Estimating Physiological Thresholds with Continuous Two-Phase Regression

David M. Nickerson[1]
Douglas E. Facey[2,3,*]
Gary D. Grossman[3]
[1]Department of Statistics, [2]Department of Zoology, and [3]School of Forest Resources, University of Georgia, Athens, Georgia 30602

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Abstract
Abrupt changes in the relationship between physiological responses and environmental parameters yield data that frequently cannot be described with a single regression equation. Many approaches used to deal with this problem result in incomplete description of the data and imprecise approximations of the physiological threshold(s) at which the relationship changes. We describe a technique for determining the best continuous two-phase, straight-line regression model and for statistically estimating the point at which the relationship between the independent and dependent variables changes (i.e., threshold point).

Introduction

Physiological thresholds often are characterized by abrupt changes in the relationship between an environmental parameter and the physiological response to that parameter. For example, the lower and upper limits of the thermal neutral zone of an endotherm mark the ambient temperatures at which the animal's metabolic rate increases above basal level to maintain constant body temperature (fig. 1). Data that include such a threshold cannot be explained by a single linear regression because the relationship between independent and dependent variables changes abruptly. It would be valuable to our understanding of physiology, however, to statistically describe these relationships and to accurately determine the threshold(s) at which the relationship changes. Statistically, such thresholds are called join points.

A review of *Physiological Zoology* from 1983 to 1987 indicated that more

* Present address: Department of Biology, Erskine College, Due West, South Carolina 29639.

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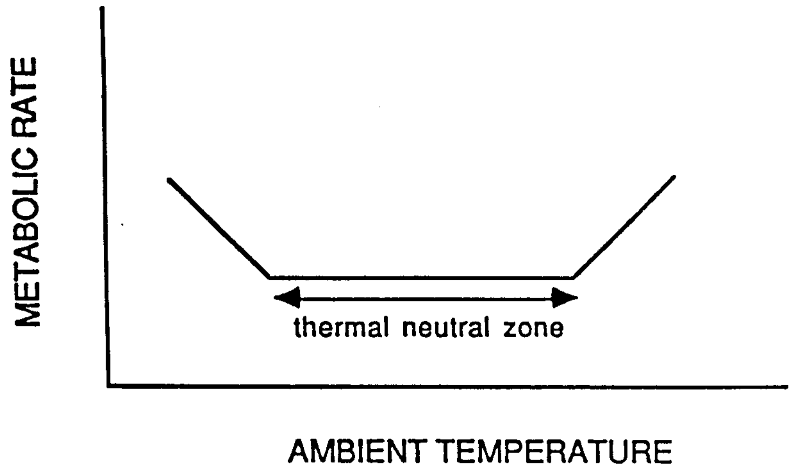


Fig. 1. Example of the effect of ambient temperature on the metabolic rate of an endotherm. The upper and lower limits of the thermal neutral zone represent thresholds at which the endotherm must increase its energy expenditure above the basal rate to maintain body temperature.

than 30 papers reported data with abrupt changes between the independent and dependent variables. In only one instance did the authors use a statistical method that provided a statistically valid description of the entire data set (Mover, Ar, and Hellwing [1986] cited the work of Hudson [1966]). Some authors presented two-phase relationships, also called split-line relationships, without a precise description of how the data were fitted and the join point estimated (Hennemann 1983, fig. 1; Rintamaki et al. 1983, figs. 2, 3; White 1983, fig. 10; Brent et al. 1984, fig. 1; Eppley 1984, fig. 8; Hinds and MacMillen 1985, fig. 1; Genoud and Bonaccorso 1986, fig. 1).

In general, researchers have used one of four approaches in trying to describe data that include a threshold, or join point. One approach is to fit one segment of the data by least-squares regression and leave the remaining segment(s) undescribed (Booth 1984, figs. 1, 4; Booth 1985, fig. 1; Byman 1985, figs. 3, 4; Thompson 1985, fig. 1; Buttemer et al. 1986, figs. 1, 2; Geiser 1987, fig. 4; Haim and Fairall 1987, fig. 1; Lovegrove 1987, fig. 2; Shoemaker et al. 1987, fig. 3). A second approach is to fit regressions to all data segments, but not constrain the lines to meet (Bartholomew, Vleck, and Bucher 1983, fig. 2; Kleinhaus et al. 1985, fig. 2; Frumkin, Pinshow, and Weinstein 1986, figs. 1, 2; Williams 1986, figs. 3, 4; Foley and Hume 1987, fig. 5). In this approach the join point is occasionally approximated by extending the regressions until they meet (Contreras 1986, figs. 2, 3). In the third approach, the data are not fit statistically and the join point is estimated by "eye" (Booth 1984, figs. 2, 3; Williams and Ricklefs 1984, fig. 3; Booth 1985, figs. 2, 3; Kaiser and Bucher 1985, fig. 2; Vogt 1986, fig. 3; Knight 1987, fig. 3; Obst, Nagy, and Ricklefs 1987, fig. 1). This yields an approximation of the join point rather than a precise estimate. Although all these approaches provide a description of the data, none of them include a statistically precise determination of the join point—an important behavioral or physiological threshold. Statistical estimation of the join point would allow comparison of thresholds among different organisms or studies. A fourth, and less common, approach has been to test a series of regressions using predetermined intervals along the *X*-axis, and then to select the combination that results in the lowest total error sum of squares (John-Alder, Garland, and Bennett 1986, fig. 1). This approach probably results in a valid description of the data but may not yield the "best" fit because the intervals at which the data are tested may be determined arbitrarily. In this study we present a technique that can identify the best fit for a continuous two-phase, straight-line regression model as well as estimate the join point. We present the necessary equations for a computer program and include a simple example to permit the testing of such a program. These procedures have been presented in the statistical literature (see Hudson 1966), and similar techniques have been discussed with respect to entomological data (Perry 1982). However, our review of recent issues of *Physiological Zoology* suggests that many physiologists collect data suitable for continuous two-phase regression models but are unaware of these procedures.

Methods

Description of the Iterative Method to Fit the Best Continuous Two-Phase, Straight-Line Regression

Specification of Model. Before attempting to find the best two-phase, segmented, straight-line model for a particular data set, a significant change must exist in the observed relationship between the independent (x) and dependent (y) variables. Otherwise, attempts at finding the best model may be futile as well as misleading (e.g., see Feder 1975). With this caveat in mind, from a sample of size n, the relationship between x and y for each $i = 1, \ldots, n$ may be expressed as

$$\begin{aligned} y_i &= \beta_0 + \beta_1 \times x_i + e_i, \quad \text{if } x_i \leqq A, \text{ and} \\ y_i &= \beta'_0 + \beta'_1 \times x_i + e_i, \quad \text{if } x_i > A, \end{aligned} \tag{1}$$

where β_0 and β_1 represent the y-intercept and slope of the first phase, respectively, β'_0 and β'_1 represent the y-intercept and slope of the second phase, respectively, and A represents the abscissa of the join point. For the sake of continuity, we also apply the restriction that

$$\beta_0 + \beta_1 \times A = \beta'_0 + \beta'_1 \times A, \tag{2}$$

to assure that the two lines join at the value $x = A$. Here the error terms (i.e., e_i's for $i = 1, \ldots, n$) are independent and identically distributed normal random variables with mean equal to zero and a constant variance.

There are several important implications of model (1). First, there is an abrupt change in the relationship between x and y occurring either at the point $x = A$ or at the level of the response $y = \beta_0 + \beta_1 \times A$. Second, the restriction given in equation (2) enables an unambiguous and statistically valid estimate of the abscissa of the join point, A. Solving equation (2) for A yields

$$A = (\beta_0 - \beta'_0)/(\beta'_1 - \beta_1). \tag{3}$$

Third, the model and restriction require estimation of only four of the five parameters (β_0, β_1, β'_0, β'_1, and A) because the final parameter can be solved for with equation (2).

We will use a least-squares criterion to determine the best continuous two-phase, straight-line regression. Hence, we wish to choose the two-phase regression line, including the continuity restriction, that minimizes the sum of the squared deviations between the observed and predicted values of y at a given x. This sum of squares is usually referred to as SSE (sum of squared errors), and the minimum SSE model is the solution that most closely fits the data when one assumes the model is continuous and has two phases.

Determining the Best Continuous Two-Phase, Straight-Line Model. Let us assume that the x's are ordered from lowest to highest, thus $x_1 \leqq x_2 \leqq \ldots \leqq x_n$. Next, consider two possibilities regarding the abscissa of the join point, A. The first is that A is between two consecutive values of x, x_j and x_{j+1}. The second is that A corresponds exactly to the x-coordinate of one of the data points, x_j.

If we assume the first possibility (i.e., $x_j < A < x_{j+1}$), then the least-squares solution simply becomes two separate "ordinary" least-squares (OLS) solutions, and the join point can be determined by equation (3), where the estimated β's replace the actual β's. This essentially means that the data are separated into two disjoint parts. The first part includes all x_i and y_i pairs up to and including x_j and y_j, whereas the second part contains all x_i and y_i pairs from x_{j+1} and y_{j+1} onward. Let n_j and n'_j be the number of observations in the first and second parts of the data set, respectively. From the first part of the data (x_1 to x_j) we simply obtain the least-squares fit for a straight line. This determines our estimates of β_0 and β_1, which we label b_0 and b_1, respectively. Similarly, from the second part of the data set (x_{j+1} to x_n) we obtain the least-squares fit of a straight line that includes our estimates of β'_0 and β'_1, which we label b'_0 and b'_1. Then, from equation (3), we determine the estimate of the abscissa of the join point, A, by replacing the β's with the b's. This estimate of A is labeled a. We may write the least-squares solution for this case ($x_j < A < x_{j+1}$) as

$$b_0 = \bar{y}_j - b_1 \times \bar{x}_j;\ b_1 = \mathrm{SS}^j_{xy}/\mathrm{SS}^j_{xx}; \qquad (4)$$

$$b'_0 = \bar{y}_{j'} - b'_1 \times \bar{x}_{j'};\ b'_1 = \mathrm{SS}^{j'}_{xy}/\mathrm{SS}^{j'}_{xx}; \qquad (5)$$

and

$$a = (b_0 - b'_0)/(b'_1 - b_1); \qquad (6)$$

where

$$\bar{y}_j = (\textstyle\sum^j_{i=1} y_i)/n_j;\ \bar{x}_j = (\sum^j_{i=1} x_i)/n_j;$$

$$\bar{y}_{j'} = (\textstyle\sum^n_{i=j+1} y_i)/n_{j'};\ \bar{x}_{j'} = (\sum^n_{i=j+1} x_i)/n_{j'};$$

$$\mathrm{SS}^j_{xy} = \textstyle\sum^j_{i=1} (y_i - \bar{y}_j) \times (x_i - \bar{x}_j);\ \mathrm{SS}^j_{xx} = \sum^j_{i=1} (x_i - \bar{x}_j)^2;$$

$$\mathrm{SS}^{j'}_{xy} = \textstyle\sum^n_{i=j+1} (y_i - \bar{y}_{j'}) \times (x_i - \bar{x}_{j'});$$

and

$$\mathrm{SS}^{j'}_{xx} = \textstyle\sum^n_{i=j+1} (x_i - \bar{x}_{j'})^2.$$

We have assumed thus far that the abscissa of the join point, A, was between x_j and x_{j+1}. If indeed the estimated join point is between these two consecutive x's, then the SSE is the sum of the individual SSEs from the two phases of the model, that is,

$$\mathrm{SSE}_j = \textstyle\sum^j_{i=1} [y_i - (b_0 + b_1 \times x_i)]^2 + \sum^n_{i=j+1} [y_i - (b'_0 + b'_1 \times x_i)]^2.$$

However, if the estimated join point is not between x_j and x_{j+1} (i.e., $a \leqq x_j$ or $a \geqq x_{j+1}$), then our solution is invalid.

The second possibility regarding the abscissa of the join point, A, is that it occurs exactly at x_j. The least-squares solution for this case differs slightly from that of the previous case (i.e., $x_j < A < x_{j+1}$), and this difference occurs for one of two reasons. The first is that in the case of $x_j < A < x_{j+1}$ there are an infinite number of possibilities for A, whereas for the case of $A = x_j$ there is only one possibility. The second reason for a different solution occurs in the minimization of SSE. For the case of $A = x_j$, the minimization of SSE is complex because certain derivatives do not exist (see Hudson 1966, p. 1105, n. ii). The least-squares solution for this case becomes a modification of the two separate OLS solutions from the previous case and is usually referred to as the "constrained" least squares (CLS) solution. This essentially means that the two OLS solutions are obtained as in the case when $x_j < A < x_{j+1}$, and then the b's are adjusted (i.e., constrained) so that the two estimated lines join at a point with an x-coordinate $= x_j$. We may write the least-squares solution for this case as

$$b_0^* = b_0 - (s/t) \times (n_j \times \mathrm{SS}_{xx}^j)^{-1} \times \textstyle\sum_{i=1}^{j} [(x_i - x_j) \times x_i], \tag{7}$$

$$b_1^* = b_1 + (s/t) \times (n_j \times \mathrm{SS}_{xx}^j)^{-1} \times \textstyle\sum_{i=1}^{j} (x_i - x_j), \tag{8}$$

$$b_0^{*\prime} = b_0' + (s/t) \times (n_{j'} \times \mathrm{SS}_{xx}^{j'})^{-1} \times \textstyle\sum_{i=j+1}^{n} [(x_i - x_j) \times x_i], \tag{9}$$

and

$$b_1^{*\prime} = b_1' - (s/t) \times (n_{j'} \times \mathrm{SS}_{xx}^{j'})^{-1} \times \textstyle\sum_{i=j+1}^{n} (x_i - x_j), \tag{10}$$

where

$$s = (b_0 + b_1 \times x_j) - (b_0' + b_1' \times x_j),$$

and

$$t = (n_j \times \mathrm{SS}_{xx}^j)^{-1} \times \textstyle\sum_{i=1}^{j} (x_i - x_j)^2 + (n_{j'} \times SS_{xx}^{j'})^{-1} \times \textstyle\sum_{i=j+1}^{n} (x_i - x_j)^2.$$

Note here that the constrained estimators satisfy the continuity condition, that is,

$$b_0^* + b_1^* \times x_j = b_0^{*\prime} + b_1^{*\prime} \times x_j.$$

For the constrained case ($A = x_j$), SSE is computed as follows:

$$\mathrm{SSE}_j^* = \textstyle\sum_{i=1}^{j} [y_i - (b_0^* + b_1^* \times x_i)]^2 + \textstyle\sum_{i=j+1}^{n} [y_i - (b_0^{*\prime} + b_1^{*\prime} \times x_i)]^2.$$

It is unnecessary, however, to consider the constrained solution if we obtain a valid unconstrained solution for the interval x_j to x_{j+1}. This is true because the SSE for the valid unconstrained solution (SSE_j) will always be less than the SSE for the constrained solution (SSE_j^*). ($SSE_j^* = SSE_j + [s^2/t]$, and therefore $SSE_j^* > SSE_j$.) Hence, a valid unconstrained solution will always be the solution of choice for a given interval x_j to x_{j+1}. Consequently, for each interval x_j to x_{j+1} we have a method for choosing the best continuous two-phase, straight-line regression (i.e., either a constrained or unconstrained solution).

A necessary condition for the use of this technique is that a significant change exist in the observed relationship between x and y. Therefore, the abscissa of the join point, A, must be somewhere between the lowest and highest x values for which we can fit a straight line to the left and to the right, respectively. (We cannot fit a straight line to the left of the second unique x value or to the right of the next-to-last unique x value because we must have at least two unique values for x in order to fit a straight line. Therefore, A must lie between the second and the next-to-last unique values for x, or at one of these points.) Hence, a thorough search for A requires that we begin at the second unique x. Let us suppose that x_2 satisfies this condition. Then, upon setting $j = 2$, we would follow the method outlined previously for the interval x_2 to x_3. After determining the best continuous two-phase, straight-line regression for this interval and computing SSE (either SSE_2 for the unconstrained case or SSE_2^* for the constrained case), we would then consider all remaining intervals including the interval whose end point is the second-to-last unique x value. (Further, for the sake of completeness, we should also consider the constrained case for $A = x_{n-1}$.) This yields a set of solutions and their associated SSEs—one for each consecutive pair of x's under consideration. Our overall best solution in terms of least squares will be the solution with the smallest SSE. In practice, it may be unnecessary to search the entire range of x values. After a plot of the data is examined, the search may be limited to those x values that reasonably could contain the abscissa of the join point, A.

Hypotheses and Related Test Statistics: Slope Parameters

After determining the best continuous two-phase model, we may be interested in testing the slope parameters, β_1 and β'_1, to see whether either is significantly different from zero. Recall that β_1 is the slope of the first phase of the model ($x_i \leqq$ the abscissa of the join point, A) and is estimated by b_1, whereas β'_1 is the slope of the second phase ($x_i > A$) and is estimated by b'_1.

The implication of the null hypothesis $H_0{:}\beta_1 = 0$ is that the complete model in equation (1), for each $i = 1, \ldots, n$, reduces to

$$y_i = \beta_0, \quad \text{if } x_i \leqq A, \text{ and}$$
$$y_i = \beta_0' + \beta_1' \times x_i, \quad \text{if } x_i > A, \tag{11}$$

where the continuity restriction from equation (2) becomes

$$\beta_0 = \beta_0' + \beta_1 \times A. \tag{12}$$

The implication of the null hypothesis $H_0: \beta_1' = 0$, however, is that the complete model in equation (1), for each $i = 1, \ldots, n$, reduces to

$$y_i = \beta_0 + \beta_1 \times x_i, \quad \text{if } x_i \leqq A, \text{ and}$$
$$y_i = \beta_0', \quad \text{if } x_i > A, \tag{13}$$

where the continuity restriction from equation (2) becomes

$$\beta_0 + \beta_1 \times A = \beta_0'. \tag{14}$$

To test these two hypotheses separately, we rely on the method of fitting complete and reduced models; the reduced model is dictated by the null hypothesis in question. Here, we determine whether the increase in SSE, going from the complete to the reduced model, is significantly large. If the increase in SSE is significantly large, then the null hypothesis can be rejected and we conclude that the complete model does a significantly better job of fitting the data than the reduced model. If the increase in SSE is not significantly large, however, then there is insufficient evidence that the null hypothesis is false, and the reduced model, therefore, fits the data adequately.

The procedure for fitting the complete model has already been outlined. The procedure for fitting the two reduced models is identical to that for the complete model with the following modifications to the parameters, estimates, and computations of SSE.

If we assume that for some $j = 1, \ldots, n$, $x_j < A < x_{j+1}$, then for the reduced model under $H_0: \beta_1 = 0$, b_0' and b_1' are defined as in equation (5), while

$$b_0 = (\textstyle\sum_{i=1}^{j} y_i)/n_j,$$

and

$$a = (b_0 - b_0')/b_1'.$$

Further, under $H_0:\beta_1 = 0$, if $x_j < a < x_{j+1}$, then

$$SSE_j = \sum_{i=1}^{j} (y_i - b_0)^2 + \sum_{i=j+1}^{n} [y_i - (b'_0 + b'_1 \times x_i)]^2.$$

If $a \leqq x_j$ or $a \geqq x_{j+1}$, then we have an invalid fit and the unconstrained solution is invalid, and we must consider the constrained solution.

If, however, we assume that $A = x_j$, then for the reduced model under $H_0:\beta_1 = 0$, $b_0^{*\prime}$ and $b_1^{*\prime}$ are defined as in equations (9) and (10), respectively, whereas

$$b_0^* = b_0 - (1/n_j) \times (s/t),$$

$$s = b_0 - b'_0 - b'_1 \times x_j,$$

and

$$t = (1/n_j) + (n_{j'} \times SS_{xx}^{j'})^{-1} \times \sum_{i=j+1}^{n} (x_i - x_j)^2.$$

In addition, under $H_0:\beta_1 = 0$, if A is constrained at x_j, then

$$SSE_j^* = \sum_{i=1}^{j} (y_i - b_0^*)^2 + \sum_{i=j+1}^{n} [y_i - (b_0^{*\prime} + b_1^{*\prime} \times x_i)]^2.$$

If we again assume that for some $j = 1, \ldots, n$, $x_j < A < x_{j+1}$, then for the reduced model under $H_0:\beta'_1 = 0$, b_0 and b_1 are defined as in equation (4), whereas

$$b'_0 = (\textstyle\sum_{i=j+1}^{n} y_i)/n_{j'},$$

and

$$a = (b'_0 - b_0)/b_1.$$

Further, under $H_0:\beta'_1 = 0$, if $x_j < a < x_{j+1}$, then

$$SSE_j = \sum_{i=1}^{j} [y_i - (b_0 + b_1 \times x_i)]^2 + \sum_{i=j+1}^{n} (y_i - b'_0)^2.$$

If $a \leqq x_j$, or $a \geqq x_{j+1}$, then this unconstrained solution is not valid and we must consider the constrained solution ($A = x_j$).

If we assume that $A = x_j$, then for the reduced model under $H_0:\beta'_1 = 0$, b_0^* and b_1^* are defined as in equations (7) and (8), respectively, whereas

TABLE 1
Sample data for fitting a continuous two-phase, straight-line regression

	i							
Coordinate	1	2	3	4	5	6	7	8
y_i	.5	1.0	2.0	2.5	2.0	2.0	1.0	.5
x_i	2	3	4	5	6	7	8	9

$$b_0^{*\prime} = b_0 + (1/n_{j'}) \times (s/t),$$

$$s = b_0 + b_1 \times x_j - b'_0,$$

and

$$t = (n_j \times SS_{xx}^j)^{-1} \times \textstyle\sum_{i=1}^j (x_i - x_j)^2 + (1/n_{j'}).$$

Further, under $H_0{:}\beta'_1 = 0$, if A is constrained at x_j, then

$$SSE_j^* = \textstyle\sum_{i=1}^j [y_i - (b_0^* + b_1^* \times x_i)]^2 + \sum_{i=j+1}^n (y_i - b_0^{*\prime})^2.$$

To test $H_0{:}\beta_1 = 0$, we first obtain the best complete model of the form in equation (1) and determine the associated SSE. Next we obtain the best reduced model of the form in equation (11) and determine the associated SSE. We can now calculate the following test statistic:

$$F = \frac{(SSE_{\text{reduced model}} - SSE_{\text{complete model}})/1}{SSE_{\text{complete model}}/(n-4)}. \qquad (15)$$

This test statistic (under $H_0{:}\beta_1 = 0$) will have an F-distribution with 1 numerator degree of freedom and $n - 4$ denominator degrees of freedom. A standard F-table can then be used for significance testing of this value.

To test the hypothesis $H_0{:}\beta'_1 = 0$, our reduced model takes the form of equation (13). We obtain the best reduced model of the form in equation (13) and determine its SSE. We then calculate F using equation (15) and test for significance using the appropriate F-tables.

An additional question of interest may be whether the slopes of the two phases are significantly different ($H_0{:}\beta_1 = \beta'_1$). This hypothesis, in conjunction with the continuity restriction (the lines must meet at the join point,

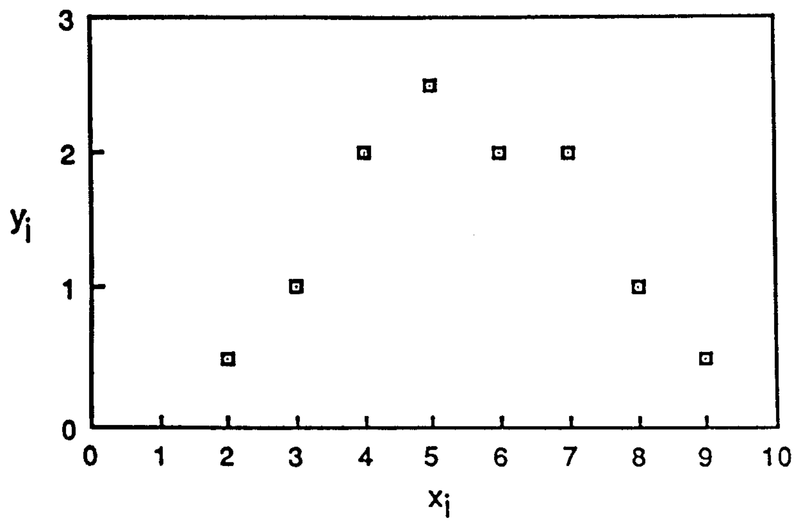


Fig. 2. Graphic representation of the data presented in table 1. These data are appropriate for a continuous two-phase, straight-line regression.

A), is equivalent to $H_0\!:\!\beta_0 = \beta'_0,\ \beta_1 = \beta'_1$. In other words, is our two-phase continuous straight-line model significantly better at describing the data than a single straight-line model? Although this null hypothesis is reasonable, it possesses several serious mathematical problems that are due mainly to the behavior of the abscissa of the join point, A (see Feder 1975). These problems occur because, if one straight line adequately describes the data, then trying to fit a two-phase segmented straight line model will result in an unstable estimate of A.

Example

Estimation

To illustrate the necessary calculations, and to permit checking of computer programs based on this paper, we shall consider a simple example using the data that appear in table 1 and figure 2. The first pair of consecutive x values that we consider is x_2 and x_3. The results of the calculations follow. Recall that n_j and n'_j represent the number of observations below and above the presumed join point, respectively. For $x_2 < A < x_3$, or, in our example, $3 < A < 4$:

$$n_2 = 2;\ \bar{x}_2 = 2.5;\ \bar{y}_2 = 0.75;\ SS^2_{xx} = 0.5;\ SS^2_{xy} = 0.25;$$

$$b_1 = 0.25/0.5 = 0.5;\ b_0 = 0.75 - (0.5) \times (2.5) = -0.5;$$

$$n_{2'} = 6; \bar{x}_{2'} = 6.5; \bar{y}_{2'} = 1.67; SS_{xx}^{2'} = 17.5; SS_{xy}^{2'} = -6.0;$$

$$b_1' = -6.0/17.5 = -0.34; b_0' = 1.67 - (-0.34) \times (6.5) = 3.88\ ;$$

and

$$a = (-0.5 - 3.88)/(-0.34 - 0.5) = 5.21.$$

Here, a (the estimate of the abscissa of the join point, A) does not fall within the range of x_2 to x_3 ($5.21 > 4$), and, hence, we have an invalid solution. Consequently, we must examine the constrained case where A occurs at x_2. The calculations follow. For $A = x_2$ or $a = 3$:

$$\textstyle\sum_{i=1}^{2} (x_i - x_2) = -1; \sum_{i=1}^{2} (x_i - x_2) \times x_i = -2; \sum_{i=1}^{2} (x_i - x_2)^2 = 1;$$

$$\textstyle\sum_{i=3}^{8} (x_i - x_2) = 21; \sum_{i=3}^{8} (x_i - x_2) \times x_i = 154; \sum_{i=3}^{8} (x_i - x_2)^2 = 91;$$

$$s = (-0.5 + 0.5 \times 3) - (3.90 - 0.34 \times 3) = -1.88;$$

$$t = (2 \times 0.5)^{-1} \times 1 + (6 \times 17.5)^{-1} \times 91 = 1.88;$$

$$b_0^* = -0.5 - (-1.88/1.88) \times (2 \times 0.5)^{-1} \times (-2) = -2.50;$$

$$b_1^* = 0.5 + (-1.88/1.88) \times (2 \times 0.5)^{-1} \times (-1) = 1.50;$$

$$b_0^{*\prime} = 3.90 + (-1.88/1.88) \times (6 \times 17.5)^{-1} \times (154) = 2.43;$$

$$b_1^{*\prime} = -0.34 - (-1.88/1.88) \times (6 \times 17.5)^{-1} \times (21) = -0.1429;$$

and

$$SSE_2^* = 2.64.$$

The next pair of consecutive x values that we consider is x_3 and x_4. The results of the calculations follow. For $x_3 < A < x_4$, or $4 < A < 5$:

$$n_3 = 3; \bar{x}_3 = 3.0; \bar{y}_3 = 1.17; SS_{xx}^{3} = 2.0; SS_{xy}^{3} = 1.5;$$

$$b_1 = 1.5/2.0 = 0.75; b_0 = 1.17 - (0.75) \times (3.0) = -1.08;$$

TABLE 2
Types of solutions and associated SSEs for continuous two-phase, straight-line regressions fitting data in table 1

Interval	Interval Values	Solution Type	SSE
$x_2 \leqq A < x_3$	$3 \leqq A < 4$	CLS	2.6429
$x_3 \leqq A < x_4$	$4 \leqq A < 5$	OLS	.2417
$x_4 \leqq A < x_5$	$5 \leqq A < 6$	OLS	.2250
$x_5 \leqq A < x_6$	$6 \leqq A < 7$	OLS	.7167
$x_6 \leqq A < x_7$	$7 \leqq A < 8$	CLS	1.2690
$x_7 \leqq A < x_8$[a]	$8 \leqq A < 9$	CLS	2.7768

Note. A = abscissa of join point.
[a] A CLS solution is the only one possible in this interval because there is only one x value to the right of x_7. To determine this regression line, simply replace x_6 with x_7 in the CLS solution for the interval $x_6 \leqq A < x_7$.

$$n_{3'} = 5;\ \bar{x}_{3'} = 7.0;\ \bar{y}_{3'} = 1.6;\ SS_{xx}^{3'} = 10.0;\ SS_{xy}^{3'} = -5.0;$$

$$b_1' = -5.0/10.0 = -0.5;\ b_0' = 1.6 + (0.5) \times (7.0) = 5.1;$$

and

$$a = (-1.08 - 5.1)/(-0.5 - 0.75) = 4.95.$$

Here, a is within the range of x_3 to x_4 $(4 < 4.95 < 5)$; hence, the solution is valid. Consequently, we need not examine the case of $A = x_3$, and we may compute SSE as

$$SSE_3 = 0.24.$$

The remainder of the possible solutions as well as these first two examples are summarized in table 2. We can see in table 2 that the OLS solution for the interval $x_4 \leqq A < x_5$ has the lowest SSE among the possible solutions that allow only for a continuous two-phase, straight-line model. Consequently, this solution is the best continuous two-phase, straight-line regression. The abscissa of the join point, A, is estimated to occur at $x = 5.16$, and the complete model is

TABLE 3
Types of solutions and associated SSEs for reduced models (H_0:$\beta_1 = 0$)

Interval	Interval Values	Solution Type	SSE
$x_1 \leqq A < x_2$[a]	$2 \leqq A < 3$	CLS	4.2173
$x_2 \leqq A < x_3$	$3 \leqq A < 4$	CLS	4.1794
$x_3 \leqq A < x_4$	$4 \leqq A < 5$	CLS	3.9744
$x_4 \leqq A < x_5$	$5 \leqq A < 6$	CLS	3.5679
$x_5 \leqq A < x_6$	$6 \leqq A < 7$	CLS	3.1908
$x_6 \leqq A < x_7$	$7 \leqq A < 8$	CLS	2.8387
$x_7 \leqq A < x_8$[b]	$8 \leqq A < 9$	CLS	3.2143

Note. A = abscissa of join point.
[a] For this reduced model we only need a minimum of one point to the left of A. Therefore, we may consider this additional interval.
[b] A CLS solution is the only one possible in this interval because there is only one x value to the right of x_7. To determine this regression line, simply replace x_6 with x_7 in the CLS solution for the interval $x_6 \leqq A < x_7$.

$$y_i = -0.95 + 0.7\,x_i, \quad \text{if } x_i \leqq 5.16, \text{ and}$$
$$y_i = 5.5 - 0.55\,x_i, \quad \text{if } x > 5.16.$$

Tests of β_1

To illustrate the necessary calculations for a hypothesis of the form described previously, let us again consider the data in table 1. Here, we will only consider the hypothesis H_0:$\beta_1 = 0$; the hypothesis H_0:$\beta_1' = 0$ can be tested in an analogous fashion. Because we have obtained the complete model for this case, the next step in the testing of H_0:$\beta_1 = 0$ is to fit a reduced model of the form shown in equation (11) by the methods described previously. These results are shown in table 3.

Table 3 shows that the solution for the interval of x_6 to x_7 has the smallest SSE among the possible solutions. Consequently, the best reduced model is

$$y_i = 1.66, \quad \text{if } x_i \leqq 7, \text{ and}$$
$$y_i = 5.84 - 0.60\,x_i, \quad \text{if } x_i > 7.$$

Next, we test to determine whether the reduced model is significantly different from the complete model by computing the F-statistic as shown in equation (15):

$$F = \frac{(2.8387 - 0.2250)/1}{0.2250/(8-4)} = 46.47.$$

From an F-table, we find that the critical F-value with 1 numerator and 4 denominator degrees of freedom at the $\alpha = 0.01$ level is 21.20, and consequently we reject the hypothesis $H_0: \beta_1 = 0$ at the 0.01 level. (The observed significance level of the test is actually 0.0024.) We conclude, therefore, that the complete model is significantly better than the reduced model.

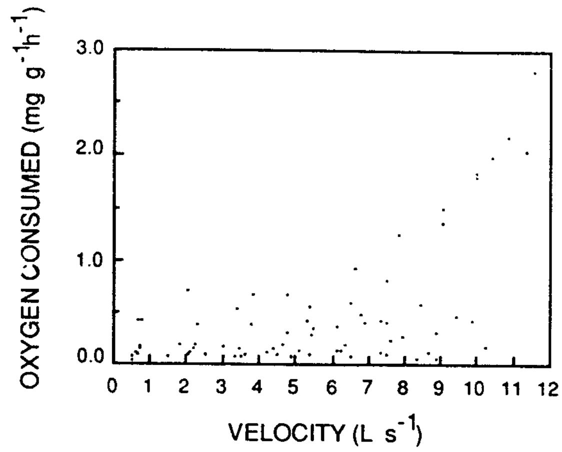
Application to Physiological Data

Figure 3*a* shows the effect of water velocity on the oxygen consumption rate of longnose dace (*Rhinichthys cataractae*) at 10°C during fall. This benthic stream fish is able to hold position without swimming up to some "critical velocity" (sensu Matthews 1985) but must swim to hold position at higher velocities. This change in behavior results in a sudden increase in the rate of oxygen consumption at the critical velocity and is reflected in the data, which suggest a two-phase relationship with the join point at a velocity between 6 and 9 body lengths per second ($L\ s^{-1}$). Using the procedures described earlier, we begin at the lowest x_j value in the data set and follow the iterative method through all possible x_j to x_{j+1} intervals, determining an unconstrained and a constrained solution for each interval. The best fit for the data among regressions that are continuous two-phase, straight-line models (the solution with the lowest SSE) was the unconstrained solution with A occurring between x_{58} ($x = 8.6667\ L\ s^{-1}$) and x_{59} ($x = 8.9041\ L\ s^{-1}$). The value of A was calculated to be $8.7082\ L\ s^{-1}$. The complete model, therefore, is

$$\begin{aligned} y &= 0.150476 + 0.0305627\,x, \quad \text{if } x \leqq 8.7082, \text{ and} \\ y &= -5.677 + 0.69976\,x, \quad \text{if } x > 8.7082. \end{aligned} \tag{16}$$

Both phases of this solution are shown in figure 3*b*. The SSE of this complete model is 8.2752, and there are $71 - 4 = 67$ df. Exponential and logarithmic fits to these same data yielded SSEs of 10.148 and 11.470, indicating that the two-phase model is a better fit to these data than either of these curvilinear models.

Next, we wish to test whether the slope of the first phase of our solution is significantly different from zero. The slope of the second phase clearly is a)



b)

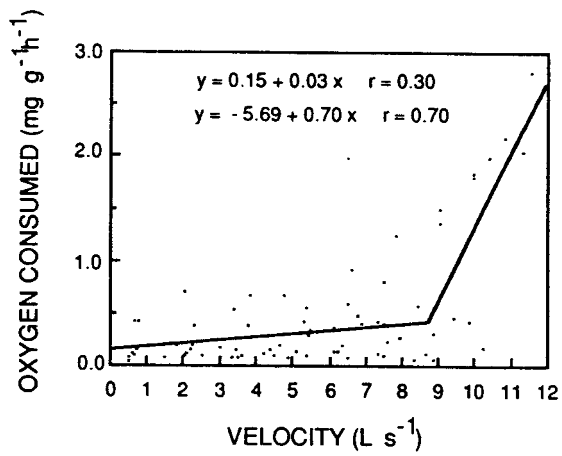


Fig. 3. a, *Data showing the effect of water velocity on the oxygen consumption of longnose dace, and* b, *the best continuous two-phase, straight-line regression describing these data.*

greater than zero; hence, we will not present the test for it. The reduced model, then, is determined by assuming that the slope of the first phase of the model is equal to zero and the best fit solution yields the following:

$$y = 0.290895, \quad \text{if } x \leqq 8.6086, \text{ and}$$
$$y = -5.981 + 0.72861\,x, \quad \text{if } x > 8.6086. \tag{17}$$

The SSE of this reduced model is 8.6273, and there are 71 − 3 = 68 df. From equation (15), $F = 2.8508$, which is lower than the F-table value for $F^{0.05}_{1,68}$ and indicates a lack of significant difference between the complete and reduced models. Hence, the slope of the first phase of our two-phase model is not significantly different from zero. We conclude, therefore, that oxygen consumption rates of longnose dace did not increase significantly with increasing velocity at velocities below the join point of our complete model, but that oxygen consumption rates did increase significantly at higher velocities.

Additional Applications

Two or More Join Points

The application of this method is not limited to continuous two-phase regression situations in which there is only one join point. For generalizations to two or more join points and general polynomials in x, consult Hudson (1966).

Comparison of Two or More Groups

Suppose we determine the best continuous two-phase, straight-line regression for each of two or more sets of data, perhaps representing data from different species, different sexes, different seasons, and so on. We may wish to determine whether or not the regressions differ significantly among groups. An application of the complete- versus reduced-model technique will allow us to test the hypothesis H_0:no difference among the groups. First, we must determine the best continuous two-phase, straight-line regression for each group. These separate regressions constitute the complete model. The SSE of the complete model will be the sum of the individual SSEs of all of the two-phase regressions, and the degrees of freedom for the complete model SSE will be the sum of the degrees of freedom associated with the individual SSEs. (Each individual SSE will have as its degrees of freedom the number of observations in the group minus four.) Next, we combine the data of all groups and determine the best single continuous two-phase, straight-line regression for the combined data set. This regression represents the reduced model. Next, we compute

$$F = \frac{(\text{SSE}_{\text{reduced model}} - \text{SSE}_{\text{complete model}})/(4 \times (g-1))}{\text{SSE}_{\text{complete model}}/(N - 4 \times g)}, \qquad (18)$$

where N is the total number of observations in the combined data set, and g is the number of groups. The F-statistic in equation (18) has an F-distribution with $4 \times (g-1)$ numerator degrees of freedom and $(N-4 \times g)$ denominator degrees of freedom.

As an example, we consider the oxygen-consumption-versus-water-velocity data for longnose dace during spring, but the data will be separated according to sex. We will consider only identifiable males and females (some fish were not sexable).

First we consider only the data for females (31 data points), determine the best continuous two-phase, straight-line regression using the methods described earlier, obtain the abscissa of the join point, and calculate the associated SSE. We then do the same for males (39 data points). Together, these continuous two-phase solutions make up our complete model:

females:

$$y = 0.1760 + 0.00930\,x, \quad \text{if } x \leqq 8.5805, \text{ and}$$
$$y = -11.347 + 1.35220\,x, \quad \text{if } x > 8.5805;$$

males:

$$y = 0.17796 + 0.0512\,x, \quad \text{if } x \leqq 7.3267, \text{ and}$$
$$y = -4.5360 + 0.6946\,x, \quad \text{if } x > 7.3267;$$

$$\text{SSE}_{\text{complete}} = \text{SSE}_{\text{F}} + \text{SSE}_{\text{M}} = 0.81831 + 6.88588 = 7.70419;$$

$$\text{df}_{\text{complete}} = (31 - 4) + (39 - 4) = 62.$$

Next, we follow an identical procedure for the combined data set to determine the reduced model:

$$y = 0.09770 + 0.061368\,x, \quad \text{if } x \leqq 8.4432, \text{ and}$$
$$y = -7.9916 + 1.0195\,x, \quad \text{if } x > 8.4432;$$

$$\text{SSE}_{\text{reduced}} = 11.0161;$$

$$\text{df}_{\text{reduced}} = 70 - 4 = 66.$$

We now test the hypothesis, H_0:no difference between the models for males and females, by calculating F according to equation (18):

$$F = \frac{(11.0161 - 7.70419)/4}{7.70419/62} = 6.6632\,.$$

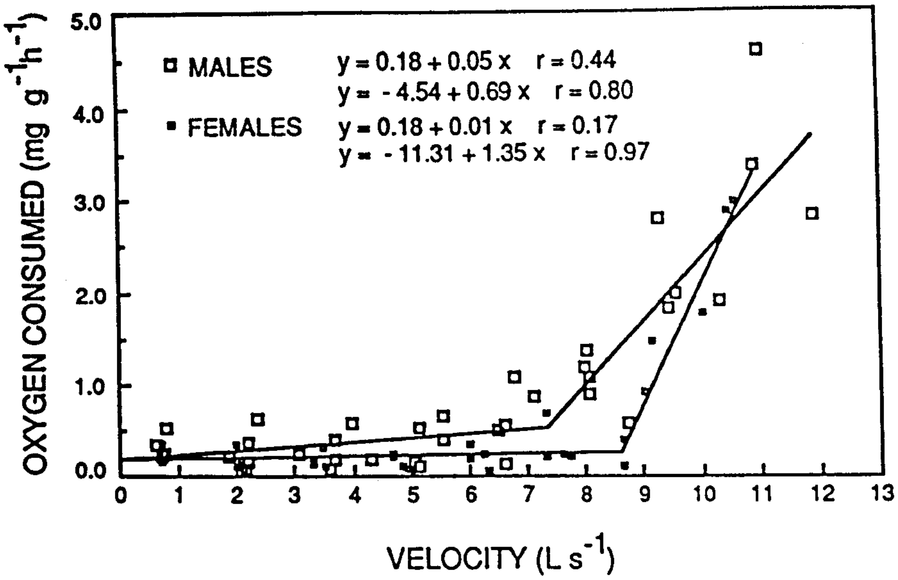


Fig. 4. Continuous two-phase, straight-line regressions describing the effect of water velocity on the oxygen consumption of male and female longnose dace.

This F is greater than the F-table value ($\alpha = 0.05$) with 4,62 df ($P = 0.0002$), and, thus, the complete and reduced models are significantly different. Consequently, the relationship between oxygen consumption and water velocity during spring at 10°C is significantly different for males and females. See figure 4 for a plot of the data for each sex and the associated estimated regression lines.

Conclusions

Continuous two-phase, straight-line regression may be appropriate for physiological data that exhibit thresholds. It seems that many physiologists are unaware of the statistical procedures for dealing with this problem and, hence, may lose valuable information from their data sets. By applying the methods contained herein, researchers can determine the continuous two-phase, straight-line model that best fits the data. They also can provide a statistically valid estimate of the threshold at which the relationship between the environmental variable and the measured physiological response changes.

If the true relationship between the independent and dependent variable is believed to be discontinuous, then a fit of lower SSE may be obtained with a model in which the two segments are not required to meet within the "critical" range of the independent variable (see Yeager and Ultsch [1989] for such a solution). The critical range of the independent variable is those values of x to the right of the rightmost x value of the first line segment and to the left of the leftmost x value of the second line segment. Within this critical range lies the threshold level of the independent variable, which, for a discontinuous model, cannot be estimated with any more precision than to say that it lies in this range. Further, such a solution leaves the relationship between the dependent and independent variables undefined within this critical range.

Therefore, if the underlying model is believed to be a continuous two-phase, straight-line model, then employ the methods of this article to fit such a model and obtain estimates of the slopes, intercepts, and the threshold value. If the underlying model is believed to be a discontinuous two-phase, straight-line model, then employ the methods of Yeager and Ultsch (1989) to fit such a model and obtain estimates of the slopes, intercepts, and a range of possible values for the threshold value. However, if the choice between a continuous or discontinuous two-phase, straight-line model is unclear, then try the following method.

Find both the best continuous and discontinuous two-phase, straight-line models and determine the associated SSEs. Since the discontinuous model is less restrictive than the continuous one, the discontinuous model will always have an SSE less than or equal to that for the continuous model. If the SSEs are equal, then the two fits will be identical. If the discontinuous model has an SSE strictly less than that for the continuous model, then the discontinuous model will produce a fit with the problem noted above.

Then, compare the two SSEs and subjectively determine whether difference is significantly large. If the difference is not great, choose the continuous model; if the difference is considerable, choose the discontinuous model.

Unfortunately, there does not exist a statistically valid test of such a hypothesis. However, you can be assured that if the true underlying model is continuous, then the continuous and discontinuous fits should be close; if the true underlying model is discontinuous, then the fits should be quite different.

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