**Wekiva Basin MFL Draft Report -Comments on behalf of Orlando Utilities Commission 2-14-24:**

**Previous comments made during MFL meetings and emailed to Andrew Sutherland 1/25/24:**

1) Arcadis on behalf of OUC submitted comments dated Oct. 19, 2018 and Dec. 11, 2018 on the HSPF and HEC-RAS models developed for the Wekiva River Basin MFL. These comments are posted on the District website. We do not see a memo prepared by the District that addresses these or other public comments. It also doesn't appear that any changes were made in the final modeling report to address these comments. There is a memo addressing the peer reviewers comments, but we do not believe these responses fully address our concerns. Please let us know if there is a response memo that can be posted to the website.
2) Do we know the likely cause or causes of the apparent deviations in the patterns of change for spring flow and spring level for some springs? (The deviation is particularly notable for Rock Springs in Figure 9 of the draft report MFL reevaluation report where after the x-axis tick mark in 2016 the flow data appear to be generally rising while the level data appear to be generally falling.)
3) The Minimum Frequent High (FH) and Minimum Average (MA) for the Little Wekiva River were not met under the no-pumping condition, making these metrics not useful for establishing MFLs. Do we know the likely cause or causes of these event-based metrics not working for this system? It would be good to understand how the Hardwood Swamp can persist at elevations above the modeled no-pumping condition hydrology considered necessary for maintenance of this habitat type. Could this be related to seepage or maintenance of unmeasured saturation or water levels existing in backwater areas of the floodplain (e.g., overtopped natural levees and relatively impermeable sediments in the floodplain)? Similarly, understanding how the thick organic soils (normally used in establishing the MA) can persist despite lack of support from the modeled no-pumping condition hydrology would be useful to understand.
4) The FH and MA were also deemed inappropriate for Rock Spring/Run because if used they would have allowed much larger flow reductions than those typically found to be protective for springs, rivers, or lakes. Do we know the likely cause or causes of these event-based metrics not being appropriate for this system?

**Additional Comments based on reviewing the draft MFL report:**

5) Since the recommended MFL condition in the basin equals average pumping for the period of 2014-2018, and any pumping above that amount is believed to create impacts, are impacts currently being observed based on the 2023 pumping which would help verify the recommended MFL condition?
6) Does the Lake Prevatt connection to the UFA influence the springs in the Wekiva Basin? Since the Prevatt MFL is currently being re-evaluated and peer reviewer comments have been made to incorporate a larger drainage basin which would bring more flow to the lake, could this potentially affect the UFA and the Wekiwa Springs analysis for the Wekiva Basin MFL?

7) The Wekiva Basin MFL POR did not include Hurricane Ian in 2022. Has the District compared the current levels in the basin to average POR levels or the end of POR levels to see if any adjustments to the long-term predictions may be warranted?
8) Some inflows have been reduced to the Wekiva Basin for a number of years due to septic-to-sewer projects and FDEP nutrient reduction limits for treated wastewater discharges within the basin. There are also septic to sewer projects currently taking place near the Wekiva State Park in Seminole County. Has the District considered this change when assessing whether pumping is causing flow reductions within the basin?
9) From the draft MFL report, Table 1 provides a good qualitative summary of the description of the variable nature of data collection frequency and data gaps for the water level and flow gaging stations used for the Wekiva River basin MFLs, but Table 2 summarizes discharge statistics as if the entire period of record was used. Was any weighting by data frequency used? For some of these, wouldn't the POR discharge largely reflect more recent sampling at a higher frequency? For example, Rock Springs POR dates back to 1931 but measurements were rare until 1999 when they became continuous, so wouldn't the summary statistics be heavily influenced by the 1999-present data instead of the entire POR?
10) Comparisons of two different y-axis on the same graph (i.e., Figures 6, 8, 9, and 10) can be problematic. In these cases the water level range has been compressed to prevent the points from overlapping the discharge points to a great extent. Two graphs temporally-aligned and immediate above one another with their own floating (allowed to vary y-axis) might make any patterns easier to see.
11) A suggestion to check subject verb agreement in this sentence on page 26 "Urban land, which includes residential, industrial and commercial uses, make up approximately 27.7% of basin area." (Perhaps "lands" would be better than "land" for the verb "make up".
12) A suggestion that an Oxford comma may be helpful after prairie in sentence on page 27 "The most common communities in the Rock Springs sub-basin are uplands, hardwood swamp, hydric hammock, wet prairie and forested flatwoods depressions (Table 6)."
13) This statement on page 54 represents a fairly critical assumption: "SJRWMD acknowledges that the MFLs analyses assume that hydrological history will repeat itself. Given the uncertainties in future rainfall and temperature predictions by global climate models, this assumption is thought to be appropriate but needs to be regularly tested by implementing an adaptive management strategy." Although adaptive management is a reasonable response to relatively high uncertainty, perhaps some quantification of current climate change projections for rainfall and ET at least could be provided as part of a sensitivity analysis to violation of this assumption.
14) In the sentence on page 61 "This cyclic wet/dry regime imparts a unique chemical environment that has promotes nutrient cycling and supports floodplain biotic communities (Wharton et al. 1982).", the word "has" appears to be redundant.
15) For the rivers listed in "Table 13. Return intervals for 30-day flooding events for hardwood swamp communities at 14 Florida river system transects.", presumably these are considered unimpacted or minimally impacted systems in order to serve as reference rivers for the SWIDS development?
16) On page 96 in the statement "the freeboard is expresses as "greater than"", it is recommended the verb be changed to "expressed".

17) In Appendix B, “The HSPF model was calibrated from 2003 to 2016, and the unsteady HEC-RAS model was calibrated between the period of 1/20/2009 to 7/20/2009.” These time periods seem relatively short for calibration, particularly the six months for the HEC-RAS. Is a justification provided for the short periods and are there any concerns about statistical inference based on these relatively short calibration periods?
18) In Appendix B “Hargraves-Samani method” should probably be “Hargreaves-Samani method”
19) In Appendix B, the Annual PET in Figure 5 appears to show a downtrend over the period studied. Is there a statistically-significant downtrend? If so, does this nonstationarity in the data cause any concerns with respect to the inference from the models. That is, if there is a trend in PET that continues at what point would we be extrapolating beyond calibration conditions? (As a side note, based on review of other datasets, it appears that the maximum and minimum daily temperatures have both been trending up over this period and that variability between daily high and low may be in the process of becoming less variable over time which could have implications for the calculation of PET. (The Hargreaves equation uses the difference between daily high and low temperature where larger daily ranges are assumed to allow more ET.)
20) In Appendix B, Figure 12 may have a misspelling in the title on the graphic that mentions “Old Railroad Brigde”.
21) In one of the supporting documents to Appendix B (Seong, C.H. and A.E. Wester. 2019. Wekiva River hydrology and hydraulic modeling for minimum flow and level evaluations. SJRWMD Final Report. Online resource, accessed 2024-02-10. https://www.sjrwmd.com/static/mfls/MFL-Wekiva/Technical_Report_WekivaMFL_2019_0417.pdf), we noticed that Figures 43-49 from this report positioned the simulated stage on the y-axis and observed on the x-axis. We strongly recommend putting the observed on the y and the simulated on the x for the reasons explained in this report: Pineiroa, G., S. Perelmanb, J. P. Guerschmanb, J.M. Parueloa. 2008 How to evaluate models: Observed vs. predicted or predicted vs. observed? Ecological Modelling 216: 316–322. The comparison of observed vs. predicted should only be made to the 1:1 line to evaluate model bias and fit when observed is plotted on the y-axis, not the x.
22) Reviewing Figures 43-49 noted above, assessment of the observed vs. modeled plot is impaired by the axes chosen for the plot as discussed above. However, most of the plots show bias in that the simulated values tend to be above the actual values. Based on the consistency of these departures and the short period of evaluation (i.e., six months), what are the implications for statistical inference?
23) In Seong and Wester (2019) missing data for Miami, Palm, Rock, Sanlando, Starbuck, and Wekiva were filled using the Line of Organic Correlation method which is appropriate. However, Helen, Island (needs capitalization in text “Helen, island, and Sulphur springs have relatively…”), and Sulphur springs were filled using linear regression. Why use linear regression for gap-filling when it is known to not preserve the characteristics of the probability distribution of the data (as noted Helsel and Hirsch 2002 as cited earlier in this report)?
24) The method used for “remaining springs” is a little unclear. It is stated “The flows of these springs were estimated using the ratio of mean flows of observation data with the corresponding mean flows of nearby springs.” Is the idea that nearby data rich springs with similar flows for dates for data poor springs would be used for extending the record by establishing a proportional relationship? Was only a single spring chosen to represent each data poor spring?

25) In Appendix F, the approach of investigating Indicators of Hydrologic Alteration as an alternative view of changes in hydrology between the no pumping and current pumping is very beneficial because of the complexity of hydrologic variability in flowing water systems that may not be fully characterized by existing MFL approaches. There are a few questions related to its application here that we would appreciate clarification on:
    a. Appendix F includes the text "According to IHA developers, a deviation factor at or above 10% (i.e., 0.10) is an indicator that instream habitat is sensitive to and could be harmed by flow reduction (Richter et al. 2011)." A brief review of this paper found that the authors stated that changes in "daily flow alterations" less than or equal to 10% would provide a "high level of protection" and the "natural structure and function of the riverine ecosystem will be maintained with minimal changes. The authors indicate that daily flow alteration changes between 11-20% are expected to cause "moderate changes in structure and minimal changes in function" while changes >20% are predicted to cause major changes in structure and function. Two questions are raised here, first, does the District view a change in any deviation factor as equivalent to the "daily flow alterations" specified in this publication or if not, is there other information making the two concepts essentially equal for practical applications. Secondly, is the Appendix F conclusion that the IHA results indicate that the current pumping condition is not overly constraining because some of the deviations are greater than 10% consistent with the idea that up to 10% of change is expected to cause "minimal changes" to the natural structure and function? (This may be clarified somewhat in a statement in Appendix E where the 10% is "deemed protective for large river systems with outstanding biological / ecological attributes (Acreman and Ferguson 2010; Richter et al. 2011)".)
    b. Additional detail about the resampling method used to assess significance for the EFC parameters would be helpful. Presumably, the results for the NP and CP groups were randomly assigned to groups and the median difference recalculated 1000 times to develop a confidence interval and a one-tailed probability value is provided, but clarification would be appreciated.
    c. Were there any efforts made to control experiment-wise error in the resampling method used for the IHA Parameters and the EFC Parameters? If not, the following concern may apply to both tables. For example, for the 32 EFC components in Table F-3, 15 are bolded as "significant" at an apparent alpha of 0.05. However, if these are 32 independent tests performed simultaneously then the probability that at least one will yield false significance at a test alpha of 0.05 would be 83.4%, i.e., highly likely. One alternative would be to use the Bonferroni correction to control experiment-wise error which would drop the test alpha to 0.05/32 = 0.0015625. At this test alpha only up to 4 of the 32 appear to be significant (determination for 2 of the 4 is uncertain based on the number of decimal places presented in the report). For Table F-2, Appendix F indicates 14 of the 30 IHA Parameters are significant at (presumably) a test error rate of 0.05. With a Bonferroni correction this would be 0.05/30 = 0.0017, the number still significant would drop to 9 of the 30.

26) In Appendix C, we recommend a change from “effect” to “affect” in this sentence: “Magnitude and duration components define the critical ecological events that effect species at an individual level…”
27) In Appendix C, the Wekiva Maple Island Transect included a stretch of “Hardwood swamp / hydric hammock” in the range of 660-980 station distance. Were these points included in the calculation of the mean elevation of hardwood swamp for MFL purposes or were only the pure “hardwood swamp” point elevations included? If the hybrid habitat elevations were included it could be questionable since the Hydric Hammock may reflect higher elevations and the lower elevation swamps aren’t distinguished by this combined habitat grouping. Other transects also included long stretches of the hybrid habitat types.
28) “Figure C-31. SSURGO soil map at the Wekiva Flats Transect” was obscured by a white-filled square. The same issue occurred with two other similar figures: Figure C-32. SSURGO Soil map at Maple Island Transect and Figure C-33. SSURGO soil map at Wekiva Railroad Transect.
29) We couldn’t find the Literature Cited entry in the main report for the reference “(Kozlowski 1997)” provided in Appendix C. Another one missing appeared to be: “(Rowe and Catlin 1971)”.
30) There doesn’t appear to be any text in Appendix C introducing Tables C-41 through C-48 (the velocity-related metrics). Please consider introducing them or possibly moving tables to Appendix E which references algal scour analyses, and potentially adding text there.
31) In Appendix E, the graphic caption “A clear positive relationship (increasing concentration with increasing discharge) is evident from this comparison (Figure E-48).” May be a bit strongly worded as the wide 95% confidence intervals (i.e., the line could be center-rotated flat or nearly flat within the intervals) suggest this may not be a statistically significant relationship. Some clarification on whether this relationship is statistically significant would be helpful.
32) In the Appendix E section “WRVS ASSESSMENT ATTACHMENT 2 - JANICKI ENVIRONMENTAL, INC. WATER QUALITY GRAPHS”, while it is logical to present the plots of the various water-quality constituents against time as a line plot, it is unclear why the plots of the constituents against flow are presented using lines, since lines imply some relationship between the points connected by lines (such as a temporal order) that doesn’t necessarily exist in the latter case. In addition, outliers are identified on the graphs but it isn’t clear whether outlier identification was manual or relied on an algorithm. Finally, were outliers excluded from the linear and quadratic fit lines provided on the graph?

# How to Evaluate Models: Observed vs. Predicted or Predicted vs. Observed?

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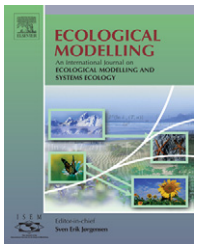

# How to evaluate models: Observed vs. predicted or predicted vs. observed?

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ABSTRACT

A common and simple approach to evaluate models is to regress predicted vs. observed values (or vice versa) and compare slope and intercept parameters against the 1:1 line. However, based on a review of the literature it seems to be no consensus on which variable (predicted or observed) should be placed in each axis. Although some researchers think that it is identical, probably because $r^2$ is the same for both regressions, the intercept and the slope of each regression differ and, in turn, may change the result of the model evaluation. We present mathematical evidence showing that the regression of predicted (in the *y*-axis) vs. observed data (in the *x*-axis) (PO) to evaluate models is incorrect and should lead to an erroneous estimate of the slope and intercept. In other words, a spurious effect is added to the regression parameters when regressing PO values and comparing them against the 1:1 line. Observed (in the *y*-axis) vs. predicted (in the *x*-axis) (OP) regressions should be used instead. We also show in an example from the literature that both approaches produce significantly different results that may change the conclusions of the model evaluation.



## 1. Introduction

Testing model predictions is a critical step in science. Scatter plots of predicted vs. observed (or vice versa) values is one of the most common alternatives to evaluate model predictions (i.e. see articles starting on pages 1081, 1124 and 1346 in *Ecology* vol. 86, No. 5, 2005). However, it is unclear if models should be evaluated by regressing predicted values in the ordinates (*y*-axis) vs. observed values in the abscissas (*x*-axis) (PO), or by regressing observed values in the ordinates vs. predicted values in the abscissas (OP). Although the $r^2$ of both regressions is the same, it can be easily shown that the slope and the intercept of these two regressions (PO and OP) differ. The analysis of the coefficient of determination ($r^2$), the slope and the intercept of the line fitted to the data provides elements for judging and building confidence on model performance. While $r^2$ shows the proportion of the total variance explained by the regression model (and also how much of the linear variation in the observed values is explained by the variation in the predicted values), the slope and intercept describe the consistency and the model bias, respectively (Smith and Rose, 1995; Mesple et al., 1996). It is interesting to note that even in widely

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**Table 1 – Number of papers published in *Ecological Modelling* in 2000 using different types of model evaluation**

| | Total papers | Papers that evaluate models | Papers plotting predicted and observed data | Using visual graph interpretation, $r^2$ or other method | Estimating intercept or slope |
|---|---|---|---|---|---|
| Predicted vs. observed (PO) | | | 11 | 6 | 5 |
| Observed vs. predicted (OP) | | | 6 | 2 | 4 |
| Both regressions | | | 2 | 1 | 1 |
| Total | 204 | 61 | 19 | 9 | 10 |

used software packages (like Statistica or Math Lab), default scatter plots available to evaluate models differ in the variable plotted in the *x*-axis. Is it important to care on what to put in each axis? Do scientists care?

Quantitative models are a common tool in ecology as shown by (Lauenroth et al., 2003), who found that 15% of the papers published in *Ecology* and 23% of the ones published in *Ecological Application* contained some dynamic quantitative modeling. In order to analyze how ecologists evaluate their quantitative models we reviewed all articles published in the journal that more focuses on quantitative modeling (*Ecological Modelling*): For year 2000 we selected the papers that used either PO or OP regressions to evaluate their models. The papers were considered in the analysis if a model was evaluated. Articles that evaluated a model using the regression of predicted vs. observed (or vice versa), were separated in two categories: those that considered slope or intercept in the analysis and those that used only visual interpretation of the data or $r^2$. We found 61 papers out of 204 published during 2000 in *Ecological Modelling* that evaluated models and 19 of them did it by regressing either PO or OP data (Table 1). Papers that did not use regression techniques evaluated model predictions mostly based on plotting observed and predicted values both in the *y*-axis, and time (or some other variable) in the *x*-axis. Thus, most papers did not present a formal evaluation of their models at the level of the prediction although they have data to do so. Almost half of the 19 papers that evaluated a model using regression techniques performed just a visual interpretation of the data or used only the $r^2$. The other half estimated the regression coefficients and compared them to the 1:1 line. Of these 19 papers, 58% regressed PO data, 32% regressed OP values and 10% did both analyses. The survey showed that regression of simulated and measured data is a frequently used technique to evaluate models, but there is no consensus on which variable should be placed in each axis.

Several methods have been suggested for evaluating model predictions, aimed in general to quantify the relative contribution of different error sources to the unexplained variance (Wallach and Goffinet, 1989; Smith and Rose, 1995; van Tongeren, 1995; Mesple et al., 1996; Monte et al., 1996; Loehle, 1997; Mitchell, 1997; Kobayashi and Salam, 2000; Gauch et al., 2003; Knightes and Cyterski, 2005). The use of regressions techniques for model evaluation has been questioned by some authors (Mitchell, 1997; Kobayashi and Salam, 2000). However, the scatter plot of predicted and observed values or vice versa is still the most frequently used approach (as shown in our survey). Thus, it seems that plotting the data and showing the dispersion of the values is important for scientists (an often undervalued issue), that probably promote authors to use graphic plots of predicted and observed data. However, we think that this approach should be complemented (not substituted) by other statistics that add important information for model evaluation as suggested further on.

In this article we show that there are conceptual and practical differences between regressing predicted in the *y*-axis vs. observed in the *x*-axis (PO) or, conversely, observed vs. predicted (OP) values to evaluate models. We argue that the latter (OP) is the correct procedure to formulate the comparison. Our approach includes both an empirical and algebraic demonstration. We also use a real example taken from the literature to further show that using a PO regression can lead to incorrect conclusions about the performance of the model being analyzed, and suggest other statistics to complement model evaluation.

## 2. Materials and methods

Since the slope and intercept derived from regressing PO or OP values differ, we investigated which of the two regressions should be used to evaluate model predictions. We constructed a *X* vector with continuous values ranging from 1 to 60.

$$X = \{1, 2, 3, \ldots 60\} \quad (1)$$

*Y* vectors were constructed to have either a linear, quadratic or logarithmic relationship with the *X* vector

$$Y_{\text{Lin}} = X + \varepsilon \quad (2)$$

$$Y_{\text{Quad}} = -0.05X^2 + 3X + \varepsilon \quad (3)$$

$$Y_{\text{Ln}} = 30\ \text{Ln}(X) + \varepsilon \quad (4)$$

where $\varepsilon$ is a random error with normal distribution (mean = 0, Stdev = 15). Both vectors *X* and *Y* are named as observed *X* and observed *Y*, since they mimic data normally observed or measured in the experiments. Using regression analyses we adjusted a linear, quadratic or logarithmic model for each *Y* vector (see examples in Fig. 1a–c, respectively):

$$\hat{Y}_{\text{Lin}} = aX + b \quad (5)$$

$$\hat{Y}_{\text{Quad}} = aX^2 + bX + c \quad (6)$$

$$\hat{Y}_{\text{Ln}} = a\ \text{Ln}(X) + b \quad (7)$$

Eqs. (5)–(7) allowed us to generate a vector of predicted values $\hat{Y}$. Each $\hat{Y}$ vector contains 60 $\hat{y}_i$ predicted values for each $x_i$

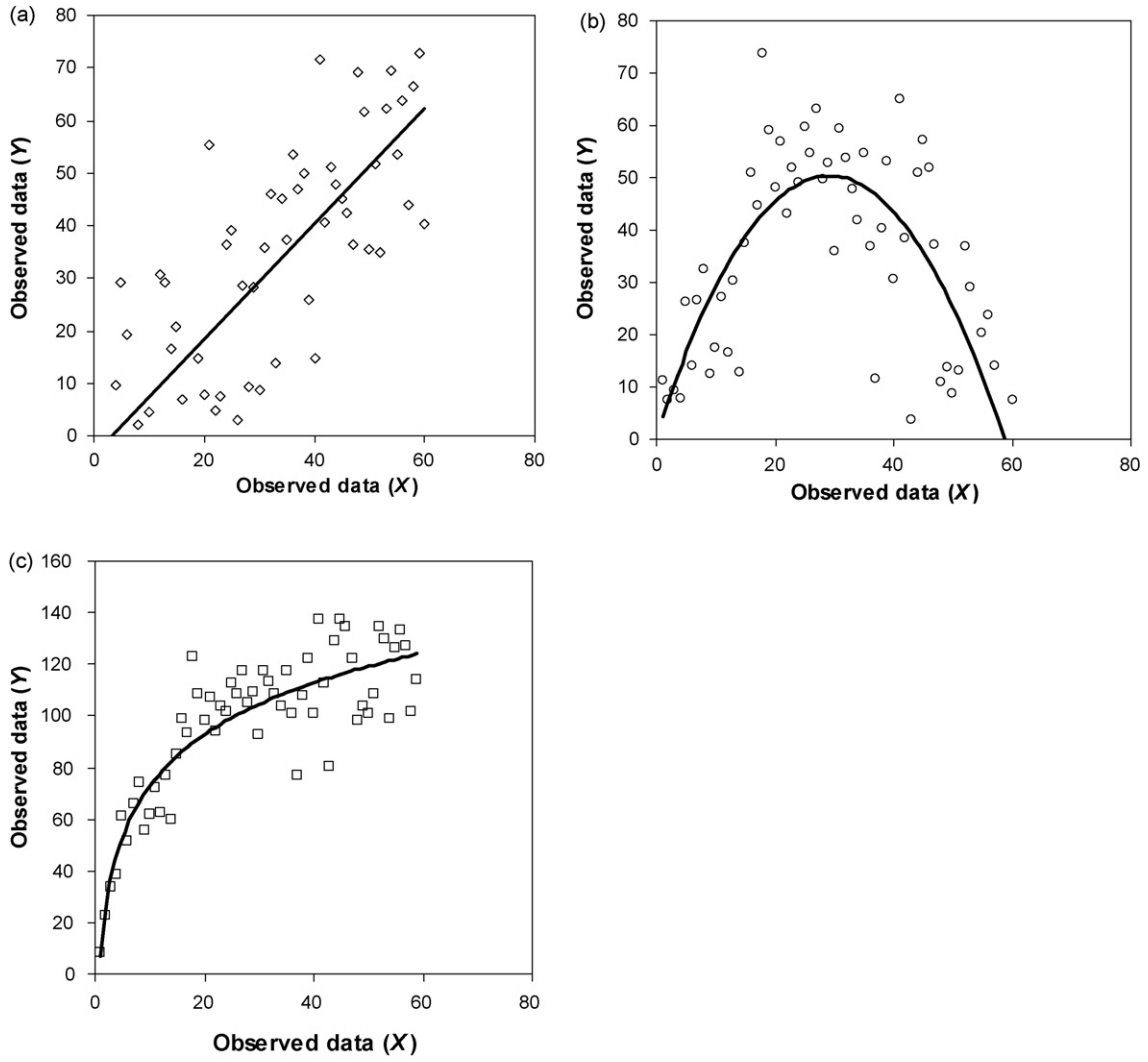


**Fig. 1 – Examples of regressions generated using X and Y vectors. (a) Linear $Y_{Lin} = X + \varepsilon$, (b) quadratic $Y_{Quad} = -0.05X^2 + 3X + \varepsilon$, and (c) logarithmic $Y_{Ln} = 30\,Ln(X) + \varepsilon$. Y vectors have a random error with normal distribution, mean = 0 and Std = 15.**

value of the X vectors. We repeated this procedure 100 times for each type of model obtaining 300 pairs of Y and $\hat{Y}$ vectors, each one with 60 elements. We evaluated model predictions ($\hat{Y}$) by plotting and calculating the linear regression equations of each paired Y (observed values) and $\hat{Y}$ (predicted values) vectors, for either PO ($\hat{y} = b_1 y + a_1$) and OP ($y = b_2 \hat{y} + a_2$) values. We then plotted the distribution of slope and intercept parameters achieved in the 100 simulations for the linear models. Since the same data were used to construct the model and to evaluate model predictions, we expect no bias in the slope nor the intercept of the regression between Y and $\hat{Y}$. Thus, $b_1$ and $b_2$ should be 1, and $a_1$ and $a_2$ should be 0.

In a second step, we further demonstrate analytically our empirical findings using basic algebra. In this mathematical approach we illustrate the relationship between $a_1$ and $a_2$, and between $b_1$ and $b_2$. We also relate both slopes to $r^2$.

Finally, we took an example from the literature and analyzed the effects of evaluating model predictions by regressing either PO or OP values. The paper by (White et al., 2000), presented regressions of predicted (in the ordinates) vs. observed (in the abscissas) (PO) values and had a table with the data used, so it was easy to generate the opposite regressions of OP values. We compared the regression parameters of both approaches and tested the hypothesis of slope = 1 and intercept = 0 to assess statistically the significance of regression parameters. This test can be performed easily with statistical computer packages with the models:

$$y_i - \hat{y}_i = a_1 + b_1 y_i + \varepsilon_i \quad (8)$$

$$\hat{y}_i - y_i = a_2 + b_2 \hat{y}_i + \varepsilon_i \quad (9)$$

The significance of the regression parameters of these models corresponds to the tests: $b_1$, $b_2 = 1$ and $a_1$, $a_2 = 0$, for either regression of PO (Eq. (8)) or OP values (Eq. (9)). If the null hypothesis for the slope is rejected the conclusion is that model predictions have no consistency with observed values. If this hypothesis is not rejected but the hypothesis for the intercept is, then the model is biased. If both null hypotheses are not rejected, then disagreement between model predictions and observed data is due entirely to the unexplained variance.

We also calculated for Whites et al.'s, data, Theil's partial inequality coefficients ($U_{bias}$, $U_{slope}$ and $U_{error}$), which separate total error of the predictions (the squared sum of the predictive error), into different components and complement the assessment of model performance made with the regression (Smith and Rose, 1995; Paruelo et al., 1998). Theil's coefficients partition the variance of observed values not explained by the predicted values (called the squared sum of the predictive error), being: $U_{bias,}$ the proportion associated with mean differences between observed and predicted values, $U_{slope}$ the proportion associated with the slope of the fitted model and the 1:1 line, and $U_{error}$ the proportion associated with the unexplained variance (see Paruelo et al., 1998, for a simple formula to calculate Theil's coefficients). Additionally, we estimated for White et al.'s data the root mean squared deviation (RMSD) as

$$\mathrm{RMSD} = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2} \tag{10}$$

which represents the mean deviation of predicted values with respect to the observed ones, in the same units as the model variable under evaluation (Kobayashi and Salam, 2000; Gauch et al., 2003).

## 3. Results and discussion

Since model predictions were tested using the same data used in their construction (the same Y vector), commonly called an evaluation of the calibration procedure, the regression of PO values is expected to have no bias from the 1:1 line. As a consequence, we expected that the parameters of the regression $\hat{y} = b_1 y + a_1$, be: $b_1 = 1$ and $a_1 = 0$. The dispersion of the data is a consequence of the random error introduced in the process of model generation. However, as shown in Fig. 2a, when regressing PO data the slope $b_1$ was always lower than 1 (and the most frequent value was similar to $r^2$) and the intercept $a_1$ was always higher than 0. Only when the regression was performed with OP data $y = b_2\hat{y} + a_2$, then $b_2 = 1$ and $a_2 = 0$ (Fig. 2b). This empirical analysis suggests that regressions to evaluate models should be performed placing observed values in the ordinates and predicted values in the abscissas (OP). The same results were obtained for the quadratic and logarithmic models (data not shown).

These results can be also demonstrated algebraically. The slope of the regression of PO values ($b_1$) can be calculated as

$$b_1 = \frac{S\hat{y}y}{Syy} \tag{11}$$

where $S\hat{y}y$ is the sum of the cross products of centered predicted and observed values and Syy is the sum of squares of centered observed values. The slope of the regression of OP values ($b_2$) can be calculated as

$$b_2 = \frac{S\hat{y}y}{S\hat{y}\hat{y}} \tag{12}$$

where $S\hat{y}\hat{y}$ is the sum of squares of centered predicted values. The coefficient of determination of the regression of PO values ($r_1^2$) is then:

$$r_1^2 = \frac{(S\hat{y}y)^2}{Syy\ S\hat{y}\hat{y}} \tag{13}$$

and the coefficient of determination of the regression of OP values ($r_2^2$) is

$$r_2^2 = \frac{(S\hat{y}y)^2}{S\hat{y}\hat{y}\ Syy} \tag{14}$$

thus, the two coefficients of determination are equal, and also related to $b_1$ and $b_2$ as

$$r_1^2 = r_2^2 = b_1 b_2 \tag{15}$$

Considering once more that our vector $\hat{Y}$ was estimated from the vector X and Eqs. (2), (3) or (4), and that because of that the relation between Y and $\hat{Y}$ is exact, with no distortion or bias, then each observed value can be defined as prediction plus a random error ($y_i = \hat{y}_i + \varepsilon_i$). Consequently:

$$\begin{aligned} S\hat{y}y &= \sum_{i=1}^{n}(\hat{y}_i - \hat{\bar{y}})(y_i - \bar{y}) = \sum_{i=1}^{n}(\hat{y}_i - \hat{\bar{y}})y_i = \sum_{i=1}^{n}(\hat{y}_i - \hat{\bar{y}})(\hat{y}_i + \varepsilon_i) \\ &= \sum_{i=1}^{n}(\hat{y}_i - \hat{\bar{y}})\hat{y}_i + \sum_{i=1}^{n}(\hat{y}_i - \hat{\bar{y}})\varepsilon_i = \sum_{i=1}^{n}(\hat{y}_i - \hat{\bar{y}})^2 = S\hat{y}\hat{y} \end{aligned} \tag{16}$$

We demonstrated that $S\hat{y}y = S\hat{y}\hat{y}$ if $y_i = \hat{y}_i + \varepsilon_i$. Thus, we confirm algebraically that for our experiment $b_2 = 1$ and that $b_1 = r^2$, founded on Eqs. (11), (12) and (15). Consequently, $b_1$ will be always smaller than 1 when any $\varepsilon_i \neq 0$. Additionally, since:

$$a_1 = \hat{\bar{y}} - b_1\bar{y}, \qquad a_2 = \bar{y} - b_2\hat{\bar{y}} \tag{16}$$

and because $b_1 = r^2$, then $a_1 = 1 - r^2$ (always >0) when observed and predicted values have the same mean (model predictions are not biased). In identical conditions $a_2 = 0$, because $b_2 = 1$. However, in real comparisons between observed and predicted values, $b_1$ will approximate $r^2$ when $b_2$ approximates to 1.

The theoretical evidence presented before shows that the proper slope and y-intercept to compare observed and predicted values must be calculated only by regressing OP data. A spurious estimate will be obtained by regressing PO values. Wrong conclusions on model performance will be drawn in the latter case. Eq. (15) also revealed that the differences between the two slopes calculated will increase as $r^2$ decreases. In addition, in Eq. (8) the error term represents the variation in the predicted values and residuals are independent of the observed values. In the second Eq. (9) the residuals are independent of the predicted values which are what we want to evaluate. This line of reasoning adds additional theoretical basis for using Eq. (9) of OP values instead of Eq. (8) of PO values in model evaluation.

The reanalysis of the data presented by (White et al., 2000), showed with real data that slope and intercept vary when regressing OP values instead of PO values, changing the results

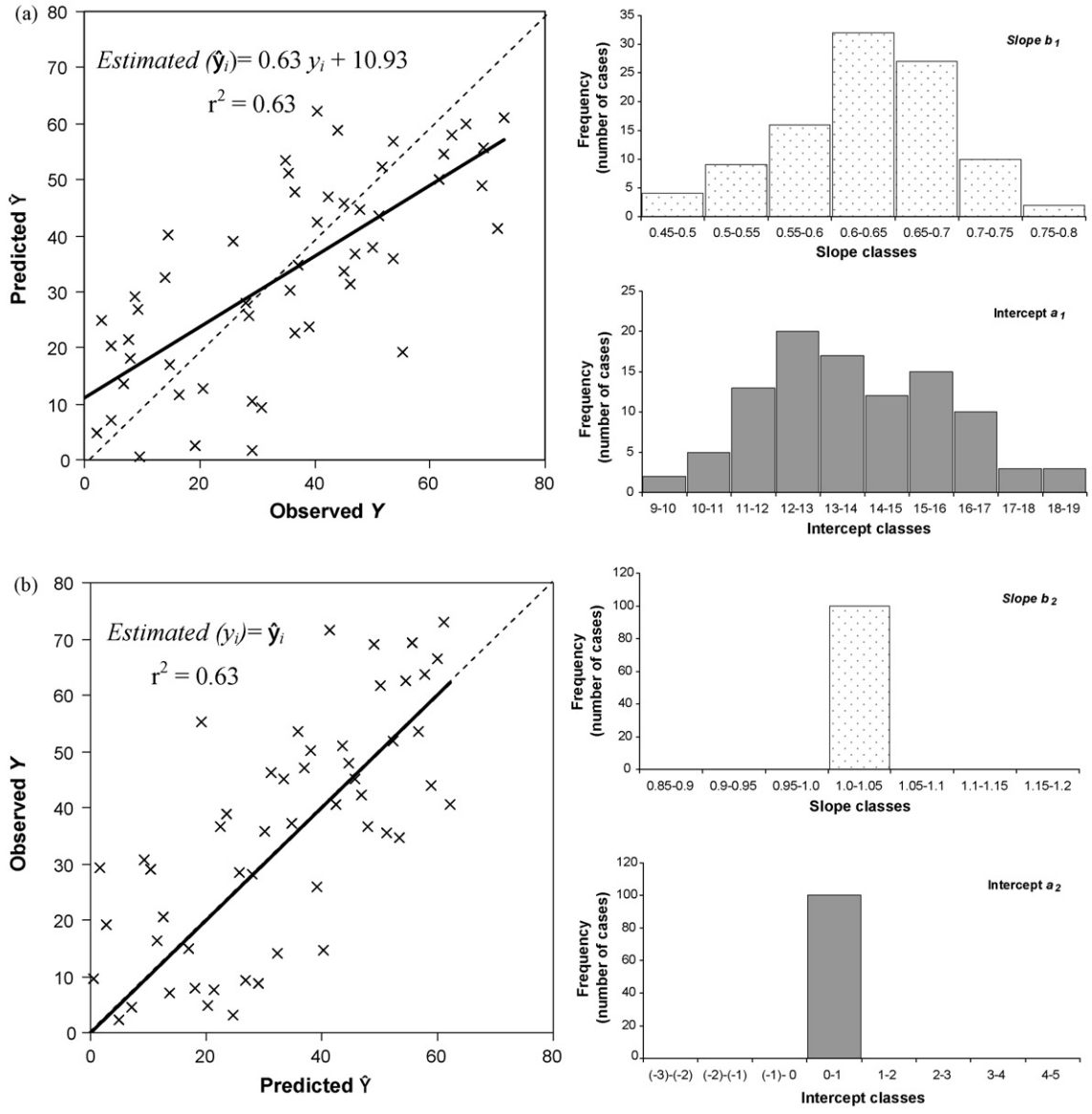


**Fig. 2 – Predicted vs. observed (a) (PO) and observed vs. predicted (b) (OP) regression scatter plots derived from the linear model presented in Fig. 1a. Regression equations are shown in the graphs. Small graphs show the distribution of slope and intercept estimates obtained from regressing 100 paired Y and Ŷ vectors either as PO (a) and OP (b).**

of the analysis. In their paper, White and collaborators used a simple physiological model for estimating biomass accumulation in New Zealand vegetation. Model predictions were compared with observed values collected in several studies. The slope of the regression of PO values of total biomass presented by the authors in their Fig. 3, differed by 0.40 units from 1, while the slope of regressing OP values differed by only 0.27 units (almost half) (Fig. 3a and b). Looking at the graphs we can state that the authors probably thought that their model overestimated observed data at low values and underestimated it at high values, thus the slope of the regression was significantly different from 1.

Opposite results are obtained when testing the significance of the intercept and the slope for both regressions. For total biomass records in White et al. (2000), the intercept and slope were significantly different from 1 and 0 when regressing PO data as the authors did ($p = 0.024$ and $p = 0.0059$, respectively), but they were both not significant with the correct regression of OP values (Table 2). The conclusions of model evaluation changed completely when exchanging the variables plotted in each axis. The regression of OP values (Fig. 3b) showed that the model had a similar bias throughout all the range of values and that the slope did not differ significantly from 1 (Table 2). Theil's coefficients also showed that most of the errors in model predictions were due to unexplained variance (77%), and not to bias or slope misleading (Table 2).

The lack of symmetry in the computation of several parameters when regressing OP or PO, has been noted by several authors, but not thoroughly examined (Kobayashi and Salam, 2000; Gauch et al., 2003). Mitchell (1997) writes in page 315: "*Prediction and observation are plotted on a scatter graph. For the*

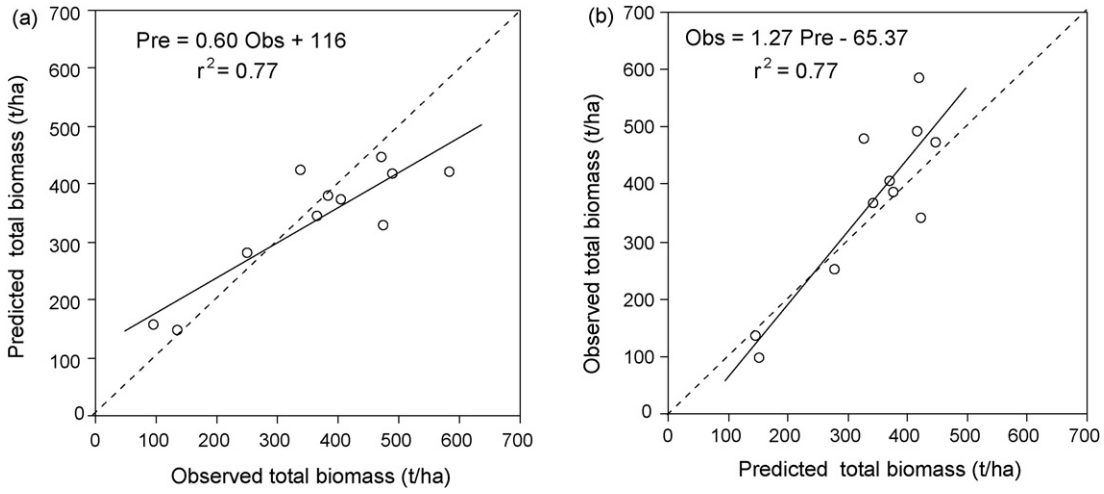


**Fig. 3 – Predicted vs. observed (a) (PO) and observed vs. predicted (b) (OP) regression scatter plots of data from White et al., 2000. (a) is Fig. 3 presented in White et al. paper's and (b) is the regression obtained with the same data but changing the variables from one axis to the other. Note that although $r^2$ is the same, regression coefficients (that describe the similarity of the regression line with the 1:1 line) change notably.**

*purpose of the arguments set out below it makes little difference whether predictions or observations are the independent variable on the x-axis*". Smith and Rose (1995) suggested in page 53 that Theil's coefficients and goodness of fit analysis are easy to perform when regressing OP values, and "*not as straightforward*" to calculate when regressing PO values. Here we have shown that this last approach is, simply, incorrect.

The validity of $r^2$ in regressions of predicted and observed values has been questioned, because it characterizes the mean deviation of observed values (placed in the y-axis) from the regression line (the regression sum of squares divided by the total sum of squares). It may have little importance to evaluate how much the observed values differ from the regression line of OP values (Kobayashi and Salam, 2000; Gauch et al., 2003). However, although the $r^2$ can be estimated by dividing the regression sum of squares by the total sum of squares, it can be also calculated from Eq. (14). This equation shows that $r^2$ also represents the proportion of the linear covariance of $y$ and $\hat{y}$, with respect to the total variance of $y$ and $\hat{y}$. In this sense, the $r^2$ indicates how much of the linear variation of observed values ($y$) is explained by the variation of predicted values ($\hat{y}$). Linearity between observed and predicted values can be tested following (Smith and Rose, 1995). Thus, the $r^2$ of OP values is a valid parameter that gives important information of model performance.

Conversely, the root mean squared error (RMSE) a commonly used statistic to show model performance (Weiss and Hays, 2004; Doraiswamy et al., 2005; Lobell et al., 2005), should not be applied for the regression of OP data, instead the root mean squared deviation (RMSD) (see Eq. (10)) should be reported (Wallach and Goffinet, 1989; Kobayashi and Salam, 2000; Gauch et al., 2003). The RMSE is a proxy of the mean deviation (not exactly the mean because it is squared and divided by $n-1$) of values in the y-axis against the regression line. When reporting the RMSE for the OP or PO regression, we are not estimating the mean deviation between estimated and predicted data. Instead, we are estimating the root mean squared error of the observed values against the regression line of observed vs. predicted values (in the case of regressing OP) and the root mean squared error of the predicted values against the regression line of predicted vs. observed values (in the case of PO). The correct comparison is to calculate the deviation of each predicted values against the 1:1 line and not against the regression line of either OP or PO. RMSE will be always smaller than RMSD and thus represents an underestimation of the real error between observed and

**Table 2 – Regression parameters and hypothesis testing for PO or OP regressions, from data presented in White et al. (2000)**

| | Predicted vs. observed (PO) | Observed vs. predicted (OP) |
|---|---|---|
| $a$ | 116.9 | −65.37 |
| Significance of Test $a=0$ | 0.024 | 0.44 |
| $b$ | 0.60 | 1.27 |
| Significance of Test $b=1$ | 0.0059 | 0.27 |
| $U_{bias}$ (%)[a] | – | 0.11 |
| $U_{slope}$ (%)[a] | – | 0.12 |
| $U_{error}$ (%)[a] | – | 0.77 |
| RMSD (tons/ha) | – | 82.6 |

Theil's partial inequality coefficients and the root mean squared deviation (RMSD) are shown when applicable. RMSD estimates the mean deviation of predicted values respect to the observed ones, in the same units as the model variable under evaluation.

[a] Theil's coefficients partition the variance of observed values not explained by the predicted values (called the squared sum of the predictive error), being: $U_{bias}$, the proportion associated with mean differences between observed and predicted values, $U_{slope}$ the proportion associated with the slope of the fitted model and the 1:1 line, and $U_{error}$ the proportion associated with the unexplained variance.

simulated values. For example, in White's and collaborators paper the RMSD was 82.6 tons/ha (Table 2), while the RMSE changed between the regression of PO and OP values (52.7 and 76.2 tons/ha, respectively), and is always smaller than RMSD.

## 4. Conclusions

We showed empirically and demonstrated analytically that model evaluation based on linear regressions should be done placing the observed values in the *y*-axis and the predicted values in the *x*-axis (OP). Model evaluation based on the opposite regression leads to incorrect estimates of both the slope and the *y*-intercept. Underestimation of the slope and overestimation of the *y*-intercept increases as $r^2$ values decrease.

We strongly recommend scientists to evaluate their models by regressing OP values and to test the significance of slope = 1 and intercept = 0. This analysis can be complemented by decomposing the variation of observed values not explained with the predictions (the squared sum of the predictive error), through calculating Theil's partial inequality coefficients (*U*). The coefficient of determination $r^2$ can be used as a measure of the proportion of the variance in observed values that is explained by the predicted values. If replicates of observed values are available then a goodness of fit test can be performed following (Smith and Rose, 1995). RMSE should not be reported for the OP regression, but the RMSD adds important information to model evaluation.

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