Bidimensional regression: Issues with interpolation

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Abstract

We investigated the interpolation of missing values in data that were fit by bidimensional regression models. This addresses a problem in spatial cognition research in which sketch maps are used to assess the veracity of spatial representations. In several simulations, we compared samples of different sizes with different numbers of interpolated coordinate pairs. A genetic algorithm was used in order to estimate parameter values. We found that artificial inflation in the fit of bidimensional regression models increased with the percent of interpolated coordinate pairs. Furthermore, samples with fewer coordinate pairs resulted in more inflation than samples with more coordinate pairs. These results have important implications for statistical models, especially those applied to the analysis of spatial data.

Keywords: regression, bidimensional regression, interpolation, sketch maps, genetic algorithm

Introduction

Bidimensional regression is a statistical technique for assessing the relationship between two configurations of related, two-dimensional data. The method was originally introduced by Tobler (1965, 1994) for the analysis of geographical data. More recently, the method has been adopted by psychology (Friedman & Kohler, 2003) and computer science (Kare, Samal, & Marx, 2010). Bidimensional regression has been used for the geometric analysis of ancient and modern maps (Tobler, 1994), fictional maps (Louwerse & Benesh, 2012), and mental maps with sighted (Schinazi, Nardi, Newcombe, Shipley, & Epstein, 2013; Weisberg, Schinazi, Newcombe, Shipley, & Epstein, 2013) and blind or visually impaired individuals (Jacobson, 1998; Jacobson & Kitchin, 1995; Schinazi, 2008). The method has also been successfully used in conjunction with eye tracking studies (Fourtassi et al., 2013), in the assessment of face familiarity (Kare et al., 2010), and in the comparison of shapes of skulls and leaves (Tobler, 1994).

Similar to unidimensional regression, bidimensional regression uses changes in one (predictor) variable to predict changes in the other (criterion) variable. This relationship is invariant to global transformations in terms of scale, rotation, and translation. Bidimensional regression is also characterized by a statistical model for which an equivalent number of predictor and criterion coordinate pairs are necessary. However, this requirement can sometimes be difficult to fulfill for situations in which the criterion variable is missing values.

Missing values can be particularly problematic for situations in which the fit of the regression model is considered as a proxy for the veracity of spatial representation. In order to account for such possibilities, participants are often given a fixed list with all the landmarks that have to be drawn (Giannopoulos, Kiefer, & Raubal, 2013; Guzmán-Muñoz & Johnson, 2008; Ishikawa, 2013; Lloyd, 2005; Uttal, Friedman, Hand, & Warren, 2010) or small cardboard pieces representing landmarks that have to be placed on blank, grid paper (Waller, Loomis, & Haun, 2004; Waller, Loomis, & Steck, 2003). These approaches have had the advantage of producing balanced sets of landmarks that can be analyzed using bidimensional regression. One possible disadvantage is that the concept of "landmark" can be defined differently depending on the situation and the individual (Raubal & Winter, 2002). In addition, these methods may constrain the data provided by participants (Kitchin & Blades, 2002) and thus inflate the overall fit of the regression model. In other studies, researchers have tried to account for the issue of missing values (representing missing landmarks) in sketch maps by developing customized algorithms that categorically or metrically evaluate landmark placement (Gardony, Brunyé, Mahoney, & Taylor, 2013). Here, we used several simulations in order to investigate the conditions under which another type of interpolation may or may not be appropriate for bidimensional regression.

One possible method for interpolating missing spatial data is to replace them with values that maximize the fit of a regression model. This is essentially the same as using the predicted values of one variable given the observed values of another variable. This method of interpolation has several advantages over other methods (e.g., eliminating participants with a large amount of missing data; Schafer and Graham, 2002). For example, interpolation maintains statistical power and uses all of the available data (Schafer

& Graham, 2002). However, this interpolation of missing values may also lead to an artificial inflation of the fit of the regression model.

For the present simulations, we used sets of coordinate pairs with numbers of values that corresponded to those typically seen in spatial cognition research (Guzmán-Muñoz & Johnson, 2008; Ishikawa & Montello, 2006; Ishikawa, 2013; Lloyd, 2005; Schinazi, 2008; Uttal et al., 2010). We predicted that the artificial inflation of the fit of the bidimensional regression models would increase as the number of values in each coordinate set decreased (given an equal proportion of interpolated values). A bidimensional regression model that is used to fit fewer points may be more flexible because of the coarseness of the "fit surface" (i.e., the shape of the function relating parameter values to the overall fit of the model). Alternatively, if each interpolated value is considered a freely varying parameter, then the model with more points may be more flexible (Lewandowsky & Farrell, 2010). Similarly, given an equal number of values overall, we expected a greater proportion of interpolated values to result in more inflation in the fit of the bidimensional regression models.

To anticipate, we found a very large, artificial inflation in the fit of bidimensional regression models after the interpolation of varying numbers of values. The number of free parameters (in terms of the number of interpolated values) did affect the extent of this inflation. However, models to which fewer values were submitted fit better than models to which more values were submitted, even though the latter models contained more free parameters. This pattern of results was also replicated using data from a real world study (see Weisberg et al., 2013).

Method

Bidimensional regression models were fit to (different) randomly generated sets of coordinate pairs using a program written in MATLAB (MathWorks®, Natick, MA, USA). Each individual number was randomly generated from a uniform distribution between -1 and 1. The first set of coordinate pairs represented the two-dimensional predictor coordinates, and the second set of coordinate pairs represented the two-dimensional criterion coordinates. One variable, "number of coordinates," was manipulated between simulations and represented the number of coordinate pairs within each set. Either 10 or 40 coordinate pairs were used for each set. The predicted values for the criterion coordinates were calculated using the following equation (Friedman & Kohler, 2003; Tobler, 1994):

$$\begin{pmatrix} A' \\ B' \end{pmatrix} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} + \begin{pmatrix} \beta_1 & -\beta_2 \\ \beta_2 & \beta_1 \end{pmatrix} \cdot \begin{pmatrix} X \\ Y \end{pmatrix}$$

Equation 1

Note that we use the four-parameter, Euclidean version of the bidimensional regression equation. Here, A' and B' represent the predicted values for the criterion coordinates, X and Y represent the randomly generated values for the predictor coordinates, α_1 and α_2 represent the intercepts for the bidimensional regression model, and β_1 and β_2 represent the slopes for the bidimensional regression model. The fit of each bidimensional regression model was evaluated by comparing the predicted and the given (i.e., randomly generated) values for the criterion coordinates and maximizing R^2:

$$R^2 = 1 - \frac{\sum[(A - A')^2 + (B - B')^2]}{\sum[(A - M_A)^2 + (B - M_B)^2]}$$

Equation 2

where M_A and M_B represent the mean values for A and B (the criterion coordinates), respectively.

We used a genetic algorithm to estimate the best fitting R^2 value because of the large number of freely varying parameters in some conditions. The estimated parameters included α_1, α_2, β_1, β_2, and parameters representing any missing coordinates. For the most part, genetic algorithms have the advantage of allowing the modeler to move toward the optimal solution while inserting enough randomness to avoid local minima (Hassan et al., 2004). Previous work has also demonstrated the performance advantages of genetic algorithms over more commonly used hill-climbing algorithms (Thrash & Thomas, 2013). In our case, the genetic algorithm began by pseudo-randomly generating 1000 "organisms" (i.e., combinations of parameter values). The starting values for the missing coordinates were constrained to [-1, 1]. The starting values for α_1 and α_2 were constrained to [-1, 1], and the starting values for β_1 and β_2 were constrained to [-10, 10]. Next, we determined the fit of every organism by calculating the R^2 value (as described above). Only the best-fitting organism (out of every eight successive organisms) was selected for reproduction (i.e., "tournament selection"; Goldberg and Deb 1991). During the reproduction stage, each organism was converted to binary code and a random crossover point was determined. These organisms were then randomly paired, and each pair of organisms randomly exchanged the bits that occurred before the randomly determined crossover point. For each bit, the probability of mutation (or switching from 0 to 1 or 1 to 0) for each organism was 0.5%. This procedure was repeated 100 times. In the end, the best-fitting organism over all iterations was maintained and used to calculate the R^2 value for each pair of coordinate pairs. Throughout the genetic algorithm, each parameter was represented by 17 bits (corresponding to a precision of approximately ±0.0001).

After estimating R^2 for the original sets of coordinate pairs, some of the criterion coordinates were randomly selected for deletion. Deleted coordinate pairs were then

# coordinates	% interpolated	M_{before}	SD_{before}	M_{after}	SD_{after}	t	SE	df	p
10	10	0.1076	0.0938	0.1849	0.1048	5.4949	0.0141	195.6008	<.0001
10	20	0.0920	0.0846	0.2247	0.0999	10.1360	0.0131	192.7549	<.0001
10	30	0.0966	0.0881	0.3118	0.1189	14.5396	0.0148	182.4707	<.0001
10	40	0.0903	0.0787	0.3709	0.1200	19.5491	0.0144	170.8757	<.0001
40	10	0.0303	0.0271	0.0929	0.0365	13.7616	0.0045	182.7430	<.0001
40	20	0.0260	0.0267	0.1444	0.0409	24.2383	0.0049	170.3885	<.0001
40	30	0.0248	0.0251	0.2044	0.0542	30.0643	0.0060	139.6256	<.0001
40	40	0.0259	0.0264	0.2516	0.0552	36.8878	0.0061	141.9366	<.0001

Table 1: Descriptive and inferential statistics for comparisons corresponding to every combination of the variables "number of coordinates" and "percent interpolated." M_{before} and M_{after} represent the mean R^2 for sets of coordinate pairs before and after interpolation, respectively. SD_{before} and SD_{after} represent the standard deviation of R^2 for sets of coordinate pairs before and after interpolation, respectively. Welch's t-tests were used to compare M_{before} to M_{after} for every condition.

replaced by values that maximized the fit of the bidimensional regression model. These coordinates were then considered additional free parameters and were estimated using the genetic algorithm as described above. The starting values for each of these coordinates were constrained to fall between -1 and 1. This procedure allowed us to compare the relationship between the original sets of coordinate pairs and the relationship between sets of coordinate pairs after interpolation.

Different numbers of coordinate pairs were deleted and replaced for each of four levels of another variable, "percent interpolated." The four levels of this variable corresponded to the deletion and replacement of 10%, 20%, 30%, and 40% of the criterion coordinates for each set of coordinate pairs.

For every factorial combination of the variables "number of coordinates" and "percent interpolated," one hundred sets of coordinate pairs were generated and manipulated in the manner described above. Two-tailed, Welch's t-tests for the comparison of samples with unequal variances (Welch, 1947) were used in order to compare the mean R^2 for each condition after interpolation to the mean R^2 for the corresponding condition before interpolation. Before comparing different conditions, we subtracted the mean R^2 before interpolation from the mean R^2 after interpolation. We then tested for main effects of and interaction between the number of coordinate pairs and percent interpolated using a 2 x 4 ANOVA.

We also replicated our pattern of results using real-world data from a model building task (see Weisberg et al, 2013). The data represented 8 predictor and criterion coordinate pairs for each of 48 participants. We eliminated one participant from consideration because of a missing data point. One, two, or three data points were randomly selected, deleted, and interpolated, representing three different conditions of the variable "percent interpolated" (i.e., 12.5%, 25%, and 37.5%). Two-tailed, Welch's t-tests were used to compare the mean R^2 for each condition after interpolation to the mean R^2 for the corresponding condition before interpolation.

In order to validate the use of the genetic algorithm in the above simulations, we also evaluated the genetic algorithm's ability to estimate known parameter values for bidimensional regression models. Initially, one set of coordinate pairs was randomly generated from uniform distributions between -1 and 1. The number of coordinate pairs in each set corresponded to the variable "number of coordinates" specified above. Then, starting values for α_1, α_2, β_1, and β_2 were randomly generated from uniform distributions. The parameters α_1 and α_2 were constrained to fall between -1 and 1, and the parameters β_1 and β_2 were constrained to fall between -10 and 10. Note that these constraints correspond to those placed on the starting values in the other simulations described above. Values for another set of coordinate pairs were then generated using these randomly generated parameter values and the initial set of coordinate pairs. We then estimated the known (previously generated) parameter values using the genetic algorithm and these two sets of coordinate pairs. The genetic algorithm was conducted in the same manner as for the other simulations (i.e., with 1000 organisms and 100 iterations). This procedure was repeated 100 times. Finally, we evaluated the genetic algorithm in terms of bias and variability in the parameter estimates. Bias in the parameter estimates was assessed by determining the degree of skew in the distribution of estimates for each parameter.

Results

As predicted, interpolation led to an artificial inflation of the bidimensional regression models (see Figure 1). For every condition, the mean R^2 after interpolation was significantly higher than the mean R^2 before interpolation (see Table 1). Given that all the initial comparisons were significantly different from chance (all *p*s < 0.0001), it is informative to investigate differences between conditions. The interaction between number of coordinate pairs and percent interpolated was marginally significant, $F(3,792) = 2.61$, $MSE = 0.007$, $p = .0504$. It appears that the rate of inflation was higher for the 10 coordinate pairs when compared to the 40 coordinate pairs.

We then investigated two specific patterns among the conditions: the difference between 10 and 40 coordinate pairs per sample in terms of inflation, and the linear relationship between percent interpolated and inflation (separately for 10 and 40 coordinate pairs). The fit of the bidimensional regression models were significantly higher with 10 coordinate pairs (*M* = 0.18; *SD* = 0.13) than with 40 coordinate pairs (*M* = 0.15; *SD* = 0.08), *F(1,792)* = 24.70, *MSE* = 0.007, *p* < .0001. In this case, additional parameters did not result in a better fit. Both linear contrasts were also found to be significant. For 10 coordinate pairs, *F(1,792)* = 53.87, *MSE* = 0.007, *p* < .0001. For 40 coordinate pairs, *F(1,792)* = 19.54, *MSE* = 0.007, *p* < .0001.

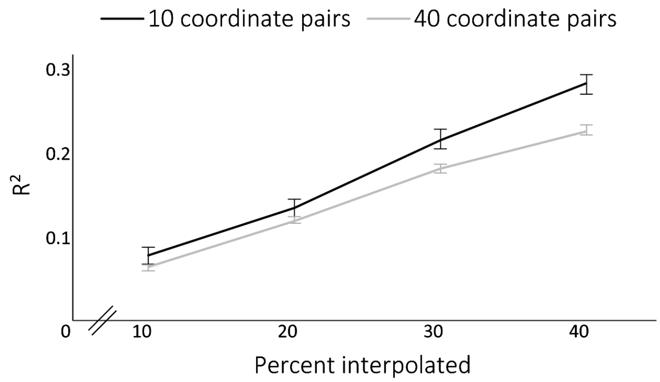

Figure 1: A graph depicting the relationship between number of coordinate pairs, percent interpolated, and the fit of the bidimensional regression models. Error bars represent the standard error of the mean R^2 for each condition.

A similar pattern of results emerged from the interpolation of data points from a real world study. Welch's t-tests found that the interpolation of one coordinate pair did not significantly inflate the R^2 value, *t(89.82)* = 0.33, *SE* = 0.035, *p* = .74; the interpolation of two coordinate pairs did significantly inflate the R^2 value, *t(88.62)* = 3.34, *SE* = 0.035, *p* < .001; and the interpolation of three coordinate pairs also significantly inflated the R^2 value, *t(87.02)* = 4.59, *SE* = 0.037, *p* < .0001.

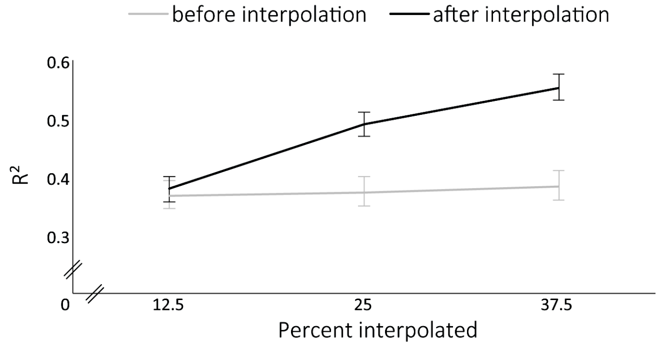

Figure 2: A graph depicting the relationship between percent interpolated and the fit of the bidimensional regression models before and after interpolation. Error bars represent the standard error of the mean R^2 for each condition

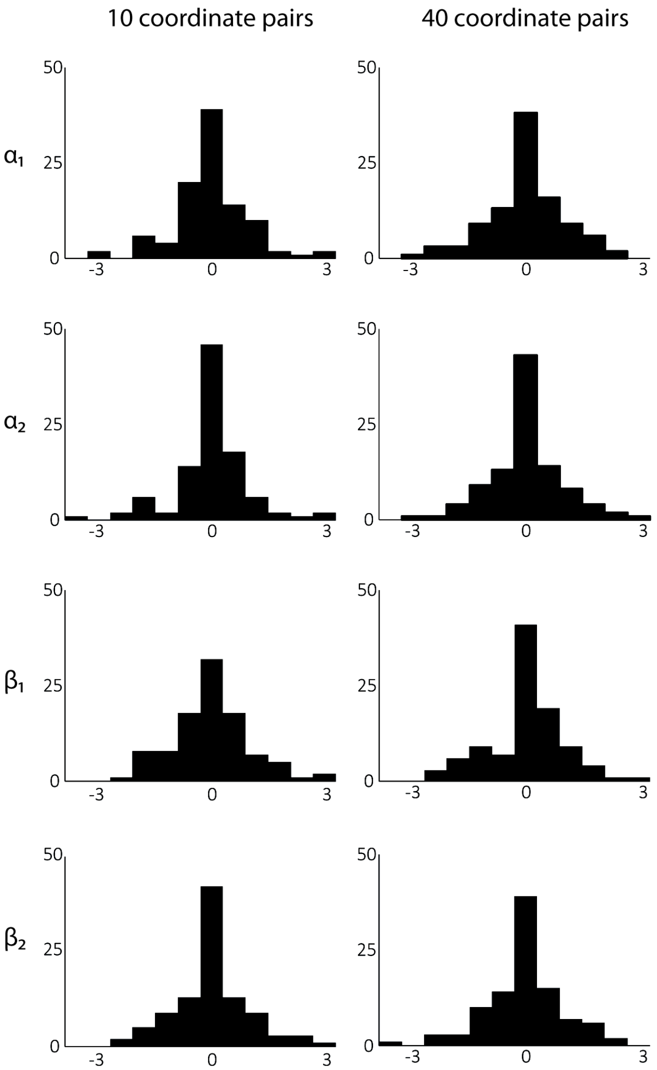

Figure 3: Histograms representing the distributions of parameter estimates by the genetic algorithm for two different levels of "number of coordinates" (i.e., 10 and 40). The x-axes represent z-scores for the (signed) difference between each parameter estimate and that parameter's known value.

	Variance		**Skew**	
	10 CP	**40 CP**	**10 CP**	**40 CP**
α_1	0.050	0.053	0.102	0.060
α_2	0.073	0.046	-0.063	-0.183
β_1	0.106	0.127	0.363	-0.259
β_2	0.141	0.136	0.322	-0.475

Table 2: Variance and skew from the distributions of the differences between the original parameter values and those estimated by the genetic algorithm. CP refers to the number of coordinate pairs in each sample.

We also examined the distributions of parameter estimates for 10 and 40 coordinate pairs separately in order to validate the use of the parameter estimation algorithm (see Figure 2). Table 2 lists the skew and variability for the unstandardized differences between estimated and original parameter values. The lack of skew indicates a lack of bias in the parameter estimates, and low variability in the parameter estimates indicates consistency. Bias and/or inconsistency in the parameter estimates would have allowed for the possibility that our patterns of results were attributable to problems with the parameter estimation algorithm.

Discussion

In the present work, we investigated the effects of interpolation on the artificial inflation of the fit of bidimensional regression models. We generated random data representing various situations that are often encountered in spatial cognition research such as the analysis of incomplete sketch maps. In order to relate to situations with differently sized data sets, we manipulated the number of coordinate pairs per sample. We also manipulated percent interpolated in order to establish the conditions under which interpolation may not be appropriate. Using a genetic algorithm, we interpolated the missing data while ensuring unbiased and consistent parameter estimates for the bidimensional regression models.

Two primary effects emerged. First, there was a linear relationship between percent interpolated and the amount of inflation in the fit of the bidimensional regression models. Specifically, inflation was higher when a greater percent of the coordinate pairs were interpolated. Second, smaller data sets produced more inflation than larger data sets despite having fewer free parameters.

These results highlight a major limitation in using interpolation as a method for compensating for missing values when using bidimensional regression. For example, the interpolation of only one coordinate pair out of ten resulted in an artificial inflation of approximately 8% on average. Such effects should be considered in spatial cognition research, given that the analyses of most sketch maps involve only a limited number of points (i.e., landmarks; Guzmán-Muñoz & Johnson, 2008; Ishikawa & Montello, 2006; Ishikawa, 2013; Lloyd, 2005; Schinazi, 2008; Schinazi et al., 2013; Uttal et al., 2010). Future studies that compare the fits of multiple regression models should also attend to the possibilities that one or more of those fits were inflated. This situation can be problematic because the precise extent to which a fit was inflated would be unknown. Thus, a comparison could artificially shift in a positive or negative direction.

These results also indicate that a larger number of coordinate pairs allows for a more reliable interpretation of a model's performance. This was evident in the significant difference between the samples with 10 and 40 coordinate pairs. Researchers are encouraged to design studies in such a way as to maximize the number of measured points. For example, this may be achieved by providing longer learning periods that allow for the acquisition of a larger number of landmarks.

We also assessed whether genetic algorithms are appropriate for fitting bidimensional regression models. The utility of this algorithm was evidenced by low skew and variance in the distribution of the parameter estimates. Additional simulations should be conducted in order to compare genetic algorithms to others that are commonly used to fit bidimensional regression models (e.g., other hill-climbing algorithms).

Future research should also consider alternative methods of interpolation that have been employed in the analysis of unidimensional data. For example, Bayesian multiple imputation (Schafer & Graham, 2002) may be useful for bidimensional data. Using assumptions such as normality of the underlying population, this method may allow for a more veridical solution to the missing data problem.

Our results may also have an interesting implication regarding the relationship between the number of coordinate pairs and the smoothness of the fit surface. One difference between 10 and 40 randomly generated coordinate pairs that are constrained to be within the same range (e.g., between -1 and 1 for the present case) is that the lower number of coordinate pairs can be more distributed. Because of this greater distribution, the movement of any one of these coordinate pairs (considered a free parameter) may have a greater effect on the prediction of a bidimensional regression model than the movement of an equivalent percent of coordinate pairs from the larger sample. Depending on the size of the difference in variability between the differently sized samples, this can override the flexibility typically afforded by the additional free parameters. Thus, a sample consisting of a larger number of coordinate pairs may result in a smoother function relating parameter values to overall model fit.

In summary, we have demonstrated artificial inflation of the fit of bidimensional regression models after interpolation for both randomly generated and real-world data sets. We have also highlighted the conditions under which this inflation is more likely to occur. The conditions that were most affected also represented those that are commonly applied in spatial cognition research.

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