'Residual diversity estimates' do not correct for sampling bias in palaeodiversity data

Article

Accepted Version

‘Residual diversity estimates’ do not correct for sampling bias in palaeodiversity data

SHORT TITLE: Do not use residuals method

WORD COUNT: 4,739

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ABSTRACT

1. It is widely accepted that the fossil record suffers from various sampling biases – diversity signals through time may partly or largely reflect the rock record – and many methods have been devised to deal with this problem. One widely used method, the 'residual diversity' method, uses residuals from a modelled relationship between palaeodiversity and sampling (sampling-driven diversity model) as 'corrected' diversity estimates, but the unorthodox way in which these residuals are generated presents serious statistical problems; the response and predictor variables are decoupled through independent sorting, rendering the new bivariate relationship meaningless.
2. Here, we use simple simulations to demonstrate the detrimental consequences of independent sorting, through assessing error rates and biases in regression model coefficients.
3. Regression models based on independently sorted data result in unacceptably high rates of incorrect and systematically, directionally biased estimates, when the true parameter values are known. The large number of recent papers that used the method are likely to have produced misleading results and their implications should be reassessed.
4. We note that the 'residuals' approach based on the sampling-driven diversity model cannot be used to 'correct' for sampling bias, and instead advocate the use of phylogenetic multiple regression models that can include various confounding factors, including sampling bias, while simultaneously accounting for statistical non-independence owing to shared ancestry. Evolutionary dynamics such as speciation are inherently

a phylogenetic process, and only an explicitly phylogenetic approach will correctly model this process.

KEY WORDS

Palaeodiversity; residuals; modeling; sampling bias; fossil record; independent sorting

INTRODUCTION

It has been well known since the time of Darwin that the fossil record is largely incomplete (Darwin 1859), prompting generations of macroevolutionary researchers to take a cautious approach when interpreting patterns of palaeodiversity through time (Raup 1972; Raup 1976; Raup 1991; Prothero 1999; Smith & McGowan 2007; Alroy 2010b). There have been many attempts to account for this sampling bias (Raup 1972; Raup 1976; Smith & McGowan 2007; Alroy 2010b), but one approach in particular, often referred to as the 'residual diversity' method, devised by Smith and McGowan (2007) (and modified by Lloyd (2012)), has been widely used (citation count ~215 to Aug 2016; Google-Scholar).

Using regression residuals as data 'corrected' for confounding factors is a widely used method in biology, social sciences, economics (King 1986; Freckleton 2002), and even in palaeodiversity studies (Raup 1976). However, Smith and McGowan's (2007) approach differs from these classical residuals approaches in one key way: the 'residuals' are generated not as regression residuals ($\varepsilon = y - \hat{y}$) from a simple regression of diversity (y) on a proxy of sampling (x), but from "*a model in which rock area at outcrop was a perfect predictor of sampled diversity*" (Smith & McGowan 2007), here referred to as the sampling-driven diversity model (SDDM). The SDDM is constructed as a regression model between y sorted from low to high values (y') and x sorted from low to high values (x'), where the relationship between these two independently sorted variables y' and x' is assumed to represent the SDD generating process – though there is no reason to assume as such. 'Residuals' are obtained as the difference between the SDDM

predictions $\hat{y}$' and the observed values y, which are then treated as the 'residual diversity estimates' (figure 1).

However, independently sorting y and x as outlined above decouples a paired, bivariate dataset, and is obviously problematic in statistics. Model fitting on decoupled data (e.g. y' and x') will lead to spurious predictions and 'residuals' as the estimated regression coefficients will be based on a forced (false) linear relationship (figure 1b). However, owing to continued wide use of the SDDM as a preferred method for identifying supposedly 'true' palaeodiversity signals (as recently as (Grossnickle & Newham 2016)), it appears that this basic statistical concept is somehow overlooked. While it has been suggested that the use of formation counts (the number of fossiliferous geological formations – a mappable unit of rock that represents a particular time and set of environments in a particular location – in a given time interval (Benton *et al.* 2011)) to 'correct' palaeodiversity time series data is unlikely to be meaningful because of substantial redundancy of the two metrics (Benton *et al.* 2011; Benton 2015), and a recent study has scrutinized the performance of SDDM residuals in accurately predicting true simulated biodiversity signals (Brocklehurst 2015), the performance of the SDDM itself has never been assessed. Here, we demonstrate the detrimental effects of decoupling data in regression modelling using simple simulations.

MATERIAL AND METHODS

We first generated random deviates, x, sampling from a normal distribution (μ = 0, σ = 1), at a sample size n = 100 (see SI for other sample sizes n = 30 and 1000). We then calculated y using a linear relationship in the form of $y = a + bx + e$, where a is the intercept, b is the slope and e is Gaussian noise. For simplicity, we fixed a = 0.4 and b = 0.6, while varying e (μ_e = 0, σ_e = 0.05, 0.1, 0.25, 0.5) – other values of a and b should return similar if not identical results (though, b = 1 would be meaningless). Following Smith and McGowan (2007), we sorted y and x independently of each other to generate y' and x', and fitted an ordinary least squares (OLS) regression model to y' on x' (SDDM). For comparison, we fitted an OLS regression model to y on x in their original paired bivariate relationship (the standard regression model, SRM), the performance of which serves as a benchmark.

To test Smith and McGowan's (2007) assertion that the SDDM is indeed "*a model in which rock area at outcrop was a perfect predictor of sampled diversity*", we evaluated whether the estimated regression coefficients α and β significantly differed from the true regression parameters, a and b, using a t-test. We repeated the procedure over 5000 simulations and calculated the percentage of times the estimated coefficients differed significantly from the true parameters. We would expect about 5% of the simulations to result in regression coefficients significantly different from the true parameters by chance alone; anything substantially above this threshold would indicate that the model has unacceptably high Type I error rates or falsely rejecting a true null hypothesis, where our null hypothesis is that the SDDM can correctly estimate the 'true' model parameters.

In addition, we tested for bias in the estimated regression slopes, i.e. whether the estimates systematically deviated from the simulation parameter b = 0.6. The mean of the 5000 slopes was subjected to a t-test against a fixed value of 0.6. If deviations were random, then we would not expect to find any significant differences between the mean slope and thew theoretical value, with all slopes randomly distributed around it.

RESULTS

SRM coefficients were significantly different from the true model parameters in only ~5% of the 5000 iterations across σ_e (figure 2a; table 1; SI), within acceptable levels of randomly detecting a statistical significance. Variation in regression lines across 5000 iterations are distributed randomly about the simulated line (figure 3a), with no significant difference between the mean regression slope and the simulation parameter b=0.6 (table 2; SI). In contrast, SDDM coefficients were significantly different from the true parameters (figure 2b) at a rate much higher than the conventionally accepted 5% (table 1; SI). The mean slope of the regression models significantly differed from the simulation parameter b, in a systematically and directional manner (figure 3b; table 2; SI) – SDDM regression coefficients are not only incorrect but grossly misleading. This systematic bias increases with increased noise in the data (table 2) – the more noise there is in the data, the more positive the relationship between y' and x' becomes.

DISCUSSION

By establishing "*a model in which rock area at outcrop was a perfect predictor of sampled diversity*", Smith and McGowan (2007) attempted to create a sampling-driven diversity model. However, their SDDM is not based on any hypothesized or empirical relationship between diversity and sampling, or formulated from first principles. This is in contrast to other well-formulated biological models such as various scaling models where the parameter of interest (i.e. scaling coefficient or the slope of the bivariate relationship) is founded on first-principle theories, e.g. the 2/3 rule for the scaling of area with mass. Rather, the SDDM is based on the assumption that y' and x' (y and x sorted independently of each other) form the expected theoretical bivariate relationship between y and x, which this study shows to be incorrect (figures 2, 3), as one would expect since there is no reason to assume such a thing.

A further and perhaps more serious problem with using a forced pairing of y' and x' is that each data point (pair of y'_i and x'_i) does not represent a natural pairing and has no meaning; the new pairing is actually y_i and x_j, where the ith and jth orders are independent of each other. For instance, using the marine generic diversity and rock area data of Smith and McGowan (2007) (figure 4), the lowest marine generic diversity is in the Cambrian, Tommotian Stage (529 – 521 million years ago [Ma]; genus count = 309), while the smallest marine rock outcrop area (after removing 0 valued data (Smith & McGowan 2007)) is from the Early Permian, Asselian/Sakmarian Stage (299 – 290 Ma; rock area = 1). Similarly, the highest diversity is recorded for the Pliocene (5.3 – 2.58 Ma; genus count = 3911)

while the largest rock area is found in the Cenomanian (100 – 94 Ma; rock area = 373). These two extreme points alone demonstrate that the paired diversity and rock area values are millions of years apart, and are independent of each other (figure 4).

This may be obvious, but independently sorting *y* and *x* has serious statistical consequences. For instance, in Smith and McGowan's (2007) data, $\log_{10}$ marine generic diversity has no significant relationship with $\log_{10}$ rock area in their original paired bivariate data (figure 4; $r^2 = 0.0398$; $p = 0.0979$), but once sorted, has a significantly strong positive relationship with $\log_{10}$ rock area sorted independently of $\log_{10}$ diversity (figure 4; $r^2 = 0.903$; $p < 0.001$). This general pattern is true in at least two more datasets (Benson *et al.* 2010; Benson & Upchurch 2013) (figures S1 and S2). The independent sorting procedure has forced a strong but false linear relationship between two variables that otherwise do not show any significant (or if significant, a very weak) relationship. In fact, two randomly generated deviates (e.g. sampled from a normal distribution) that have no relationship with each other (figure 5a), once sorted independently from lowest to highest will inevitably have a significant and strong relationship ($r^2 = \sim 1$; figure 5b). Perhaps more detrimental, is the fact that the independently sorted bivariate relationship will always be strongly positive – a simulated negative relationship between *x* and *y* (figure 5c) will have a strong and positive relationship once they are sorted independently (figure 5d).

194 In some clades (namely Mesozoic dinosaurs), diversity measures can have very
195 strongly positive relationships with some sampling metrics, such as geological
196 formation counts (β = 0.868; r^2 = 0.85; p < 0.001 (Barrett, McGowan & Page
197 2009)) or fossil collection counts (β = 0.865; r^2 = 0.79; p < 0.001 (Butler *et al.*
198 2011)) , which would justify correcting for such confounding factors, if the
199 sampling metrics were indeed non-redundant with diversity (Benton *et al.* 2011;
200 Benton *et al.* 2013). However, even in such cases, it does not change the fact that
201 the modelled relationship obtained from the SDDM will still be systematically
202 biased (figure 3), and alternative methods should be considered.
203
204 It is problematic to stipulate that this forced relationship is the 'true' relationship
205 between sampled palaeodiversity and the rock record. Our simulations show
206 that regression models fitted on independently sorted data have unacceptably
207 high Type I error rates when the data generation processes are known, meaning
208 that Smith and McGowan's (2007) approach is not statistically viable. In
209 particular, that the slopes are incorrectly estimated at very high rates (~100%
210 when σ_e = 0.5) has severe consequences in that SDDM predictions are
211 systematically biased (figures 2b, 3b), leading to erroneous 'residuals'.
212 Inferences made from such problematic 'residuals' (Smith & McGowan 2007;
213 Barrett, McGowan & Page 2009; Benson *et al.* 2010; Butler *et al.* 2011; Benson &
214 Upchurch 2013) will inevitably be misleading (Brocklehurst 2015), lacking any
215 biological or geological meaning.
216
217 Given our simulations, we strongly recommend against using the SDDM
218 approach in modelling the relationship between palaeodiversity and rock record

219 data; the standard regression using unsorted data is a sensible option. However,
220 using the residuals of a regression model as data for subsequent analyses has
221 also long been known to introduce biased statistical estimates (King 1986;
222 Freckleton 2002). Successive series of modelling removes variance and degrees
223 of freedom from subsequent model parameter estimation, so the final models
224 and statistical analyses do not account for the removed errors appropriately
225 (King 1986). Instead, one can directly model the confounding effects along with
226 effects of interest (e.g. environment, climate, etc) through multiple regressions
227 (OLS, GLMs or generalized least squares [GLS]). In the context of palaeodiversity
228 studies, one can fit a multiple regression model using some diversity metric as
229 the response variable and sampling proxy as a confounding covariate, alongside
230 additional predictor variables such as sea level, temperature, etc. The resulting
231 model coefficients for the environmental predictors would be the effects of
232 interest after accounting for the undesired effects of rock availability. Since
233 diversity measures are frequently taken as counts, it is advisable to use models
234 that appropriately account for errors in count data, such as the Poisson or
235 negative binomial models (O'Hara & Kotze 2010). Whether or not to include time
236 series terms (e.g. autoregressive [AR] terms) depends on the level of serial
237 autocorrelation in the time series data and on sample size; palaeontological time
238 series tend to be short, with 30 time bins or fewer being fairly typical (Mesozoic
239 dinosaurs only span a maximum of 26 geological stages (Butler *et al.* 2011;
240 Benson & Mannion 2012)), in which case complex models face the risks of over-
241 parameterisation. Model selection procedures using the Akaike Information
242 Criterion (Akaike 1973) or similar indices can help make this decision (Burnham
243 & Anderson 2002). However, we do not lightly advocate the use of time series

modelling, especially if the dependent variable, sampled diversity, is in the form of counts, in which case appropriate time series methods are severely under-developed (but see generalised linear autoregressive moving average [GLARMA] models (Dunsmuir & Scott 2015) or Poisson exponentially weighted moving average [PEWMA] models (Brandt *et al.* 2000)), but more importantly since there are more appropriate alternative methods, i.e. phylogenetic approaches (Sakamoto, Benton & Venditti 2016).

Fundamentally, macroevolutionary studies aim to increase our understanding of evolutionary processes (speciation and extinction through time), rather than the resulting patterns or phenomena (sampled diversity, e.g. richness). Thus, we should seek to characterize the process using biologically meaningful and interpretable models instead of describing the patterns. Further, simply exploring error in the fossil record in itself seems rather fruitless because uncertainty depends on the questions being posed; palaeontological studies of macroevolution should be no different than other statistical approaches in the natural sciences in that uncertainty is assessed while exploring the phenomena of interest (Benton 2015). Explicitly phylogenetic approaches (e.g. (Lloyd *et al.* 2008; Didier, Royer-Carenzi & Laurin 2012; Stadler 2013; Stadler *et al.* 2013; Sakamoto, Benton & Venditti 2016) offer the best and most appropriate means to tackle questions of evolutionary processes. Especially when extrinsic causal mechanisms for changes in biodiversity are tested using regression models, ignoring phylogeny is in serious violation of statistical independence (Felsenstein 1985; Harvey & Pagel 1991). It is also worth noting that subsampling approaches (e.g. Alroy's SQS (Alroy 2010a; Alroy 2010b; Alroy

2010c)) are gaining wide popularity as modern methods to account for sampling bias, they are not without problems (Hannisdal *et al.* 2016), and certainly do not take shared ancestry described by phylogeny into account, thus also suffering statistical non-independence (Felsenstein 1985; Harvey & Pagel 1991), and can frequently result in incorrect interpretation of the data. For instance, while recent studies using binned time series approaches (including SDDM and SQS) have led to mixed conclusions regarding the long-term demise of dinosaurs before their final extinction at the Cretaceous-Paleogene (K-Pg) boundary 66 million years ago (Ma) (Barrett, McGowan & Page 2009; Lloyd 2012; Brusatte *et al.* 2015), an explicitly phylogenetic Bayesian analysis has strongly suggested that dinosaurs were indeed in a long-term decline tens of millions of years prior to the K-Pg mass extinction event, in which speciation rate was exceeded by extinction rate and dinosaurs were increasingly incapable of replacing extinct taxa with new ones (Sakamoto, Benton & Venditti 2016). Such evolutionary dynamics cannot be identified using time-binned (tabulated) data. Phylogenetic mixed modelling approaches (Hadfield 2010) further allow the incorporation of confounding variables such as sampling but also environmental effects (Sakamoto, Benton & Venditti 2016). Therefore, in order to advance our understanding of the evolutionary dynamics of biodiversity, speciation and extinction through time (or the underlying process generating the observed patterns in sampled diversity, e.g. taxon richness), while accounting for sampling and phylogenetic non-independence, it is imperative that we have an abundance of large-scale comprehensive phylogenetic trees of fossil (and extant) taxa.

ACKNOWLEDGEMENTS

We thank Jo Baker, Ciara O'Donovan and Henry Ferguson-Gow for discussion and insightful comments. We also thank Neil Brocklehurst and Michel Laurin for reviewing this manuscript and providing helpful commentary. We have no conflicts of interest.

DATA ACCESSIBILITY

This manuscript does not include data.

FUNDING

MS and CV are funded by Leverhulme Trust Research Project Grant RPG-2013-185 (awarded to CV). MJB is funded by Natural Environment Research Council Standard Grant NE/I027630/1.

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413

SUPPORTING INFORMATION

SI-text. Supporting information and results pertaining to the effects of sample size (Tables S1 and S2) as well as examples of discrepancies between original paired bivariate relationship and the independently sorted relationship from the literature (Figs S1 and S2).

TABLES

Table 1. Type I error rates (%) for SRM (Standard Regression Model) and SDDM (Sampling-Driven Diversity Model) estimates (intercept α and slope β) across residual error (σ_e).

σ_e	SRM		SDDM	
	α	β	α	β
0.05	5.34	4.90	26.1	28.5
0.10	4.84	4.92	40.2	48.4
0.25	4.82	4.78	57.3	91.3
0.50	5.48	5.14	68.7	100.0

Table 2. *t*-test results between mean regression slopes of 5000 iterations and the theoretical slope $b = 0.6$, for SRM (Standard Regression Model) and SDDM (Sampling-Driven Diversity Model) across residual error (σ_e).

σ_e	SRM			SDDM		
	mean-slope	***t*-value**	***p*-value**	**mean-slope**	***t*-value**	***p*-value**
0.05	0.6	1.230	0.220	0.602	20.9	0
0.10	0.6	-1.790	0.073	0.607	46.0	0
0.25	0.6	-0.042	0.967	0.646	131.0	0
0.50	0.6	0.685	0.493	0.775	244.0	0

FIGURES

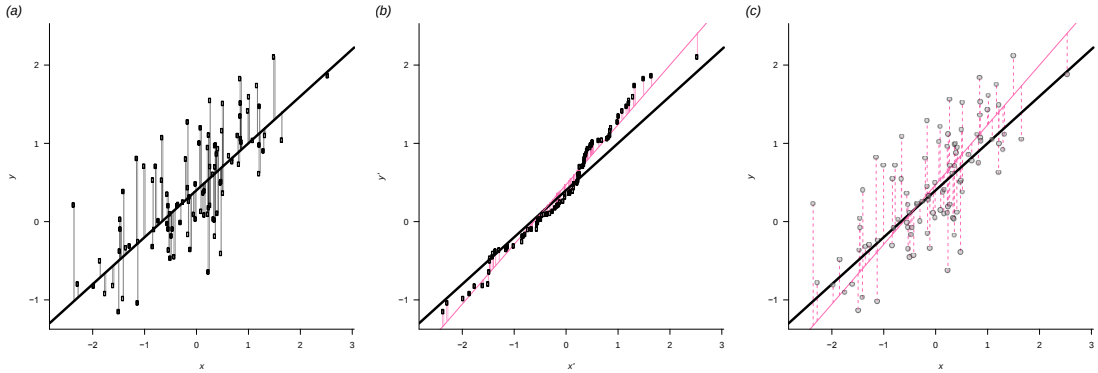


Figure 1. Procedure for generating 'residuals' from a sampling-driven diversity model. (a) A paired, bivariate dataset x (sampling proxy) and y (sampled diversity) was simulated so that x is randomly drawn from a normal distribution ($\mu = 0$, $\sigma = 1$) and y is calculated as $y = a + bx + e$ where $a = 0.4$, $b = 0.6$ and e is noise ($\mu = 0$, $\sigma = 0.5$). The thick black line is the expected relationship $Y = a + bx$. Vertical lines represent the true residuals or deviations in y from the thick line. (b) Following Smith and McGowan (2007) x and y are sorted from low to high values independent of each other (x' and y' respectively), and an ordinary least squares (OLS) regression model (pink line) is fitted to y' on x'. Despite the pink line supposedly representing the data generating process, it is clear that it is not a good estimator of the true known generating process, the thick line. (c) The OLS model from (b) is used as the sampling-driven diversity model (SDDM) or the expected relationship between y and x, from which 'residuals' are computed as the deviations in y from the pink line (vertical pink dotted lines). It is immediately clear that there is a substantial difference between the true residuals (a) and the SDDM 'residuals' (c).

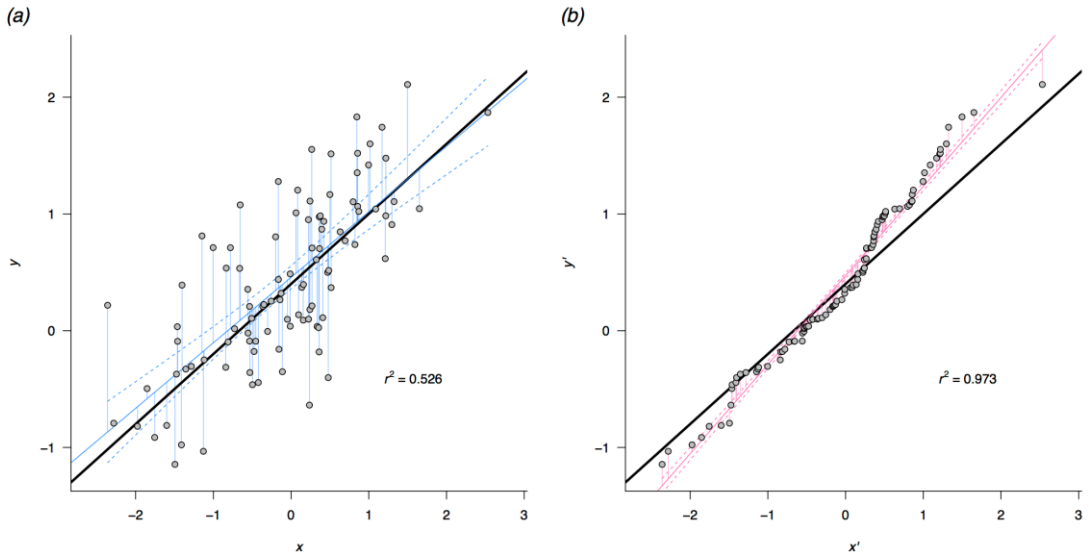


Figure 2. Regression modelling on a decoupled bivariate dataset fails to estimate the simulation slope parameter. (*a*) A bivariate dataset (*y* and *x*) was generated so as to follow a theoretical relationship (thick line) with intercept $a = 0.4$, slope $b = 0.6$ and noise (e [$\mu_e = 0$, $\sigma_e = 0.5$]). The best-fit regression line (blue) is not significantly different from the theoretical line (dashed 95% confidence intervals encompass the thick line; see table 1 for Type I error rates over 5000 simulations), with *y* and *x* forming a moderately strong relationship ($r^2 = 0.526$) appropriate for the degree of *e* modelled. Regression model residuals (vertical lines) show no structure, as expected. (*b*) The bivariate data in (*a*) were sorted independently of each other (*y*' and *x*'), to which a regression model was fitted. The best-fit sampling-driven diversity model (SDDM) regression line (pink) deviates strongly from the theoretical relationship (dashed 95% confidence intervals do not encompass the thick line; table 1), and *y*' and *x*' form a very strong (but false) linear relationship ($r^2 = 0.973$). Regression residuals (vertical lines) show clear structure. One pair of model comparison out of 5000 simulations is shown.

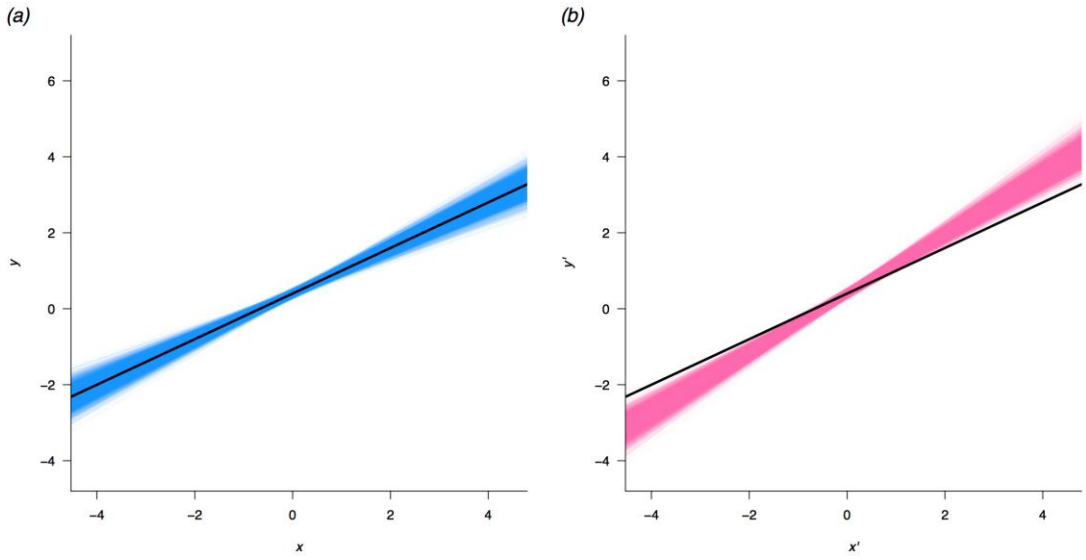
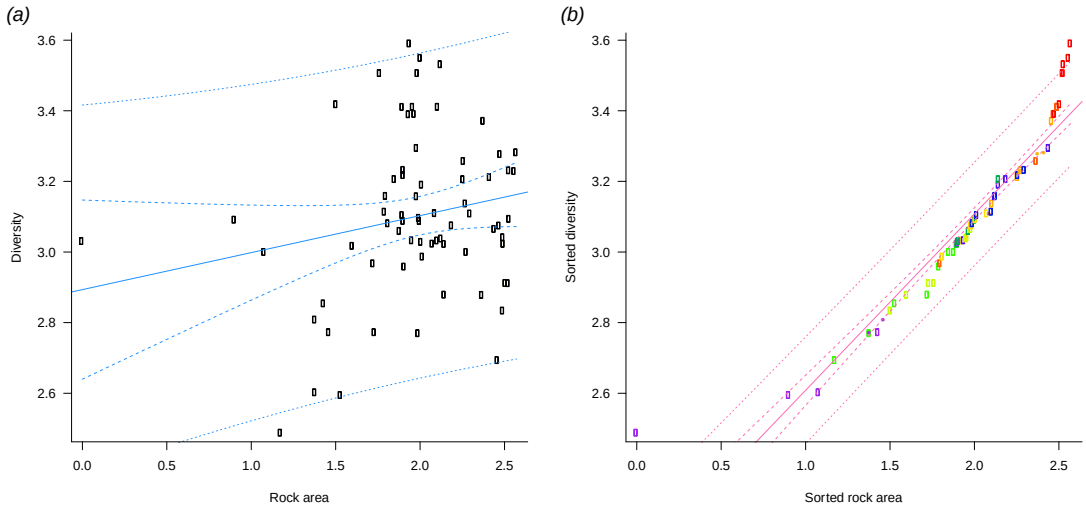


Figure 3. SDDM regression predictions are systematically biased. (*a*) Standard regression lines (blue) for 5000 simulated datasets at $\sigma_e = 0.5$ deviate randomly around the theoretical relationship (thick line) with the mean slope showing no significant difference from the theoretical slope $b = 0.6$ (table 2). (*b*) SDDM regression lines on decoupled datasets (pink) deviate systematically away from the theoretical relationship (thick line), with a significant difference between the mean regression slope and the theoretical slope (table 2).



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477 Figure 4. The difference between the original paired, bivariate relationship (a)
478 and the forced, false relationship (b) shown using the data from Smith and
479 McGowan (2007). Log-transformed marine generic diversity has a non-
480 significant and weak relationship with log-transformed rock area (β = 0.105; r^2 =
481 0.0398; p = 0.0979; a). However, once diversity and rock area are sorted
482 independently of each other following Smith and McGowan (2007), then the
483 relationship becomes significant and strong (β = 0.499; r^2 = 0.903; p < 0.001; b).
484 Points are coloured according to their geological age with cooler colours on the
485 older and warmer colours on the younger ends of the time scale. Filled and
486 outline colours in (b) correspond to the ages of the rock record and diversity
487 respectively, and demonstrate visually the mismatch between *y*' and *x*'. Dashed
488 lines are confidence intervals, while dotted lines are prediction intervals.

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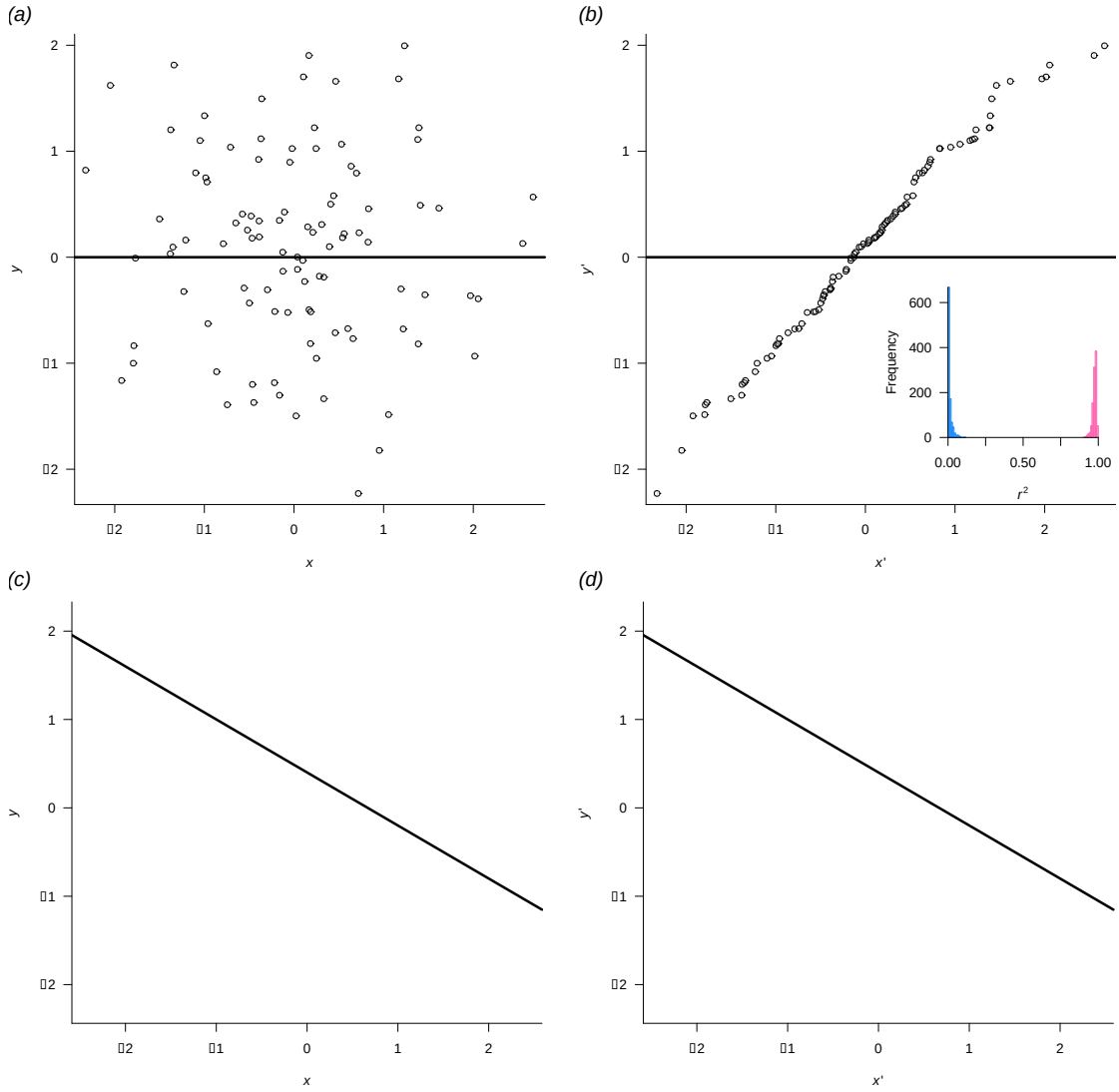

Figure 5. Independently sorting any two variables results in a forced positive relationship. (*a*) Two randomly generated variables *y* and *x* show no significant relationships across 1000 simulations, with the slopes of the regression lines (blue) distributed around the expected slope of zero. (*b*) When regression models are fitted on independently sorted datasets (*y*' and *x*'), estimated slopes are significantly different from the expected value of zero, and result in a strong positive relationship (r^2 = ~1; inset pink) despite the unrelated nature of the original datasets (r^2 = ~0; inset blue). (*c*) A bivariate dataset (*y* and *x*) was generated so as to follow a theoretical relationship (thick line) with intercept a = 0.4, slope b = -0.6 and noise (e [μ_e = 0, σ_e = 0.5]). Standard regression lines (blue)

deviate randomly around the theoretical relationship with the mean slope showing no significant difference from the theoretical slope b = -0.6. (d) However once sorted independently, regression lines (pink) deviate systematically away from the theoretical relationship, with all estimated slopes being positive. Thus SDDM slope estimates are systematically and directionally biased.