

Bill Shipley, November 4 2015

Evaluation of the structural equations model described in the document entitled  
“March 2015 proposed approach for Minnesota’s sulfate standard to protect wild  
rice” by the Minnesota Pollution Control Agency, dated March 24, 2015.

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### Background qualifications

I am the author of 16 papers published in peer-reviewed scientific journals dealing with the development (Shipley, 1997, 1999a; Shipley, 1999b; Shipley, 2000a, 2003a, b, 2009, 2013) or ecological application of structural equations modelling (Shipley & Meziane, 1998; McKenna & Shipley, 1999; Meziane & Shipley, 1999a, b, 2001; Shipley *et al.*, 2005; Vile *et al.*, 2006; Thomas *et al.*, 2007; Sonnier *et al.*, 2010) and am the author of a scientific monograph, published by Cambridge University Press on structural equations modeling (Shipley, 2000b). The second edition of this book will be published in April 2016.

### Scientific evaluation

In any predictive model such as proposed in the report by Minnesota Pollution Control Agency (hereafter called the MPCA report), there are two important questions to ask: (1) What is the “within-sample” predictive ability of the model? (2) Can the predictions of the model be extended to new observations (i.e. observations that were not used to develop the model)? I explain each of these in turn, their relationship to the statistical analysis in the report, and my summary conclusions for each.

#### *The “within-sample” predictive ability*

In order to evaluate the within-sample predictive ability of a statistical model, we need a statistical measure of the degree of difference between the observed values of the dependent variable (here, porewater sulfide concentration) and the values that are predicted by the model (Equation 2 in the MPCA report). In other words, if the model predicts a value of (say) 100 micrograms/L, then what is the range of the true (observed) values in the data? A model whose predicted values are consistently higher

or lower than the actual values is said to be statistically “biased”. A model whose predicted values are not consistently high or low, but whose predicted values are far from the actual values is said to be statistically “imprecise” and to lack predictive ability.

There are different ways of quantifying this “within-sample” predictive ability and the authors of the MCPA report use the “model  $R^2$ ” as a measure of “within-sample” predictive ability. This statistic is the proportion of the total variance in the observed values that is captured by the predictive model, and varies from 0 to 1. A value of 0 means that the model has no predictive capacity (you can get just a good a prediction by ignoring the model completely). A value of 1 means that the model perfectly predicts the observed values (you would get exactly the same values if you use the prediction equation as if you actually measured porewater sulfide concentration directly). Equivalently,  $1-R^2$  measures the proportion of the total variance that is *not* captured by the predictive model.

The authors report a “model  $R^2$ ” value of 0.44 on page 13<sup>1</sup> and so the proportion of the total variance in the observed porewater sulfide concentration that is *not* captured by the model is  $1-0.44=0.66$ . This is a first indication that the within-sample predictive ability of the model is poor since more variance in the actual values of porewater sulfide concentration is left unexplained than the proportion that the model succeeds in capturing. Actually, although not explicitly stated in the MCPA report, the authors must have first transformed all of their original variables to logarithms<sup>2</sup> and so the reported model  $R^2$  of 0.44 actually refers to the logarithm of porewater sulfide; this means that the  $R^2$  using the original units would be even lower. This is a rather poor level of “within-sample” predictive ability.

In principle, the authors should also have reported the “95% confidence intervals of the observations” which gives the upper and lower bounds in which 95% of the observed values would fall for a given

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<sup>1</sup> This is actually for a multiple regression but the authors state (pages 12, 13) that the SEM-derived equation is essentially equal to this multiple regression.

<sup>2</sup> Two reasons: First, Equation 3 is presented as an allometric equation but the model is linear, not multiplicative and so the logarithms of the variables must have been used. Second, Figure 9 is shown with logarithmic axes.

prediction. Since the authors don't give this information, we can get an approximate idea of this range by looking at Figure 9 of the MCPA report, in which each point gives each actual observed porewater sulfide concentration (x axis) and the value predicted by the model (y axis). Note that the axes on this graph are on a logarithmic scale. The horizontal red dotted line in this Figure 9 (i.e. that cuts the y axis at a value of 165) shows when the model predicted value of porewater sulfide is at the critical level of 165. The actual observed concentrations of porewater sulfide in samples whose predicted value is 165 (judging visually, since the exact values are not provided in the MCPA report) range from around 24 to around 3020 micrograms/L. This range covers almost the entire range of observed values in the data set. In other words, when the model predicts that a lake will have a porewater sulfide concentration at the target value of 165 (and therefore would be judged in an acceptable range), about half the time the actual concentration will be more than this (i.e. has a porewater sulfide concentration that puts Wild Rice at risk) and can even reach concentrations that are over 18 times higher than predicted.

There are other problems in the "within-sample" predictive ability of this model that are clear from Figure 9 of the MCPA report. An unbiased model will have (i) the points distributed equally above and below the solid blue diagonal line (this is the line along which the observed and predicted values are equal) and (ii) the scatter above and below this line will be of the same magnitude all along this line. In fact, we see that above about 250 micrograms/L, there is no longer any relationship between the observed values (x axis) and the model predicted values (y axis); the observed values go up to over 3000 but the model predictions never go over about 414. Even when the actual observed values are as low as 20 micrograms/L the model predictions go up to almost the maximum values of around 414, and certainly above the target value of 165 micrograms/L. There is therefore clear model bias in these data.

***My conclusion, based on the regression fit of the MCPA's Equation 3, their (almost) equivalent SEM-derived equation 2, and their Figure 9, is that this prediction equation has quite poor "within-sample"***

***predictive ability and could not reliably distinguish between lakes whose porewater sulfide concentration is below or above the critical value.***

*Can the predictions of the model be extended to new observations (i.e. observations that were not used to develop the model)?*

Everything said above refers to the “within-sample” predictive ability. In other words, it tells us how well the model can predict the actual porewater sulfide concentrations when we already know the answer, because the predictions are based on the same observations that were used to develop the model. What we really want to know is the extent to which the prediction equation could predict the actual porewater sulfide concentrations in the sediment of some new lake (or the same lakes at some new time). In order to judge this, we first have to know if the underlying causal processes that are involved in generating the independent variables in our predictive equations, and generating these new porewater sulfide concentrations, are the same as those assumed when developing the original predictive model or not? If the answer is “yes” then we can use our equation, assuming that it has acceptable within-sample predictive ability. If the answer is “no” then it is critical to know the cause – effect links between the four variables in the predictor equation. If some of the predictor variables in the equation do not actually cause changes in porewater sulfide concentrations then the predictor equation might not correctly predict porewater sulfide concentrations when used in new observations even if its “within-sample” predictive ability is high.

There are two ways to decide. One way is to perform controlled experiments in which we experimentally and directly manipulate each of the predictor variables (surface water sulfate, sediment iron, sediment organic content) and see if this changes the measured porewater sulfide concentration. However, the authors only experimentally manipulated one of these variables (surface water sulfate). They found that experimentally changing the surface water sulfate did change the porewater sulfide concentration. Since

we have no experimental evidence showing a causal effect from each of the other two predictor variables and porewater sulfide concentration, we cannot simply assume that the causal relationships between these two variables and porewater sulfide concentration would remain the same in new observations.

The other way to decide is to propose an hypothesis linking these predictor variables to porewater sulfide concentration as a system of cause – effect relationships and test this causal hypothesis using a statistical method known as structural equations modelling (SEM). If the SEM properly represents the actual cause – effect links between the variables in the model then the observed pattern of “covariation” between the variables will be the same as the pattern of “covariation” between the variables that is predicted by the SEM, except for random sampling variation. A statistician would say: “if the causal processes generating the data are correctly represented in the structural equations, then the sample covariance matrix will equal the model predicted covariance matrix, up to sampling fluctuations”. Therefore, instead of experimental manipulations, one would propose how the predictor variables and porewater sulfide in the prediction equation interact as a causal system. In order to claim that the predictor equation should continue to apply to new samples, it is necessary that the predictor variables be causes, rather than effects, of porewater sulfide or simply variables that covary with porewater sulfide because they share common causes with porewater sulfide. The authors do propose an SEM (Figure 7 of the MCPA report) and the three proposed predictor variables for the predictor equation (sediment organic carbon, sediment iron and surface water sulfate concentrations) are each (indirect) causes of porewater sulfide in this proposed SEM.

To measure the degree of difference between the observed and predicted covariance matrices, the authors of the MCPA report use the “maximum likelihood chi-square statistic”. The greater the difference between the observed and predicted covariance matrices, the larger the value of this

statistic. One can calculate the probability of any given degree of difference between these two matrices arising purely by chance due to sampling fluctuations; this is called the “null probability”. If this is the case, then the “null probability” of the SEM will be high; the usual criterion is that this null probability be above 0.05.

The hypothesised causal model is shown in Figure 7 of the MCPA report. The reported null probability of this SEM (Appendix 1) is 0.36 and so this would be evidence in favour of accepting the hypothesis that the causal relationships among the predictor variables in Nature are as specified by the SEM. This, in turn, would provide justification for assuming that the predictor equation would continue to provide the same (poor) level of predictive ability in new observations.

However, there are three key problems with the SEM in Figure 7 of the MCPA report, which make me doubt that the analysis was done correctly.

Problem 1: the possibility of alternative viable structural equation models.

The SEM is shown graphically in Figure 7 (page 12) based on a “simplified” multivariate causal hypothesis that is presented in Figure 5 (page 10). Appendix 1 (pages 23 – 24) presents further statistical details of the model. The SEM in Figure 7 presents one of several other models that were evaluated (page 11, final paragraph) but these alternative models are not presented in the report nor is any information given concerning their statistical fit to the empirical data or why they were rejected in favour of the model presented in Figure 7. This lack of information on alternative models is worrisome because if alternative structural equations models exist that cannot be rejected based on standard statistical criteria then this means that there might be viable alternative causal explanations for the empirical data. If some of these alternative, but acceptable, models do not have each of the predictor variables as causes of porewater sulfide, then this raises doubts about the ability of the predictor equation to generalize to new conditions.

Problem 2: incorrect model degrees of freedom.

The appendix (page 23) lists 3 “degrees of freedom” for the SEM. The degrees of freedom, along with the maximum likelihood chi-square statistic, jointly determine the null probability and thus the statistical significance of the fit between the model and the data. It is only because the multivariate causal hypothesis represented by the SEM in Figure 7 could not be statistically rejected that the SEM can be considered as a viable causal representation of the biological process. This statistical justification is given in Appendix 1 (page 23) when it reports that the model chi-squared statistic is 3.23, the model degrees of freedom are 3, and therefore that that probability of observing at least this degree of difference between the model and the data by chance, assuming that the model is correct, is high (0.3572).

The degrees of freedom for any SEM are given by the following formula:

$$df = \frac{v(v+1)}{2} - p$$

Here, “v” is the number of observed variables in the model (there are 6 observed variables in Figure 7) and “p” is the number of “free parameters” in the model. A “free parameter” is a parameter (a path coefficient, a variance, a covariance) whose value must be estimated from the data rather than imposed based on the causal hypothesis. In Figure 7 there are 8 path coefficients, 3 exogenous variances (for sediment iron, sediment organic carbon, and surface water sulfate) and 3 endogenous error variances (associated with the remaining 3 variables). There are no free covariances indicated in Figure 7.

Therefore, there are 7 degrees of freedom for this model. However, the model degrees of freedom reported in the Appendix were 3 rather than 7. Therefore, the model shown in Figure 7 is not the same model as reported in the appendix yet the decision to accept it is based on the results reported in the appendix.



Problem 3: The path coefficients in Figure 7 do not match those reported in Appendix 1

Another reason to believe that the SEM in Figure 7 is not the same as the SEM reported in Appendix 1 is that some of the values of the path coefficients in Figure 1 do not match those reported in the first table of the Appendix (page 23). For instance the direct effect of Sediment iron on porewater iron is given as 0.79 in Appendix 1 (a standardized value of 0.40) but in Figure 7 the value is given as 0.77. A bigger discrepancy is the direct effect of surface water sulfate on porewater sulfide. Figure 7 reports a value of 0.57 but Appendix 1 reports a value of 0.14.

**In summary, I cannot know if the causal assumptions represented in Figure 7, which (if correct) would justify using the prediction equation on new observations, are correct or not because I am not convinced that the correct SEM (i.e. the one in Figure 7) was actually tested. In other words, even if the prediction equation had good “within-sample” predictive ability (it doesn’t), we could not know if we could apply this equation to new observations (i.e. new lakes, or the same lakes after surfacewater sulfate concentrations have been limited by legislation).**

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## Curriculum vitae

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### Degrees

BSc (honors) Bishop's University, 1983

PhD University of Ottawa, 1987

### Evidence of professional impact

#### (1) Editorships/scientific committees

North American Editor: <i>Annals of Botany</i> since 2001
Subject editor: <i>Global Ecology and Biogeography</i> 2010-2014
Subject editor: <i>Ecoscience</i> since 2011
Editor: <i>Ecology and Ecological Monographs</i> - 2002 -2005
Editor: <i>Population and Community Biology series</i> , Springer Publishing 2005 - 2007
Editor: <i>Canadian Journal of Botany</i> 1996-1998
Member of the College of Reviewers for the Canada Research Chairs since 2001
Member of Grant Selection Committee 18 (Ecology and Evolution) of NSERC 1998-2001
External evaluator for the Centre National de Recherche Scientifique (France) 2002

#### (2) Prizes and awards

Prix de la recherche et de la création (UdeS) 2006
Research scholarship MENRT from French Government 1999

#### (3) Invited speaker

Intensive course in structural equation modelling, Wageningen University (Netherlands), 2015
Workshop: Theories and Methods in Spatial Community Modelling Lausanne (Switzerland) 2015
Intensive course in structural equation modelling, CNRS Montpellier (France), 2015
Workshop of Case Studies of Causal Discovery with Model Search. Carnegie Mellon University, Pittsburgh. 2013
Eco-Stats Symposium, Sydney, Australia, 2013
Exploratories Research Group, Eisenach, Germany 2012
Institute of Ecology, University of Jena, Germany 2012

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UFZ Helmholtz Centre for Environmental Research, Halle Germany 2012
Workshop in "Current Perspectives in Functional Ecology", Amsterdam 2008
Nordic Informatics Network in the Agricultural Sciences invited lecturer. Mustiala Finland 2007
FastTrack Initiative on Plant Functional Traits (Alicante, Spain) 2007
GLOBIMED workshop, Placencia Spain. 2006
Virginia Tech 2005
Ecological Society of America (Montréal 2005)
Ecological Society of America 3-8 August 2003, Savannah Georgia USA.
16th Annual Conference, Ecological Society of Germany, Switzerland & Austria. May 28 - June 1 2003, Copenhagen.
McDonnell Foundation Workshop Dallas, Texas USA January 9-11 2003
Santa Fe Institute USA /May 22-26, 2002
Montpellier (France) 1998
Ecological Society of America 1997
Utrecht (Holland) 1997

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**Peer-reviewed articles (total) : 108**

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