

Introduction of a new measure for detecting poor fit due to omitted nonlinear terms in SEM

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Abstract The model chi-square that is used in linear structural equation modeling compares the fitted covariance matrix of a target model to an unstructured covariance matrix to assess global fit. For models with nonlinear terms, i.e., interaction or quadratic terms, this comparison is very problematic because these models are not nested within the saturated model that is represented by the unstructured covariance matrix. We propose a novel measure that quantifies the heteroscedasticity of residuals in structural equation models. It is based on a comparison of the likelihood for the residuals under the assumption of heteroscedasticity with the likelihood under the assumption of homoscedasticity. The measure is designed to respond to omitted nonlinear terms in the structural part of the model that result in heteroscedastic residual scores. In a small Monte Carlo study, we demonstrate that the measure appears to detect omitted nonlinear terms reliably when falsely a linear model is analyzed and the omitted nonlinear terms account for substantial nonlinear effects. The results also indicate that the measure did not respond when the correct model or an overparameterized model were used.

Keywords Heteroscedasticity · Monte Carlo study · Nonlinear model · Structural equation modeling · Interaction effect · Quadratic effect

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1 Introduction

Over the last three decades, structural equation modeling (SEM) has become a popular statistical technique for modeling relationships between unobservable, latent variables. The structural relationships between such variables are typically formulated in linear model equations, and the latent variables are measured with errors by a measurement model that carries observable variables known as indicators. SEM has become available to a large community of researchers by the release of software packages for covariance structure analysis such as Amos (Arbuckle 1997), EQS (Bentler 1995; Bentler and Wu 1993), LISREL (Jöreskog and Sörbom 1993, 1996), or Mplus (Muthén and Muthén 2007).

While ordinary SEM incorporates linear relationships among latent variables, applied researchers sometimes wish to estimate an SEM with nonlinear terms in the latent variables, for example, models with latent interaction effects (cf. Barendse et al. 2010; Schermelleh-Engel et al. 2010) or quadratic effects. The model chi-square that is used in ordinary SEM compares the fitted covariance matrix or fitted mean vector of a target model to an unstructured covariance matrix or mean vector to assess global fit (cf. Jak et al. 2010 and King-Kallimanis et al. 2010 for evaluation of measurement bias in nested models using χ^2 difference tests; cf. Geiser et al. 2010 for evaluation of multitrait-multimethod change models). For structural equation models with nonlinear terms, this comparison is problematic because these models are not nested within the saturated model that is represented by the unstructured covariance matrix (Jöreskog and Yang 1996). For that reason, the assessment of the overall model fit for a nonlinear SEM has been an unresolved problem up to the present.

In this paper, we propose to use residual information to evaluate whether the structural part of a model is consistent with the data. Nonlinear terms that have been omitted in the structural part of a model result in residuals which contain nonlinear random terms. These nonlinear terms can cause the residual to be non-normally distributed and heteroscedastic. To illustrate this, consider two residual variables e_1 and e_2 given by

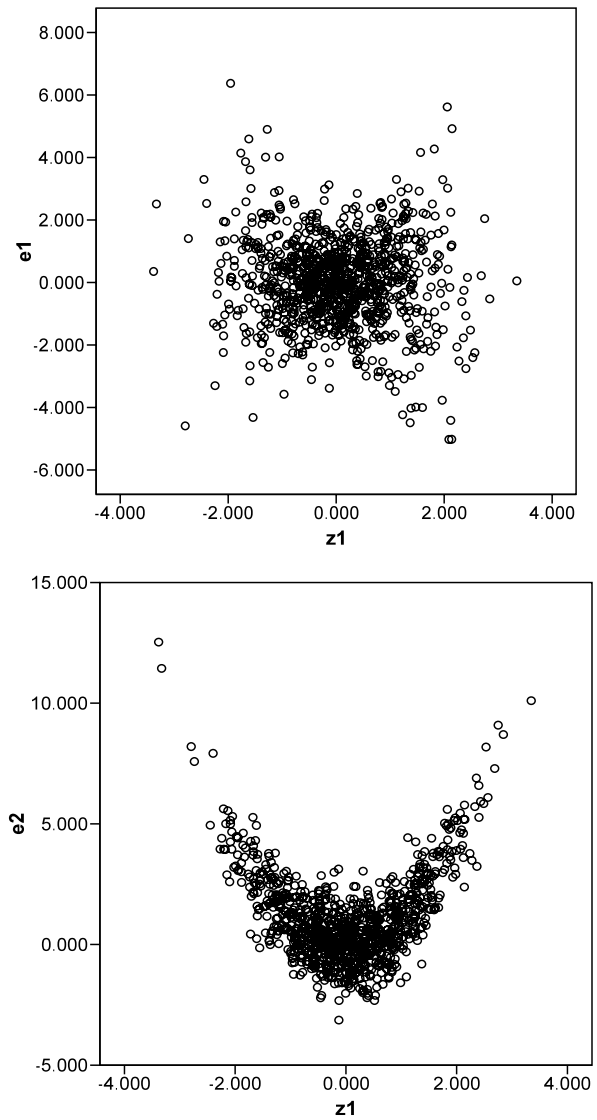
$$\begin{aligned} e_1 &= z_1 z_2 + z_3 \\ e_2 &= z_1^2 + z_3 - 1 \end{aligned} \quad (1)$$

where z_1, z_2, z_3 are mutually uncorrelated, standard normally distributed variables. Both residual variables have zero means: $E(e_1) = E(e_2) = 0$. For e_1 , there is deviation from normality because of the product term $z_1 z_2$, for e_2 there is deviation from normality because of the quadratic term z_1^2 . The variable e_1 is uncorrelated with both z_1 and z_2 , and the variable e_2 is uncorrelated with z_1 . If we draw random samples for e_1 and e_2 and plot each sample against z_1 , we obtain the following scatter plots as shown in Fig. 1.

In the first graph, the plot shows that the residual scores of e_1 are heteroscedastic, with the variances of the scores being larger the more z_1 deviates from zero. In the second graph, there is curvilinearity combined with some heteroscedasticity, with the variances of the residual scores being larger when z_1 is close to zero.

Klein and Moosbrugger (2000) developed the LMS (Latent Moderated Structural Equations) method that can handle SEM with nonlinear terms such as squares or

Fig. 1 Scatter plots for residuals with nonlinear model components



products of latent predictor variables. LMS is an ML estimation procedure and has been implemented in the commercial software package Mplus (Muthén and Muthén 2007). As is the standard for many types of statistical models and also for LMS, residual scores, that is, scores of disturbance terms and measurement errors, are assumed to be normally distributed and homoscedastic.

The idea of this paper is to construct a measure that can help detect a possible misfit of the structural part of the model by evaluating whether the residual scores are homoscedastic. In the following section, we will develop such a measure. It quantifies the degree of heteroscedasticity in order to detect hidden nonlinearity in a model structure.

2 A measure of heteroscedasticity for residual scores

In this section, we propose a measure Z_{het} that quantifies the heteroscedasticity of residuals. It is based on the comparison of the likelihood for the residuals under the assumption of heteroscedasticity with the likelihood for the residuals under the assumption of homoscedasticity. The measure is designed to respond to omitted nonlinear terms in the structural part of a model when these terms result in heteroscedastic residual scores.

We assume that residual scores e_1, \dots, e_n on a residual variable e are available, that is, one residual score for each case in the sample. When a model has been analyzed, such residual scores can often be readily computed from the model equations by using the estimated parameters, factor scores, and observed scores on the indicators. We further assume that the n residual scores have been sampled from n independent univariate normal distributions¹ with zero means but possibly different variances:

$$\begin{pmatrix} e_1 \\ \vdots \\ e_n \end{pmatrix} \sim N^* \left(\begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} \sigma_1^2 & & \\ & \ddots & \\ & & \sigma_n^2 \end{pmatrix} \right). \tag{2}$$

The distribution of the e_1, \dots, e_n is homoscedastic if the n variance parameters $\sigma_1^2, \dots, \sigma_n^2$ are all equal, and otherwise it is heteroscedastic. We first consider the log-likelihood LL_{hom} for the residual scores under the assumption of homoscedasticity. If $\sigma^2 = \sigma_1^2 = \dots = \sigma_n^2$ holds, the log-likelihood for the residuals is

$$LL_{\text{hom}} = -\frac{n}{2} \ln(2\pi) - \frac{n}{2} \ln(\hat{\sigma}^2) - \frac{n}{2}, \tag{3}$$

where $\hat{\sigma}^2$ is the ML estimate for the variance parameter for a normal distribution with zero population mean from a sample of n observations. Next, we consider the log-likelihood LL_{het} for the residual scores under the assumption of heteroscedasticity. Under heteroscedasticity, and when it is assumed that for each case the residual score has been drawn from a normal distribution with arbitrary variance and zero mean, the ML estimates for the n variances are $\hat{\sigma}_i^2 = e_i^2, i = 1, \dots, n$ (Stuart et al. 1999, p. 552). With n free variance parameters $\sigma_1^2, \dots, \sigma_n^2$, the log-likelihood LL_{het} is then derived as

$$LL_{\text{het}} = -\frac{n}{2} \ln(2\pi) - \frac{1}{2} \sum_i \ln(e_i^2) - \frac{n}{2}. \tag{4}$$

The difference between LL_{het} and LL_{hom} is

$$LL_{\text{het}} - LL_{\text{hom}} = \frac{n}{2} \ln(\hat{\sigma}^2) - \frac{1}{2} \sum_i \ln(e_i^2) = -\frac{1}{2} \sum_i \ln[(e_i/\hat{\sigma})^2]. \tag{5}$$

¹For technical reasons, we have to assume that the value zero is excluded for any of the e_1, \dots, e_n , which is why we denote the above normal distribution by N^* instead of N . The properties of this modified normal distribution, its moments, and likelihood are the same as they are for the regular normal distribution.

The last equation shows that the difference between LL_{het} and LL_{hom} is a function of the rescaled residual scores $(e_i/\hat{\sigma})$. If the n variances $\sigma_1^2, \dots, \sigma_n^2$ are all equal (homoscedastic case), and if n is large enough such that $\hat{\sigma}$ is close to the population parameter σ , the standardized residual scores $(e_i/\hat{\sigma})$ are drawn from an (approximate) standard normal distribution. With additional algebra that is given in the Appendix, the expected value, the variance, and the standard deviation of the difference $2(LL_{\text{het}} - LL_{\text{hom}})$ can then be derived, under the assumption of homoscedasticity: If $\sigma_1^2 = \dots = \sigma_n^2$, we have

$$\begin{aligned} E[2(LL_{\text{het}} - LL_{\text{hom}})] &\approx 1.270n, \\ \text{Var}[2(LL_{\text{het}} - LL_{\text{hom}})] &\approx 4.936n, \\ SD[2(LL_{\text{het}} - LL_{\text{hom}})] &\approx 2.222\sqrt{n}. \end{aligned} \tag{6}$$

We can now define a surrogacy measure Z_{het} by

$$Z_{\text{het}} = \left(- \sum_i \ln[(e_i/\hat{\sigma})^2] - 1.270n \right) / \left(2.222\sqrt{n} \right). \tag{7}$$

The measure Z_{het} quantifies the heteroscedasticity of the residual scores on a Z-scale. We recommend using it as a descriptive measure rather than as a formal test. When sample size n is large, the statistic Z_{het} is approximately standard normally distributed. For a detailed explanation of this, see the Appendix. An absolute value of Z_{het} that lies clearly above 1.96 may be interpreted as a very strong sign of heteroscedasticity. This value marks the upper 2.5% cut-off for a standard normal distribution.

3 Simulated examples

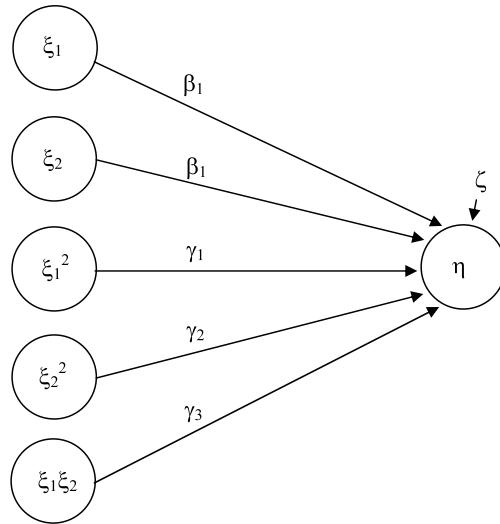
In this section, we illustrate the use of the measure Z_{het} for the detection of omitted nonlinear terms in a structural equation model by a set of examples. For the application of the measure Z_{het} to SEM, it is assumed that the measurement models for the latent variables are all valid and have normally distributed errors. For several simulation conditions to follow, we consider a basic nonlinear structural model

$$\eta_i = \alpha + \beta_1\xi_{1i} + \beta_2\xi_{2i} + \gamma_1\xi_{1i}^2 + \gamma_2\xi_{2i}^2 + \gamma_3\xi_{1i}\xi_{2i} + \zeta_i, \tag{8}$$

where η is a latent dependent variable (criterion variable), α is an intercept term, ξ_1 and ξ_2 are latent predictor variables, ζ is a disturbance variable, β_1 and β_2 are linear effect coefficients, γ_1 and γ_2 are quadratic effect coefficients, and γ_3 is the coefficient of the interaction term. We also consider a basic measurement model

$$\begin{pmatrix} x_{1i} \\ x_{2i} \\ x_{3i} \\ x_{4i} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \lambda_{21} & 0 \\ 0 & 1 \\ 0 & \lambda_{42} \end{pmatrix} \begin{pmatrix} \xi_{1i} \\ \xi_{2i} \end{pmatrix} + \begin{pmatrix} \delta_{1i} \\ \delta_{2i} \\ \delta_{3i} \\ \delta_{4i} \end{pmatrix}, \quad y_i = \eta_i, \tag{9}$$

Fig. 2 Path diagram of nonlinear structural equation



with four indicators x_1 , x_2 , x_3 , x_4 for the two latent predictors ξ_1 and ξ_2 , and one indicator y for the latent criterion η . Figure 2 illustrates the structural part of the model; the measurement part has been omitted in the picture.

For a set of simulated examples, we selected the values for the coefficients as $\alpha = 1.0$, $\beta_1 = 0.2$, $\beta_2 = 0.3$, the values for the variances and covariance of the latent predictors as $\phi_{11} = 1.0$, $\phi_{22} = 1.0$, $\phi_{12} = 0.3$, the variance of the disturbance term as $\psi = 0.2$, the loading parameters as $\lambda_{21} = \lambda_{42} = 0.8$, and the error variances as $\theta_{11} = \theta_{22} = \theta_{33} = \theta_{44} = 0.36$.

The coefficients of the nonlinear effects were varied across five conditions in the data generating model: A linear model with $\gamma_1 = \gamma_2 = \gamma_3 = 0$ (Condition I), a model with small quadratic effects with $\gamma_1 = 0.1$, $\gamma_2 = 0.2$, $\gamma_3 = 0$ (Condition II), a full model with $\gamma_1 = 0.1$, $\gamma_2 = 0.2$, $\gamma_3 = 0.5$ (Condition III), a model with strong quadratic effects with $\gamma_1 = 0.3$, $\gamma_2 = 0.5$, $\gamma_3 = 0$ (Condition IV), and a model with an interaction effect with $\gamma_1 = \gamma_2 = 0$, $\gamma_3 = 0.5$ (Condition V). For each of the five conditions, 1000 cases were randomly generated, where the predictors, the disturbance term, and the errors were sampled from normal distributions.

Then, each model was analyzed in three different ways using the Mplus software: As a linear model with γ_1 , γ_2 , γ_3 set to zero, as a quadratic model with only γ_3 set to zero, and as a full model. The linear coefficients β_1 and β_2 were always included in the analysis model. For the Mplus analysis, we rearranged the syntax such that the structural part of the model was represented by a latent variable f3. This is illustrated in Fig. 3, which shows the Mplus code for the full model.

The factor scores option ("Save = FS;") was used to obtain ML-based factor scores for the latent variable f3. f3 technically represents the criterion variable η of the analysis model, but without the disturbance term ζ . The Mplus factor scores for f3 were calculated under the assumption that the exogeneous factors and the residuals of the measurement model are all normally distributed. The factor scores for f3 were then subtracted from the scores for y to obtain residual scores for ζ for the Mplus

```

TITLE: Full model with two latent variables
DATA: FILE IS lin.dat;
VARIABLE: NAMES ARE y1-y5;
ANALYSIS: TYPE = RANDOM;
          ALGORITHM = INTEGRATION;

MODEL:   f1 BY y1-y2;
          f2 BY y3-y4;
          flxf2 | f1 XWITH f2; !interaction term
          f11 | f1 xwith f1; !quadratic term
          f22 | f2 xwith f2; !quadratic term

          f3 ON f1 f2 f11 f22 flxf2;
              !factor f3 used to represent the structural part
          f3@0; !f3 has no residual
          [f3*]; !f3 has an intercept

          ! code example when model has 1 indicator for eta
          f3 BY y5;
          [y5@0]; !intercept of y5 is set to zero
          ! residual: e=y5-f3

          ! code example when model has 3 indicators for eta
          ! f4 ON f3@1; !f4 represents latent criterion
          eta
          ! f4 BY y5-y7;
          ! [y5@0];
          ! residual: e=f4-f3

OUTPUT: TECH1 TECH8;
SAVEDATA: FILE IS SCORE.DAT;
          Save = FS;
          !creates ML factor scores in file score.dat

```

Fig. 3 Mplus code for nonlinear model with latent variable f_3 representing the structural part of the model, and with factor scores saving option

analysis model. In each analysis, the heteroscedasticity measure Z_{het} was calculated to see if it indicates heteroscedastic residuals as a consequence of an ill-specified nonlinear model part. The results of the analyses are given in Table 1.

We illustrate the calculation of Z_{het} for the value in the upper left corner of the table: Mplus produces a file with factor scores for f_3 . The factor scores for f_3 are subtracted from the scores for the indicator y for each case to obtain residual scores e_i . The residual scores are then divided by the standard deviation of the residual scores, squared, and log-transformed by using the natural logarithm. From this, the sum

$$-\sum_i \ln((e_i/\hat{\sigma})^2) = 1224.4 \quad (10)$$

is calculated. For the expected value and the standard deviation in (6), we obtain the values $1270 = 1.270 \times 1000$ and $70.27 = 2.222 \times \sqrt{1000}$, respectively. By applying (7), we obtain for Z_{het} :

$$Z_{\text{het}} = (1224.4 - 1270)/70.27 = -0.65. \quad (11)$$

Table 1 Values for the measure Z_{het} for five different data-generating models (Conditions I to V) that were analyzed under three different model structures (linear, quadratic, full model)

	Linear analysis model $\gamma_1 = \gamma_2 = \gamma_3 = 0$	Quadratic analysis model γ_1, γ_2 free, $\gamma_3 = 0$	Full analysis model $\gamma_1, \gamma_2, \gamma_3$ free
<i>Condition I</i>			
Data generated for linear model with $\gamma_1 = \gamma_2 = \gamma_3 = 0$	$Z_{\text{het}} = -0.65$	$Z_{\text{het}} = -0.51$	$Z_{\text{het}} = -0.46$
<i>Condition II</i>			
Data generated for model with small quadratic effects, $\gamma_1 = 0.1$, $\gamma_2 = 0.2$, $\gamma_3 = 0$	$Z_{\text{het}} = 0.26$	$Z_{\text{het}} = -1.08$	$Z_{\text{het}} = -0.90$
<i>Condition III</i>			
Data generated for full model with $\gamma_1 = 0.1$, $\gamma_2 = 0.2$, $\gamma_3 = 0.4$	$Z_{\text{het}} = 3.53$	$Z_{\text{het}} = -0.92$	$Z_{\text{het}} = -0.03$
<i>Condition IV</i>			
Data generated for model with strong quadratic effects, $\gamma_1 = 0.3$, $\gamma_2 = 0.5$, $\gamma_3 = 0$	$Z_{\text{het}} = 3.48$	$Z_{\text{het}} = 1.82$	$Z_{\text{het}} = 1.62$
<i>Condition V</i>			
Data generated for model with interaction effect, $\gamma_1 = 0$, $\gamma_2 = 0$, $\gamma_3 = 0.5$	$Z_{\text{het}} = 3.69$	$Z_{\text{het}} = 1.30$	$Z_{\text{het}} = 0.09$

The results for the measure Z_{het} showed that when the true model was strongly non-linear (Conditions III, IV, V) but was analyzed as a linear model (first column), the measure Z_{het} clearly responded to the heteroscedastic residual that resulted from the ill-specified analysis model: The measure Z_{het} attained values between 3.48 and 3.69. Thus, as expected, the measure responded to hidden nonlinearity in the model structure as a result of omitted nonlinear terms. When the data were analyzed by using the correct model (diagonal elements in Table 1), the measure Z_{het} correctly did not respond and the values lay between -0.65 and $+1.08$. As expected, when a model was analyzed by an overparameterized model, Z_{het} did not respond: When the true linear model (Condition I) was analyzed as a quadratic or full model, the absolute value of Z_{het} decreased somewhat; when the quadratic model (Condition II) was analyzed as a full model, Z_{het} changed only from -1.08 to -0.90 ; when the second quadratic model (Condition IV) was analyzed as a full model, Z_{het} decreased from 1.82 to 1.62; when the interaction model (Condition V) was analyzed as a full model, Z_{het} was only 0.09. However, Z_{het} did not respond when the quadratic model (Condition II) was analyzed as a linear model, which might be due to the fact that the quadratic effects were comparatively small under Condition II. Also, Z_{het} did not

respond when the full model (Condition III) was analyzed as a quadratic model or when the interaction model (Condition V) was analyzed as a purely quadratic model. This is not so surprising when one considers the fact that quadratic terms can partially account for the variance of an interaction term when the predictors are correlated (cf. Ganzach 1997). In the Mplus examples, we only considered a model with one indicator for the criterion variable for η . However, the Mplus syntax could be readily extended to models with multiple indicators, where in the syntax the latent factor f3 again represents the structural part and where an additional factor f4 is specified that represents the latent criterion η . The residual variable e for the measure \mathbf{Z}_{het} is then $e = f4 - f3$. We expect that the measure \mathbf{Z}_{het} will then respond to heteroscedasticity similarly, although detailed simulation results for this case still await further exploration.

4 Discussion

A novel measure for the detection of heteroscedasticity was proposed that can relate to nonlinear terms which have possibly been omitted in the structural part of a model. We demonstrated that the measure appears to detect omitted nonlinear terms when falsely a linear model is used and the omitted nonlinear terms account for substantial nonlinear effects. Also, the results indicate that the measure correctly does not respond when the correct model or an overparameterized model is used. This is a desirable feature, as the application does not recommend including additional nonlinear terms when it is not necessary.

The measure mainly responds when there is heteroscedasticity left that cannot be explained or captured by any of the remaining nonlinear terms in the model. Although the results for the small number of simulated examples cannot yet be generalized, they give some indication that the measure \mathbf{Z}_{het} may be useful to detect nonlinear model parts that have been omitted in the model structure and do account for a considerable amount of variance. This feature might be useful for the exploration of linear SEM with a large number of predictors and a large number of possible interaction terms.

Future simulation studies with a more detailed variation of conditions are required to further examine the sensitivity and power of the measure \mathbf{Z}_{het} . The current version of the measure has only been examined for models with one indicator for the latent criterion. It is expected that the method can be extended to models with multiple indicators, where the measure \mathbf{Z}_{het} is then computed for the residual ζ of the latent criterion. Such an extension awaits future research. Also, it is planned to apply the method to empirical data sets and further evaluate its feasibility.

Appendix

We derive the expectation and variance for the expression

$$2[LL_{\text{het}} - LL_{\text{hom}}] = - \sum_i \ln[e_i^2 / \hat{\sigma}^2]. \quad (12)$$

Under the assumption of homoscedasticity, the residuals e_i have been drawn from a normal distribution with variance σ^2 . When sample size n is large, the variance estimate $\hat{\sigma}^2$ is very close to the population variance σ^2 , and

$$2[LL_{\text{het}} - LL_{\text{hom}}] \approx - \sum_i \ln[e_i^2/\sigma^2]. \quad (13)$$

By use of the central limit theorem, $2[LL_{\text{het}} - LL_{\text{hom}}]$ then follows an approximate normal distribution with the expectation and variance given by

$$\begin{aligned} \mu &= E[2[LL_{\text{het}} - LL_{\text{hom}}]] = nE[-\ln(Z^2)] = n \int_{IR} -\ln(z^2)\varphi(z) dz, \\ \text{Var}[2[LL_{\text{het}} - LL_{\text{hom}}]] &= n(E[\ln(Z^2)^2] - \mu^2) = n \left(\int_{IR} \ln(z^2)^2 \varphi(z) dz - \mu^2 \right), \end{aligned} \quad (14)$$

where Z is a standard normal variate and $\varphi(z)$ is the density of the standard normal distribution. By use of numerical integration, these quantities are computed as

$$E[2[LL_{\text{het}} - LL_{\text{hom}}]] \approx 1.270n, \quad \text{and} \quad \text{Var}[2[LL_{\text{het}} - LL_{\text{hom}}]] \approx 4.936n. \quad (15)$$

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