Correcting the Root Mean Squared Error of Approximation under Missingness

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Abstract

Missing data is a frequent occurrence in both small and large datasets. Among other things, missingness may be a result of coding or computer error, participant absences, or it may be intentional, as in a planned missingness design. Whatever the cause, the problem of how to approach a dataset with missing values is of much relevance in scientific research. We discuss missingness as it relates to fit indices in Structural Equation Modeling, specifically its interaction with the Root Mean Squared Error of Approximation (RMSEA). We use data simulation to show that RMSEA has a downward bias with missing data, yielding skewed fit values. Two alternative formulas for RMSEA calculation are proposed: one correcting degrees of freedom and one using Kullback-Leibler divergence to result in an RMSEA calculation which is independent of missingness for misspecified models. Simulations are conducted in Java, with results indicating that the Kullback-Leibler divergence provides a better correction for RMSEA calculation.

Keywords: missing data, structural equation modeling, fit indices, KL divergence

Correcting the Root Mean Squared Error of Approximation under Missingness

Structural Equation Modeling (SEM; Baltes, Reese, & Nesselroade, 1988) is a ubiquitous and powerful analytic technique for the analysis of multivariate data. Many models can be fit within the SEM paradigm, including simple GLM-based methods like regression and ANOVA (see for example Miller, 1997), and more complex techniques ranging from factor analysis (Mulaik & Press, 1972) to non-linear growth mixture models (Grimm, Ram, & Estabrook, 2010). Models are usually assessed in part using fit indices describing how well the data fits the model. Fit indices typically compare the proposed model to either a saturated model or both a saturated and an independence model. Saturated models include all possible means, variances and covariances, and represent the best possible fit of a covariance structure to the data, while independence models include only means and variances (i.e., assume all covariances are zero) and represent the worst reasonable fit of a covariance structure. Fit indices like Root Mean Square Error of Approximation (RMSEA; Steiger & Lind, 1980) describe absolute misfit of a model relative to the saturated model, while indices like the Comparative Fit Index (CFI) and Tucker Lewis Index (Tucker & Lewis, 1973) place the proposed model on a continuum between the saturated and independence models.

Since its initial inception as a model of simple covariances, the theory surrounding SEM has greatly expanded to include multi-level modeling (Heck, 2001), mixture modeling (Muthén & Shedden, 1999), non-linearity (Grimm & Ram, 2009), and many others. One important extension is the implementation of Full-Information Maximum Likelihood (FIML; cf. Finkbeiner, 1979) estimation. Early SEM packages relied solely on observed moment matrices (e.g., covariance matrices, mean vectors, SSCP matrices) as input, requiring researchers to convert their data into the appropriate matrices and handle missing data, ordinal data, and other complexities prior to model fitting. More modern SEM packages can use FIML to handle raw data, eschewing user-generated data reduction in favor of fitting the model to each row of the data individually. This allows SEM to

handle missing values by applying the model to whatever values are observed for a particular row of data. FIML is robust to missingness under both the missing completely at random (MCAR) and missing at random (MAR) mechanisms (Rubin, 1976; Little & Rubin, 1987), yielding unbiased parameter estimates under ignorable missingness conditions and perform better than other missing data methods, such as similar response pattern imputation or listwise deletion (Enders & Bandalos, 2001).

While the methods by which we fit SEM have changed, the methods by which we assess the fit of these models has not. Most of the common fit indices used to assess model fit make assumptions about the models being compared and the data that underly them, namely that they contain full rank covariance matrices with single values for sample size and degrees of freedom. To the extent that a particular model uses raw data under FIML and is affected by missingness, these assumptions are decidedly false and thus bias fit indices. For example, RMSEA measures the amount of noncentrality per the product of sample size and degrees of freedom. When the data are complete, the product of adjusted sample size and degrees of freedom contain one measure of the total amount of information in the sample. When some portion of the data are missing, the χ^2 will decrease while the sample size and degrees of freedom values stay constant, which reduces the absolute value of the RMSEA statistic and make fit appear to be better than it would be with complete data.

This artificial improvement in model fit has been noted in previous research (i.e. Davey, 2005; Hoyle, 2012), with no known solution. Despite this, using fit statistics in the presence of missing data remains common practice. Google Scholar search indicates approximately 30% of articles (or 8,930/30,361) that cited one of two popular articles with recommended "rules of thumb" for RMSEA (Browne & Cudeck, 1993; Hu & Bentler, 1999) also include either "missing" or "full information". While this search is imperfect and nowhere near exhaustive, it gives some background toward the widespread use of fit

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statistics in SEM and, more importantly, the widespread use of fit statistics in SEM with missing data.

Summary of this article

In this article, we will first discuss the problem that missing data introduces into the realm of model fit indices in SEM, focusing on RMSEA. We then introduce two possible solutions and explain the mathematical basis of each. Next, we present data simulations and data plots used to illustrate the problem and demonstrate in what ways the proposed solutions are better than the naive RMSEA equation. Discussion includes reasons for corrections, implications of the problem of missingness in SEM, limitations, and future directions.

Method

Mathematical Basis of Correction

For full data, the RMSEA for a proposed model is defined as

$$RMSEA_{uncorrected} = \sqrt{\max\left(0, \frac{\chi^2 - df}{(N-1)df}\right)}$$

where df is the difference in degrees of freedom between the proposed model and a saturated normal model, N the number of participants, and χ^2 the difference in the minus two log likelihood between the proposed and saturated models for the given data set. Without model misspecification, the χ^2 index will be distributed as a central χ^2 distribution with df degrees of freedom, and the fraction will have an expected value of zero, with decreasing variance as N increases. If the model is misspecified, χ^2 follows a non-central χ^2 distribution and will grow proportional to N, and the fraction will converge towards a fixed non-zero number in expectation.

As a data set has an increasing amount of missingness, the minus two log likelihoods of both the proposed and saturated models will decrease. In consequence, the χ^2 will

decrease while df and N remain constant, which results a better RMSEA value for increasing missingness. In effect, the RMSEA is unaffected by missingness without model misspecification, but will reduce (i.e., improve) with missingness under misspecification.

To be able to use the RMSEA as a measure of existing misfit, the RMSEA value needs to be constant on different missingness levels if the model is misspecified. Therefore, changes in χ^2 due to missingness need to be reflected somewhere in the calculation. We propose two methods to achieve this. For the first, let p be the rate of non-missing data points, i.e., p=1 for complete data, p=0.5 if half of the measurements are missing, and p=0 for completely missing data. Under a missingness of p, χ^2 is distributed as p times a non-central χ^2 distribution with df degrees of freedom times. This distribution has a mean of $N \cdot df \cdot p$ instead of mean $N \cdot df$ as in the non-missing case. Following the original idea of the RMSEA, we subtract the mean in the numerator and divide by the mean in the denominator. This results in our first suggestion for an RMSEA under missingness:

$$RMSEA_{df\ corrected} = \sqrt{\max\left(0, \frac{\chi^2 - pdf}{pNdf}\right)}$$

As a second suggestion, instead of correcting the mean subtracted, we correct the distribution. Instead of using the difference of the minus two log likelihoods for the model and the saturated model, we suggest to use 2N times the Kullback-Leibler (Kullback & Leibler, 1951) divergence between the two distributions,

$$KL = \operatorname{Trace}\left(\Sigma^{-1}S\right) + \left(\mu - m\right)^{T} \Sigma^{-1} \left(\mu - m\right) - k - \ln\left(\frac{|S|}{|\Sigma|}\right)$$

where Σ and μ are the model distribution and S and m the saturated model distribution, and k the number of variables (i.e., the dimensionality of the distributions). Note that the KL coincides with the χ^2 value for complete data sets, but does not change in expectation under missingness if $S \neq \Sigma$ in the population. Using $2N \cdot KL$ instead of χ^2 , N needs to be replaced by pN in the RMSEA equation to obtain a term under the square root that is mathematically guaranteed to be constant in expectation for all values of p:

$$RMSEA_{KL\ corrected} = \sqrt{\max\left(0, \frac{p \cdot N \cdot KL - df}{pNdf}\right)}$$

Note that even though the fraction is guaranteed to have a constant expectation for different missingness rates, the expression under the square root (which includes the max operator) may show an increasing expectation with p if the distribution of the fraction includes negative results. However, the actual center of the distribution is not changed; the effect is just due to the non-negative values being moved to zero. The median and mode of the distribution stays constant.

Simulation Design

To demonstrate the mathematical results and compare the three RMSEA calculations under missingness, we simulated data and fit it with a misspecified model. The simulation study utilized two 2-variable SEMs created in Ω nyx (von Oertzen, Brandmaier, & Tsang, in press). In the model used for data generation, two observed variables were created, each with variance one and covariance between them set at intervals ranging from 0.0 to 0.9 (Figure 1). The second model (Figure 2) is similar to the first, with two observed variables, each with freely estimated variance and a covariance constrained to a value of 0.0.

This second model was then used to fit the simulated data. The model was chosen as simple as possible to isolate the effect of missingness under misspecification on the three suggested RMSEA variants.

In addition to generating raw data, simulation setup included a structured environment in which missing values could be simulated. All data were simulated with N=1000, and missing value ratios ranged from 0.0 to 0.75, increasing in increments of 0.05. All simulation conditions were repeated for 1000 trials.

Following data generation, two types of missing data were simulated: data missing completely at random (MCAR) and data missing at random (MAR). MCAR data were simulated by randomly deleting variables by way of introducing a random number generator into the model. A uniformly distributed random real number between 0.0 and 1.0 was generated, and if that number was smaller than the missingness ratio specified in

that specific trial block (where the missingness ratio ranged in value from 0.0 to 0.75), a missing value occurred. The program looped through each participant and each variable within each participant, such that any variable for any participant could be set as missing.

For data MAR, the missingness simulation was set up differently. Because data MAR depends on values of non-missing data, missingness was introduced among the second variable only, resulting in a range of total missingness of half the amount of what it was for MCAR. The total missingness ratio hence ranged from 0.0 to 0.4, because one, rather than two, variables could have designated missing values. The way in which we modeled data MAR involved the introduction of a sigmoid function

$$f(x) = \frac{1}{1 + e^{-x}}$$

into the simulation. The sigmoid function was used to generate a missing probability of the second variable that depended on the x-value of the first variable. Depending on the total missing ratio (miss) aimed at for the second variable, the sigmoid function was rescaled to pass through miss at the intersection with the vertical axis. For total missingness ratios below 0.5, the function started at zero, passed through miss at the y-axis, and reached an asymptote of $2 \cdot miss$ for high x-values. For missingness rations above 0.5, the function started at $2 \cdot miss - 1$, i.e., at twice the distance of miss from a value of 1. It then passed miss at the y-axis and finally reached an asymptote of 1. The value x of the function is the value of the first variable generated for a given participant and trial. To put this in an equation, for an x-value of the first variable and an overall missingness rate of miss, the missing probability missProb for the second variable was computed as

$$missProb = \begin{cases} \frac{2miss}{1 + e^{-x}} & 0.0 \le miss \le 0.5\\ \frac{2(1 - miss)}{1 + e^{-x}} + 2miss - 1 & 0.5 \le miss \le 1.0 \end{cases}$$

Observe that the two cases coincide for miss = 0.5, where the missing probability is the unaltered sigmoid function. Also observe that due to the symmetry of the sigmoid function, the expected missing probability under a normally distributed x is miss in all cases.

Analogously to the data MCAR, simulation values for data MAR were deleted at random according to whether a random number between 0 and 1 was less than *missProb* for a specific participant and trial. If the number was smaller than *missProb*, then the value for data in the second variable was set to missing.

After creating the missingness, data was fitted to the second, misspecified model which had fixed zero covariance between the two variables using Ω nyx. The uncorrected, df corrected, and KL corrected RMSEA were then computed for the estimation result. All simulation conditions were repeated for 1000 trials. Data generation and calling the Ω nyx SEM program was done in Java.

Results

Plot Descriptions

Results are presented visually by condition, with one plot per type of missingness (MCAR vs. MAR) and observed covariance between variables. The horizontal (x) axes of each plot represent the percent of data missing, while the vertical (y) axes of each plot represent RMSEA. The standard error of the values given in the plots ranged from 0.0002 to 0.002. To aid in the interpretation of these simulations, we follow general guidelines in the literature to define RMSEA values less than 0.05 to indicate good fit, greater than 0.1 to indicate poor fit, and values in between 0.05 and 0.1 to indicate mediocre fit (Browne & Cudeck, 1993). A line for RMSEA of 0.05 is included where necessary.

Simulation results revealed consistent patterns for RMSEA calculations. RMSEA values were most strongly related to model misspecification (i.e., the strength of the correlation between variables that was constrained to zero in the misspecified model), but also showed effects of missingness patterns (MCAR vs. MAR). For both covariance value of 0.0 and 0.125, MAR and MCAR data generally yielded similar patterns.

MAR, cov = 0.125. For data MAR with a covariance of 0.125 between variables (Figure 3), the uncorrected RMSEA values scale linearly with missingness. For the data

simulation conducted here, a missingness percentage of zero results in an RMSEA value of approximately 0.065, which indicates that the model has mediocre fit. With only 30% missingness, however, the RMSEA value drops below 0.05, indicating "good" fit. With an additional decline of 20% of data reported, 50% missingness total, we see the RMSEA value decreases by almost two one-hundredths, confirming the linearly declining pattern observed. The df corrected RMSEA calculation also shows a decline with increasing missingness, although not as drastically as the uncorrected values. KL corrected RMSEA values remain constant across all levels of missingness, with only a slight increase near 35% missingness.

MCAR, cov = 0.125. For data MCAR with a covariance value of 0.125 between variables (Figure 4), we see a similar pattern as was observed with the MAR data condition above. In these calculations, however, the trends are even more dramatic. Note the difference in scale between the MCAR and MAR conditions; as previously described, data that we simulated to be MAR can have missing percentages only half of what missingness percentages in data simulated as MCAR. Uncorrected RMSEA values continue to decline linearly as missingness percentage increases. With increasing percentages of missing data, uncorrected values reach the .05 cutoff rather quickly and continue to decline far below the original RMSEA value of approximately 0.065. Values for df corrected RMSEA decline and reach the 0.05 cutoff value and thus cross the threshold into the range of RMSEA values indicating "good" fit.

MAR and MCAR, cov = 0.9. As model misspecification increases, the resulting patterns observed become more pronounced. In the 0.9 covariance condition, the trend in the data is maintained, with uncorrected values scaling downward as the percentage of missingness increases, df corrected values being less linearly dependent on missing percentages, and KL corrected values being almost completely independent of missingness. Figures 5 and 6 display results for data simulation when model covariance cov = 0.9 under MAR and MCAR data conditions, respectively. The mean of the KL corrected RMSEA increases slightly for high missingness values. This is due to the floor effect in which df and

KL corrected values are found using the maximum operator. This results in only positive RMSEA values being reported, skewing the mean in a positive direction. When the expression beneath the square root sign is evaluated and is thus no longer required to be positive, the floor effect is eliminated.

MAR and MCAR, cov = 0.0. For models with no model misspecification (i.e., those with no covariance between variables), we observe no decline in RMSEA values for any of the three calculations. Instead, uncorrected RMSEA values remain constant at a level of almost zero, even as missingness increase. The proposed calculation values, for both df corrected and KL corrected, increase slightly as missingness increases. When missing percentage values reach 35-40%, both MAR and MCAR KL corrected values show an increase in terms of RMSEA value. See Figures 7 and 8 for these results.

Results Summary

Among models with some misspecification, we see a a downward bias with the uncorrected RMSEA calculation, a trend which is reduced for the df corrected RMSEA and eliminated for the KL corrected RMSEA. This trend appears among both MCAR and MAR data simulations among models with both low (cov = 0.125) and high (cov = 0.9) model misspecification.

For the models having no misspecification, an upward trend for KL and df corrected values is observed when missingness values are high, but not when they are low. In this case, the uncorrected RMSEA is the best choice. However, in practical situations models are almost never exactly correctly specified.

Discussion

The RMSEA as defined by Steiger and Lind (1980) normalizes the χ^2 index. Under the null hypothesis that the data is generated by a population distribution described exactly by the model, this index follows a χ^2 distribution regardless of the missingness in the data set. Therefore, as expected, we find in our simulation that the uncorrected RMSEA is constant in expectation for every missingness condition. Thus, under the null hypothesis, the uncorrected RMSEA does exactly what we expect it to do. We also find that both suggested corrections in this case exaggerate the model misfit, although even under strong missingness the RMSEA remains below typically used cut-off criteria for "good" model fit.

However, RMSEA was created to evaluate misspecified models. In fact, if we want a test whether a model is perfectly specified, we could use the Likelihood-Ratio test. The logic of the RMSEA is that models are never perfectly specified, and in fact would be useless if they were, since simplification is an integral part of statistical modeling. The RMSEA is a quantification of the degree of misspecification that allows us to talk about "slightly" misspecified models that still work as desired in most cases. With misspecification, the uncorrected RMSEA is no longer guaranteed to be constant. This is evident in our simulations, where the uncorrected RMSEA decreases with higher amounts of missingness. Therefore, a misspecified model yields an artificially low RMSEA value indicating "good" model fit for datasets with high degrees of missingness. It is therefore necessary to correct the RMSEA in cases where missingness is present. We showed mathematically that the KL corrected RMSEA index is unaffected by missingness and therefore provides a better indicator of model fit, a result which was further evident in our simulations.

Limitations

Although the data simulations strongly support that KL corrected RMSEA values are unaffected by missingness, further investigation is needed for more general models. The model used in our simulation was very simple, having only two observed variables to underline the conceptual point and to examine initially two potential corrections. In most cases, such models are oversimplified and do not adequately represent more complicated datasets. Increasing the complexity of data simulation models and reassessing RMSEA

trends will allow for broader confirmation of the effectiveness of KL corrected RMSEA as a modified fit index. Additionally, all RMSEA corrections cause an artificial increase under the null hypothesis of a perfectly specified model. This needs to be taken into consideration despite the fact that, as mentioned above, RMSEA was not created for scenarios in which no misspecification is present.

A possible objection to implementing the KL correction for RMSEA lies in the realization that, in presence of missingness, corrected RMSEA values indicate worse model fit than uncorrected values. Though the rationale for an RMSEA correction is rooted in theory and practice, it may be hard to accept that RMSEA values traditionally reported imply artificially good fit for models with missingness. Accepting the KL correction will force researchers to reassess model fit, and there may be resistance if KL corrected RMSEA values point to a different conclusion than uncorrected RMSEA values had indicated previously. Considering that the typically used cut-off values are based on experience without using the correction, it may be reasonable to re-think the typical cut-off values. Changing the RMSEA calculation under missingness en masse, with higher RMSEA values considered acceptable, may lessen resistance to such a change. RMSEA values may then become comparable across different levels of missingness, and preference will no longer be given to models where missing data rates are high.

Summary and Future Directions

To summarize, we see that a naive application of the RMSEA for data with missingness, for which the RMSEA is not designed, results in exaggerated model fit (i.e. RMSEA values that are too low). It is possible that researchers hence were too optimistic about the fit of their model if their data contained missing values. The RMSEA can easily be corrected by replacing the χ^2 with the KL divergence in the RMSEA equation, the intuitive continuation of the RMSEA into data missingness cases.

Informing researchers about the benefits of an RMSEA correction and its ability to

handle missing data may encourage the use of SEM in the presence of missingness. In order to do this, it is important to provide the scientific community easy access to the correction. A feasible solution is writing a package for R which includes wrapper tools that will extract data from existing functions and calculate RMSEA corrected values. In this line, we attach a small R script to this article that implements the equations for the KL and the df corrected RMSEA values based on the estimation results. The script is available in the additional materials, the code for the script can be found in the supplementary information. Although likely more difficult, integrating the KL correction into existing data software tools, such as Ω nyx, SPSS and SAS, or popular R packages, such as OpenMx, lavaan, or sem, would be useful for encouraging and supporting widespread use of corrected RMSEA estimates.



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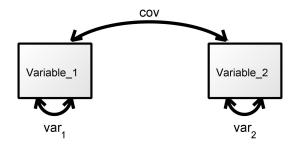


Figure 1. Model used for data generation. The cov values range from 0.0 to 0.9 in the simulation.





Figure 2. Model used to fit data. The covariance value between variables 1 and 2 is fixed to zero, which is a misspecification if the data was generated with nonzero covariance.



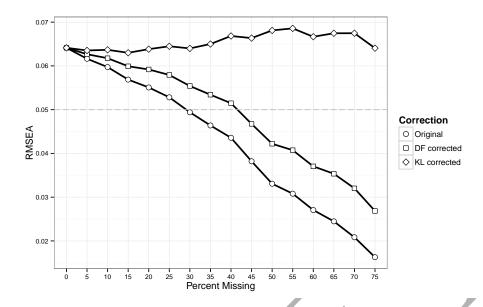


Figure 3. Simulation results for data generated with a covariance of 0.125 and data missing at random. While KL corrected RMSEA values remain mostly constant across levels of missingness, uncorrected and df corrected RMSEA yield artificially improved model fit. Standard errors ranged from 0.0002 (left) to 0.002 (right).

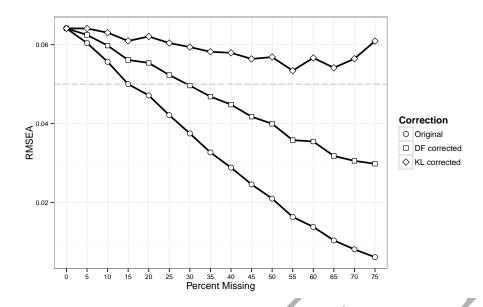


Figure 4. Simulation results for data generated with a covariance of 0.125 and data missing completely at random. Again, KL corrected RMSEA values stay mostly constant across levels of missingness, while uncorrected and df corrected RMSEA yield artificially improved model fit. Standard errors ranged from 0.0002 (left) to 0.002 (right).

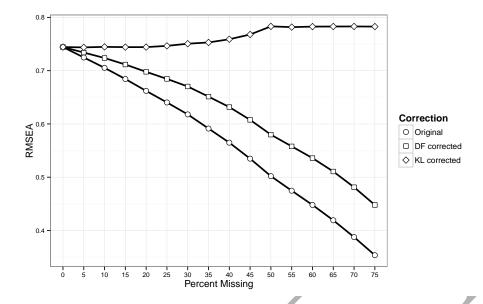


Figure 5. Simulation results for data generated with a covariance of 0.9 and data missing at random. Again, KL corrected RMSEA values remain mostly constant across levels of missingness and uncorrected and df corrected RMSEA yield artificially improved model fit. Standard errors ranged from 0.0002 (left) to 0.002 (right).

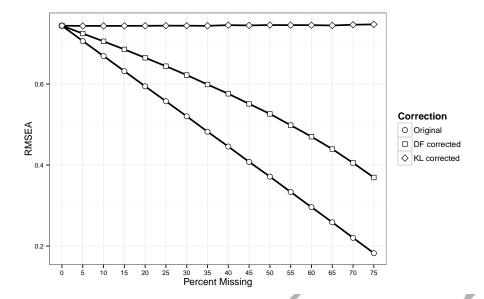


Figure 6. Simulation results for data generated with a covariance of 0.9 and data missing completely at random. Again, KL corrected RMSEA values remain mostly constant across levels of missingness and uncorrected and df corrected RMSEA yield artificially improved model fit. Standard errors ranged from 0.0002 (left) to 0.002 (right).

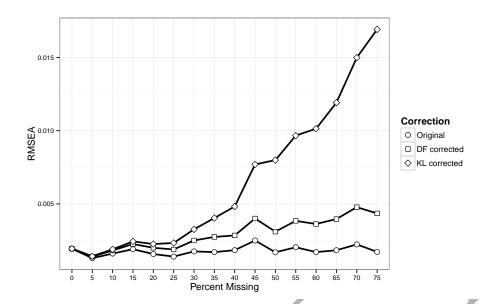


Figure 7. Simulation results for data generated with no model misspecification and data missing at random. As expected, results stay close to zero. Corrected RMSEA indices start increasing for high missingness rates. Standard errors were around 0.0001. When evaluating RMSEA values in this condition, keep note of the small scale of the y-axis.

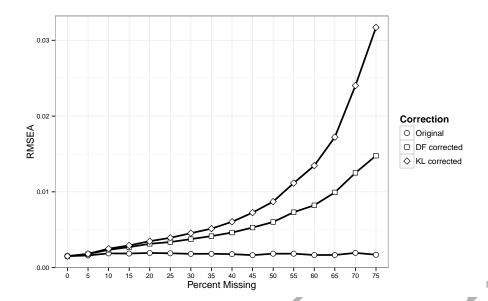


Figure 8. Simulation results for data generated with no model misspecification and data missing completely at random. As expected, results stay close to zero. Corrected RMSEA indices start increasing for high missingness rates. Standard errors were around 0.0001. When evaluating RMSEA values in this condition, keep note of the small scale of the y-axis.