Models as Approximations:
How Random Predictors and Model Violations
Invalidate Classical Inference in Regression

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August 19, 2014

Dedicated to Halbert White (†2012)

Abstract

We review and interpret the early insights of Halbert White who over thirty years ago inaugurated a form of statistical inference for regression models that is asymptotically correct even under “model misspecification,” that is, under the assumption that models are approximations rather than generative truths. This form of inference, which is pervasive in econometrics, relies on the “sandwich estimator” of standard error. Whereas linear models theory in statistics assumes models to be true and predictors to be fixed, White’s theory permits models to be approximate and predictors to be random. Careful reading of his work shows that the deepest consequences for statistical inference arise from a synergy — a “conspiracy” — of nonlinearity and randomness of the predictors which invalidates the ancillarity argument that justifies conditioning on the predictors when they are random. Unlike the standard error of linear models theory, the sandwich estimator provides asymptotically correct inference in the presence of both nonlinearity and heteroskedasticity. An asymptotic comparison of the two types of standard error shows that discrepancies between them can be of arbitrary magnitude. If there exist discrepancies, standard errors from linear models theory are usually too liberal even though occasionally they can be too conservative as well. A valid alternative to the sandwich estimator is provided by the “pairs bootstrap”; in fact, the sandwich estimator can be shown to be a limiting case of the pairs bootstrap. We conclude by giving meaning to regression slopes when the linear model is an approximation rather than a truth. — In this review we limit ourselves to linear least squares regression, but many qualitative insights hold for most forms of regression.

Keywords: Ancillarity of predictors; First and second order incorrect models; Model misspecification; Econometrics; Sandwich estimator; Pairs bootstrap.

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1 Introduction

The classical Gaussian linear model reads as follows:

\[ y = X\beta + \epsilon, \quad \epsilon \sim \mathcal{N}(0_N, \sigma^2 I_{N \times N}) \quad (y, \epsilon \in \mathbb{R}^N, \ X \in \mathbb{R}^{N \times (p+1)}, \ \beta \in \mathbb{R}^{p+1}). \] (1)

Important for the present focus are two aspects of how the model is commonly interpreted: (1) the model is assumed correct, that is, the conditional response means are a linear function of the predictors and the errors are independent, homoskedastic and Gaussian; (2) the predictors are treated as known constants even when they arise as random observations just like the response. Statisticians have long enjoyed the fruits that can be harvested from this model and they have taught it as fundamental at all levels of statistical education. Curiously little known to many statisticians is the fact that a different framework is adopted and a different statistical education is taking place in the parallel universe of econometrics. For over three decades, starting with Halbert White’s (1980a,b;1981;1982) seminal articles, econometricians have used multiple linear regression without making the many assumptions of classical linear models theory. While statisticians use assumption-laden exact finite sample inference, econometricians use assumption-lean asymptotic inference based on the so-called “sandwich estimator” of standard error. In our experience most statisticians have heard of the sandwich estimator but do not know its purpose, use, and underlying theory. A first goal of the present exposition is therefore to convey an understanding of the assumption-lean framework of basic econometrics in a language that is intelligible to statisticians. The approach is to interpret linear regression in a semi-parametric fashion as extracting the parametric linear part of a general nonlinear response surface. The modeling assumptions can then be reduced to i.i.d. sampling from largely arbitrary joint \((\vec{X}, Y)\) distributions that satisfy a few moment conditions. It is in this assumption-lean framework that the sandwich estimator produces asymptotically correct standard errors.

A second goal of this exposition is to connect the assumption-lean econometric framework to a form of statistical inference in linear models that is known to statisticians but appreciated by few: the “pairs bootstrap.” As the name indicates, the pairs bootstrap consists of resampling pairs \((\vec{a}_i, y_i)\), in contrast to the “residual bootstrap” which resamples residuals \(r_i\). Among the two, the pairs bootstrap is the less promoted even though asymptotic theory exists to justify both under different assumptions (see, for example, Freedman 1981, Mammen 1993). It is intuitively clear that the pairs bootstrap can be asymptotically justified in the assumption-lean framework, and for this reason it produces standard error estimates that solve the same problem as the sandwich estimator. Indeed, we establish a connection that shows the sandwich estimator to be the asymptotic limit of the \(M\)-of-\(N\) pairs bootstrap when \(M \to \infty\). We will use the general term “assumption-lean estimator” to refer to either the sandwich estimator or the pairs bootstrap estimator of standard error.

A third goal of this article is to theoretically and practically compare the assumption-lean estimators with the linear models estimator. We define a ratio of asymptotic variances — “RAV” for short — that describes the discrepancies between the two types of standard error estimators in the asymptotic limit. If there exists a discrepancy, \(RAV \neq 1\), it will be assumption-lean estimators (sandwich or pairs bootstrap) that are asymptotically correct, and the linear models estimator is...
then indeed asymptotically incorrect. If $\text{RAV} \neq 1$, there exist deviations from the linear model in the form of nonlinearities and/or heteroskedasticities. If $\text{RAV} = 1$, the linear models estimator is asymptotically correct, but this does not imply that the linear model is correct, the reason being that nonlinearities and heteroskedasticities can conspire to produce a coincidentally correct size for the linear models estimator. Importantly, the $\text{RAV}$ is specific to each regression coefficient because the discrepancies between the two types of standard error estimators vary from coefficient to coefficient.

A fourth goal is to estimate the $\text{RAV}$ for use as a test statistic. We derive an asymptotic null distribution to test the presence of model violations that invalidate the classical standard error of a specific coefficient. While the result can be called a “misspecification test” in the tradition of econometrics, it is more usefully viewed as guidance to the better standard error. The sandwich estimator comes with a cost — vastly increased non-robustness — which makes it desirable to use the linear models standard error when possible. However, a procedure that chooses the type of standard error depending on the outcome of a pre-test raises new performance issues that require future research. (Simpler is Angrist and Pischke’s proposal (2009) to choose the larger of the two standard errors; their procedure forfeits the possibility of detecting the classical standard error as too conservative. MacKinnon and White (1985) on the other hand recommend using a sandwich estimator even if no misspecification is detected.)

A fifth and final goal of this article is to propose answers to questions and objections that would be natural to statisticians who hold the following tenets:

1. Models need to be “nearly correct” for inference to be meaningful. The implication is that assumption-lean standard errors are misguided because inference in a “misspecified model” is meaningless.

2. Predictors in regression models should or can be treated as fixed even if they are random.

   Here the implication is that inference which treats predictors as random is unprincipled or at a minimum superfluous.

A strong proponent of the first tenet is the late David Freedman (2006). While his insistence on intellectual honesty and rigor is admirable, we will counter argue based on White (1980a,b; 1981; 1982) that inference under misspecification can be meaningful and rigorous. To begin with, we should avoid the negative rhetoric of the term “misspecification”. An alternative view, to be discussed below, can be summarized as follows:

1. Models are always approximations, not truths (Box 1979; Cox 1995).

2. If models are approximations, it is still possible to give regression slopes meaningful interpretations.

3. If models are approximations, it is prudent to use inference that is less dependent on model correctness.

In fact, neither of the second and the third point depends on the degree of approximation: meaningful interpretation and valid inference can be provided for regression slopes whether models are good or bad approximations. (This is of course not to say that every regression analysis is meaningful!)

The second tenet above, conditionality on predictors, has proponents to various degrees. More forceful ones hold that conditioning on the predictors is a necessary consequence of the ancillarity
principle; others hold that the principle confers license, not a mandate. The ancillarity principle says in simplified terms that valid inference results from conditioning on statistics whose distribution does not involve the parameters of interest. When the predictors in a regression are random, their distribution is ancillary for the regression parameters, hence conditioning on the predictors is necessary or at least permitted. This argument, however, fails when the parametric model is only an approximation and the predictors are random. It will be seen that under these circumstances the population slopes do depend on the predictor distribution which is hence not ancillary. This effect does not exist when the conditional mean of the response is a linear function of the predictors or the predictors are truly nonrandom.

This article continuous as follows: Section 2 illustrates discrepancies between standard error estimates with real data examples. Section 3 sets up the semi-parametric population framework in which LS approximation extracts the parametric linear component. Section 4 shows how nonlinear conditional expectations invalidate ancillarity of the predictor distribution. Sections 5 derive a decomposition of asymptotic variance of LS estimates into contributions from noise and from nonlinearity, and central limit theorems associated with the decomposition. Section 6 introduces the sandwich estimator of standard error and shows how it is a limiting case of the $M$-of-$N$ pairs bootstrap. Section 7 expresses parameters, estimates, asymptotic variances and CLTs in the language of predictor adjustment. This is critical in order to arrive at expressions that speak to individual predictors in a transparent fashion. In Section 8 the language of adjustment allows us to define the $RAV$, that is, the ratio of proper (assumption-lean) and improper (linear models-based) asymptotic variances and to analyze conditions under which linear models theory yields standard errors that are too liberal (often) or too conservative (rarely). Section 9 turns the $RAV$ into a simple test statistic with an asymptotically normal null distribution under “well-specification”. The penultimate Section 10 proposes an answer to the question of what the meaning of regression coefficients is when the linear model is only an approximation. The final Section 11 has a brief summary and ends with a pointer to problematic aspects of the sandwich estimator. Throughout we use precise notation for clarity. The notation may give the impression of a technical article, but all technical results are elementary and all limit theorems are stated informally without regularity conditions.

2 Discrepancies between Standard Errors Illustrated

Table 1 shows regression results for a dataset in a sample of 505 census tracts in Los Angeles that has been used to examine homelessness in relation to covariates for demographics and building usage (Berk et al. 2008). We do not intend a careful modeling exercise but show the raw results of linear regression to illustrate the degree to which discrepancies can arise among three types of standard errors: $SE_{lin}$ from linear models theory, $SE_{boot}$ from the pairs bootstrap ($N_{boot} = 100,000$) and $SE_{sand}$ from the sandwich estimator (according to MacKinnon and White’s (1985) HC2 proposal). Ratios of standard errors that are far from +1 are shown in bold font.

The ratios $SE_{sand}/SE_{boot}$ show that the sandwich and bootstrap estimators are in good agreement. Not so for the linear models estimates: we have $SE_{boot}, SE_{sand} > SE_{lin}$ for the predictors.
Table 1: Comparison of Standard Errors for the LA Homeless Data.

|                  | \(\hat{\beta}_j\) | \(SE_{lin}\) | \(SE_{boot}\) | \(SE_{sand}\) | \(t_{lin}\) | \(t_{boot}\) | \(t_{sand}\) |
|------------------|---------------------|---------------|---------------|---------------|-------------|-------------|-------------|
| Intercept        | 0.760               | 22.767        | 16.505        | 16.209        | 0.726       | 0.712       | 0.981       | 0.033       | 0.046       | 0.047       |
| MedianInc ($\text{\$K}$) | -0.183              | 0.187         | 0.114         | 0.108         | 0.610       | 0.576       | 0.944       | -0.977      | -1.601      | -1.696      |
| PercVacant       | 4.629               | 0.901         | 1.385         | 1.363         | 1.531       | 1.513       | 0.988       | 5.140       | 3.341       | 3.396       |
| PercMinority     | 0.123               | 0.176         | 0.165         | 0.164         | 0.937       | 0.932       | 0.995       | 0.701       | 0.748       | 0.752       |
| PercResidential  | -0.050              | 0.171         | 0.112         | 0.111         | 0.653       | 0.646       | 0.988       | -0.292      | -0.446      | -0.453      |
| PercCommercial   | 0.737               | 0.273         | 0.390         | 0.397         | 1.438       | 1.454       | 1.011       | 2.700       | 1.892       | 1.857       |
| PercIndustrial   | 0.905               | 0.321         | 0.577         | 0.592         | 1.801       | 1.843       | 1.023       | 2.818       | 1.570       | 1.529       |

PercVacant, PercCommercial and PercIndustrial, and \(SE_{boot}, SE_{sand} < SE_{lin}\) for Intercept, MedianInc ($1000), PercResidential. Only for PercMinority is \(SE_{lin}\) off by less than 10% from \(SE_{boot}\) and \(SE_{sand}\). The discrepancies affect outcomes of some of the \(t\)-tests: Under linear models theory the predictors PercCommercial and PercIndustrial have commanding \(t\)-values of 2.700 and 2.818, respectively, which are reduced to unconvincing values below 1.9 and 1.6, respectively, if the pairs bootstrap or the sandwich estimator are used. On the other hand, for MedianInc ($\text{\$K}$) the \(t\)-value \(-0.977\) from linear models theory becomes borderline significant with the bootstrap or sandwich estimator if the plausible one-sided alternative with negative sign is used.

Table 2 illustrates discrepancies between types of standard errors with the Boston Housing data (Harrison and Rubinfeld 1978) which will be well known to many readers. Again, we dispense with the question as to whether the analysis is meaningful and focus on the comparison of standard errors. Here, too, \(SE_{boot}\) and \(SE_{sand}\) are mostly in agreement as they fall within less than 2% of each other, an exception being CRIM with a deviation of about 10%. By contrast, \(SE_{boot}\) and \(SE_{sand}\) are larger than their linear models cousin \(SE_{lin}\) by a factor of about 2 for RM and LSTAT, and about 1.5 for the intercept and the dummy variable CHAS. On the opposite side, \(SE_{boot}\) and \(SE_{sand}\) are less than 3/4 of \(SE_{lin}\) for TAX. For several predictors there is no substantial discrepancy among all three standard errors: ZN, NOX, B, and even for CRIM, \(SE_{lin}\) falls between the somewhat discrepant values of \(SE_{boot}\) and \(SE_{sand}\).

We conclude: (1) \(SE_{boot}\) and \(SE_{sand}\) are in substantial agreement; (2) \(SE_{lin}\) on the one hand and \{(\(SE_{boot}\), \(SE_{sand}\)\) on the other hand can show substantial discrepancies; (3) the discrepancies are specific to predictors.

3 The Semi-Parametric Population Framework

3.1 Targets of Estimation

Before standard errors can be meaningfully compared it is necessary to describe the semi-parametric framework and define targets of estimation. The latter will no longer be parameters in a generative model but statistical functionals that are well-defined for a large nonparametric class of data distributions. A seminal work that inaugurated this approach is P.J. Huber’s 1967 article whose
Table 2: Comparison of Standard Errors for the Boston Housing Data.

|         | \(\hat{\beta}_j\) | \(SE_{lin}\) | \(SE_{boot}\) | \(SE_{sand}\) | \(SE_{boot}^{sand}\) | \(SE_{sand}^{lin}\) | \(t_{lin}\) | \(t_{boot}\) | \(t_{sand}\) |
|---------|---------------------|--------------|--------------|--------------|---------------------|---------------------|-------------|-------------|-------------|
| (Intercept) | 36.459 | 5.103 | 8.038 | 8.145 | 1.575 | 1.596 | 1.013 | 7.144 | 4.536 | 4.477 |
| CRIM    | -0.108 | 0.033 | 0.035 | 0.031 | 1.055 | 0.945 | 0.896 | -3.287 | -3.115 | -3.478 |
| ZN      | 0.046  | 0.014 | 0.014 | 0.014 | 1.005 | 1.011 | 1.006 | 3.382 | 3.364 | 3.345 |
| INDUS   | 0.021  | 0.061 | 0.051 | 0.051 | 0.832 | 0.823 | 0.990 | 0.334 | 0.402 | 0.406 |
| CHAS    | 2.687  | 0.862 | 1.307 | 1.310 | 1.517 | 1.521 | 1.003 | 3.118 | 2.056 | 2.051 |
| NOX     | -17.767 | 3.820 | 3.834 | 3.827 | 1.004 | 1.005 | 0.998 | -4.651 | -4.634 | -4.643 |
| RM      | 3.810  | 0.418 | 0.848 | 0.861 | 2.030 | 2.060 | 1.015 | 9.116 | 4.490 | 4.426 |
| AGE     | 0.001  | 0.013 | 0.016 | 0.017 | 1.238 | 1.263 | 1.020 | 0.052 | 0.042 | 0.042 |
| DIS     | -1.476 | 0.199 | 0.214 | 0.217 | 1.075 | 1.086 | 1.010 | -7.398 | -6.882 | -6.812 |
| RAD     | 0.306  | 0.066 | 0.063 | 0.062 | 0.949 | 0.940 | 0.990 | 4.613 | 4.858 | 4.908 |
| TAX     | -0.012 | 0.004 | 0.003 | 0.003 | 0.736 | 0.723 | 0.981 | -3.280 | -4.454 | -4.540 |
| PTRATIO | -0.953 | 0.131 | 0.118 | 0.118 | 0.899 | 0.904 | 1.005 | -7.283 | -8.104 | -8.060 |
| B       | 0.009  | 0.003 | 0.003 | 0.003 | 1.026 | 1.009 | 0.984 | 3.467 | 3.379 | 3.435 |
| LSTAT   | -0.525 | 0.051 | 0.100 | 0.101 | 1.980 | 1.999 | 1.010 | -10.347 | -5.227 | -5.176 |

The behavior of maximum likelihood estimation under nonstandard conditions. The “nonstandard conditions” are essentially arbitrary distributions for which certain moments exist.

In a population framework for regression with random predictors the ingredients are random variables \(X_1, \ldots, X_p\) and \(Y\), where \(Y\) is singled out as the response. For now the only assumption is that these variables have a joint distribution \(P = P(dy, dx_1, \ldots, dx_p)\) whose second moments exist and whose predictors have a full rank covariance matrix. We write \(\vec{X} = (1, X_1, \ldots, X_p)^T\) for the column random vector consisting of the predictor variables, with a constant 1 prepended to accommodate an intercept term. Values of the random vector \(\vec{x} = (1, x_1, \ldots, x_p)^T\) will be denoted by lower case \(\vec{x}\). We write any function \(f(X_1, \ldots, X_p)\) of the predictors equivalently as \(f(\vec{X})\) as the prepended constant 1 is irrelevant. Correspondingly we also use the notations \(P = P(dy, dx)\), \(P(dx)\), \(P(dy|dx)\) and \(P = P_{Y,\vec{X}}, P_{\vec{X}}, P_{Y|\vec{X}}\), respectively. Nonsingularity of the predictor covariance matrix is equivalent to nonsingularity of the cross-moment matrix \(E[\vec{X} \vec{X}^T]\).

Among functions of the predictors, an important one is the best \(L_2(P)\) approximation to the response \(Y\), which is the conditional expectation of \(Y\) given \(\vec{X}\):

\[
\mu(\vec{X}) := \arg\min_{f(\vec{X}) \in L_2(P)} E[(Y - f(\vec{X}))^2] = E[Y | \vec{X}].
\]
Figure 1: Illustration of the decomposition (5).

Among linear functions \( l(\tilde{X}) = \beta^T\tilde{X} \) of the predictors, one stands out as the best linear \( L_2(P) \) approximation or the population LS linear approximation to \( Y \):

\[
\beta(P) := \arg\min_{\beta \in \mathbb{R}^{p+1}} E[(Y - \beta^T\tilde{X})^2] = E[\tilde{X}\tilde{X}^T]^{-1}E[\tilde{X}Y].
\]  

(4)

The right hand expression follows from the normal equations \( E[\tilde{X}\tilde{X}^T]\beta - E[\tilde{X}Y] = 0 \) that are the stationarity conditions for minimizing the population LS criterion \( E[(Y - \beta^T\tilde{X})^2] = -2\beta^T E[\tilde{X}Y] + \beta^T E[\tilde{X}\tilde{X}^T]\beta + \text{const.} \)

By abuse of terminology, we use the expressions “population coefficients” for \( \beta(P) \) and “population approximation” for \( \beta(P)^T\tilde{X} \), omitting the essential terms “linear” and “LS” or “\( L_2(P) \)” to avoid cumbersome language. We will often write \( \beta \), omitting the argument \( P \) when it is clear from the context that \( \beta = \beta(P) \).

The population coefficients \( \beta = \beta(P) \) form a statistical functional that is defined for a large class of data distributions \( P \). How \( \beta(P) \) relates to the classical linear model will be discussed in Section 5.2.
3.2 The Noise-Nonlinearity Decomposition

The response $Y$ has the following natural decompositions:

$$
Y = \beta^T \tilde{X} + (\mu(\tilde{X}) - \beta^T \tilde{X}) + (Y - \mu(\tilde{X}))
$$

These equalities define the random variables $\eta = \eta(\tilde{X})$, called **nonlinearity**, $\epsilon$, called **noise**, and

$$
\delta = \epsilon + \eta,
$$

for which there does not exist a standard term, hence the name “total deviation” (from linearity) may suffice. An attempt to depict the decompositions (5) for a single predictor is given in Figure 1.

The noise $\epsilon$ is not assumed homoskedastic, and its conditional distributions $P(d\epsilon|\tilde{X})$ can be quite arbitrary except for being centered and having second moments almost surely:

$$
E[\epsilon|\tilde{X}] = 0,
$$

$$
\sigma^2(\tilde{X}) := V[\epsilon|\tilde{X}] = E[\epsilon^2|\tilde{X}] < \infty.
$$

In addition to the **conditional variance** $\sigma^2(\tilde{X})$, we will need the **conditional mean squared error** $m^2(\tilde{X})$ of the population LS linear function, and its variance-bias$^2$ decomposition associated with (6):

$$
m^2(\tilde{X}) := E[\delta^2|\tilde{X}] = \sigma^2(\tilde{X}) + \eta^2(\tilde{X}).
$$

3.3 Interpretations and Properties of the Decompositions

Equations (5) above can be given the following **semi-parametric interpretation**:

$$
\mu(\tilde{X}) = \beta^T \tilde{X} + \eta(\tilde{X}).
$$

Thus the proposed purpose of linear regression is to extract the parametric part of the response surface and provide statistical inference for the parameters even in the presence of a nonparametric part.

To make the decomposition (10) identifiable one needs an orthogonality constraint:

$$
E[(\beta^T \tilde{X}) \eta(\tilde{X})] = 0.
$$

For $\eta(\tilde{X})$ as defined in (5), this equality follows from the more general fact that the nonlinearity $\eta(\tilde{X})$ is uncorrelated with all predictors. Because we will need similar facts for $\epsilon$ and $\delta$ as well, we state them all at once:

$$
E[\tilde{X} \eta] = 0, \quad E[\tilde{X} \epsilon] = 0, \quad E[\tilde{X} \delta] = 0.
$$
Proofs: The nonlinearity $\eta$ is uncorrelated with the predictors because it is the population residual of the regression of $\mu(\bar{X})$ on $\bar{X}$ according to (13) below. The noise $\epsilon$ is uncorrelated with $\bar{X}$ because $E[\bar{X}\epsilon] = E[\bar{X}E[\epsilon|\bar{X}]] = 0$. Finally, $\delta$ is uncorrelated with $\bar{X}$ because $\delta = \eta + \epsilon$. — As a consequence of the inclusion of an intercept in $\bar{X}$, centering follows as a special case of (11):

$$E[\epsilon] = E[\eta] = E[\delta] = 0.$$  (12)

### 3.4 Error Terms in Econometrics

In econometrics, where random predictors are prevalent, there exists a need to specify how error terms relate stochastically to the predictors. While statisticians would assume errors to be independent of predictors, there is a tendency in econometrics to assume “orthogonality” only, that is, absence of correlation: $E[error \cdot \bar{X}] = 0$. This weaker condition, however, inadvertently permits nonlinearities as part of the “error” because nonlinearities $\eta$ are indeed uncorrelated with the predictors according to (11), though not independent from them. Thus econometricians’ error terms appear to be the total deviations $\delta = \epsilon + \eta$. The unusual property of $\delta$ as “error term” is that generally $E[\delta|\bar{X}] \neq 0$ in the assumption-lean framework, even though $E[\delta] = 0$ holds always.

The implications may not always be clear, as the following two examples show: Hausman (1978), in an otherwise groundbreaking article, seems to imply that $E[error \cdot \bar{X}] = 0$ is equivalent to $E[error|\bar{X}] = 0$ (ibid., p.1251, (1.1a)), which it isn’t. White’s (1980b, p.818) famous article on heteroskedasticity-consistent standard errors also uses the weaker orthogonality assumption, but he is clear that his misspecification test addresses both nonlinearity and heteroskedasticity (ibid., p.823). He is less clear about the fact that “heteroskedasticity-consistent” standard errors are also “nonlinearity-consistent”, even though this is spelled out clearly in his lesser-known article on “Using Least Squares to Approximate Unknown Regression Functions” (White 1980a, p.162-3). For this reason the latter article is the more relevant one for us even though it uses an idiosyncratic framework. As nonlinearity is the more consequential model deviation than heteroskedasticity, the synonym “heteroskedasticity-consistent estimator” for the sandwich estimator is somewhat misleading.

What statisticians are more likely to recognize as “error” is $\epsilon$ as defined above; yet they will have misgiving as well because $\epsilon$ is the deviation not from the fitted approximate model but from the true response function. We therefore call it “noise” rather than “error.” The noise $\epsilon$ is not independent of the predictors either, but because $E[\epsilon|\bar{X}] = 0$ it enjoys a stronger orthogonality property than the nonlinearity $\eta$: $E[g(\bar{X})\epsilon] = 0$ for all $g(\bar{X}) \in L_2(P)$. For full independence one would need the property $E[g(\bar{X})h(\epsilon)] = 0$ for all centered $g(\bar{X}), h(\epsilon) \in L_2(P)$, which is not generally the case.

**Facts:**

- **The error $\epsilon$ is independent of $\bar{X}$ iff the conditional distribution of $\epsilon$ given $\bar{X}$ is the same across predictor space:** $E[f(\epsilon)|\bar{X}] \overset{P}= E[f(\epsilon)] \forall f(\epsilon) \in L_2(P)$ (which implies heteroskedasticity).
- **The nonlinearity $\eta$ is independent of $\bar{X}$ iff it vanishes:** $\eta \overset{P}= 0$.
- **The total deviation $\delta$ is independent of $\bar{X}$ iff both the error $\epsilon$ is independent of $\bar{X}$ and $\eta \overset{P}= 0$.**
As technically simple as these facts are, they show that stochastic independence of errors and predictors is a strong assumption that rules out both nonlinearities and heteroskedasticities. (This form of independence is to be distinguished from the assumption of i.i.d. errors in the linear model where the predictors are fixed.) A hint of unclarity in this regard can be detected even in White (1980b, p.824, footnote 5) when he writes “specification tests ... may detect only a lack of independence between errors and regressors, instead of misspecification.” However, violation of independence to first order is nonlinearity and to second order it is heteroskedasticity, which are “misspecification” to first and second order, respectively. Tests could respond to some higher order violations of independence between errors and predictors, but the primary ones are misspecifications of first and second order. Thus independence and well-specification are crucially linked when the predictors are random.

4 Non-Ancillarity of the Predictor Distribution

We show in detail that the principle of predictor ancillarity does not hold when models are approximations rather than generative truths. For some background on ancillarity, see Appendix A.

It is clear that the population coefficients $\beta(P)$ do not depend on all details of the joint $(Y, \tilde{X})$ distribution. For one thing, they are blind to the errors $\epsilon$. This follows from the fact that $\beta(P)$ is
also the best linear $L_2(P)$ approximation to $\mu(\mathbf{X})$:

$$
\beta(P) = \arg\min_{\beta \in \mathbb{R}^{p+1}} E[(\mu(\mathbf{X}) - \beta^T \mathbf{X})^2] = E[\mathbf{X} \mathbf{X}^T]^{-1} E[\mathbf{X} \mu(\mathbf{X})].
$$

(13)

This may be worth spelling out in detail:

**Lemma:** The LS functional $\beta(P)$ depends on $P$ only through the conditional mean function and the predictor distribution; it does not depend on the conditional error distribution. That is, for two data distributions $P_1(dy, d\mathbf{x})$ and $P_2(dy, d\mathbf{x})$ the following holds:

$$
P_1(d\mathbf{x}) = P_2(d\mathbf{x}), \quad \mu_1(\mathbf{x}) \equiv \mu_2(\mathbf{x}) \implies \beta(P_1) = \beta(P_2).$$

The next and most critical question is whether $\beta(P)$ depends on the predictor distribution at all. If the ancillarity argument for predictors is to be believed, the distribution of the predictors should be unrelated to $\beta(P)$. The facts, however, are as follows:

**Proposition:** The LS functional $\beta(P)$ does not depend on the predictor distribution if and only if $\mu(\mathbf{x})$ is linear. More precisely, for a fixed measurable function $\mu_0(\mathbf{x})$ consider the class of data distributions $P$ for which $\mu_0(\cdot)$ is a version of their conditional mean function: $E[Y|\mathbf{X}] = \mu(\mathbf{X}) \overset{P}{=} \mu_0(\mathbf{X})$. In this class the following holds:

$$
\begin{align*}
(2a) \quad \mu_0(\cdot) \text{ is nonlinear} \implies & \exists P_1, P_2 : \beta(P_1) \neq \beta(P_2), \\
(2b) \quad \mu_0(\cdot) \text{ is linear} \implies & \forall P_1, P_2 : \beta(P_1) = \beta(P_2).
\end{align*}
$$

(For the simple proof details, see Appendix B.2.) In the nonlinear case (2a) the clause $\exists P_1, P_2 : \beta(P_1) \neq \beta(P_2)$ is driven solely by differences in the predictor distributions $P_1(d\mathbf{x})$ and $P_2(d\mathbf{x})$ because $P_1$ and $P_2$ share the mean function $\mu_0(\cdot)$ while their conditional error distributions are irrelevant by Lemma.

The proposition is much more easily explained with a graphical illustration: Figure 2 shows single predictor situations with a nonlinear and a linear mean function, respectively, and the same two predictor distributions. The two population LS lines for the two predictor distributions differ in the nonlinear case and they are identical in the linear case. (This appears first in White (1980a, p.155-6); to see the correspondence, identify $Y$ with his $g(Z) + \epsilon$.)

The relevance of the proposition is that in the presence of nonlinearity the LS functional $\beta(P)$ depends on the predictor distribution, hence the predictors are not ancillary for $\beta(P)$. The concept of ancillarity in generative models has things upside down in that it postulates independence of the predictor distribution from the parameters of interest. In a semi-parametric framework where the model is only an approximation and the parameters are statistical functionals, the matter presents itself in reverse: It is not the parameters that affect the predictor distribution; rather, it is the predictor distribution that affects the parameters.

The loss of predictor ancillarity has practical implications: Consider two empirical studies that use the same predictor and response variables. If their statistical inferences about $\beta(P)$ seem superficially
Figure 3: Illustration of the interplay between predictors’ high-density range and nonlinearity: Over the small range of $P_1$ the nonlinearity will be undetectable and immaterial for realistic sample sizes, whereas over the extended range of $P_2$ the nonlinearity is more likely to be detectable and relevant.

If at this point one is tempted to recoil from the idea of models as approximations and revert to the idea that models must be well-specified, one should expect little comfort: The very idea of well-specification is a function of the high-density range of predictor distributions because over a small range a model has a better chance of appearing “well-specified” for the simple reason that small ranges allow better approximations. This is illustrated by Figure 3: the narrow range of the predictor distribution $P_1(d\bar{x})$ is the reason why the linear approximation is excellent, that is, the model is very nearly “well specified”, whereas the wide range of $P_2(d\bar{x})$ is the reason for the gross “misspecification” of the linear approximation. This is a general issue that cannot be resolved by calls for more “substantive theory” in modeling: Even the best of theories have limited ranges of
validity as has been shown by the most successful theories known to science, those of physics.

5 Observational Datasets, Estimation, and CLTs

5.1 Notation for Observations Datasets

Moving from populations to samples and estimation, we introduce notation for “observational data”, that is, cross-sectional data consisting of i.i.d. cases \((Y_i, X_{i1}, ..., X_{ip})\) drawn from a joint multivariate distribution \(P(dy, dx_1, ..., dx_p)\) \((i = 1, 2, ..., N)\). (Note that White (1980a,b) permits “i.n.i.d.” sampling, that is independent but not identically distributed observations. His theory imposes technical moment conditions that limit the degree to which the distributions deviate from each other. We use the simpler i.i.d. condition for greater clarity but lesser generality.)

We collect the predictors of case \(i\) in a column \((p+1)\)-vector \(\vec{X}_i = (1, X_{i1}, ..., X_{ip})^T\), prepended with 1 for an intercept. We stack the \(N\) samples to form random column \(N\)-vectors and a random predictor \(N \times (p+1)\)-matrix:

\[
Y = \begin{bmatrix} Y_1 \\ \vdots \\ Y_N \end{bmatrix}, \quad X_j = \begin{bmatrix} X_{1j} \\ \vdots \\ X_{Nj} \end{bmatrix}, \quad X = [1, X_1, ..., X_p] = \begin{bmatrix} \vec{X}_1^T \\ \vdots \\ \vec{X}_N^T \end{bmatrix}.
\]

Similarly we stack the values of the mean function \(\mu(\vec{X}_i)\), of the nonlinearity \(\eta(\vec{X}_i)\), of the errors \(\epsilon_i = Y_i - \mu(\vec{X}_i)\), of the total deviations \(\delta_i\) from linearity, and of the error standard deviations \(\sigma(\vec{X}_i)\) to form random column \(N\)-vectors:

\[
\mu = \begin{bmatrix} \mu(\vec{X}_1) \\ \vdots \\ \mu(\vec{X}_N) \end{bmatrix}, \quad \eta = \begin{bmatrix} \eta(\vec{X}_1) \\ \vdots \\ \eta(\vec{X}_N) \end{bmatrix}, \quad \epsilon = \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_N \end{bmatrix}, \quad \delta = \begin{bmatrix} \delta_1 \\ \vdots \\ \delta_N \end{bmatrix}, \quad \sigma = \begin{bmatrix} \sigma(\vec{X}_1) \\ \vdots \\ \sigma(\vec{X}_N) \end{bmatrix}.
\]

The definitions of \(\eta(\vec{X}), \epsilon\) and \(\delta\) in (5) translate to vectorized forms:

\[
\eta = \mu - X\beta, \quad \epsilon = Y - \mu, \quad \delta = Y - X\beta.
\]

It is important to keep in mind the distinction between population and sample properties. In particular, the \(N\)-vectors \(\delta, \epsilon\) and \(\eta\) are not orthogonal to the predictor columns \(X_j\) in the sample. Writing \(\langle \cdot, \cdot \rangle\) for the usual Euclidean inner product on \(\mathbb{R}^N\), we have in general \(\langle \delta, X_j \rangle \neq 0, \langle \epsilon, X_j \rangle \neq 0, \langle \eta, X_j \rangle \neq 0\), even though the associated random variables are orthogonal to \(X_j\) in the population:

\[
E[\delta X_j] = E[\epsilon X_j] = E[\eta(\vec{X})X_j] = 0.
\]

The sample linear LS estimate of \(\beta\) is the random column \((p+1)\)-vector

\[
\hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1, ..., \hat{\beta}_p)^T = \arg\min_{\beta} \| Y - X\beta \|_2^2 = (X^TX)^{-1}X^TY.
\]
Randomness stems from both the random response $Y$ and the random predictors in $X$. Associated with $\hat{\beta}$ are the following:

- the hat or projection matrix: $H = X^T (X^T X)^{-1} X^T$,
- the vector of LS fits: $\hat{Y} = X \hat{\beta} = H Y$,
- the vector of residuals: $r = Y - X \hat{\beta} = (I - H) Y$.

The vector $r$ of residuals is distinct from the vector of total deviations $\delta = Y - X \beta$ which arises from $\beta = \beta(P)$.

5.2 Decomposition of the LS Estimate According to Noise and Nonlinearity

When the predictors are random and linear regression is interpreted semi-parametrically as the extraction of the best linear approximation to a nonlinear response surface, the sampling variation of the LS estimate $\hat{\beta}$ can be additively decomposed into two components: one component due to error $\epsilon$ and another component due to nonlinearity interacting with randomness of the predictors. This decomposition is a direct reflection of the decomposition $\delta = \epsilon + \eta$, according to (5) and (15). We give elementary asymptotic normality statements for each part of the decomposition. The relevance of the decomposition is that it explains what the pairs bootstrap estimates, while the associated asymptotic normalities are necessary to justify the pairs bootstrap.

In the classical linear models theory, which conditions on $X$, the target of estimation is $E[\hat{\beta} | X]$. When $X$ is treated as random and nonlinearity is permitted, the target of estimation is the population LS solution $\beta = \beta(P)$ defined in (4). In this case, $E[\hat{\beta} | X]$ is a random vector that is naturally placed between $\hat{\beta}$ and $\beta$:

$$\hat{\beta} - \beta = (\hat{\beta} - E[\hat{\beta} | X]) + (E[\hat{\beta} | X] - \beta)$$

This decomposition corresponds to the decomposition $\delta = \epsilon + \eta$ as the following lemma shows.

Definition and Lemma: We define “Estimation Offsets” or “EOs” for short as follows:

- **Total EO**: $\hat{\beta} - \beta = (X^T X)^{-1} X^T \delta$,
- **Error EO**: $\hat{\beta} - E[\hat{\beta} | X] = (X^T X)^{-1} X^T \epsilon$,
- **Nonlinearity EO**: $E[\hat{\beta} | X] - \beta = (X^T X)^{-1} X^T \eta$.

The equations follow from the decompositions (15), $\epsilon = Y - \mu$, $\eta = \mu - X \beta$, $\delta = Y - X \beta$, and these facts:

$$\hat{\beta} = (X^T X)^{-1} X^T Y, \quad E[\hat{\beta} | X] = (X^T X)^{-1} X^T \mu, \quad \beta = (X^T X)^{-1} X^T (X \beta).$$

The first equality is the definition of $\hat{\beta}$, the second uses $E[Y | X] = \mu$, and the third is a tautology.

The variance/covariance matrix of $\hat{\beta}$ has a canonical decomposition with regard to conditioning on $X$:

$$V[\hat{\beta}] = E[V[\hat{\beta} | X]] + V[E[\hat{\beta} | X]].$$
Figure 4: Error-less Response: The filled and the open circles represent two “datasets” from the same population. The $x$-values are random; the $y$-values are a deterministic function of $x$: $y = \mu(x)$ (shown in gray).
Left: The true response $\mu(x)$ is nonlinear; the open and the filled circles have different LS lines (shown in black). Right: The true response $\mu(x)$ is linear; the open and the filled circles have the same LS line (black on top of gray).

This decomposition reflects the estimation decomposition (17) and $\delta = \epsilon + \eta$ in view of (18):

$$
\begin{align*}
V[\hat{\beta}] &= V[(X^T X)^{-1} X^T \delta], \\
E[V[\hat{\beta} | X]] &= E[V[(X^T X)^{-1} X^T \epsilon | X]], \\
V[E[\hat{\beta} | X]] &= V[(X^T X)^{-1} X^T \eta].
\end{align*}
$$

(Note that in general $E[(X^T X)^{-1} X^T \eta] \neq 0$ even though $E[X^T \eta] = 0$ and hence $(X^T X)^{-1} X^T \eta \rightarrow 0$ a.s.)

5.3 Random $X$ and Nonlinearity as a Source of Sampling Variation

Linear models theory is largely about sampling variability due to error $V[\hat{\beta} | X]$. The fact that there exists another source of sampling variability is little known: nonlinearity in the presence of random predictors, as expressed by $V[E[\hat{\beta} | X]]$ in (5.2). It may be useful to isolate this source and illustrate it in a situation that is free of error: Consider a response that is a deterministic noiseless but nonlinear function of the predictors: $Y = \eta(\mathbf{X})$. (This may be a realistic situation when outcomes from expensive deterministic simulation experiments are modeled based on inputs.)
Assume therefore $\epsilon = 0$ but $\eta \neq 0$, hence there exists sampling variability in $\hat{\beta}$ which is solely due to the nonlinearity $\eta$: $\hat{\beta} - \beta = (X^TX)^{-1}X^T\eta$ in conjunction with the randomness of the predictors — the “conspiracy” in the title of this article.

Figure 4 illustrates the situation with a single-predictor example by showing the LS lines fitted to two “datasets” consisting of $N = 5$ predictor values each. The random differences between datasets cause the fitted line to exhibit sampling variability under nonlinearity (left hand figure), which is absent under linearity (right hand figure). Compare this figure with the earlier Figure 2: mathematically the effects illustrated in both are identical; Figure 2 shows the effect for different populations (theoretical $X$ distributions) while Figure 4 shows it for different datasets (empirical $X$ distributions). Thus nonlinearity creates complications on two interconnected levels: (1) in the definition of the population LS parameter, which becomes dependent on the predictor distribution, and (2) through the creation of sampling variability due to $E[\hat{\beta} | X]$ which becomes a true random vector. (A more striking illustration in the form of an animation is available to users of the R language by executing the following line of code: source("http://stat.wharton.upenn.edu/~buja/src-conspiracy-animation2.R").)

The case of error free but nonlinear response is of interest to make another point regarding statistical inference: If classical linear models theory conditions on the predictors and assumes erroneously that the response surface is linear, it is not so that the resulting procedures do “not see” see the sampling variability caused by nonlinearity, but they misinterpret it as due to error. The consequences of the confusion of errors and nonlinearities for statistical inference will be examined in Section 8.3. This misinterpretation also seeps into the residual bootstrap as it assumes the residuals to originate from exchangeable errors only. By comparison, the pairs bootstrap gets statistical inference right even in the error-free nonlinear case, at least asymptotically. It receives its justification from the following central limit theorems.

5.4 Assumption-Lean Central Limit Theorems

The three EOs of Section 5.2 arise from the decomposition (5): $\delta = \epsilon + \eta$. The respective CLTs draw on the analogous conditional second moment decomposition $m^2(\bar{X}) = \sigma^2(\bar{X}) + \eta^2(\bar{X})$ (9). The asymptotic variance/covariance matrices have the well-known sandwich form:

**Proposition:** The three EOs follow central limit theorems under usual multivariate CLT assumptions:

\[
N^{1/2} (\hat{\beta} - \beta) \overset{D}{\rightarrow} N \left( 0, E[\bar{X} \bar{X}^T]^{-1} E[\delta^2 \bar{X} \bar{X}^T] E[\bar{X} \bar{X}^T]^{-1} \right)
\]

\[
N^{1/2} (\hat{\beta} - E[\hat{\beta} | X]) \overset{D}{\rightarrow} N \left( 0, E[\bar{X} \bar{X}^T]^{-1} E[\epsilon^2 \bar{X} \bar{X}^T] E[\bar{X} \bar{X}^T]^{-1} \right)
\]

\[
N^{1/2} (E[\hat{\beta} | X] - \beta) \overset{D}{\rightarrow} N \left( 0, E[\bar{X} \bar{X}^T]^{-1} E[\eta^2 \bar{X} \bar{X}^T] E[\bar{X} \bar{X}^T]^{-1} \right)
\]

The proof is standard, but here is an outline for the first case, if only to show how the sandwich
form of the asymptotic variance arises. Using $E[\delta \bar{X}] = 0$ from (12) we have:

$$N^{1/2}(\hat{\beta} - \beta) = \left(\frac{1}{N} X^T X\right)^{-1} \left(\frac{1}{N^{1/2}} X^T \delta\right)$$

$$= \left(\frac{1}{N} \sum \bar{X}_i \bar{X}_i^T\right)^{-1} \left(\frac{1}{N^{1/2}} \sum \bar{X}_i \delta_i\right)$$

$$\xrightarrow{D} E[\bar{X} \bar{X}^T]^{-1} N\left(0, E[\delta^2 \bar{X} \bar{X}^T]\right)$$

$$= N\left(0, E[\bar{X} \bar{X}^T]^{-1} E[\delta^2 \bar{X} \bar{X}^T] E[\bar{X} \bar{X}^T]^{-1}\right) ,$$

Note: The center parts of the first two asymptotic sandwich covariances can equivalently be written as

$$E[m^2(\bar{X}) \bar{X} \bar{X}^T] = E[\delta^2 \bar{X} \bar{X}^T], \quad E[\sigma^2(\bar{X}) \bar{X} \bar{X}^T] = E[\epsilon^2 \bar{X} \bar{X}^T], \quad (20)$$

which follows from $m^2(\bar{X}) = E[\delta^2 | \bar{X}]$ and $\sigma^2(\bar{X}) = E[\epsilon^2 | \bar{X}]$ according to (8) and (9).

The proposition can be specialized in a few ways to cases of partial or complete well-specification:

- **First order well-specification**: When there is no nonlinearity, $\eta(\bar{X}) \overset{P}{=} 0$, then

$$N^{1/2}(\hat{\beta} - \beta) \xrightarrow{D} N\left(0, E[\bar{X} \bar{X}^T]^{-1} E[\epsilon^2 \bar{X} \bar{X}^T] E[\bar{X} \bar{X}^T]^{-1}\right)$$

The sandwich form of the asymptotic variance/covariance matrix is solely due to heteroskedasticity.

- **First and second order well-specification**: When additionally homoskedasticity holds, $\sigma^2(\bar{X}) \overset{P}{=} \sigma^2$, then

$$N^{1/2}(\hat{\beta} - \beta) \xrightarrow{D} N\left(0, \sigma^2 E[\bar{X} \bar{X}^T]^{-1}\right)$$

The familiar simplified form is asymptotically valid under first and second order well-specification but without the assumption of Gaussian errors.

- **Deterministic nonlinear response**: $\sigma^2(\bar{X}) \overset{P}{=} 0$, then

$$N^{1/2}(\hat{\beta} - \beta) \xrightarrow{D} N\left(0, E[\bar{X} \bar{X}^T]^{-1} E[\eta^2 \bar{X} \bar{X}^T] E[\bar{X} \bar{X}^T]^{-1}\right)$$

The sandwich form of the asymptotic variance/covariance matrix is solely due to nonlinearity and random predictors.

### 6 The Sandwich Estimator and the $M$-of-$N$ Pairs Bootstrap

Empirically one observes that standard error estimates obtained from the pairs bootstrap and from the sandwich estimator are generally close to each other. This is intuitively unsurprising as they both estimate the same asymptotic variance, that of the first CLT in (30). A closer connection between them will be established below.
6.1 The Plug-In Sandwich Estimator of Asymptotic Variance

According to (19) the asymptotic variance of the LS estimator $\hat{\beta}$ is

$$AV[\hat{\beta}] = E[\bar{XX}^T]^{-1} E[\delta^2 \bar{XX}^T] E[\bar{XX}^T]^{-1}. \quad (21)$$

The sandwich estimator is then the plug-in version of (21) where $\delta^2$ is replaced by residuals and population expectations $E[...]$ by sample means $\hat{E}[...]$:

$$\hat{E}[\bar{XX}^T] = \frac{1}{N} \sum_{i=1}^N \bar{X}_i \bar{X}_i^T = \frac{1}{N} (X^T X)$$
$$\hat{E}[r^2 \bar{XX}^T] = \frac{1}{N} \sum_{i=1}^N r_i^2 \bar{X}_i \bar{X}_i^T = \frac{1}{N} (X^T D_r^2 X),$$

where $D_r^2$ is the diagonal matrix with squared residuals $r_i^2 = (Y_i - \bar{X}_i \hat{\beta})^2$ in the diagonal. With this notation the simplest and original form of the sandwich estimator of asymptotic variance can be written as follows (White 1980a):

$$\hat{AV}_{sand} := \hat{E}[\bar{XX}^T]^{-1} \hat{E}[r^2 \bar{XX}^T] \hat{E}[\bar{XX}^T]^{-1} = N (X^T X)^{-1} (X^T D_r^2 X) (X^T X)^{-1} \quad (22)$$

The sandwich standard error estimate for the $j$'th regression coefficient is therefore obtained as

$$\hat{SE}_{sand}[\hat{\beta}_j] := \frac{1}{N^{1/2}} (\hat{AV}_{sand})_{jj}^{1/2}. \quad (23)$$

For this simplest version ("HC" in MacKinnon and White (1985)) obvious modifications exist. For one thing, it does not account for the fact that residuals have on average smaller variance than errors. An overall correction factor $(N/(N - p - 1))^{1/2}$ in (23) would seem to be sensible in analogy to the linear models estimator ("HC1" ibid.). More detailed modifications have been proposed whereby individual residuals are corrected for their reduced conditional variance according to $V[r_i | X] = \sigma^2(1 - H_{ii})$ under homoskedasticity and ignoring nonlinearity ("HC2" ibid.). Further modifications include a version based on the jackknife ("HC3" ibid.) using leave-one-out residuals. An obvious alternative is estimating asymptotic variance with the pairs bootstrap, to which we now turn.

6.2 The $M$-of-$N$ Pairs Bootstrap Estimator of Asymptotic Variance

To connect the sandwich estimator to its bootstrap counterpart we need the $M$-of-$N$ bootstrap whereby the resample size $M$ is allowed to differ from the sample size $N$. It is at this point important not to confuse

- $M$-of-$N$ resampling with replacement, and
- $M$-out-of-$N$ subsampling without replacement.

In resampling the resample size $M$ can be any $M < \infty$, whereas for subsampling it is necessary that the subsample size $M$ satisfy $M < N$. We are here concerned with bootstrap resampling, and we will focus on the extreme case $M \gg N$, namely, the limit $M \to \infty$. 

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Because resampling is i.i.d. sampling from some distribution, there holds a CLT as the resample size grows, $M \to \infty$. It is immaterial that in this case the sampled distribution is the empirical distribution $P_N$ of a given dataset $\{(\tilde{X}_i, Y_i)\}_{i=1\ldots N}$, which is frozen of size $N$ as $M \to \infty$.

**Proposition:** For any fixed dataset of size $N$, there holds a CLT for the $M$-of-$N$ bootstrap as $M \to \infty$. Denoting by $\beta_M^*$ the LS estimate obtained from a bootstrap resample of size $M$, we have

$$M^{1/2}(\beta_M^* - \hat{\beta}) \overset{D}{\to} \mathcal{N}(0, \hat{E}[\tilde{X} \tilde{X}^T]^{-1} \hat{E}[(Y - \tilde{X}^T \hat{\beta})^2 \tilde{X} \tilde{X}^T] \hat{E}[\tilde{X} \tilde{X}^T]^{-1}) \quad (M \to \infty). \quad (24)$$

This is a straight application of the CLT of the previous section to the empirical distribution rather than the actual distribution of the data, where the middle part (the “meat”) of the asymptotic formula is based on the empirical counterpart $r_i^2 = (Y_i - \tilde{X}_i^T \hat{\beta})^2$ of $\delta^2 = (Y - \tilde{X}^T \beta)^2$. A comparison of (22) and (24) results in the following:

**Corollary:** The sandwich estimator (22) is the asymptotic variance estimated by the limit of the $M$-of-$N$ pairs bootstrap as $M \to \infty$ for a fixed sample of size $N$.

As an inferential method the pairs bootstrap is obviously more flexible and richer in possibilities than the sandwich estimator. The latter is limited to providing a standard error estimate assuming approximate normality of the parameter estimate’s sampling distribution. The bootstrap distribution, on the other hand, can be used to generate confidence intervals that are often second order correct (the literature on this topic is too rich to list, so we point only to the standard bootstrap reference Efron and Tibshirani (1994)).

Further connections are mentioned by MacKinnon and White (1985): Some forms of the sandwich estimator were independently derived by Efron (1982, p.18-19) using the infinitesimal jackknife, and by Hinkley (1977) using what he calls a “weighted jackknife”. See Weber (1986) for a concise comparison in the fixed-$X$ linear models framework limited to the problem of heteroskedasticity. A richer context for the relation between the jackknife and bootstrap is given by Wu (1986)

## 7 Adjusted Predictors

The adjustment formulas of this section serve to express the slopes of multiple regressions as slopes in simple regressions using adjusted single predictors. The goal is to analyze the discrepancies between asymptotically proper and improper standard errors of regression estimates in Section 8. The result will be tests that indicate for each predictor separately whether the linear models standard error is invalidated by “misspecification”.

### 7.1 Adjustment in populations

To express the population LS regression coefficient $\beta_j = \beta_j(P)$ as a simple regression coefficient, let the adjusted predictor $X_{j*}$ be defined as the “residual” of the population regression of $X_j$, used as
the response, on all other predictors. In detail, collect all other predictors in the random $p$-vector
\[ \mathbf{X}_j = (1, X_1, ..., X_{j-1}, X_{j+1}, ..., X_p)^T, \]
and let $\beta_{j*}$ be the coefficient vector from the regression of $X_j$ onto $\mathbf{X}_j$:
\[ \beta_{j*} = \arg\min_{\beta \in \mathbb{R}^p} E[(X_j - \beta^T \mathbf{X}_j)^2] = E[\mathbf{X}_j \mathbf{X}_j^T]^{-1} E[\mathbf{X}_j X_j]. \]
The adjusted predictor $X_{j*}$ is the residual from this regression:
\[ X_{j*} = X_j - \mathbf{X}_j^T \beta_{j*}. \tag{25} \]

The representation of $\beta_j$ as a simple regression coefficient is as follows:
\[ \beta_j = \frac{E[Y X_{j*}]}{E[X_{j*}^2]} = \frac{E[\mu(\mathbf{X}) X_{j*}]}{E[X_{j*}^2]} \tag{26}. \]

### 7.2 Adjustment in samples

To express estimates of regression coefficients as simple regressions, we collect all predictor columns other than $X_j$ in a $N \times p$ random predictor matrix $\mathbf{X}_j = (1, ..., X_{j-1}, X_{j+1}, ...)$ and define
\[ \hat{\beta}_{j*} = \arg\min_{\beta \in \mathbb{R}^p} \|X_j - X_j \hat{\beta}\|^2 = (X_j^T X_j)^{-1} X_j^T X_j. \]
Using the hat notation “$\hat{\cdot}$” to denote sample-based adjustment to distinguish it from population-based adjustment “$\cdot$”, we write the sample-adjusted predictor as
\[ X_{j\hat{}} = X_j - X_j \hat{\beta}_{j\hat{}} = (I - H_j) X_j. \tag{27} \]
where $H_j = X_j (X_j^T X_j)^{-1} X_j^T$ is the associated projection or hat matrix. The $j$’th slope estimate of the multiple linear regression of $Y$ on $X_1, ..., X_p$ can then be expressed in the well-known manner as the slope estimate of the simple linear regression without intercept of $Y$ on $X_{j\hat{}}$:
\[ \hat{\beta}_j = \frac{\langle Y, X_{j\hat{}} \rangle}{\|X_{j\hat{}}\|^2}. \tag{28} \]

In the proofs (see the Appendix) we also need notation for each observation’s population-adjusted predictors: $X_{j*} = (X_{1j*}, ..., X_{Nj*})^T = X_j - X_j \beta_{j*}$. The following distinction is elementary but important: The component variables of $X_{j*} = (X_{ij*})_{i=1...N}$ are i.i.d. as they are population-adjusted, whereas the component variables of $X_{j\hat{}} = (X_{ij\hat{}})_{i=1...N}$ are dependent as they are sample-adjusted. As $N \to \infty$ for fixed $p$, this dependency disappears asymptotically, and we have for the empirical distribution of the values $\{X_{ij}\}_{i=1...N}$ the obvious convergence in distribution:
\[ \{X_{ij}\}_{i=1...N} \overset{D}{\longrightarrow} X_{j*} \overset{D}{=} X_{j\hat{}} \quad (N \to \infty). \]
7.3 Adjustment for Estimation Offsets and Their CLTs

The vectorized formulas for estimation offsets (17) can be written componentwise using adjustment as follows:

**Total EO:** \[ \hat{\beta}_j - \beta_j = \frac{\langle X_j \hat{\beta}_j, \delta \rangle}{\|X_j\|_2^2}, \]

**Error EO:** \[ \hat{\beta}_j - E[\hat{\beta}_j|X] = \frac{\langle X_j \hat{\beta}_j, \epsilon \rangle}{\|X_j\|_2^2}, \] \hspace{1cm} (29)

**Nonlinearity EO:** \[ E[\hat{\beta}_j|X] - \beta_j = \frac{\langle X_j \hat{\beta}_j, \eta \rangle}{\|X_j\|_2^2}. \]

Asymptotic normality can also be expressed for each \( \hat{\beta}_j \) separately using population adjustment:

**Corollary:**

\[ N^{1/2}(\hat{\beta}_j - \beta_j) \xrightarrow{D} \mathcal{N} \left( 0, \frac{E[m^2(X_j \hat{\beta}_j^2)]}{E[X_j^2]^2} \right) = \mathcal{N} \left( 0, \frac{E[\delta^2 X_j^2]}{E[X_j^2]^2} \right) \]

\[ N^{1/2}(\hat{\beta}_j - E[\hat{\beta}_j|X]) \xrightarrow{D} \mathcal{N} \left( 0, \frac{E[\sigma^2(X_j \hat{\beta}_j^2)]}{E[X_j^2]^2} \right) = \mathcal{N} \left( 0, \frac{E[\epsilon^2 X_j^2]}{E[X_j^2]^2} \right) \]

\[ N^{1/2}(E[\hat{\beta}_j|X] - \beta_j) \xrightarrow{D} \mathcal{N} \left( 0, \frac{E[\eta^2(X_j \hat{\beta}_j^2)]}{E[X_j^2]^2} \right) \] \hspace{1cm} (30)

These are not new results but reformulations for the components of the vector CLTs (19). The equalities in the first and second case are based on (20). The asymptotic variances of (30) are the subject of next section.

8 Asymptotic Variances — Proper and Improper

The following prepares the ground for an asymptotic comparison of linear models standard errors with correct assumption-lean standard errors. We know the former to be potentially incorrect in the presence of nonlinearity and/or heteroskedasticity, hence a natural question is: by how much can linear models standard errors deviate from valid assumption-lean standard errors? We look for an answer in the asymptotic limit, which frees us from issues related to how the standard errors are estimated.

8.1 Proper Asymptotic Variances in Terms of Adjusted Predictors

The CLTs (30) contain three asymptotic variances, one for the estimate \( \hat{\beta}_j \) and two for the contributions due to error and due to nonlinearity according to \( m^2(\hat{X}) = \sigma^2(\hat{X}) + \eta(\hat{X}) \). These asymptotic
variances are of the same functional form, which suggests using generic notation for all three. We therefore define:

**Definition:**
\[
\text{AV}^{(j)}_{\text{lean}}[f^2(\bar{X})] := \frac{E[f^2(\bar{X})X_{j^*}^2]}{E[X_{j^*}^2]} \tag{31}
\]

Using \( m^2(\bar{X}) = \sigma^2(\bar{X}) + \eta^2(\bar{X}) \) from (9), we obtain a decomposition of asymptotic variance suggested by (30):

\[
\begin{align*}
\text{AV}^{(j)}_{\text{lean}}[m^2(\bar{X})] &= \text{AV}^{(j)}_{\text{lean}}[\sigma^2(\bar{X})] + \text{AV}^{(j)}_{\text{lean}}[\eta^2(\bar{X})] \\
\frac{E[m^2(\bar{X})X_{j^*}^2]}{E[X_{j^*}^2]^2} &= \frac{E[\sigma^2(\bar{X})X_{j^*}^2]}{E[X_{j^*}^2]^2} + \frac{E[\eta^2(\bar{X})X_{j^*}^2]}{E[X_{j^*}^2]^2} \tag{32}
\end{align*}
\]

### 8.2 Improper Asymptotic Variances in Terms of Adjusted Predictors

Next we write down an asymptotic form for the conventional standard error estimate from linear models theory in the assumption-lean framework. This asymptotic form will have the appearance of an asymptotic variance but it will generally be improper as its intended domain of validity is the assumption-loaded framework of linear models theory. This “improper” asymptotic variance derives from an estimate \( \hat{\sigma}^2 \) of the error variance, usually \( \hat{\sigma}^2 = \|Y - X\hat{\beta}\|^2/(N-p-1) \). In the assumption-lean framework with both heteroskedastic error variance and nonlinearity, \( \hat{\sigma}^2 \) has the following limit for fixed \( p \): 

\[
\hat{\sigma}^2 \overset{P}{\to} E[m^2(\bar{X})] = E[\sigma^2(\bar{X})] + E[\eta^2(\bar{X})], \quad N \to \infty.
\]

Squared standard error estimates for coefficients are, in matrix form and adjustment form, as follows:

\[
\hat{V}_{\text{lin}}[\hat{\beta}] = \hat{\sigma}^2 (X^TX)^{-1}, \quad \hat{SE}_{\text{lin}}^2[\hat{\beta}_j] = \frac{\hat{\sigma}^2}{\|X_{j^*}\|^2}. \tag{33}
\]

Their scaled limits under lean assumptions are as follows:

\[
N \hat{V}_{\text{lin}}[\hat{\beta}] \overset{P}{\to} E[m^2(\bar{X})] E[\bar{X}\bar{X}^T]^{-1}, \quad N \hat{SE}_{\text{lin}}^2[\hat{\beta}_j] \overset{P}{\to} \frac{E[m^2(\bar{X})]}{E[X_{j^*}^2]}. \tag{34}
\]

We call these limits “improper asymptotic variances”. Again we can use (9) \( m^2(\bar{X}) = \sigma^2(\bar{X}) + \eta^2(\bar{X}) \) for a decomposition and therefore introduce generic notation where \( f^2(\bar{X}) \) is a placeholder for any one among \( m^2(\bar{X}), \sigma^2(\bar{X}) \) and \( \eta^2(\bar{X}) \):

**Definition:**
\[
\text{AV}^{(j)}_{\text{lin}}[f^2(\bar{X})] := \frac{E[f^2(\bar{X})]}{E[X_{j^*}^2]} \tag{35}
\]

Hence this the improper asymptotic variance of \( \hat{\beta}_j \) and its decomposition:
\[
\begin{align*}
AV_{lin}^{(j)}[m^2(\tilde{X})] &= AV_{lin}^{(j)}[\sigma^2(\tilde{X})] + AV_{lin}^{(j)}[\eta^2(\tilde{X})] \\
\frac{E[m^2(\tilde{X})]}{E[X_j^2]} &= \frac{E[\sigma^2(\tilde{X})]}{E[X_j^2]} + \frac{E[\eta^2(\tilde{X})]}{E[X_j^2]}
\end{align*}
\] (36)

### 8.3 Comparison of Proper and Improper Asymptotic Variances: RAV

We examine next the discrepancies between proper and improper asymptotic variances by forming their ratio. It will be shown that this ratio can be arbitrarily close to 0 and to \(\infty\). It can be formed separately for each of the versions corresponding to \(m^2(\tilde{X})\), \(\sigma^2(\tilde{X})\) and \(\eta^2(\tilde{X})\). For this reason we introduce a generic form of the ratio:

**Definition:** *Ratio of Asymptotic Variances, Proper/Improper.*

\[
\text{RAV}_{j}\left[f^2(\tilde{X})\right] := \frac{AV_{lin}^{(j)}[f^2(\tilde{X})]}{AV_{lin}^{(j)}[f^2(\tilde{X})]} = \frac{E[f^2(\tilde{X})X_j^2]}{E[f^2(\tilde{X})]E[X_j^2]}
\] (37)

Again, \(f^2(\tilde{X})\) is a placeholder for each of \(m^2(\tilde{X})\), \(\sigma^2(\tilde{X})\) and \(\eta^2(\tilde{X})\). The overall \(\text{RAV}_j[m^2(\tilde{X})]\) can be decomposed into a weighted average of \(\text{RAV}_j[\sigma^2(\tilde{X})]\) and \(\text{RAV}_j[\eta^2(\tilde{X})]\):

**Lemma:** *RAV Decomposition.*

\[
\text{RAV}_j[m^2(\tilde{X})] = w_\sigma \text{RAV}_j[\sigma^2(\tilde{X})] + w_\eta \text{RAV}_j[\eta^2(\tilde{X})]
\]

\[
w_\sigma := \frac{E[\sigma^2(\tilde{X})]}{E[m^2(\tilde{X})]}, \quad w_\eta := \frac{E[\eta^2(\tilde{X})]}{E[m^2(\tilde{X})]}, \quad w_\sigma + w_\eta = 1.
\] (38)

Implications of this decomposition will be discussed below. Structurally, the three ratios \(\text{RAV}_j\) can be interpreted as inner products between the normalized squared random variables

\[
\frac{m^2(\tilde{X})}{E[m^2(\tilde{X})]}, \quad \frac{\sigma^2(\tilde{X})}{E[\sigma^2(\tilde{X})]}, \quad \frac{\eta^2(\tilde{X})}{E[\eta^2(\tilde{X})]}
\]

on the one hand, and the normalized squared adjusted predictor

\[
\frac{X_j^2}{E[X_j^2]}
\]

on the other hand. These inner products, however, are *not* correlations, and they are *not* bounded by \(+1\); their natural bounds are rather 0 and \(\infty\), both of which can generally be approached to any degree as will be shown in Subsection 8.5.
8.4 The Meaning of $RAV$ 

The ratio $RAV_j[m^2(\bar{X})]$ shows by what multiple the proper asymptotic variance deviates from the improper one:

- If $RAV_j[m^2(\bar{X})] = 1$, then $\hat{SE}_{lin}[\hat{\beta}_j]$ is asymptotically correct;
- if $RAV_j[m^2(\bar{X})] > 1$, then $\hat{SE}_{lin}[\hat{\beta}_j]$ is asymptotically too small/optimistic;
- if $RAV_j[m^2(\bar{X})] < 1$, then $\hat{SE}_{lin}[\hat{\beta}_j]$ is asymptotically too large/pessimistic.

If, for example, $RAV_j[m^2(\bar{X})] = 4$, then, for large sample sizes, the proper standard error of $\hat{\beta}_j$ is about twice as large as the improper standard error of linear models theory. If, however, $RAV_j[m^2(\bar{X})] = 1$, it does not imply that the model is well-specified because heteroskedasticity and nonlinearity can conspire to make $RAV_j[m^2(\bar{X})] = 1$ even though neither $\sigma^2(X) = \text{const}$ nor $\eta(\bar{X}) = 0$; see the decomposition lemma in Subsection 8.3. If, for example, $m^2(\bar{X}) = \sigma^2(\bar{X}) + \eta^2(\bar{X}) = m^2_0$ constant while neither $\sigma^2(\bar{X})$ is constant nor $\eta^2(\bar{X})$ vanishes, then $RAV_j[m^2_0] = 1$ and the linear models standard error is asymptotically correct, yet the model is “misspecified.” Well-specification to first and second order, $\eta(\bar{X}) = 0$ and $\sigma^2(\bar{X}) = \sigma^2_0$ constant, is a sufficient but not necessary condition for asymptotic validity of the conventional standard error.

8.5 The Range of $RAV$

As mentioned $RAV$ ratios can generally vary between 0 and $\infty$. The following proposition states the technical conditions under which these bounds are sharp. The formulation is generic in terms of $f^2(\bar{X})$ as placeholder for $m^2(\bar{X})$, $\sigma^2(\bar{X})$ and $\eta^2(\bar{X})$. The proof is in Appendix B.3.

Proposition:
(a) If $X_j*$ has unbounded support on at least one side, that is, if $P[X_j*^2 > t] > 0 \forall t > 0$, then
\[
\sup_f RAV_j[f^2(\bar{X})] = \infty. \tag{39}
\]

(b) If the closure of the support of the distribution of $X_j*$ contains zero (its mean) but there is no pointmass at zero, that is, if $P[X_j*^2 < t] > 0 \forall t > 0$ but $P[X_j*^2 = 0] = 0$, then
\[
\inf_f RAV_j[f^2(\bar{X})] = 0. \tag{40}
\]

As a consequence, it is in general the case that $RAV_j[m^2(\bar{X})]$, $RAV_j[\sigma^2(\bar{X})]$ and $RAV_j[\eta^2(\bar{X})]$ can each range between 0 and $\infty$. (A slight subtlety arises from the constraint imposed on $\eta(\bar{X})$ by orthogonality (11) to the predictors, but it does not invalidate the general fact.)
The proposition involves only some plausible conditions on the distribution of $X_j$, not all of $\bar{X}$. This follows from the fact that the dependence of $RAV_j[f^2(\bar{X})]$ on the distribution of $\bar{X}$ can be reduced to dependence on the distribution of $X_j^2$ through conditioning:

$$RAV_j[f^2(\bar{X})] = \frac{E[f_j^2(X_j) X_j^2]}{E[f_j^2(X_j) | X_j^2]}$$

where $f_j^2(X_j) := E[f^2(\bar{X}) | X_j^2]$. (41)

The problem then boils down to a single-predictor situation in $X = X_j$ which lends itself to graphical illustration. Figure 5 shows a family of functions $f^2(x)$ that interpolates the range of the $RAV$ from 0 to $\infty$ for $X \sim N(0, 1)$. (Details are in Appendix B.4.)

Even though the $RAV$ is not a correlation, it is nevertheless a measure of association between

![Figure 5: A family of functions $f_t^2(x)$ that can be interpreted as heteroskedasticities $\sigma^2(X_j)$, squared nonlinearities $\eta^2(X_j)$, or conditional MSEs $m^2(X_j)$: The family interpolates $RAV$ from 0 to $\infty$ for $x = X_j \sim N(0, 1)$. The three solid black curves show $f_t^2(x)$ that result in $RAV=0.05$, 1, and 10. (See Appendix B.4 for details.) $RAV = \infty$ is approached as $f_t^2(x)$ bends ever more strongly in the tails of the $x$-distribution. $RAV = 0$ is approached by an ever stronger spike in the center of the $x$-distribution.](image)
Figure 6: The effect of heteroskedasticity on the sampling variability of slope estimates: The question is how the misinterpretation of the heteroskedasticities as homoskedastic affects statistical inference. Left: High error variance in the tails of the predictor distribution elevates the true sampling variability of the slope estimate above the linear models standard error (RAV[σ²(X)] > 1).
Center: High error variance near the center of the predictor distribution lowers the true sampling variability of the slope estimate below the linear models standard error (RAV[σ²(X)] < 1).
Right: The error variance oscillates in such a way that the linear models standard error is coincidentally correct (RAV[σ²(X)] = 1).

f_j^2(X_j.) and X_j.². Unlike correlations, it exists for f² = const > 0 as well, in which case RAV = 1. It indicates a positive association between f²(X) and X_j.² for RAV > 1 and a negative association for RAV < 1. This is borne out by Figure 5: large values RAV > 1 are obtained when f_j^2(X_j.) is large for X_j. far from zero, and small values RAV < 1 are obtained when f²(X_j.) is large for X_j. near zero.

So far we discussed and illustrated the properties of RAV_j in terms of an X̄-conditional function f²(X̄) which could be any of m²(X̄), σ²(X̄) and η²(X̄). Next we illustrate in terms of potential data situations: Figure 6 shows three heteroskedasticity scenarios and Figure 7 three nonlinearity scenarios. These examples allow us to train our intuitions about the types of heteroskedasticities and nonlinearities that drive the overall RAV_j[m²(X̄)]. Based on the RAV decomposition lemma (38) of Subsection 8.3 according to which RAV[m²(X̄)] is a mixture of RAV[σ²(X̄)] and RAV[η²(X̄)], we can state the following:

- Heteroskedasticities σ²(X̄) with large average variance E[σ²(X̄) | X_j.²] in the tail of X_j.² imply an upward contribution to the overall RAV_j[m²(X̄)]; heteroskedasticities with large average variance concentrated near X_j.² = 0 imply a downward contribution to the overall RAV_j[m²(X̄)].

- Nonlinearities η²(X̄) with large average values E[η²(X̄) | X_j.²] in the tail of X_j.² imply an upward contribution to the overall RAV_j[m²(X̄)]; nonlinearities with large average values concentrated near X_j.² = 0 imply a downward contribution to the overall RAV_j[m²(X̄)].
Figure 7: The effect of nonlinearities on the sampling variability of slope estimates: The three plots show three different error-free nonlinearities; each plot shows for one nonlinearity 20 overplotted datasets of size $N = 10$ and their fitted lines through the origin. The question is how the misinterpretation of the nonlinearities as homoskedastic random errors affects statistical inference.

Left: Strong nonlinearity in the tails of the predictor distribution elevates the true sampling variability of the slope estimate above the linear models standard error ($RAV[\eta^2(X)] > 1$).
Center: Strong nonlinearity near the center of the predictor distribution lowers the true sampling variability of the slope estimate below the linear models standard error ($RAV[\eta^2(X)] < 1$).
Right: An oscillating nonlinearity mimics homoskedastic random error to make the linear models standard error coincidentally correct ($RAV[\eta^2(X)] = 1$).

These facts also suggest the following: in practice, large values $RAV_j > 1$ are generally more likely than small values $RAV_j < 1$ because both large conditional variances and nonlinearities are often more pronounced in the extremes of predictor distributions. This seems particularly natural for nonlinearities which in the simplest cases will be convex or concave. In addition it follows from the $RAV$ decomposition lemma (38) that for fixed relative contributions $w_\sigma > 0$ and $w_\eta > 0$ either of $RAV_j[\sigma^2(\tilde{X})]$ or $RAV_j[\eta^2(\tilde{X})]$ is able to single-handedly pull $RAV_j[m^2(\tilde{X})]$ to $+\infty$, whereas both have to be close to zero to pull $RAV_j[m^2(\tilde{X})]$ toward zero. These considerations are of course no more than heuristics and practical common sense, but they may be the best we can hope for to understand the prevalence of situations in which the linear models standard error is too small.

9 The Sandwich Estimator in Adjusted Form and a $RAV$ Test

The goal is to write the sandwich estimator of standard error in adjustment form and use it to estimate the $RAV$ with plug-in for use as a test to decide whether the standard error of linear models theory is adequate. In adjustment form we obtain one test per predictor variable. These tests belong in the class of “misspecification tests” for which there exists a literature in econometrics starting with Hausman (1978) and continuing with White (1980a,b; 1981; 1982) and others. The tests of Hausman and White are largely global rather than coefficient-specific, which ours is. Test
proposed here has similarities to White’s (1982, Section 4) “information matrix test” as it compares two types of information matrices globally, while we compare two types of standard errors one coefficient at a time. The parameter-specific tests of White (1982, Section 5), however, take a different approach altogether: they compare two types of coefficient estimates rather than standard error estimates. The test procedures proposed here have a simplicity and flexibility that may be missing in the extant literature. The flexibility arises from being able to exclude normality of errors from the null hypothesis, which we find important as otherwise most misspecification tests respond to non-normality much of the time rather than nonlinearity and heteroskedasticity.

9.1 The Adjustment Form of the Sandwich Estimator and the $R \hat{A}V_j$ Statistic

To begin with, the adjustment versions of the asymptotic variances in the CLTs (30) can be used to rewrite the sandwich estimator by replacing expectations $E[...]$ with means $\hat{E}[...]$, the population parameter $\beta$ with its estimate $\hat{\beta}$, and population adjustment $X_j*$ with sample adjustment $X_{j*}$:

$$\hat{A}V_{sand}^{(j)} = \frac{\hat{E}[(Y - \bar{X}^T \hat{\beta})^2 X_{j*}^2]}{\hat{E}[X_{j*}^2]^2} = N \frac{\langle (Y - \bar{X} \hat{\beta})^2, X_{j*}^2 \rangle}{\|X_{j*}\|^4}$$  (42)

The squaring of $N$-vectors is meant to be coordinate-wise. Formula (42) is not a new estimator of asymptotic variance; rather, it is an algebraically equivalent re-expression of the diagonal elements of $\hat{A}V_{sand}$ in (22) above: $\hat{A}V_{sand}^{(j)} = (\hat{A}V_{sand})_{j,j}$. The sandwich standard error estimate (23) can therefore be written as follows:

$$\hat{SE}_{sand}(\hat{\beta}_j) = \frac{\langle (Y - \bar{X} \hat{\beta})^2, X_{j*}^2 \rangle^{1/2}}{\|X_{j*}\|^2}.$$  (43)

The usual standard error estimate from linear models theory is (33):

$$\hat{SE}_{lin}(\hat{\beta}_j) = \frac{\hat{\sigma}}{\|X_{j*}\|} = \frac{\|Y - X \hat{\beta}\|}{(N-p-1)^{1/2} \|X_{j*}\|}.$$  (44)

In order to translate $RAV_j[m^2(\bar{X})]$ into a practically useful diagnostic, an obvious first attempt would be forming the ratio $\hat{SE}_{sand}(\hat{\beta}_j)/\hat{SE}_{lin}(\hat{\beta}_j)$, squared. However, $\hat{SE}_{lin}(\hat{\beta}_j)$ has been corrected for fitted degrees of freedom, whereas $\hat{SE}_{sand}(\hat{\beta}_j)$ has not. For greater comparability one would either correct the sandwich estimator with a factor $(N/(N-p-1))^{1/2}$ (MacKinnon and White 1985) or else “uncorrect” $\hat{SE}_{lin}(\hat{\beta}_j)$ by replacing $N-p-1$ with $N$ in the variance estimate $\hat{\sigma}^2$. Either way one obtains the natural plug-in estimate of $RAV_j$:

$$RAV_j := N \frac{\langle (Y - X \hat{\beta})^2, X_{j*}^2 \rangle}{\|Y - X \hat{\beta}\|^2 \|X_{j*}\|^2} = \frac{\hat{E}[(Y - \bar{X}^T \hat{\beta})^2 X_{j*}^2]}{\hat{E}[(Y - \bar{X}^T \hat{\beta})^2] \hat{E}[X_{j*}^2]},$$  (45)

This diagnostic quantity can be used as a test statistic, as will be shown next.

9.2 A $RAV_j$ Test

There exist several ways to generate inference based on the $RAV_j$, three of which we discuss in this section. We start with an asymptotic result that can be used for retention intervals under a null
hypothesis of well-specification.

**Proposition:** If the total deviations \( \delta_i \) are independent of \( \tilde{X}_i \) (not assuming normality of \( \delta_i \)) we have:

\[
N^{1/2} (R\hat{AV}_j - 1) \overset{D}{\rightarrow} N\left(0, \frac{E[\delta^4]}{E[\delta^2]^2} \frac{E[X_{j*}^4]}{E[X_{j*}^2]^2} - 1\right)
\]

If one assumes \( \delta_i \sim N(0, \sigma^2) \), then the asymptotic variance simplifies using \( E[\delta^4]/E[\delta^2]^2 = 3 \).

As always we ignore moment conditions among the assumptions. A proof outline is in Appendix B.5.

According to (46) it is the kurtoses (= the standardized fourth moments - 3) of the error \( \delta \) and of the adjusted predictor \( X_{j*} \) that drive the asymptotic variance of \( R\hat{AV}_j \) under the null hypothesis. We note:

**Fact 1:** Because standardized fourth moments are always \( \geq 1 \) by Jensen’s inequality, the asymptotic variance is \( \geq 0 \), as it should be. The minimal standardized fourth moment of +1 is attained by a two-point distribution symmetric about 0. Thus a zero asymptotic variance of \( R\hat{AV}_j \) is achieved when both the error distribution and the adjusted predictor distribution are two-point masses.

**Fact 2:** The larger the kurtosis of \( \delta \) or \( X_{j*} \), the less likely it is that first and second order model misspecification can be detected because the larger the asymptotic standard errors will be. It is an important fact that elevated kurtosis of \( \delta \) and \( X_{j*} \) obscures nonlinearity and heteroskedasticity. Yet, if such misspecification can be detected in spite of elevated kurtoses, it is news worth knowing.

**Fact 3:** A test of the stronger hypothesis that includes normality of \( \delta \) is obtained by setting \( E[\delta^4]/E[\delta^2]^2 = 3 \) rather than estimating it. However, the resulting test turns into a non-normality test much of the time. As non-normality can be diagnosed separately with normality tests or normal quantile plots of the residuals, we recommend keeping normality out of the null hypothesis and test independence of \( \delta \) and \( X_{j*} \) alone.

The asymptotic result of the proposition provides insights, but unfortunately it is in our experience not suitable for practical application. The standard procedure would be to estimate the asymptotic null variance of \( R\hat{AV}_j \) and use it to form a retention interval around the null value \( RAV_j = 1 \). The problem is that the null distribution of \( R\hat{AV}_j \) in finite datasets can be non-normal in such a way that is not easily overcome by obvious tools such as logarithmic transformations.

Not all is lost, however, because non-asymptotic simulation-based approaches to inference exist for the type of null hypothesis in question. Because the null hypothesis is independence between the total deviation \( \delta \) and the adjusted predictor \( X_{j*} \), a permutation test offers itself. To this end it is necessary that \( N \gg p \), and the test will not be exact. The reason is that one needs to estimate the total deviations \( \delta_i \) with residuals \( r_i \) and the population adjusted predictor values \( X_{i,j*} \) with sample adjusted predictor values \( X_{i,j*} \). This test is for the weak hypothesis that does not include normality.
of $\delta_i$ and therefore permits general (centered) error distributions. A retention interval should be formed directly from the $\alpha/2$ and $1-\alpha/2$ quantiles of the permutation distribution. Quantile-based intervals can be asymmetric according to the skewness and other idiosyncrasies of the permutation distribution. Computations inside the permutation simulation are cheap: Once standardized squared vectors $r_j^2/\|r_j\|^2$ and $X_j^\varepsilon/\|X_j^\varepsilon\|^2$ are formed, a draw from the conditional null distribution of $\hat{\delta}_{AV_j}$ is obtained by randomly permuting one of the vectors and forming the inner product with the other vector. Finally, the approximate permutation distributions can be readily used to diagnose the non-normality of the conditional null using normal quantile plots (see Appendix C for examples).

Tables 3 and 4 show the results for the two datasets of Section 2. Values of $\hat{\delta}_{AV_j}$ that fall outside the middle 95% range of their permutation null distributions are marked with "*".

### Table 3: Permutation Inference for $\hat{\beta}_{AV_j}$ in the LA Homeless Data (10,000 permutations).

|           | $\hat{\beta}_{AV_j}$ | $SE_{lin}$ | $SE_{sand}$ | $\hat{\beta}_{AV_j}$ | 2.5% Perm. | 97.5% Perm. |
|-----------|------------------------|------------|-------------|------------------------|------------|-------------|
| Intercept | 0.760                  | 22.767     | 16.209      | 0.495*                 | 0.567      | 3.228       |
| MedianInc (1000) | -0.183               | 0.187      | 0.108       | 0.318*                 | 0.440      | 5.205       |
| PercVacant | 4.629                 | 0.901      | 1.363       | 2.071                  | 0.476      | 3.852       |
| PercMinority | 0.123                | 0.176      | 0.164       | 0.860                  | 0.647      | 2.349       |
| PercResidential | -0.050              | 0.171      | 0.111       | 0.406*                 | 0.568      | 3.069       |
| PercCommercial | 0.737                | 0.273      | 0.397       | 2.046                  | 0.578      | 2.924       |
| PercIndustrial | 0.905                | 0.321      | 0.592       | 3.289*                 | 0.528      | 3.252       |

### Table 4: Permutation Inference for $\hat{\delta}_{AV_j}$ in the Boston Housing Data (10,000 permutations).

|           | $\hat{\beta}_{AV_j}$ | $SE_{lin}$ | $SE_{sand}$ | $\hat{\beta}_{AV_j}$ | 2.5% Perm. | 97.5% Perm. |
|-----------|------------------------|------------|-------------|------------------------|------------|-------------|
| CRIM      | -0.108                 | 0.033      | 0.031       | 0.776                  | 0.511      | 3.757       |
| ZN        | 0.046                  | 0.014      | 0.014       | 1.006                  | 0.820      | 1.680       |
| INDUS     | 0.021                  | 0.061      | 0.051       | 0.671*                 | 0.805      | 1.957       |
| CHAS      | 2.687                  | 0.862      | 1.310       | 2.255*                 | 0.722      | 1.905       |
| NOX       | -17.767                | 3.820      | 3.827       | 0.982                  | 0.848      | 1.556       |
| RM        | 3.810                  | 0.418      | 0.861       | 4.087*                 | 0.793      | 1.816       |
| AGE       | 0.001                  | 0.013      | 0.017       | 1.553*                 | 0.860      | 1.470       |
| DIS       | -1.476                 | 0.199      | 0.217       | 1.159                  | 0.852      | 1.533       |
| RAD       | 0.306                  | 0.066      | 0.062       | 0.857                  | 0.830      | 1.987       |
| TAX       | -0.012                 | 0.004      | 0.003       | 0.512*                 | 0.767      | 1.998       |
| PTRATIOD  | -0.953                 | 0.131      | 0.118       | 0.806*                 | 0.872      | 1.402       |
| B         | 0.009                  | 0.003      | 0.003       | 0.995                  | 0.786      | 1.762       |
| LSTAT     | -0.525                 | 0.051      | 0.101       | 3.861*                 | 0.803      | 1.798       |

10 The Meaning of Regression Slopes in the Presence of Nonlinearity

An objection against using linear fits in the presence of nonlinearities is that slopes lose their common interpretation: no longer is $\beta_j$ the average difference in $Y$ associated with a unit difference in $X_j$
at fixed levels of all other \(X_k\). Yet, there exists a simple alternative interpretation that is valid and intuitive even in the presence of nonlinearities, both for the parameters of the population and their estimates from samples: slopes are weighted averages of case-wise slopes or pairwise slopes. This holds for simple linear regression and also for multiple linear regression for each predictor after linearly adjusting it for all other predictors. This is made precise as follows:

- **Sample estimates:** In a multiple regression based on a sample of size \(N\), consider the LS estimate \(\hat{\beta}_j\): this is the empirical simple regression slope through the origin with regard to the empirically adjusted predictor \(X_j^\bullet\) (for \(j \neq 0\) as we only consider actual slopes, not the intercept, but assume the presence of an intercept). To simplify notation we write \((x_1, ..., x_N)^T\) for \(X_j^\bullet\), as well as \((y_1, ..., y_N)^T\) for the response vector \(Y\) and \(\hat{\beta}\) for the LS estimate \(\hat{\beta}_j\). Then the representation of \(\hat{\beta}\) as a weighted average of case-wise slopes is

\[
\hat{\beta} = \sum_i w_i b_i, \quad \text{where} \quad b_i := \frac{y_i}{x_i} \quad \text{and} \quad w_i := \frac{x_i^2}{\sum_i x_i'^2}, \quad (47)
\]

are case-wise slopes and weights, respectively.

The representation of \(\hat{\beta}\) as a weighted average of pairwise slopes is

\[
\hat{\beta} = \sum_{ik} w_{ik} b_{ik}, \quad \text{where} \quad b_{ik} := \frac{y_i - y_k}{x_i - x_k} \quad \text{and} \quad w_{ik} := \frac{(x_i - x_k)^2}{\sum_{i'k'} (x_{i'} - x_{k'})^2}, \quad (48)
\]

are pairwise slopes and weights, respectively. The summations can be over \(i \neq k\) or \(i < k\). See Figure 8 for an illustration.

- **Population parameters:** In a population multiple regression, consider the slope parameter \(\beta_j\) of the predictor variable \(X_j\). It is also the simple regression slope through the origin with regard to the population-adjusted predictor \(X_j^\bullet\), where again we consider only actual slopes, \(j \neq 0\), but assume the presence of an intercept. We now write \(X\) instead of \(X_j^\bullet\) and \(\beta\) instead of \(\beta_j\). The population regression is thus reduced to a simple regression through the origin.

The representation of \(\beta\) as a weighted average of case-wise slopes is

\[
\beta = \mathbb{E}[WB], \quad \text{where} \quad B := \frac{Y}{X} \quad \text{and} \quad W := \frac{X^2}{\mathbb{E}[X^2]}
\]

are case-wise slopes and case-wise weights, respectively.

For the representation of \(\beta\) as a weighted average of pairwise slopes we need two independent copies \((X, Y)\) and \((X', Y')\) of the predictor and response:

\[
\beta = \mathbb{E}[WB] \quad \text{where} \quad B := \frac{Y - Y'}{X - X'} \quad \text{and} \quad W := \frac{(X - X')^2}{\mathbb{E}[(X - X')^2]}
\]

are pairwise slopes and weights, respectively.

These formulas provide intuitive interpretations of regression slopes that are valid without the first order assumption of linearity of the response as a function of the predictors. They support the
Figure 8: Case-wise and pairwise average weighted slopes illustrated: Both plots show the same six points (the “cases”) as well as the LS line fitted to them (fat gray). The left hand plot shows the case-wise slopes from the mean point (open circle) to the six cases, while the right hand plot shows the pairwise slopes between all 15 pairs of cases. The LS slope is a weighted average of the case-wise slopes on the left according to (47), and of the pairwise slopes on the right according to (48).

intuition that, even in the presence of a nonlinearity, a linear fit can be used to infer the overall direction of the association between the response and the predictors.

The above formulas were used and modified to produce alternative slope estimates by Gelman and Park (2008), also with the “Goal of Expressing Regressions as Comparisons that can be Understood by the General Reader” (see their Sections 1.2 and 2.2). Earlier, Wu (1986) used generalizations from pairs to tuples of size \( r \geq p+1 \) for the analysis of jackknife and bootstrap procedures (see his Section 3, Theorem 1). The formulas have a history in which Stigler (2001) includes Edgeworth, while Berman (1988) traces it back to a 1841 article by Jacobi written in Latin.

11 Summary

In this article we compared statistical inference from classical linear models theory with inference from econometric theory. The major differences are that the former is a finite-sample theory that relies on strong assumptions and treats the predictors as fixed even when they are random, whereas the latter uses asymptotic theory that relies on few assumptions and treats the predictors as random. On a practical level, inferences differ in the type of standard error estimates they use: linear models theory is based on the “usual” standard error which is a scaled version of the error standard deviation,
whereas econometric theory is based on the so-called “sandwich estimator” of standard error which derives from an assumption-lean asymptotic variance. In comparing and contrasting the two modes of statistical inference we observe the following:

- As econometric theory does not assume the correctness of the linearity and homoskedasticity assumptions of linear models theory, a new interpretation of the targets of estimation is needed: Linear fits estimate the best linear approximation to a usually nonlinear response surface.

- If statisticians are willing to buy into this semi-parametric view of linear regression, they will accept sandwich-based inference as asymptotically correct. — If they are unwilling to go down this route, they must have strong belief in the correctness of their models and/or rely on diagnostic methodology to ascertain that linearity and homoskedasticity assumptions are not violated in ways that affect “usual” statistical inference.

- While regression is rich in model diagnostics, a more targeted approach in this case may be based on misspecification tests which are well-established in econometrics. We described one such test which permits testing the adequacy of the linear models standard error, one coefficient at a time.

- The discrepancies between standard errors from assumption-rich linear models theory and assumption-lean econometric theory can be of arbitrary magnitude in the asymptotic limit, but real data examples indicate discrepancies by a factors of 2 to be common. This is obviously relevant because such factors can change a t-statistic from significant to insignificant and vice versa.

- The pairs bootstrap is seen to be an alternative to the sandwich estimate of standard error. The latter is the asymptotic limit in the $M$-of-$N$ bootstrap as $M \rightarrow \infty$.

Assumption lean inference is not without its problems. A major issue is its non-robustness: compared to the standard error from linear models theory the sandwich standard error relies on higher order moments. The non-robustness is fundamentally a consequence of the LS method, which may suggest that solutions should be obtained through a revival of robustness theory.
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A Ancillarity

The facts as layed out in Section 4 amount to an argument against conditioning on predictors in regression. The justification for conditioning derives from an ancillarity argument according to which the predictors, if random, form an ancillary statistic for the linear model parameters $\beta$ and $\sigma^2$, hence conditioning on $X$ produces valid frequentist inference for these parameters (Cox and Hinkley 1974, Example 2.27). Indeed, with a suitably general definition of ancillarity, it can be shown that in any regression model the predictors form an ancillary. To see this we need an extended definition of ancillarity that includes nuisance parameters. The ingredients and conditions are as follows:

1. $\theta = (\psi, \lambda)$: the parameters, where $\psi$ is of interest and $\lambda$ is nuisance;
2. $S = (T, A)$: a sufficient statistic with values $(t, a)$;
3. $p(t, a; \psi, \lambda) = p(t | a; \psi) p(a; \lambda)$: the condition that makes $A$ an ancillary.

We say that the statistic $A$ is ancillary for the parameter of interest, $\psi$, in the presence of the nuisance parameter, $\lambda$. Condition (3) can be interpreted as saying that the distribution of $T$ is a mixture with mixing distribution $p(a | \lambda)$. More importantly, for a fixed but unknown value $\lambda$ and two values $\psi_1, \psi_0$, the likelihood ratio

$$\frac{p(t, a; \psi_1, \lambda)}{p(t, a; \psi_0, \lambda)} = \frac{p(t | a; \psi_1)}{p(t | a; \psi_0)}$$

has the nuisance parameter $\lambda$ eliminated, justifying the conditionality principle according to which valid inference for $\psi$ can be obtained by conditioning on $A$.

When applied to regression, the principle implies that in any regression model the predictors, when random, are ancillary and hence can be conditioned on:

$$p(y, X; \theta) = p(y | X; \theta) p_X(X),$$

where $X$ acts as the ancillary $A$ and $p_X$ as the mixing distribution $p(a | \lambda)$ with a “nonparametric” nuisance parameter that allows largely arbitrary distributions for the predictors. (The predictor distribution should grant identifiability of $\theta$ in general, and non-collinearity in linear models in particular.) The literature does not seem to be rich in crisp definitions of ancillarity, but see, for example, Cox and Hinkley (1974, p.32-33). For the interesting history of ancillarity see the articles by Stigler (2001) and Aldrich (2005).

As explained in Section 4, the problem with the ancillarity argument is that it holds only when the regression model is correct. In practice, whether models are correct is never known.
\section*{B Proofs}

\subsection*{B.1 Proof of the Lemma in Section 3.4}

- Error $\epsilon$: Assuming constancy of the conditional distribution we obtain independence of the errors as follows:

\[ E[f(\epsilon)g(\tilde{X})] = E[E[f(\epsilon)|\tilde{X}]g(\tilde{X})] = E[E[f(\epsilon)]g(\tilde{X})] = E[f(\epsilon)]E[g(\tilde{X})] \]

Conversely, if the conditional distribution of the errors is not constant, there exists $f(\epsilon)$ such that $E[f(\epsilon)|\tilde{X}] > E[f(\epsilon)]$ for $\tilde{X} \in A$ for some $A$ with $P[A] > 0$. Let $g(\tilde{X}) = 1_A(\tilde{X})$, and it follows $E[f(\epsilon)g(\tilde{X})] > E[f(\epsilon)]E[g(\tilde{X})]$.

- Nonlinearity $\eta$: The conditional distribution of $\eta$ given $\tilde{X}$ is a point mass. The same argument as for errors applies, but restricted to point masses. Because $E[\eta] = 0$ (due to the presence of an intercept) the point masses must be at zero.

- Total deviation $\delta = \epsilon + \eta$: Again, the conditional distribution must be identical across predictor space, which results in both of the previous cases.

\subsection*{B.2 Proofs of the Proposition in Section 4}

The linear case is trivial: if $\mu_0(\tilde{X})$ is linear, that is, $\mu_0(\tilde{x}) = \beta^T \tilde{x}$ for some $\beta$, then $\beta(P) = \beta$ irrespective of $P(d\tilde{x})$ according to (13). The nonlinear case is proved as follows: For any set of points $\tilde{x}_1, ... \tilde{x}_{p+1} \in \mathbb{R}^{p+1}$ in general position and with 1 in the first coordinate, there exists a unique linear function $\beta^T \tilde{x}$ through the values of $\mu_0(\tilde{x}_i)$. Define $P(d\tilde{x})$ by putting mass $1/(p+1)$ on each point; define the conditional distribution $P(dy|\tilde{x}_i)$ as a point mass at $y = \mu_0(\tilde{x}_i)$; this defines $P$ such that $\beta(P) = \beta$. Now, if $\mu_0(\cdot)$ is nonlinear, there exist two such sets of points with differing linear functions $\beta_1^T \tilde{x}$ and $\beta_2^T \tilde{x}$ to match the values of $\mu_0(\cdot)$ on these two sets; by following the preceding construction we obtain $P_1$ and $P_2$ such that $\beta(P_1) = \beta_1 \neq \beta_2 = \beta(P_2)$.

\subsection*{B.3 Proof of the Proposition of Section 8.5}

An important difference between $\eta^2(\tilde{X})$ and $\sigma^2(\tilde{X})$ is that nonlinearities are constrained by orthogonalities to the predictors, whereas conditional error variances are not.

Consider first nonlinearities $\eta(\tilde{X})$: We construct a one-parameter family of nonlinearities $\eta_k(\tilde{X})$ for which $\sup_k \text{RAV}_j[\eta_k^2] = \infty$ and $\inf_k \text{RAV}_j[\eta_k^2] = 0$. Generally in the construction of examples, it must be kept in mind that nonlinearities are orthogonal to (adjusted for) all other predictors: $E[\eta(\tilde{X})\tilde{X}] = 0$. To avoid uninsightful complications arising from adjustment due to complex dependencies among the predictors, we construct an example for simple linear regression with a single predictor $X_1 = X$ and an intercept $X_0 = 1$. W.l.o.g. we will further assume that $X_1$ is centered (population adjusted for $X_0$, so that $X_{1a} = X_1$) and standardized. In what follows we write $X$ instead of $X_1$, and the assumptions are $E[X] = 0$ and $E[X^2] = 1.$


**Proposition:** Define a one-parameter family of nonlinearities as follows:

\[
\eta_t(X) = \frac{1_{|X|>t} - p(t)}{\sqrt{p(t)(1 - p(t))}}, \quad \text{where} \quad p(t) := P[|X| > t]. \tag{49}
\]

We assume that \(p(t) > 0 \ \forall t > 0\). (We have \(1 - p(t) > 0\) for sufficiently large \(t\).) Assume further that the distribution of \(X\) is symmetric about 0, so that \(E[\eta_t(X)X] = 0\). Then we have:

\[
\lim_{t \to \infty} RAV[\eta_t^2] = \infty;
\]

\[
\lim_{t \downarrow 0} RAV[\eta_t^2] = 0 \quad \text{if the distribution of } X \text{ has no atom at the origin: } P[X = 0] = 0.
\]

By construction these nonlinearities are centered and standardized, \(E[\eta_t(X)] = 0\) and \(E[\eta_t(X)^2] = 1\). They are also orthogonal to \(X\), \(E[\eta_t(X)X] = 0\), due to the assumed symmetry of the distribution of \(X\), \(P[X > t] = P[X < -t]\), and the symmetry of the nonlinearities, \(\eta_t(-X) = \eta_t(X)\).

Consider next heteroskedastic error variances \(\sigma^2_t(X)\): The above construction for nonlinearities can be re-used. As with nonlinearities, for \(RAV[\sigma^2_t(X)]\) to rise with no bound, the conditional error variance \(\sigma^2_t(X)\) needs to place its large values in the unbounded tail of the distribution of \(X\). For \(RAV[\sigma^2_t(X)]\) to reach down to zero, \(\sigma^2_t(X)\) needs to place its large values in the center of the distribution of \(X\).

**Proposition:** Define a one-parameter family of heteroskedastic error variances as follows:

\[
\sigma^2_t(X) = \frac{(1_{|X|>t} - p(t))^2}{p(t)(1 - p(t))}, \quad \text{where} \quad p(t) = P[|X| > t], \tag{50}
\]

and we assume that \(p(t) > 0\) and \(1 - p(t) > 0 \ \forall t > 0\). Then we have:

\[
\lim_{t \to \infty} RAV[\sigma^2_t] = \infty;
\]

\[
\lim_{t \downarrow 0} RAV[\sigma^2_t] = 0 \quad \text{if the distribution of } X \text{ has no atom at the origin: } P[X = 0] = 0.
\]
We abbreviate $\bar{p}(t) = 1 - p(t)$ in what follows.

\[
\begin{align*}
\text{RAV}[\eta] &= \mathbb{E} [\eta(X)^2 X^2] \\
&= \frac{1}{p(t)\bar{p}(t)} \mathbb{E} \left[ (1_{|X| > t} - \bar{p}(t))^2 X^2 \right] \\
&= \frac{1}{p(t)\bar{p}(t)} \mathbb{E} \left[ (1_{|X| > t} - 2 \cdot 1_{|X| > t} p(t) + p(t)^2) X^2 \right] \\
&= \frac{1}{p(t)\bar{p}(t)} \mathbb{E} \left[ (1_{|X| > t}) (1 - 2 p(t)) + p(t)^2) X^2 \right] \\
&= \frac{1}{p(t)\bar{p}(t)} \left( \mathbb{E} \left[ 1_{|X| > t} X^2 \right] (1 - 2 p(t)) + p(t)^2) \right) \\
&\geq \frac{1}{p(t)\bar{p}(t)} (p(t) t^2 (1 - 2 p(t)) + p(t)^2) \quad \text{for } p(t) \leq \frac{1}{2} \\
&= \frac{1}{p(t)} \left( t^2 (1 - 2 \bar{p}(t)) + \bar{p}(t) \right) \\
&\geq t^2 (1 - \bar{p}(t)) + \bar{p}(t) \sim t^2 \quad \text{as } t \uparrow \infty.
\end{align*}
\]

For the following we note $1_{|X| > t} - p(t) = -1_{|X| \leq t} + \bar{p}(t)$:

\[
\begin{align*}
\text{RAV}[\eta] &= \mathbb{E} [\eta(X)^2 X^2] \\
&= \frac{1}{p(t)\bar{p}(t)} \mathbb{E} \left[ (1_{|X| \leq t} - \bar{p}(t))^2 X^2 \right] \\
&= \frac{1}{p(t)\bar{p}(t)} \mathbb{E} \left[ (1_{|X| \leq t} - 2 \cdot 1_{|X| \leq t} \bar{p}(t) + \bar{p}(t)^2) X^2 \right] \\
&= \frac{1}{p(t)\bar{p}(t)} \mathbb{E} \left[ (1_{|X| \leq t}) (1 - 2 \bar{p}(t)) + \bar{p}(t)^2) X^2 \right] \\
&= \frac{1}{p(t)\bar{p}(t)} \left( \mathbb{E} \left[ 1_{|X| \leq t} X^2 \right] (1 - 2 \bar{p}(t)) + \bar{p}(t)^2) \right) \\
&\leq \frac{1}{p(t)\bar{p}(t)} (\bar{p}(t) t^2 (1 - 2 \bar{p}(t)) + \bar{p}(t)^2) \quad \text{for } \bar{p}(t) \leq \frac{1}{2} \\
&= \frac{1}{p(t)} \left( t^2 (1 - 2 \bar{p}(t)) + \bar{p}(t) \right) \\
&\sim t^2 + \bar{p}(t) \quad \text{as } t \downarrow 0,
\end{align*}
\]

assuming $\bar{p}(0) = P[X = 0] = 0$.

### B.4 Details for Figure 5

We write $X$ instead of $X_j$, and assume it has a standard normal distribution, $X \sim N(0, 1)$, whose density will be denoted by $\phi(x)$. In Figure 5 the base function is, up to scale, as follows:

\[
f(x) = \exp \left( -\frac{t}{2} \frac{x^2}{2} \right), \quad t > -1.
\]
The second equality on each line holds under the null hypothesis of independent \( \delta \). Conveniently, \( f(x)\phi(x) \) and \( f^2(x)\phi(x) \) are both normal densities (up to normalization) for \( t > -1 \):

\[
\begin{align*}
  f(x)\phi(x) &= s_1 \phi_{s_1}(x), & s_1 &= (1 + t/2)^{-1/2}, \\
  f^2(x)\phi(x) &= s_2 \phi_{s_2}(x), & s_2 &= (1 + t)^{-1/2},
\end{align*}
\]

where we write \( \phi_s(x) = \phi(x/s)/s \) for scaled normal densities. Accordingly we obtain the following moments:

\[
\begin{align*}
  E[f(X)] &= s_1 E[1|N(0,s_1^2)] = s_1 = (1 + t/2)^{-1/2}, \\
  E[f(X)X^2] &= s_1 E[X^2|N(0,s_1^2)] = s_1^3 = (1 + t/2)^{-3/2}, \\
  E[f^2(X)] &= s_2 E[1|N(0,s_2^2)] = s_2 = (1 + t)^{-1/2}, \\
  E[f^2(X)X^2] &= s_2 E[X^2|N(0,s_2^2)] = s_2^3 = (1 + t)^{-3/2},
\end{align*}
\]

and hence

\[
RAV[f^2(X)] = \frac{E[f^2(X)X^2]}{E[f^2(X)]E[X^2]} = s_2^2 = (1 + t)^{-1}
\]

Figure 5 shows the functions as follows: \( f(x)^2/E[f^2(X)] = f(x)^2/s_2 \).

### B.5 Proof of Asymptotic Normality of \( \hat{RAV}_j \), Section 9

We recall (45) for reference in the following form:

\[
RAV_j = \frac{1}{N} \langle (Y - X\hat{\beta})^2, X_j^* \rangle.
\]

For the denominators it is easy to show that

\[
\frac{1}{N} \| Y - X\hat{\beta} \|^2 \xrightarrow{P} E[\delta^2], \\
\frac{1}{N} \| X_j^* \|^2 \xrightarrow{P} E[X_j^*^2].
\]

For the numerator a CLT holds based on

\[
\frac{1}{N^{1/2}} \langle (Y - X\hat{\beta})^2, X_j^* \rangle = \frac{1}{N^{1/2}} \langle (Y - X\beta)^2, X_j^* \rangle + O_P(N^{-1/2}).
\]

For a proof outline see Details below. It is therefore sufficient to show asymptotic normality of \( \langle \delta^2, X_j^*^2 \rangle \). Here are first and second moments:

\[
\begin{align*}
  E[\frac{1}{N} \langle \delta^2, X_j^*^2 \rangle] &= E[\delta^2 X_j^*^2] = E[\delta^2] E[X_j^*^2], \\
  V[\frac{1}{N^{1/2}} \langle \delta^2, X_j^*^2 \rangle] &= E[\delta^4 X_j^*^4] - E[\delta^2 X_j^*^2]^2 = E[\delta^4] E[X_j^*^4] - E[\delta^2]^2 E[X_j^*^2]^2.
\end{align*}
\]

The second equality on each line holds under the null hypothesis of independent \( \delta \) and \( \hat{X} \). For the variance one observes that we assume that \( \{(Y_i, X_i)\}_{i=1...N} \) to be i.i.d. sampled pairs, hence \( \{(\delta_i, X_{ij}^*^2)\}_{i=1...N} \) are i.i.d. sampled pairs as well. Using the denominator terms (52) and Slutsky’s theorem, we arrive at the first version of the CLT for \( \hat{RAV}_j \):

\[
N^{1/2} (\hat{RAV}_j - 1) \xrightarrow{D} \mathcal{N} \left( 0, \frac{E[\delta^2]}{E[\delta^2]^2} \frac{E[X_j^*^4]}{E[X_j^*^2]^2} - 1 \right)
\]
With the additional null assumption of normal errors we have \( E[\delta^4] = 3E[\delta^2]^2 \), and hence the second version of the CLT for \( \mathbf{RAV}_j \):

\[
N^{1/2}(\mathbf{RAV}_j - 1) \xrightarrow{D} \mathcal{N}\left(0, \frac{E[X_{\mathbf{j}}^4]}{E[X_{\mathbf{j}}^2]^2} - 1\right).
\]

Details for the numerator (53), using notation of Sections 7.1 and 7.2, in particular \( X_{\mathbf{j}} = X_j - X_j \beta_{\mathbf{j}} \) and \( X_{\mathbf{j}} = X_j - X_j \hat{\beta}_{\mathbf{j}} \):

\[
\left\langle (Y - X \hat{\beta})^2, X_{\mathbf{j}}^2 \right\rangle = \left\langle (Y - X \beta - X(X\hat{\beta} - \beta))^2, (X_{\mathbf{j}} - X_j(\hat{\beta}_{\mathbf{j}} - \beta_{\mathbf{j}}))^2 \right\rangle \\
= \left\langle \delta^2 + (X(\hat{\beta} - \beta))^2 - 2 \delta (X(\hat{\beta} - \beta)), X_{\mathbf{j}}^2 + (X_j(\hat{\beta}_{\mathbf{j}} - \beta_{\mathbf{j}}))^2 - 2 X_{\mathbf{j}}(X_j(\hat{\beta}_{\mathbf{j}} - \beta_{\mathbf{j}})) \right\rangle \\
= \left\langle \delta^2, X_{\mathbf{j}}^2 \right\rangle + \ldots
\]

Among the 8 terms in “...”, each contains at least one subterm of the form \( \hat{\beta} - \beta \) or \( \hat{\beta}_{\mathbf{j}} - \beta_{\mathbf{j}} \), each being of order \( O_P(N^{-1/2}) \). We first treat the terms with just one of these subterms to first power, of which there are only two, normalized by \( N^{1/2} \):

\[
\frac{1}{N^{1/2}} \left\langle -2 \delta (X(\hat{\beta} - \beta)), X_{\mathbf{j}}^2 \right\rangle = -2 \sum_{k=0}^{m} \left( \frac{1}{N^{1/2}} \sum_{i=1}^{m} \delta_i X_{i,k} X_{i,j} \right) (\hat{\beta}_j - \beta_j) \\
= \sum_{k=0}^{m} O_P(1) O_P(N^{-1/2}) = O_P(N^{-1/2}),
\]

\[
\frac{1}{N^{1/2}} \left\langle \delta^2, -2 X_{\mathbf{j}}(X_j(\hat{\beta}_{\mathbf{j}} - \beta_{\mathbf{j}})) \right\rangle = -2 \sum_{k \neq j} \left( \frac{1}{N^{1/2}} \sum_{i=1}^{m} \delta_i^2 X_{i,j} X_{i,k} \right) (\hat{\beta}_{\mathbf{j},k} - \beta_{\mathbf{j},k}) \\
= \sum_{k \neq j} O_P(1) O_P(N^{-1/2}) = O_P(N^{-1/2}).
\]

The terms in the big parens are \( O_P(1) \) because they are asymptotically normal. This is so because they are centered under the null hypothesis that \( \delta_i \) is independent of the predictors \( \mathbf{X}_i \): In the first term we have

\[
E[\delta_i X_{i,k} X_{i,j}] = E[\delta_i] E[X_{i,k} X_{i,j}] = 0
\]
due to \( E[\delta_i] = 0 \). In the second term we have

\[
E[\delta_i^2 X_{i,j} X_{i,k}] = E[\delta_i^2] E[X_{i,j} X_{i,k}] = 0
\]
due to \( E[X_{i,j} X_{i,k}] = 0 \) as \( k \neq j \).

We proceed to the 6 terms in (54) that contain at least two \( \beta \)-subterms or one \( \beta \)-subterm squared. For brevity we treat one term in detail and assume that the reader will be convinced that the other 5 terms can be dealt with similarly. Here is one such term, again scaled for CLT purposes:

\[
\frac{1}{N^{1/2}} \left\langle (X(\hat{\beta} - \beta))^2, X_j^2 \right\rangle = \sum_{k,l=0}^{m} \left( \frac{1}{N} \sum_{i=1}^{m} X_{i,k} X_{i,l} X_{i,j}^2 \right) N^{1/2} (\hat{\beta}_k - \beta_k)(\hat{\beta}_l - \beta_l) \\
= \sum_{k,l=0}^{m} \text{const} \cdot O_P(1) O_P(N^{-1/2}) = O_P(N^{-1/2}).
\]

The term in the parenthesis converges in probability to \( E[X_{i,k} X_{i,l} X_{i,j}^2] \), accounting for “\( \text{const} \)”; the term \( N^{1/2} (\hat{\beta}_k - \beta_k) \) is asymptotically normal and hence \( O_P(1) \); and the term \( (\hat{\beta}_l - \beta_l) \) is \( O_P(N^{-1/2}) \) due to its CLT.
Details for the denominator terms (52): It is sufficient to consider the first denominator term.

\[ \frac{1}{N} \| Y - X\hat{\beta} \|^2 = \frac{1}{N} Y^T (I - H) Y \]
\[ = \frac{1}{N} \left( \| Y \|^2 - Y^T H Y \right) \]
\[ = \frac{1}{N} \| Y \|^2 - \left( \frac{1}{N} \sum Y_i \bar{X}_i^T \right) \left( \frac{1}{N} \sum \bar{X}_i \bar{X}_i^T \right)^{-1} \left( \frac{1}{N} \sum \bar{X}_i Y_i \right) \]
\[ \overset{P}{\rightarrow} E[Y^2] - E[Y \bar{X}] E[\bar{X} \bar{X}^T]^{-1} E[\bar{X} Y] \]
\[ = E[Y^2] - E[Y \bar{X}^T \beta] \]
\[ = E[(Y - \bar{X}^T \beta)^2] \quad \text{due to} \quad E[(Y - \bar{X}^T \beta) \bar{X}] = 0 \]
\[ = E[\delta^2]. \]

The calculations are the same for the second denominator term, substituting \( X_j \) for \( Y \), \( X_{-j} \) for \( X \), \( \bar{X}_j \) for \( \delta \), and \( \beta_{-j} \) for \( \beta \).
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Figure 9: Permutations distributions of $\hat{RAV}_j$ for the LA Homeless Data

Figure 10: Permutations distributions of $\hat{RAV}_j$ for the Boston Housing Data