) bootstrap where \(m\) can be of the same order as \(n\) or even larger, subsampling validity usually requires \(m = o(n)\). We refer the reader to Politis and Romano [1994] for details. Subsampling is more generally applicable than empirical and multiplier bootstrap schemes, allowing for valid inference even with stationary dependent data. In \texttt{maars}, subsampling can be run as follows:

```r
# obtain maars obj. w/ subsampling variance
maars_var_sub <- mod_fit %>%
comp_var(boot_sub = list(B = 1e3, m = 200))
```

### 4.3 Putting it all together: Summarizing the results

In Section 4.1 and Section 4.2, we have demonstrated how the \texttt{maars} package can be used to compute the variance of the coefficients estimates based on the sandwich estimator, the bootstraps, and subsampling. Although we have presented the code for each of the methods separately for instructive purposes, all of these variance estimators can be computed simultaneously through a single call of the \texttt{comp_var()} function as follows:

```r
# obtain maars obj. w/ all methods
maars_var <- mod_fit %>%
comp_var(
  boot_emp = list(B = 1e3, m = 505),
  boot_mul = list(B = 1e3),
  boot_sub = list(B = 1e3, m = 200),
  boot_res = list(B = 1e3))
```

The \texttt{maars}\_\texttt{var} object (i.e., of class \texttt{maars}\_\texttt{lm}) by default supports the generic \texttt{print()} and \texttt{summary()} methods in \texttt{R} that are typically called on \texttt{lm()} objects, for instance. In fact, for our newly created \texttt{maars}\_\texttt{var} object, a natural first step in the \texttt{maars} inferential workflow is for the user to simply run the generic \texttt{print()} method. This can be used to generate a summary of the OLS estimates and of the assumptions behind each of the variance estimation methods that have been employed:

```r
# print obj.
print(maars_var)
```

As shown in the left panel of Figure 2, this method essentially returns an augmented version of the typical \texttt{print()} called on an \texttt{lm} object. Besides the OLS estimates, for each variance estimation methods that has been used in \texttt{comp_var()}, the assumptions (e.g., homoscedasticity)
and parameters chosen (e.g., \( n \), \( B \), and \( m \)) are displayed. We hope our default feature of explicitly presenting assumptions will become a de facto standard for most statistical modeling in R.

The computed inferential statistics can be obtained as follows:

```r
# summarise obj.
summary(maars_var)
```

Figure 2: Model diagnostics for the `maars_var` object. Left panel: Partial console output of `print(maars_var)`. Right panel: Partial console output of `summary(maars_var)`.

As shown in the right panel of Figure 2, calling the `summary()` method on a `maars_lm` object prints a stacked series of tibbles in a similar format as returned by the `tidy()` function in the `broom` package [Robinson et al., 2020]. They are based on the different variance estimation methods, together with the related sets of assumptions. The result of a \( \chi^2 \) test for testing the null hypothesis that the OLS coefficients are all equal to 0 is reported at the bottom of the printed output. We make use of the `cli` package [Csárdi, 2021] to produce well-structured console output for both the `print()` and `summary()` methods.

In order to simplify downstream manipulation of the results, the generic methods present in `maars` have `tidy` analogues. For example, the user can obtain the set of OLS estimates and variance estimates in the form of a tibble by running `get_summary(maars_var)`. More specifically, these functions begin with a consistent `get` prefix and return tidy tibble objects for data, ggplot2 objects for plots. By tidy tibble output we mean data in which every column is a variable, every row is an observation, and every cell is a single value [Wickham, 2014]. We believe that this tidy grammar for function naming enables efficient further analysis of results using the `tidyverse` or similar R packages.
5 Visual diagnostic tools

Using the `maars.var` object that we created in Section 4, the user can readily inspect the model’s fit via model diagnostic plots by calling the `plot()` method and its related tidy analogue `get_plot()`. These functions return eight graphical diagnostics. Six of them correspond to the same output that is generated by calling `plot(mod_fit)`. These are the same plots returned from the classical `lm()` object but returned as `ggplot2` objects. The two additional diagnostics are presented in Figure 3. The diagnostic in the left panel displays the widths of the different 95% confidence intervals for the OLS coefficients estimates. This graphical tool allows the user to visually compare the variance estimators computed using `comp_var`. Recall that the `lm()` and the residual bootstrap based variance estimator are only valid under a well-specified linear model, whereas the empirical, multiplier bootstrap, and subsampling variance estimator are model-free. Therefore, the visual comparison of estimated variances (as in the left panel of Figure 3) already provides evidence of misspecification, if any. The last diagnostic, which is shown in the right panel of Figure 3, presents the distribution of the OLS estimates on the bootstrapped data sets. Through this tool, the user can compare the distribution of the estimates via a normal Q-Q plot to visually check whether sample size is large enough to justify the asymptotic regime.

Figure 3: Model diagnostics for the `maars.var` object. Left panel: 95% confidence intervals based on the different variance estimation methods. Right panel: Normal Q-Q plot based on the OLS estimates obtained via empirical bootstrap.

The `maars` package also includes the three graphical diagnostic tools proposed in Buja et al. [2019b]. When the regression model is correctly specified, the regression coefficients do not depend on the distribution of \( X \); see Buja et al. [2019b, Proposition 4]. Equivalently, variations in the OLS estimates under reweighting of \( X \) would suggest that the model is not well-specified. In `maars`, we have implemented the graphical model diagnostics tools through which one can investigate whether the OLS assumptions are broken. These tools, which were proposed by Buja et al. [2019b], supplement of the model diagnostics returned by `lm()`.

The key idea behind these model diagnostics is to study how the OLS estimates vary under arbitrary reweighting of \( X \). It is hard visualize such a diagnostic with arbitrary reweighting and hence we restrict to reweighting along certain regressors, as in Buja et al. [2019b]. Although
restrictive, the resulting plots provide intuitive understanding of misspecification in data. For reweighting along the $j$-th regressor $X(j)$, $1 \leq j \leq d$, we do the following two operations:

**DT.1** Select a grid of $K$ values (or centers) $c_{1,j}, \ldots, c_{K,j}$ on the support of $X(j)$.

**DT.2** For each center $c_{\ell,j}$, $1 \leq \ell \leq K$, compute the weighted least squares estimator

$$
\hat{\beta}_\ell = \arg \min_{\theta \in \mathbb{R}^d} \sum_{i=1}^n (Y_i - X_i^T \theta)^2 e^{-(X_i(j) - c_{\ell,j})^2/(2\gamma^2)}.
$$

Intuitively, this is the least squares estimator that gives more weight to observations that have $j$-th regressor values close to $c_{\ell,j}$.

The procedure consists of fitting $K$ regressions. This will give us one curve and for comparison, we also run the same procedure on bootstrapped data leading to $\hat{\beta}_\ell^*$, $1 \leq \ell \leq K$. The tibble containing the OLS estimates based on the reweighting procedure can be obtained using the following function:

```r
# regression based on reweighting of regressors
coeff_rwgt <- mod_fit %>%
  diag_fit_reg_rwgt(B = 300, terms_to_rwgt = names(la_county)[-1])
```

In the package, we have developed two types of grids for **DT.1**. The default grid of reweighting centers in **DT.1** is based on the deciles of $X(j)$ as in Buja et al. [2019b]. Alternatively, the user can select a grid of evenly spaced values between $X(1)(j)$ and $X(n)(j)$. For **DT.2**, maars uses $\gamma = (\sum_{i=1}^n (X_i(j) - \overline{X}(j))^2/(n - 1))^{1/2}$. To assist the data scientist in interpreting the results of the refitting procedure, Buja et al. [2019b] have proposed using the following three graphical model diagnostics tools.

- **focal slope**: Consider changes in coefficient of interest $\hat{\beta}_\ell(k)$ to the reweighting of each of the regressors $X(j)$, $1 \leq j \leq d$; this provides insights into the interactions between regressor $X(k)$ and all other regressors $X(j)$.

- **nonlinearity detection**: Consider changes in $\hat{\beta}_\ell(k)$ to the reweighting of its own regressor $X(k)$; this provides insights into marginal nonlinear behaviors of the response surface.

- **focal reweighting variable**: Consider changes in all coefficients $\hat{\beta}_\ell(j)$ to the reweighting of a given regressor $X(k)$.

For further information and interpretations of these types of diagnostics, see Buja et al. [2019b, Section 5]. The three types of graphical diagnostics can be obtained in maars as follows.

```r
# focal slope for "PercVacant"
mod_fit %>%
  diag_foc_slope(coeff_rwgt, 'PercVacant')
# nonlinearity detection
mod_fit %>%
  diag_nl_detect(coef_rwgt)
# focal reweighting var. for "PercVacant"
mod_fit %>%
  diag_foc_rwgt(coef_rwgt, 'PercVacant')
```

A sample output of the focal slope diagnostics is shown in Figure 4. These plots show how the OLS estimate of the prevalence of vacant lots (PercVacant) in our running example for 300 bootstrapped data sets (gray lines) vary under reweighting of all regressors (plot panel titles). The changes observed in the means of the estimates (black lines in the middle of each panel) indicate
that the model is unlikely to be well-specified. In particular, these plots suggest the presence of an interaction between *PercVacant* and other regressors such as *Perc Minority*, *Perc Residential*, and *Median Inc* ($1000). In the plot in the bottom right corner, which depicts the estimate of *Perc Vacant* under reweighting of its own regressor, we observe that the reweighted estimates are far larger than the unweighted ones on the original data (blue dashed line).

![Figure 4: Focal slope](image)

6 Teaching by example: vignettes

As previously noted, *maars* is developed as a pedagogical (and research) tool to convey the rich techniques and concepts for OLS under model misspecification. Specifically, per *DP.4* we emphasize teaching these concepts through guided case studies using tidy *maars* workflows. Our goal is to showcase these case studies as vignettes on our official package website.

These vignettes take two main forms. First, we take the core *research* papers upon which *maars* is based and reproduce tables and plots from them [Buja et al., 2019a,b]. The intent here is to make the latest theoretical research in OLS under model misspecification accessible to the data scientist in a hands-on manner. Second, we provide *lesson plan* vignettes for these inferential techniques. For example, we know that both empirical and multiplier bootstrap are valid under model misspecification, but how different are they in practice? A systematic way to approach this question in a classroom setting (and beyond) is to observe that they contain the number of bootstrap replications, $B$, as a common parameter. Under a simulated misspecified linear model, we demonstrate using a tidy *maars* workflow how to plot the confidence interval coverage, and average confidence width for these two estimators, as a function of the common parameter $B$. The tidy *maars* grammar helps illustrate how to efficiently and consistently prototype these concepts in R, particularly to new students. We currently have two such case studies available and plan to extend this to a much a larger repository of research and pedagogical vignettes in the near future.
7 Open-source best practices

Our goal in developing the maars package is for it to be a standard R workflow for OLS inference under the model misspecification framework described in Buja et al. [2019a,b], and related literature. Per DP.5, we have strived to implement and adapt to open-source best practices to ensure an inclusive community for all users and contributors.

In developing the maars package, we have setup benchmarking using the bench package [Hester, 2020]. We plan to conduct high-precision benchmarking of the core maars package functionality, and to assist in future code efficiency profiling efforts. Similarly, we currently test our statistical functionality and error handling using the testthat package [Wickham, 2011]. Moreover, testing is built into the development cycle through cross-platform continuous integration using Github Actions. We use the tidyverse contributing guide and code of conduct to ensure that new contributors have ample guidance on the maars package development practices.

8 Conclusion and future work

In this paper, we introduce the maars package functionality to perform OLS inference under model misspecification. The maars package is designed to implement the key inferential ideas from Buja et al. [2019a,b] in a tidy R workflow.

The maars package is built on five core software design principles (see DP.1–DP.5). These design principles affect the day-to-day model-free inferential workflow. They also influence the way in which users can contribute to the existing maars functionality. The main tools for statistical inference in this framework are based on different variance estimation methods. These variance estimation tools in maars include closed-form variance estimators and standard errors computed using resampling techniques. By default maars provides valid hypothesis testing under model misspecification, i.e., reporting $\chi^2$ tests rather than $F$ tests. To help diagnose issues under the misspecified setting, there are a number of visualization tools readily accessible to maars user. These currently include the focal slope graphs of regressor variables [Buja et al., 2019b] and the Q-Q plots.

The maars package is still in active development and the final version we envision includes more tools related to misspecification. Implementation of analysis of variance (ANOVA) under misspecification and conformal inference based prediction [Vovk et al., 2005, Section 2.3] is in testing phase and will be added to the package soon. Further future work includes other variants of inference under dependent and time series data (beyond subsampling) as well as cluster robust standard errors. Finally, we want to extend the functions to GLMs, the Cox proportional hazards model, and inference after data exploration, e.g., PoSI [Kuchibhotla et al., 2020]. We intend to demonstrate new package functionalities through more illustrative case study vignettes.

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