Statistical Models for Limiting Nutrient Relations in Inland Waters
Author(s): Mark S. Kaiser, Paul L. Speckman and John R. Jones
Source: *Journal of the American Statistical Association*, Vol. 89, No. 426 (Jun., 1994), pp. 410-423
Published by: Taylor & Francis, Ltd. on behalf of the American Statistical Association
Stable URL: https://www.jstor.org/stable/2290841
Accessed: 21-05-2025 00:30 UTC

Statistical Models for Limiting Nutrient Relations in Inland Waters

Mark S. KAISER, Paul L. SPECKMAN, and John R. JONES*

The ecological theory of limiting factors holds that the observed level of response in a biological process will be governed by the input factor in least supply—the limiting factor. This theory has formed the basis for numerous attempts by aquatic ecologists to describe the relation between the biological productivity of inland waters and the availability of plant nutrients required for algal growth. Regression analysis has been the primary statistical tool used in the development of such relations, yet any statistical model that represents the limiting effect of some explanatory factor as an expectation contradicts the substantive theory of limiting factors. Limnological data not resulting in an adequate regression of chlorophyll on phosphorus have been viewed as failing to support the limiting effect of this nutrient on algal biomass in lakes. But when represented by a more appropriate model, such data may be seen to provide similar evidence for the relation of chlorophyll to phosphorus as does data resulting in a strong regression. Data from limnological studies often exhibit a scatter of points distributed in the shape of a triangle lying beneath an upper boundary. Appropriate models for such data are introduced to describe the upper boundary or potential limit, the distribution of points falling below the limit, and the degree of random error. An application of the EM algorithm provides marginal maximum likelihood estimates of the parameters in the more complex models considered. Several results are given for the models, including a goodness-of-fit diagnostic and estimation of the large-sample parameter covariance matrix. Application of the models is illustrated by fitting empirical relationships between chlorophyll and the plant nutrient phosphorus in temperate lakes.

KEY WORDS: EM algorithm; Limit function; Marginal maximum likelihood; Mixture distributions.

1. INTRODUCTION

An early and basic tenet of ecological science is the Law of Limiting Factors, also known as Liebig's Law of the Minimum (Blackman 1905; Liebig 1840). This principle holds that when a biological process, such as growth or photosynthesis, depends on several input factors, the speed of the process is governed by the slowest factor. Recast in modern convention, the law of limiting factors implies that the biomass of a particular organism in an ecosystem is potentially constrained by any of the factors critical to its growth and reproduction (Pianka 1978). The one factor that is least available will be the active constraint and is then called the limiting factor. Any of the necessary components of growth and reproduction have the potential to be the limiting factor at a given point in time and space. As a result, knowledge of the level of one potentially limiting factor does not necessarily lead to knowledge about the level of biological production, unless that factor is actually the active constraint across time, space, and all of the individual organisms in a community. But the level of one potentially limiting factor does set an upper limit to the level of production, a limit determined by the production possible were that potentially limiting factor to become the sole active limiting factor.

Aquatic ecologists have used the concept of limiting factors to explain empirical relations between the fertility of temperate zone lakes, as measured by the abundance of algal biomass, and the concentration of major plant nutrients in those lakes. Simple linear regression has been used to describe the relation between the photosynthetic pigment algal chlorophyll (a measure of algal biomass) and total phosphorus (a major plant nutrient), typically after log transformation of both variables. A number of published regressions for lakes in Japan and North America showed a strong relation between log chlorophyll and log phosphorus, with values of r^2 from .90 to .95 (see, for example, Dillon and Rigler 1974; Jones and Bachmann 1976; and Sakamoto 1966). Experimental studies provided evidence that the plant nutrient phosphorus was frequently the limiting factor for algal growth in some north temperate zone lakes (see, for example, Fuhs, Demmerie, Canelli, and Chen 1972 and Schindler 1977). The prevailing view among limnologists became that linear regressions described the limitation of algal growth by phosphorus. We argue that this interpretation is based on a misconception of the way in which the law of the minimum translates into a statistical model for observations. Regardless, normal linear regression models of (transformed) chlorophyll on phosphorus have provided the basis for lake management practices. For example, based in large part on evidence from such models, the governments of Canada and the United States entered into agreements to decrease phosphorus inputs from human activity to control eutrophication in the Great Lakes (Chapra and Robertson 1977). In the United States, a number of both federal and local initiatives were implemented to control phosphorus inputs from treated waste water effluent. The effectiveness of these programs is still being debated.

The use of empirical chlorophyll–phosphorus regression equations to predict productivity in lakes has proven troublesome. Since the mid-1970s, limnologists have gathered a great deal of data from many lakes and regions of the world. Although some sets of data reflected chlorophyll–phosphorus models similar to published examples, many did not (Smith and Shapiro 1981). In general, residual variability in simple

* Mark S. Kaiser is Assistant Professor, Department of Statistics, Iowa State University, Ames, IA 50011. Paul L. Speckman is Associate Professor, Department of Statistics, and John R. Jones is Professor of Limnology, School of Natural Resources, University of Missouri, Columbia, MO 65211. Part of this work was completed while Kaiser served as Mathematical Statistician, National Fisheries Contaminant Research Center, U.S. Fish and Wildlife Service, Columbia, MO 65201. The authors thank Matthew F. Knowlton for helping to introduce us to this problem and for stimulating discussions and criticism, Roger Bachmann and Lorin Hatch for graciously granting permission to use their data, and several anonymous referees, an associate editor, and the editor for providing helpful comments.

regressions of chlorophyll on phosphorus was greater than investigators believed it should be. Figure 1 shows plots of chlorophyll and phosphorus from two data sets. The left panels of Figure 1 show data from one of the early chlorophyll-phosphorus regressions cited previously, and the right panels show data from a more recent study. In the upper half of the figure, these data are presented under log transformation of both chlorophyll and phosphorus; in the lower half of the figure, the same data are plotted in original units of measurement. Ordinary least squares fits of the data are provided by the dashed lines, shown in the lower panels under transformation to original scale. Both regressions using log data are significant, but the amount of residual variability differs markedly; r^2 values are .91 for the data on the left and .24 for the data on the right. There is strong substantive reason to believe that both sets of data can be considered to be generated from the same model, as will be discussed in Section 2. The solid lines shown in the lower panels of Figure 1 will also be discussed later in this article.

That chlorophyll concentration is generally related to phosphorus concentration in temperate waters is untested, but ecologists recognize that several potentially limiting factors interact temporally and spatially to regulate algal biomass in most aquatic systems. Factors other than phosphorus that may limit algal biomass in lakes include other essential elements such as nitrogen and carbon, predation on algae by zooplankton (which may in turn be regulated by fish), and light availability, which is affected by various physical and biological processes. In addition, algal communities may be composed of a number of species with different physiological requirements, making the concept that algal biomass in an entire lake is limited by a single factor an over-simplified view of algal communities (Dodds, Johnson, and Priscu 1989). The view that phosphorus is the active limiting factor in the majority of lakes has been subjected to closer scrutiny in the past decade than at any time since the initial chlorophyll–phosphorus regressions were published. There is growing evidence that nitrogen is the major limiting factor in some Asian lakes (Jones, Knowlton, and Swar 1989). In a series of 54 experiments conducted to determine whether phytoplankton growth in 8 mountain lakes was limited by phosphorus, nitrogen, both concomitantly,

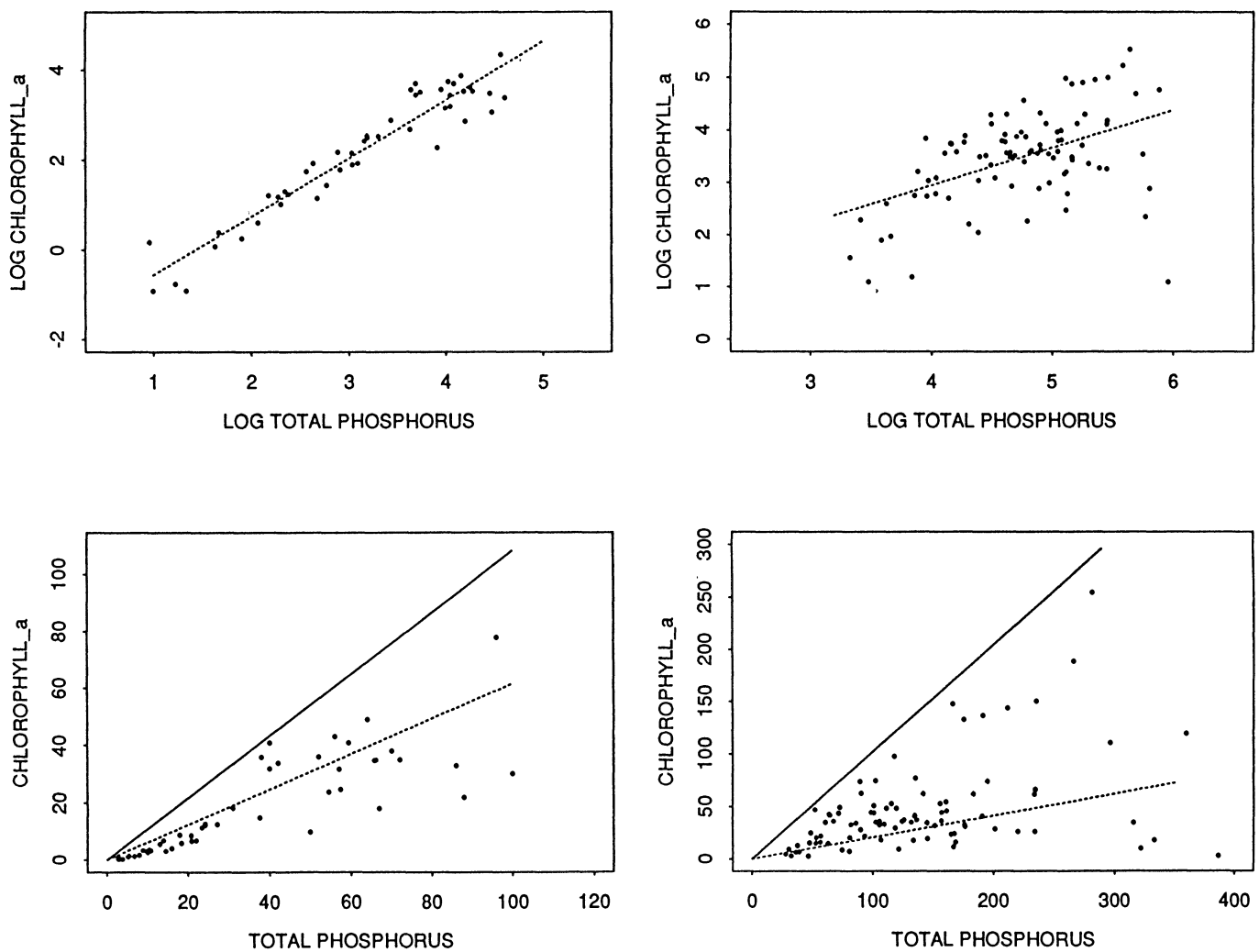

Figure 1. Data Sets From Two Limnological Studies. Data for the left-side panels are from Dillon and Rigler (1975). Data for the right-side panels were provided by Roger Bachmann and Lorin Hatch of Iowa State University. The upper plots show data under log transformation of both variables; the lower plots use original units (mg/m^3). See the text for a complete explanation.

or neither, phosphorus was determined to be the sole limiting factor on only 5 occasions; phosphorus and nitrogen, either alone or in combination were determined to be limiting on 23, or less than half, of the occasions (Morris and Lewis 1988).

Although phosphorus alone is not adequate to explain the regulation of algal growth in most lakes, in most cases phosphorus has continued to provide a better relation with chlorophyll than any other single potentially limiting factor. As a result, limnologists have attempted to construct improved models through the addition of other potentially limiting factors as explanatory variables in multiple linear regression. These attempts have met with little or no success (Hoyer and Jones 1983; Prairie, Duarte, and Kalff 1989; Smith and Shapiro 1981). Other approaches aimed at improving the basic relation between chlorophyll and phosphorus have included nonlinear models (McCauley, Downing and Watson 1989) and division of observations into groups based on nitrogen to phosphorus ratios (see, for example, Prepas and Trew 1983). None of these attempts has yielded a broadly applicable approach.

A major thesis of this article is that the source of difficulties with application of chlorophyll–phosphorus regressions to lake management lies in the fact that the law of the minimum does not translate into a regression model; we use the term "regression model" to refer to any model that has as its focus the description of conditional expectations over a range of values for the conditioning agent. As an alternative, we present models that directly reflect the substantive theory of limiting factors.

The article is organized as follows. Our argument for our claim is presented and some pertinent characteristics of limnological studies are briefly reviewed in Section 2. Statistical models of varying complexity are introduced in Section 3. Estimation is considered in Section 4, and some examples using simulated data are presented in Section 5. Section 6 compares the estimation approach developed with simpler approaches. A goodness-of-fit diagnostic is introduced and model selection is discussed in Section 7. An application of the models is presented in Section 8, and the article concludes with a short discussion in Section 9.

2. IMPLICATIONS OF THE LAW OF LIMITING FACTORS FOR STATISTICAL MODELS

Given a set of bivariate data, it is nearly always possible to fit some model aimed at description of the central tendency of the response variable. If a suitable parametric model proves elusive or is not desired, then one can use a smoothing function to describe the situation. But any such model fails to grasp the essence of the law of the minimum, which provides no direct indication of how the expected value of a response variable should change with the level of an explanatory factor. Rather, the law of the minimum translates directly into a model for the conditional maxima of responses or, more accurately, the conditional potential maxima. An adequate modeling effort should reflect this while also considering the complex nature of limnological measurement.

2.1 Turning the Law of the Minimum into a Statistical Model

The law of the minimum implies that when a potentially limiting factor becomes active, that factor regulates the biological process in question. If the limiting factor is depleted to a level at which it is no longer available, then the process stops. If the limiting factor is increased in level, then the process will continue until the factor is once again depleted. The biological process of concern here is algal growth in a lake. Given a potentially limiting factor that is continuously active, algal biomass should be given as an exact function of the limiting factor; continuous can be taken to mean across time, space, or different algal types in the community. Random variation in observed responses would be caused only by measurement error or by the use of measured quantities that do not exactly reflect the physical mechanism of limitation. In this situation it may be reasonable to model the expected values of observed levels of production as a function of the limiting factor, assuming that residual error, caused only by imperfect observation, will be small. This clearly does not appear to be the case for the examples presented in Figure 1. In contrast, given a potentially limiting factor that is not continuously active, the observed responses could assume any values that are less than the value dictated by the potentially limiting factor were it to become active and also subject to small perturbation from imperfect observation. In this latter situation, the law of the minimum translates into a model in which the maximum of observed responses is related to the potentially limiting factor.

A statistical model derived from the law of the minimum should focus on description of the maximum responses across levels of the potentially limiting factor. Observations will fall at or below the maximum, except as affected by the error of observation. The function used to describe maximum responses may be accurately interpreted to represent the maximum potential response for given levels of the potentially limiting factor. An essential part of any such model is to provide a description for the observed response falling below the potential maximum value. Here substantive theory provides little guidance, but it is reasonable to model the pattern of observations as if they were generated by some flexible probability distribution. Formal comparison of different data sets should include both the function that describes potential maximum values and the description of the pattern of observations. Our goal is to introduce such models.

2.2 Characteristics of Limnological Survey Data

Limnological assessment of the productivity of lakes and reservoirs and the supply of critical elements that may act as potentially limiting factors involves a complex measurement problem. Our concern is with empirical models to describe data gathered from limnological surveys in which waterbodies are sampled over the course of a summer, with each individual water body providing one datum. Thus we are concerned primarily with large-scale studies that focus on the major components of variation among lakes (Collins and Sprules 1983). We see no reason that, given independent observations, the models proposed here could not be applied

to data gathered from one waterbody, but the examples we present are broad surveys.

It is common in the analysis of data from limnological surveys to use single data points that represent a seasonal mean of individual observations taken on different days. A seasonal mean for a lake is calculated as the arithmetic average of (typically) three to four measurements made during the summer months. Again, there is no reason that these models could not be applied to individual measurements, but analyses predominant in the limnological literature involve seasonal means. A consequence of using seasonal values is that for an observation to reflect the maximum level of production possible, the response must be under active limitation by that factor at each of the individual sampling dates. With the use of seasonal averages it is reasonable to expect most, if not all, data points to lie below the theoretical maximum.

Limnologists generally measure the concentration of the photosynthetic pigment chlorophyll as an estimate of algal biomass; algal biomass in turn is a reflection of primary production (Smith 1979). Similarly, the concentrations of phosphorus or other nutrients are considered convenient, but not exact (Bradford and Peters 1987), measures of nutrient supply. The relations between measured values of chlorophyll and nutrients and the actual quantities involved in biological limitation of production has been addressed in the limnological literature (see, for example, Bradford and Peters 1987; Flynn 1988; and Walker 1986). The importance for statistical modeling is that the measured quantities of chlorophyll and nutrient concentrations represent the use of surrogate variables to assess lake and reservoir production. Limnologists consider the error associated with the use of these surrogate variables to be small relative to the magnitude of the measurements themselves. Thus, in the models presented here, we take error due to the use of surrogate measures to be absorbed along with measurement error in a single error term. Measurement error is a small component of systematic variation in limnological data (Knowlton, Hoyer, and Jones 1984).

3. STATISTICAL MODELS WITH EXPLICIT LIMIT FUNCTIONS

Throughout this section we let Y_i denote a measured response variable and let x_i denote the associated level of an explanatory factor. In the examples introduced, Y_i is chlorophyll concentration and x_i is total phosphorus concentration. Our goal is to relate $\mathbf{Y}$ to $\mathbf{x}$ through the use of models that in the absence of error explicitly represent the conditional maximum of $(\mathbf{Y}|\mathbf{x})$ as a linear limit function and to incorporate a way to estimate the probabilities that various proportions of that maximum will be observed. We assume independent Y_i's.

3.1 A Five-Parameter Model

The most complete model to be discussed is given by

$$Y_i = \gamma_1(x_i - \gamma_0)U_i + \sigma\varepsilon_i, \tag{1}$$

where $x_i \in [x_a, x_b] \subset \mathbb{R}^+$, $-\infty < \gamma_0 < \infty$, $\gamma_1 > 0$, $\sigma > 0$, the U_i are iid beta (α, β) random variables, and the ε_i are iid random error terms with mean 0. We assume that the U_i and ε_i are independent and that the ε_i have an absolutely continuous distribution function, F, with corresponding density f_ε. Model (1) describes data scattered below a straight line, subject to additive random error. The linear portion of the model, $-\gamma_1\gamma_0 + \gamma_1 x_i$, will be called the limit function, or simply the limit.

The random variable U_i models dispersion of the data below the limit function. We take a parametric distribution, the beta, for the U_i. The beta family is convenient and appears flexible enough to fit a number of data sets that we have examined. A diagnostic to assess model fit is given in Section 7. The additive term ε_i is included to model the combined effects of measurement error and the use of surrogate variables. This additive error term allows individual observations to lie above the limit and avoids a restriction on the support of Y. In our applications, F will generally be taken as the standard normal distribution function. Model (1) contains five parameters: γ_0, γ_1, and σ^2 explicitly and the beta parameters α and β through the U_i.

3.2 Reduced Models

Substantive theory may dictate that the response variable Y must equal 0 when the level of the explanatory factor is 0. This leads to a model with four parameters,

$$Y_i = \gamma x_i U_i + \sigma\varepsilon_i, \tag{2}$$

with $\gamma > 0$ and x_i, U_i, ε_i, and σ as before. Model (2) is simply model (1) with γ_0 taken as 0 or, equivalently, some other known value. Under some circumstances it may be desirable to make additional restrictions in the form of the model. For example, the amount of data available may prohibit estimation of four or five parameters, yet we may wish to examine exploratory questions or determine whether the more complex models show promise as a means of analysis. A substantial reduction in the complexity of the model may be obtained by assuming that the dispersion of data falling below the limit is completely specified, and in particular that α and β both equal 1. Then

$$Y_i = \gamma x_i U_i + \sigma\varepsilon_i, \qquad U_i \sim \text{iid uniform } (0, 1). \tag{3}$$

An alternative is to assume that no observation error is present in the model so that

$$Y_i = \gamma x_i U_i, \qquad U_i \sim \text{iid beta}. \tag{4}$$

Note that if both beta parameters are taken as 1 in (4), then Y_i has a uniform distribution on $(0, \gamma x_i)$, and the maximum likelihood estimate of γ becomes simply $\max\{Y_i/x_i\}$. For any values of the beta parameters, model (4) places an absolute restriction on the support of Y_i, which, given the intended use of these models in ecological field studies, is statistically unpleasing. Also, the asymptotic result mentioned in Section 4.4 does not apply to models with no random error term, because the support of the Y_i then depends on the parameter γ. It can be easily shown that for model (4) with $U_i \sim$ iid uniform (0, 1), the limiting distribution of the maximum likelihood estimator, $\hat{\gamma}$, is exponential (cf. Kaiser 1990).

3.3 Model Formulation

To formulate models including an additive error term, let $\phi = (\alpha, \beta)$ denote the parameters of the beta distribution and

$$g(u|\phi) = u^{\alpha-1}(1-u)^{\beta-1}.$$

In addition, let $\theta = (\gamma_0, \gamma_1, \sigma)$ denote the remaining parameters and define the function

$$f(y|u, \theta, x) = f_\varepsilon\left(\frac{y - \gamma_1(x-\gamma_0)u}{\sigma}\right).$$

Then, using $C = \sigma\Gamma(\alpha)\Gamma(\beta)/\Gamma(\alpha+\beta)$, Y_i has density

$$h(y|\phi, \theta, x_i) = C^{-1}\int_0^1 g(u|\phi)f(y|u, \theta, x_i)\,du, \qquad -\infty < y < \infty. \quad (5)$$

The Y_i are independent but nonidentically distributed random variables due to the influence of the x_i, and $h(y|\phi, \theta, x_i)$ in (5) is an identifiable mixture distribution. This formulation leads naturally to consideration of the problem as one involving missing information, where the Y_i are observed but the U_i are not. In this context, the density of the complete data is

$$p(u, y|\phi, \theta, x) = C^{-1}g(u|\phi)f(y|u, \theta, x), \quad (6)$$

and the conditional density of the unobserved U_i, given the observed Y_i, is

$$k(u|y, \phi, \theta, x) = \frac{p(u, y|\phi, \theta, x)}{h(y|\phi, \theta, x)}. \quad (7)$$

Equations (5), (6), and (7) apply directly for models (1) and (2), and the major difficulty for parameter estimation is the unevaluated integral appearing in several of these expressions. Complete specification of the distribution of the mixing random variable, U_i, with $\alpha = \beta = 1$ as in model (3) simplifies computation and may eliminate this integral. The density of Y_i for model (3) is given by

$$h(y|\theta, x_i) = \sigma^{-1}\int_0^1 f(y|u, \theta, x_i)\,du = (\gamma x_i)^{-1}[F(y/\sigma) - F((y-\gamma x_i)/\sigma)], \quad (8)$$

for $-\infty < y < \infty$. Equation (8) may still contain an integral form for $F(\cdot)$ with some choices of the error distribution such as normal, but the computation of integrals defining well-known cdf's is a less arduous task than evaluation of mixtures such as (5) and may often be accomplished by a polynomial approximation. Models lacking an additive error term, such as (4), eliminate the need to deal with incomplete information, and the density of Y_i is that of a scaled beta with the scaling factor depending on x_i.

4. PARAMETER ESTIMATION

Our approach for parameter estimation is marginal maximum likelihood using the missing information principle (Hartley 1958; Orchard and Woodbury 1972), popularized and formulated as the EM algorithm by Dempster, Laird, and Rubin (1977). The EM algorithm is most appropriately applied to these models in its general form, because for many choices of F the densities (5) are not members of an exponential family. Even for a model with normally distributed errors, these densities constitute a curved, rather than a regular, exponential family.

4.1 General EM Algorithm Estimation

The general EM algorithm consists at each iteration of evaluating the expected complete data log-likelihood formed from (6) and maximizing the result with respect to the unknown parameters. Expectation is taken with respect to (7) for some fixed parameter values. If the distribution of the ε_i in models (1) or (2) is taken as normal, so that $f_\varepsilon(\cdot)$ used to define $f(\cdot)$ in (5) is the standard normal density, then the expected complete data log-likelihood becomes

$$Q(\phi, \theta|\phi_p, \theta_p) = -n\log(C) - \frac{n}{2}\log(2\pi) + (\alpha-1)\times\sum_{i=1}^n E\{\log(U_i)|y_i, \phi_p, \theta_p, x_i\} + (\beta-1)\times\sum_{i=1}^n E\{\log(1-U_i)|y_i, \phi_p, \theta_p, x_i\} - \frac{1}{2\sigma^2}\times\sum_{i=1}^n E\{(y_i - \gamma_1(x_i-\gamma_0)U_i)^2|y_i, \phi_p, \theta_p, x_i\}, \quad (9)$$

where for model (2), γ_0 is taken as 0. The success of the EM algorithm in this case stems from the fact that the M step, maximization of equation (9), separates into parts for $\phi = (\alpha, \beta)$ and $\theta = (\gamma_0, \gamma_1, \sigma)$.

Maximization for θ is accomplished by direct solution of the gradient vector, giving

$$\hat\gamma_{1(p+1)} = \frac{\sum_{i=1}^n x_i y_i E_p(U_i)\sum_{i=1}^n E_p(U_i^2) - \sum_{i=1}^n y_i E_p(U_i)\sum_{i=1}^n x_i E_p(U_i^2)}{\sum_{i=1}^n x_i^2 E_p(U_i^2)\sum_{i=1}^n E_p(U_i^2) - [\sum_{i=1}^n x_i E_p(U_i^2)]^2}, \quad (10a)$$

$$\hat\gamma_{0(p+1)} = \frac{\hat\gamma_{1(p+1)}\sum_{i=1}^n x_i E_p(U_i^2) - \sum_{i=1}^n y_i E_p(U_i)}{\hat\gamma_{1(p+1)}\sum_{i=1}^n E_p(U_i^2)}, \quad (10b)$$

and

$$\hat\sigma^2_{p+1} = n^{-1}\sum_{i=1}^n E_p[y_i - \hat\gamma_{1(p+1)}(x_i - \hat\gamma_{0(p+1)})U_i]^2, \quad (10c)$$

where in all of these equations

$$E_p[t(u_i)] = E[t(u_i)|y_i, \phi_p, \theta_p, x_i] = \int_0^1 t(u)k(u|y_i, \phi_p, \theta_p, x_i)\,du.$$

The update equations (10), although algebraically complex, are not difficult to calculate once the moments of U_i and U_i^2 conditional on (ϕ_p, θ_p) are obtained numerically. The

updates $\phi_{p+1} = (\alpha_{p+1}, \beta_{p+1})$ can be computed by evaluating the partial derivatives

$$\frac{\partial}{\partial\alpha} Q = \sum_{i=1}^{n} \int_0^1 \log(u) k(u|y_i, \phi_p, \theta_p, x_i)\, du - n[\psi(\alpha) - \psi(\alpha+\beta)],$$

$$\frac{\partial}{\partial\beta} Q = \sum_{i=1}^{n} \int_0^1 \log(1-u) k(u|y_i, \phi_p, \theta_p, x_i)\, du - n[\psi(\beta) - \psi(\alpha+\beta)],$$

$$\frac{\partial^2}{\partial\alpha^2} Q = n[\psi'(\alpha+\beta) - \psi'(\alpha)],$$

$$\frac{\partial^2}{\partial\beta^2} Q = n[\psi'(\alpha+\beta) - \psi'(\beta)],$$

and

$$\frac{\partial^2}{\partial\alpha\partial\beta} Q = n\psi'(\alpha+\beta), \tag{11}$$

where $\psi(\cdot)$ and $\psi'(\cdot)$ are the digamma and trigamma functions. Using these derivatives, a Newton–Raphson solution for $\hat{\alpha}_{p+1}$ and $\hat{\beta}_{p+1}$ may be obtained in the usual manner. The required conditional moments of $\log(U_i)$, $\log(1-U_i)$, and the digamma and trigamma functions can be evaluated numerically.

4.2 Simplifications for Reduced Models

The general EM algorithm simplifies for models containing less than five parameters. Restricting γ_0 to be 0, as in model (2), simplifies the update equations for $\theta = (\gamma, \sigma^2)$ whereas estimation of $\phi = (\alpha, \beta)$ remains unchanged.

For model (3), in which the distribution of the U_i is taken as completely specified, the gradient of the expected complete data log-likelihood may be solved analytically in terms of the standard normal cdf, $\Phi(\cdot)$, which then collapses the E and M steps of the algorithm for estimation of θ. As an alternative to model (3) with normal errors, the use of logistic errors allows rapid calculation of estimates directly from the marginal log-likelihood, which becomes

$$L = \sum_{i=1}^{n} \log[(1+\exp(-y_i/\sigma))^{-1} - (1+\exp(-(y_i-\gamma x_i)/\sigma))^{-1}] - \sum_{i=1}^{n} \log(\gamma x_i).$$

This function may be easily maximized using a direct search algorithm such as Nelder and Mead's modified simplex, the method of Hooke and Jeeves, or the method of Powell (Press, Flannery, Teukolsky, and Vetterling 1986). If σ is fixed in model (3) with either normal or logistic errors, then the algorithm reduces to simple one-dimensional bisection. Reducing the problem to this level, calculation is rapid enough to allow the use of profile likelihoods, although we have not pursued this.

4.3 Numerical Considerations

Application of the EM algorithm for this problem requires repeated numerical evaluation of eight integral equations. The integral appearing in (10) must be evaluated to obtain $k(u|y_i, \phi_p, \theta_p, x_i)$, which appears in other integrands. The conditional moments of U_i and U_i^2 are used in (10), whereas $\Gamma(\cdot)$, $\psi(\cdot)$, $\psi'(\cdot)$, and the conditional expectations of $\log(U_i)$ and $\log(1-U_i)$ are used in (11). Numerical evaluation of these integrals takes some care, because their shape and location depend on x_i and y_i, and the algorithm is sensitive with regard to the precision of these numerical calculations. Nevertheless, the quantities needed in both (10) and (11) require a single routine that allows a minor change in the integrand. Thus, although the number of numerical integrations is large, the problem amounts to evaluation of only two basic types of integrands. Given that these numerical integrations have been performed, the observed data log-likelihood is calculated as

$$\begin{aligned} L(\phi_p, \theta_p, \underset{\sim}{y}|\underset{\sim}{x}) &= \sum_{i=1}^{n} \log \int_0^1 g(u|\phi) f(y_i|u, \theta, x_i)\, du \\ &\quad - n\log(C) \\ &= n\log[\Gamma(\alpha_p+\beta_p)] \\ &\quad - n\log[\Gamma(\alpha_p)\Gamma(\beta_p)] - n\log\sigma_p \\ &\quad + \sum_{i=1}^{n} \log\{Ch(y_i|\phi_p, \theta_p, x_i)\}, \end{aligned} \tag{12}$$

because from (5), $Ch(y|\phi, \theta, x) = \int g(u|\phi) f(y|u, \theta, x) \times du$, which by (7) must be computed for use in (10) and (11). We assume convergence when $|L_{p+1} - L_p| \le \delta$. A secondary check for convergence of the estimates may also be made, using $\|(\hat{\phi}_{p+1}, \hat{\theta}_{p+1}) - (\hat{\phi}_p, \hat{\theta}_p)\| \le \delta'$. In most situations examined, convergence of the likelihood and vector of parameter estimates occurred within a small number of iterations of each other, taking both δ and δ' as .001 or .0005.

4.4 Large-Sample Behavior

A theorem given by Kaiser (1990) permits fairly general conditions for maximum likelihood estimates of ϕ and θ to be consistent and asymptotically normal. Given restriction of the x_i to a bounded interval of the real line, these conditions depend entirely on the distribution of the ε_i and an assumption of convergent information. We thus use the inverse information matrix to approximate the large-sample covariance matrix of the maximum likelihood estimate. For many incomplete data problems, the expected information is difficult to calculate, but the observed information (Efron and Hinkley 1978) may be used instead. Louis (1982) presented a general procedure for computing the observed information matrix in applications of the EM algorithm by making use of the missing information principle of Orchard and Woodbury (1972). Using the proof found in the appendix of Louis, the observed information matrix for one observation may be computed as

$$I_i(y) = E\{B_i(\hat{\eta}, y_i, U|x_i)|\, y_i, \hat{\eta}\} - E\{S_i(\hat{\eta}, y_i, U|x_i)S_i^T(\hat{\eta}, y_i, U|x_i)|\, y_i, \hat{\eta}\} + E\{S_i(\hat{\eta}, y_i, U|x_i)|\, y_i, \hat{\eta}\} \times E\{S_i(\hat{\eta}, y_i, U|x_i)|\, y_i, \hat{\eta}\}^T, \quad (13)$$

where $\eta = (\phi, \theta)$, $B_i(\eta, y, u|x)$ is the matrix with jkth element $-(\partial/\partial\eta_j\eta_k)\tilde{L}_i(\eta, y, u|x)$, $S_i(\eta, y, u|x) = \nabla\tilde{L}_i(\eta, y, u|x)$, and $\tilde{L}_i(\eta, y, u|x) = \log p(u, y|\eta, x_i)$ is the contribution of the ith observation to the complete data log-likelihood. The total observed information matrix is then given as $I.(\underset{\sim}{y}) = \sum I_i$. Necessary derivatives are easily found and expectations approximated by numerical methods as before. Using the total observed information, an approximate large-sample interval estimate for a constituent parameter of η may be formed as

$$\eta_j \pm z_{\alpha/2}\hat{\sigma}_{jj}(\underset{\sim}{y}), \quad (14)$$

where $\hat{\sigma}^2_{jj}(\underset{\sim}{y})$ is the appropriate diagonal element of $[I.(\underset{\sim}{y})]^{-1}$.

5. EXAMPLES USING SIMULATED DATA

Several examples of data simulated from models (1) and (2) are presented in Figure 2 to demonstrate the variety of situations that may be handled by these models. Solid lines represent true values of the parameters, and dashed lines represent estimated values. Known and estimated values for all of the parameters are given in Table 1.

The leftmost panels of Figure 2 illustrate the situation we envisioned when developing these models. Here the data are scattered as a triangle lying below a linear limit function except for additive error. The center panels illustrate a situation for which accurate estimation of the limit function is not intuitive, as no points lie above the limit function and few lie near it. Estimation is apparently capable of discerning this situation, in which the bulk of the probability mass for the U_i lies toward the lower end of the range (0, 1), from that described by the left panels. The rightmost panels in Figure 2 illustrate a situation similar to data generated from a simple linear regression model. Linear regression models are limiting forms of models (1) and (2), with β fixed at 1 and α tending to infinity. In addition to the true and estimated limit functions, the upper right panel of Figure 1 includes the ordinary least squares (OLS) estimate of expected values of Y as the broken line.

Taken together, the examples presented in Figure 2 indicate that the appropriateness of models such as (1) and (2) for a problem requires more than visual inspection of the data. These models were developed as the result of a strong substantive theory, and the appropriateness of their use is perhaps more dependent on the availability of suitable subject matter theory than is the use of many statistical models. We discuss statistical evaluation of the appropriateness of these models in Section 7.

6. COMPARISON WITH SIMPLER LEAST SQUARES ESTIMATORS

Estimation of parameters as described in Section 4 involves the use of numerical methods imbedded in iterative algorithms. It is natural to question whether this computational burden is worth the effort and to wonder whether simpler techniques based on least squares might not behave as well as the estimators proposed here. Our focus is on estimation of a function to describe, in the absence of additive error, the maximum response for a given covariate level. To be used for this purpose, a least squares estimate of the conditional expected response must be adjusted appropriately, which would be difficult for the case of unknown beta parameters as in (1) and (2). For models (3) and (4) with the U_i uniform, $E[Y_i] = \gamma x_i/2$, and under a uniform assumption this is also true for model (4). Thus, using either of these models, an unbiased estimate of γ may be obtained by multiplying a least squares estimate by 2. The variance of Y_i from model (3) is $(\gamma x_i)^2/12 + \sigma^2$, so it is reasonable to use a weighted least squares estimator. The simplest approach would take the weights to be proportional to $1/x_i^2$, whereas a slightly more complicated procedure would involve iteratively reweighted least squares using $(\hat{\gamma}x_i)^2/12 + \hat{\sigma}^2$ as weights at each step.

A simulation was conducted using data generated from both model (3) and model (4) with U_i uniform, to compare the efficiency of maximum likelihood estimators and these two least squares estimators. The simulation consisted of generating 1,000 data sets each from models (3) and (4), with $U_i \sim$ iid uniform (0, 1) and $\varepsilon_i \sim$ iid logistic (0, 1) in model (3). The value of γ was held at 1.5 throughout, and $x_i = \{1, 2, \ldots, 50\}$. Let $\hat{\gamma}^{(1)}$ and $\hat{\gamma}^{(2)}$ denote the maximum likelihood estimators developed from models (4) and (3), let $b_w^{(1)}$ denote the least squares estimator with weights $1/x_i^2$, and let $b_w^{(2)}$ denote the iteratively reweighted least squares estimator. Squared error loss was used to compare estimators, because the maximum likelihood estimator for model (4), which lacks a random error term, is biased. Mean observed squared errors for the four estimators with data generated from model (4) were .0017 for $\hat{\gamma}^{(1)}$, .0033 for $\hat{\gamma}^{(2)}$, .015 for $b_w^{(1)}$, and .0166 for $b_w^{(2)}$. Thus both estimators based on least squares algorithms showed an expected squared error 5 times that of the maximum likelihood estimator developed from model (3) and nearly 10 times that of the maximum likelihood estimator for the true model. Using model (3) to generate data, the mean observed squared errors were .9431 for $\hat{\gamma}^{(1)}$, .0034 for $\hat{\gamma}^{(2)}$, .0283 for $b_w^{(1)}$, and .0172 for $b_w^{(2)}$. Clearly, an estimator that assumes additive random error, $(\hat{\gamma}^{(2)})$, is preferable to an estimator that does not, $(\hat{\gamma}^{(1)})$, under reciprocal model misspecification. The expected squared error estimated in this simulation was about 8 times that of the maximum likelihood estimator for the weighted least squares estimator and 5 times the maximum likelihood estimator for the iteratively reweighted solution.

It can be shown that for model (3), which assumes a uniform distribution for the U_i and additive random error, the maximum likelihood estimator is consistent and asymptotically normal (Kaiser 1990), with Fisher information

$$I_n(\gamma) = \sum_i \left\{ \frac{x_i}{\gamma} \int \frac{f_\varepsilon^2(y - \gamma x_i)}{F(y) - F(y - \gamma x_i)}\, dy \right\} - \frac{n}{\gamma^2}. \quad (15)$$

Again using logistic errors for ease of computation, an additional simulation using model (3) was conducted with

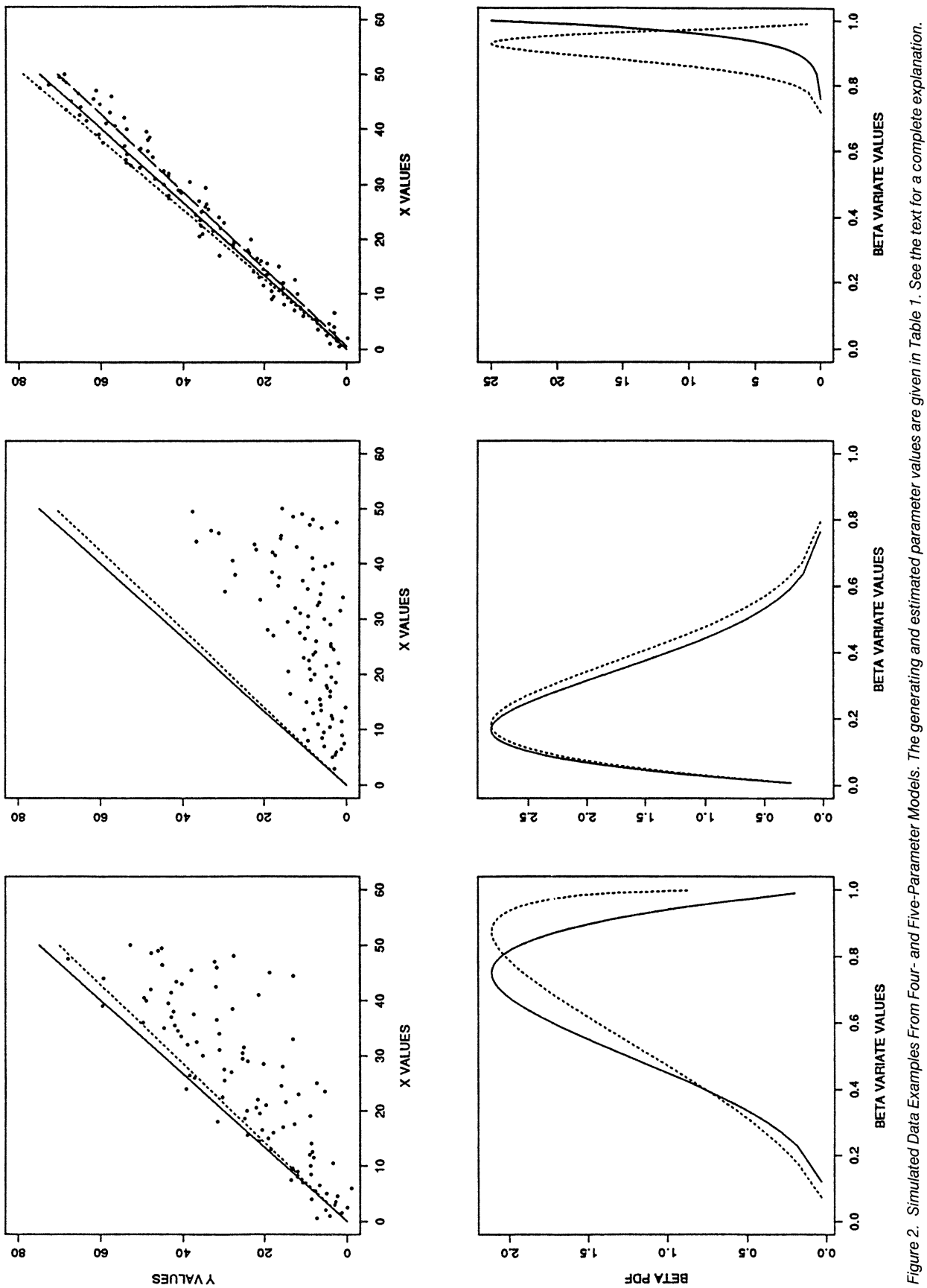

Figure 2. Simulated Data Examples From Four- and Five-Parameter Models. The generating and estimated parameter values are given in Table 1. See the text for a complete explanation.

Table 1. Parameter Values and Estimates for Simulated Data of Figure 2

Data set	α	$\hat{\alpha}$	β	$\hat{\beta}$	γ_0	$\hat{\gamma}_0$	γ_1	$\hat{\gamma}_1$	σ^2	$\hat{\sigma}^2$
Left panels	4.00	2.75	2.00	1.30	30.00	28.84	1.50	1.36	16.00	20.98
Center panels	2.00	1.98	6.00	5.44	—	—	1.50	1.42	3.00	1.86
Right panels	25.00	36.29	1.00	3.87	15.00	14.64	1.50	1.56	9.00	8.42

equally spaced x_i on the interval (0, 50]. The number of values of x was increased from 50 to 100, and the bias and variance of the maximum likelihood estimator $\hat{\gamma}^{(2)}$ was examined. Although the estimated bias was not significantly different from 0 for all sample sizes, the mean observed variance did not approach that given by (15) until 100 values of x were used. The theoretical variance calculated using (15) and the mean observed variance from 1000 simulated data sets were (.0025, .0033) for 50 values of x, (.0016, .0021) for 75 values of x, and (.0012, .0012) for 100 values of x. Observed coverage rates for a 95% interval estimate in these cases were <80%, 88%, and 96%, and p values from Kolmogorov–Smirnov tests of normality applied to parameter estimates were .013, .030, and .170.

7. MODEL SELECTION AND A GOODNESS OF FIT DIAGNOSTIC

Faced with the analysis of a single data set, it is not clear in what manner one should choose from among the possible models and under what conditions one should accept results that differ from what was expected. The answers to these questions certainly must depend in part on substantive theory, but statistical approaches should also prove useful. For example, substantive theory may indicate that if no positive level of the explanatory factor (or potentially limiting factor) is present, then no positive level of response will be present, but the converse may be more difficult to defend. That is, it may well be possible that the explanatory factor must be present at some level greater than a certain threshold before a measurable response will occur. In dealing with real data we have found the choices in model to be among (1), (2), and (3). Models with restrictions greater than (3)—that is, models lacking an additive error term—have been used to obtain starting values, but they hold little hope for a realistic description of most problems. In practice, then, the choice of model can be broken into three issues: inclusion of γ_0, inclusion of $\phi = (\alpha, \beta)$, and model adequacy.

7.1 Assessing Goodness of Fit

A graphical goodness-of-fit diagnostic may be developed based on the probability integral transformation in which we replace the parameters by estimates to calculate

$$\tilde{v}_i = \int_{-\infty}^{y_i} h(y|\hat{\phi}, \hat{\theta}, x_i)\, dy$$

$$= C^{-1} \int_{-\infty}^{y_i} \int_0^1 g(u|\hat{\phi}) f(y|u, \hat{\theta}, x_i)\, du\, dy. \quad (16)$$

Here $\hat{\phi}$ and $\hat{\theta}$ are maximum likelihood estimates, and $h(\cdot)$, $g(\cdot)$, and $f(\cdot)$ are as defined in Section 3. Note that in the case of model (3), $g(u|\phi)$ is completely specified, and $h(y|\hat{\phi}, \hat{\theta}, x_i)$ in (15) becomes $h(y|\hat{\theta}, x_i)$. The variates $\tilde{v}_i$ are calculated by means of numerical integration, the inner integrations in (16) having been previously used in estimation. The empirical cdf of the $\tilde{v}_i$ may then be graphed along with the uniform (0, 1) cdf, and measures such as the Kolmogorov–Smirnov one-sample goodness-of-fit test can be used as a guide to decision making.

This diagnostic addresses the question of whether or not a model provides an acceptable description of the data. Because the diagnostic involves the use of parameter estimates to define the cdf of the responses, and because these are not simple location and scale parameters, no probability results are offered and no attempt has been made to reduce the dimensionality of the sample to gain independence among the transformed variates. Nevertheless, we feel that the diagnostic offers a reasonable technique to address model fit based on heuristics and the fact that exact results are available for a number of specific examples using the same principle (see, for example, Quesenberry 1986).

7.2 Model Selection

In cases for which several models provide adequate descriptions of the observed data, the choice among models may be approached through the use of likelihood ratio tests. In particular, whether or not to include γ_0 as a parameter in the model and whether or not to include the parameters α and β are questions that lend themselves to likelihood ratio tests. Likelihood ratio tests may also be constructed to determine whether groups of observations should be described with separate models or a common model. Although we have no formal validation of this approach, the use of likelihood ratio tests seems reasonable here, particularly in light of the consistency and asymptotic normality of maximum likelihood estimates mentioned in Section 4.

7.3 Application to the Data of Figure 1

The use of likelihood ratio tests and the goodness-of-fit diagnostic for model selection may be illustrated using the examples of Figure 1. A plot showing the goodness-of-fit diagnostic for each of these data sets is given in Figure 3. The upper left panel of Figure 3 shows the goodness-of-fit diagnostic for fits of model (2) and model (3) to the data on the left in Figure 1. The empirical distributions for values of $\tilde{v}_i$ from (16) are plotted as dots for model (2) and as plus symbols for model (3). The Kolmogorov–Smirnov statistics were .143, .127, and .253 for models (1), (2), and (3). The diagnostic for model (1) is not shown in Figure 3 because of overlap with the line for model (2). Models (2) and (1) provide adequate descriptions of the data, but model (3) does not. The final model selection for these data was based on

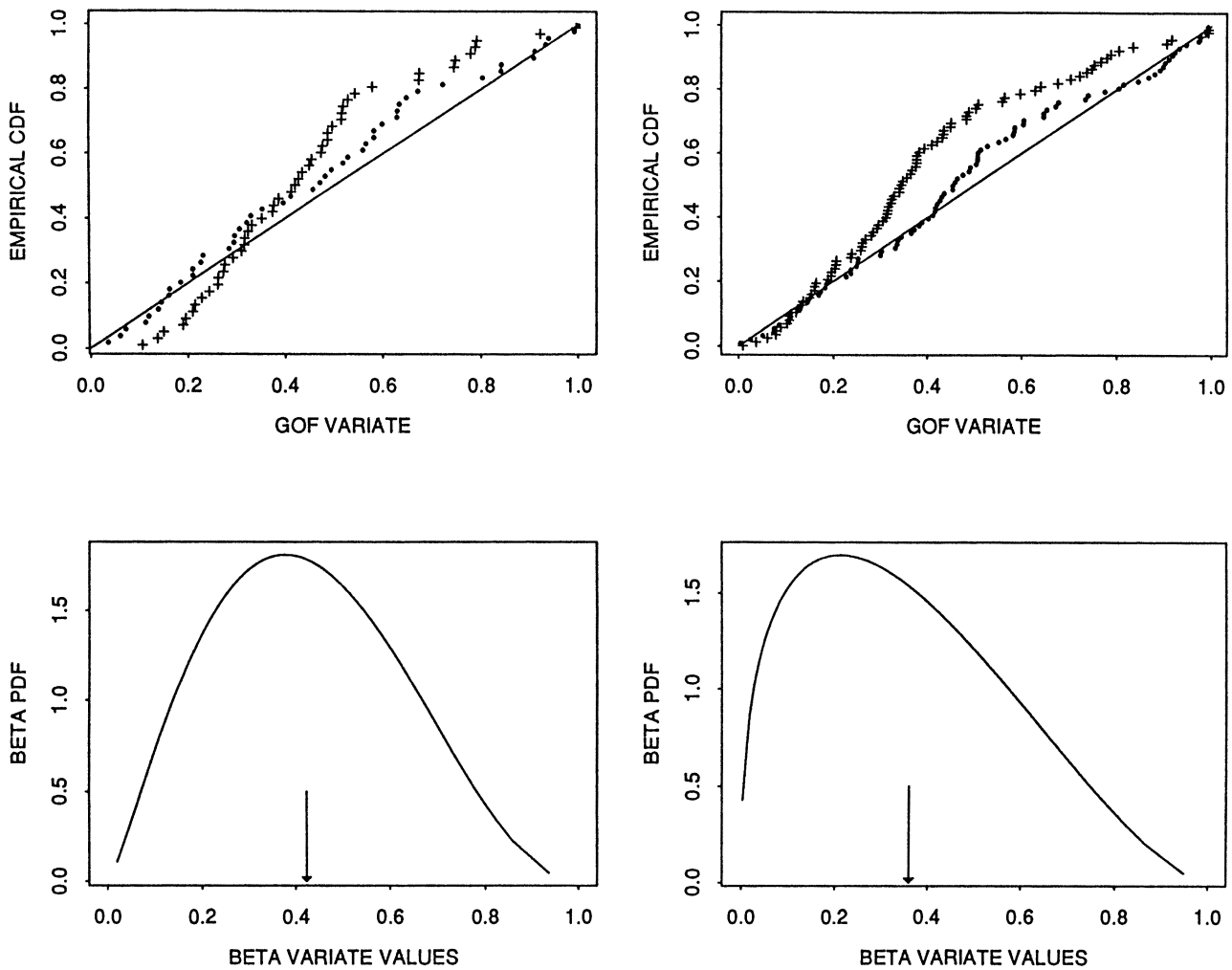

Figure 3. Plots of the Goodness-of-Fit Diagnostic and Estimated Beta Density Functions for the Data of Figure 1. The left-side panels correspond to the left side of Figure 1 (data from Dillon and Rigler 1975); the right side panels correspond to the right side of Figure 1 (data from Bachmann and Hatch).

a likelihood ratio test between models (1) and (2), a test that $\gamma_0 = 0$ in model (1). The observed data log-likelihoods were -147.2478 and -146.6341, giving a likelihood ratio test statistic of 1.227 with 1 degree of freedom. Thus the final model selected was model (2) with estimated parameters $\hat{\alpha} = 2.28$, $\hat{\beta} = 3.11$, $\hat{\gamma} = 1.09$, and $\hat{\sigma}^2 = .20$.

The upper right panel of Figure 3 shows the plotted goodness-of-fit diagnostic for fits of models (2) and (3) to the data on the right in Figure 1, using dots for model (2) and plus symbols for model (3) as before. The Kolmogorov–Smirnov statistics were .083, .099, and .254 for models (1), (2), and (3); the diagnostic for model (1) is again not shown because of overlap. Log-likelihoods were -401.1634 for model (1) and -401.5294 for model (2), resulting in a single degree of freedom likelihood ratio test statistic for $\gamma_0 = 0$ of .732; parameter estimates for model (2) were $\hat{\alpha} = 1.41$, $\hat{\beta} = 2.53$, $\hat{\gamma} = 1.02$, and $\hat{\sigma}^2 = 1.53$.

The lower panels of Figure 3 show plots of beta density functions using estimates of α and β for the two data sets. The discussions of Sections 2 and 3 indicate that these two data sets—one for which linear regression of transformed variables provided a good fit (data on the left) and one for which such regression did not provide a good fit (data on the right, see Fig. 1)—should both be considered as arising from the same model. Although as analyzed by regression these data sets provide quite disparate evidence of the strength and form of the relation between chlorophyll and phosphorus, analysis using the models proposed here results in similar conclusions for both data sets. The estimated limit functions were both very near a value of 1 (i.e., 1.09 and 1.02), and the estimated mixing distributions indicate the mean proportion of the potential maximum reached is about .4 in both cases (i.e., .42 and .38). The shapes of these distributions differ; that for the "poor regression" data is skewed to the right, whereas that for the "good regression" data exhibits a more symmetric form. The conclusion reached from a regression-based analysis would be that the data on the left in Figures 1 and 3 indicate that phosphorus is limiting for chlorophyll, whereas the data on the right in these figures provide no such evidence. Using a more appropriate model, both data sets result in a conclusion that at the maximum value of chlorophyll possible, chlorophyll and phosphorus occur in a ratio close to unity, and that the distribution of values below this maximum has a central value of about .4

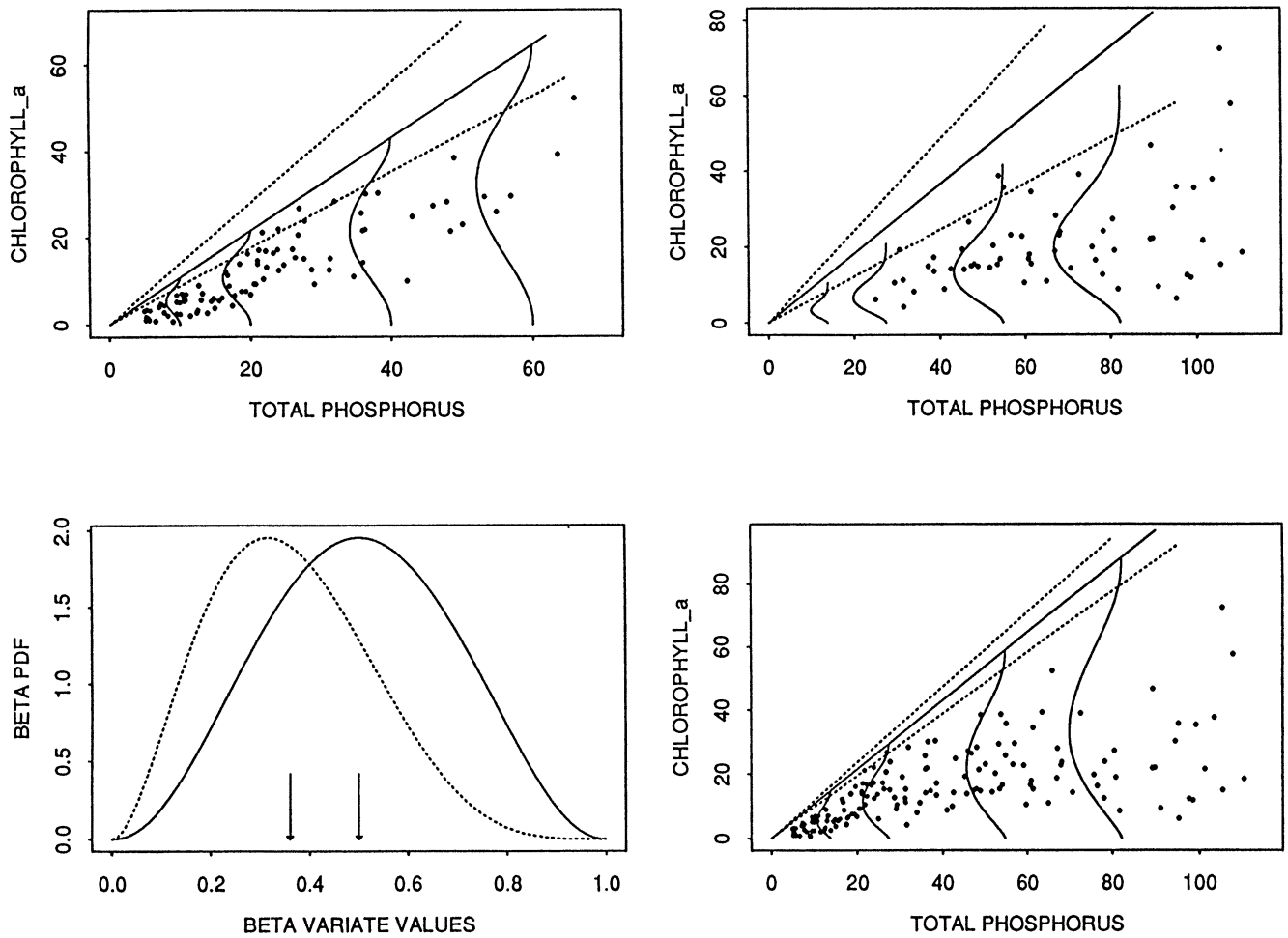

Figure 4. Seasonal Mean Chlorophyll and Phosphorus Concentrations in Reservoirs in Missouri, Grouped by Inorganic Suspended Solids Content of Water. The plotted lines show estimated limit function, limit functions for lower and upper endpoints of 90% interval estimates, and estimated distributions of observed data. Parameter estimates are given in Table 3. See the text for a complete explanation.

times the potential maximum. Differences between the two data sets are exhibited in the shapes of these estimated distributions.

8. AN APPLICATION TO PHOSPHORUS LIMITATION OF PHYTOPLANKTON GROWTH

In many limnological studies the amount of particulate matter in the water is a potential agent in the limitation of algal growth. Particulate matter reduces the availability of light to photosynthetic algal cells and may remove phosphorus from the water by binding processes (Jones and Bachmann 1978). The particulate matter of concern is inorganic material, such as clay and related material. In lakes and reservoirs this particulate matter is often measured as the concentration of inorganic suspended solids (ISS). A data set consisting of seasonal mean values of chlorophyll, total phosphorus, and ISS from reservoirs in Missouri was separated into two groups based on ISS: one group consisting of low values (ISS < 3) and the other consisting of high values (ISS > 6). Our objectives were to determine the maximum potential chlorophyll concentration for these waters, to determine the probabilities with which waters obtain various proportions of the maximum, and to determine whether differences exist in these characteristics for waters in the two ISS groups.

Results are summarized in Figure 4 and Tables 2 and 3. Table 2 contains maximized log-likelihoods and Kolmogorov distance measures for fits of models (1), (2), and (3) to the two ISS groups and to a combined data set; included are maximized log-likelihood values for a normal linear regression for each case. Based on distance measures from the goodness-of-fit diagnostic, models (1) and (2) both provide adequate fits of all three data sets, but model (3) fails to adequately fit any of the data sets; approximate critical values for the Kolmogorov–Smirnov statistic at the .05 and .10 levels are (.139 and .124), (.172 and .154), and (.108 and .097) for sample sizes of 93, 60, and 153. Based on likelihood ratio tests at the .05 level, model (2) would be selected for all three data sets: ISS < 3, ISS > 6, and the combined data.

Parameter estimates and their approximate asymptotic standard errors for model (2) fit to each ISS group and to the combined data are given in Table 3. Interpretation of these estimates may be made in terms of the estimated potential maximum and actual observed concentrations of chlorophyll for a range of phosphorus concentrations. The estimated value of γ for the two groups suggests that the

maximum potential response of algal communities to phosphorus is similar for the two ISS groups but may be slightly greater for reservoirs with low ISS ($\hat{\gamma} = 1.07$) than for reservoirs with high ISS ($\hat{\gamma} = .93$). Approximate 90% interval estimates for this parameter overlap are (.82, 1.34) for ISS < 3 and (.61, 1.21) for ISS > 6. In addition, estimated beta pdf's indicate that the proportion of maximum potential chlorophyll obtained by lakes in the two groups is nearly symmetric in distribution for low ISS lakes but positively skewed for high ISS lakes; lakes low in ISS also may be expected to reach a higher proportion of their potential maximum (.50) than lakes with high ISS values (.36), presumedly because of greater light availability. An inspection of the estimated asymptotic standard errors for $\hat{\alpha}$ and $\hat{\beta}$ (Table 2) again shows that these differences would not be "significant" as measured by a conventional statistical test.

A statistically more pleasing assessment of likeness or difference between ISS groups can be made by comparing the entire models resulting from estimation using separate groups and one pooled data set. The sum of the observed data log-likelihoods under model (2) for the two individual data sets was −467.1524, whereas that for the combined data was −489.3191, yielding a likelihood ratio statistic of 44.3333 with 4 degrees of freedom. This is strong evidence for a difference between the two ISS groups. Inspection of the parameter estimates of Table 3 suggests that this difference may be primarily a result of different distributions of the data falling below the potential maximum. But, as indicated by the approximate standard errors for the beta distribution parameter estimates, and $\hat{\beta}$ in particular, any meaningful differences in particular parameters is difficult to detect with the given sample sizes; the standard error for $\hat{\beta}$ drops dramatically for the combined data set with 153 observations.

The upper panels of Figure 4 present the data for ISS < 3 on the left, ISS > 6 on the right, and the combined data on the lower right. Included in the figures are the estimated limit functions plotted as solid lines, approximate 90% interval estimates for the limit calculated from the asymptotic standard errors plotted as dashed lines, and estimated distributions for $\gamma x_i U_i$ (the horizontal "heights" of the pdf's shown were scaled to give a visually pleasing picture). The lower left panel of Figure 3 shows the estimated beta densities of the U_i for the two ISS groups (ISS < 3, solid line; ISS > 6, dashed line).

Many limnologists may find it surprising that the estimated limit functions in Figure 4, as well as those of Figure 1, bear more resemblance to the second simulated data example of Figure 2 than to the first. In fact, none of the examples presented have any data points lying above the estimated limit function and few points even near the limit. The estimated distributions of the variables U_i in the model imply low contact on the upper end of the interval (0, 1). Substantively, the fact that each datum is a mean of three or four individual measurements may help explain these data patterns. A seasonal mean that, in the absence of observation error, falls at the limit function represents a reservoir for which algal biomass was limited by phosphorus at each sampling; that is, a reservoir in a constant state of phosphorus limitation throughout the summer. Given the dynamic behavior nearly universal to biological processes, such events would be expected to occur only rarely (Walmsley 1984). Taken in total, the results presented here indicate that continuous phosphorus limitation may occur less often than is commonly assumed. Although this conjecture has important implications for overall control of eutrophication in lakes, it in no way diminishes the role played by phosphorus in the control of algal growth. One of the key issues faced in lake and reservoir management is the assessment and control of algal blooms, periods of rapid growth in the algal community. An important issue becomes identification of the limiting factor for such growth at a critical point in time. We believe that our models, if applied to individual daily observations from a single lake, could help determine whether the potential maximum algal biomass allowed by phosphorus conditions is defined by these critical periods or other times.

Table 3. Estimated Parameter Values and Asymptotic Standard Errors (in Parentheses) for Models of Chlorophyll and Phosphorus in Reservoirs From Missouri

ISS group	$\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\hat{\sigma}^2$	Sample size
Low (<3)	3.24	3.23	1.08	.20	93
	(1.160)	(2.189)	(.159)	(.746)	
High (>6)	2.92	5.13	.91	.15	60
	(.186)	(2.95)	(.182)	(.127)	
Combined	2.42	3.28	1.08	.08	153
	(.317)	(.665)	(.062)	(.242)	

NOTE: Estimates are for fits of model (2).

9. DISCUSSION

The theory of limiting factors is important in ecology, but the problem of developing models that reflect this theory in a realistic manner has received scant attention in the statistical literature. Models that use regression functions to describe the limiting effect of an explanatory factor often give unsatisfactory results, because they do not correctly reflect the underlying ecological theory. In this article we have shown how more appropriate models can be formulated and estimated. We make no claim that our models are *the correct* statistical representation for problems involving the theory

Table 2. Maximized Log-Likelihoods and Kolmogorov Distances (in Parentheses) for Fits of Models (1), (2), and (3) to Missouri Reservoir Chlorophyll and Phosphorus Data

ISS group	Model (1)	Model (2)	Model (3)	Sample size	Normal regression
Low (<3)	−249.880 (.0757)	−251.295 (.0544)	−270.655 (.1926)	93	−272.839
High (>6)	−215.602 (.0990)	−215.856 (.0974)	−229.217 (.2360)	60	−229.294
Combined	−489.040 (.0832)	−489.319 (.0685)	−513.962 (.1193)	153	−552.528

of limiting factors, only that they do less abuse to the substantive theory than an approach that takes limitation of a biological process to be reflected as expected values.

Several related models have been proposed to describe data that exhibit the form of a triangular scatterplot in specific problems. Maller, deBoer, Joll, Anderson, and Hinde (1983) estimated the maximum foregut volume of Western rock lobsters as a function of carapace length. The model used by these authors differs from ours in treatment of random error and intercept values, and their estimation involves a nonparametric approach. Winkler (1980) described several examples from the social sciences in which plotted data assume the shape of a "rectangular triangle." Raftery (1984) introduced a multivariate distribution constructed as a finite mixture of independent exponential distributions to deal with a variety of correlation structures.

Our models are a first step, and we envision several modifications and generalizations. The separation of the estimation problem into parts for θ and ϕ and the general form of derivatives that require numerical evaluation have allowed modification of the basic algorithm to deal with change points in the limit function and error variance modeled as a function of the x's. The connections of these modifications with substantive theory are not clear and await further development. The possibility of a nonlinear limit function is intriguing and might offer a smooth alternative to the use of a change point in the limit. In addition, consideration of the case in which the U_i in these models are not identically distributed for all x_i promises to prove both useful and challenging, as does the possible use of nonadditive error structure. Finally, we hope to extend these models to include several potentially limiting factors, each of which may be active for a small portion of the data set. Suppose that x_1 and x_2 are each potentially limiting factors. Then, ignoring measurement error, $Y \leq \tau_1 x_1$ and $Y \leq \tau_2 c_2$, where τ_1 and τ_2 are unknown parameters. For a given datum, one or neither of these two factors may be the active limiting factor.

Although the data examples presented in this article involve the relationship of chlorophyll concentration to phosphorus concentration in lakes, similar examples may be found in a number of ecological disciplines. Data exhibiting the form of a triangle lying under an apparent limit function include scatterplots of fish production versus primary production (Marten and Polovina 1982), juniper girth versus ring count (Ward 1982), mercury concentration versus weight in fish (Jensen 1988), and prey taken versus prey presented in foraging experiments with aphids (Trexler, McCulloch, and Travis 1988).

Other methods than the EM algorithm could be used for estimation of our models. The desire to use an alternative method stems from the slowness of the EM algorithm. Scoring and Newton–Raphson methods were abandoned, because the Hessian matrix of the log-likelihood function was found to be positive definite only near the maximum likelihood estimate. As a result, iterations did not converge. For models with two to four parameters, the variable simplex method of Nelder and Mead (1965) may be successfully used, although this method provided little or no improvement in speed over the EM algorithm. Simplex methods are known to be inefficient in terms of the number of function evaluations required, and calculation of the observed data log-likelihood alone provides little savings in time or programming difficulty over calculation of all the integrals required for the EM algorithm.

The EM algorithm as described in Section 4 has now been programmed with several languages on different computing platforms, and it has become clear that high precision is needed in numerical calculations. As the algorithm nears convergence, lack of precision in numerical evaluation of the required integrals can lead to lack of smoothness in convergence or, in extreme cases, to decreases in the observed data log-likelihood. The estimation proposed in this article involves heavy use of numerical approximation, and there are a large number of technical details involved which have not been elaborated on here. We believe that the EM algorithm developed here could be improved through various modifications. For example, the smooth convergence of the EM algorithm suggests that a pattern move made at the end of each iteration might offer an improvement in speed. Or the algorithm could be approached from a Monte Carlo view, resulting in a version of Gibbs sampling that, for mixture problems, is very similar to a numerical version of the EM algorithm.

[*Received November 1990. Revised September 1993.*]

REFERENCES

Blackman, F. F. (1905), "Optima and Limiting Factors," *The Annals of Botany,* 19, 281–295.

Bradford, M. E., and Peters, R. H. (1987), "The Relationship Between Chemically Analyzed Phosphorus Fractions and Bioavailable Phosphorus," *Limnology and Oceanography,* 32, 1124–1137.

Canfield, D. E., Jr., and Bachmann, R. W. (1981), "Prediction of Total Phosphorus Concentrations, Chlorophyll a, and Secchi Depths in Natural and Artificial Lakes," *Canadian Journal of Fisheries and Aquatic Sciences,* 38, 414–423.

Chapra, S. C., and Robertson, A. (1977), "Great Lakes Eutrophication: The Effect of Point Source Control of Total Phosphorus," *Science,* 196, 1448–1449.

Collins, N. C., and Sprules, W. G. (1983), "Introduction to Large-Scale Comparative Studies of Lakes," *Canadian Journal of Fisheries and Aquatic Sciences,* 40, 1750–1751.

Dempster, A. P., Laird, N. M., and Rubin, D. B. (1977), "Maximum Likelihood From Incomplete Data Via the EM Algorithm," (with discussion), *Journal of the Royal Statistical Society,* Ser. B, 39, 1–38.

Dillon, P. J., and Rigler, F. H. (1974), "The Phosphorus–Chlorophyll Relationship in Lakes," *Linmology and Oceanography,* 19, 767–773.

Dodds, W. K., Johnson, K. R., and Priscu, J. C. (1989), "Simultaneous Nitrogen and Phosphorus Deficiency in Natural Phytoplankton Assemblages: Theory, Empirical Evidence, and Implications for Lake Management," *Lake and Reservoir Management,* 5, 21–26.

Efron, B., and Hinkley, D. V. (1978), "Assessing the Accuracy of the Maximum Likelihood Estimator: Observed Versus Expected Fisher Information," *Biometrika,* 65, 457–487.

Flynn, K. J. (1988), "The Concept of 'Primary Production' in Aquatic Ecology," *Limnology and Oceanography,* 33, 1215–1216.

Fuhs, G. W., Demmerie, S. D., Canelli, E., and Chen, M. (1972), "Characterization of Phosphorus Limited Plankton Algae (With Reflections on the Limiting-Nutrient Concept)," in *Nutrients and Eutrophication, Limnology, and Oceanography Special Symposium No. 1,* ed. G. E. Likens, Lawrence, Kansas, Society for Limnology and Oceanography, pp. 113–134.

Hartley, H. O. (1958), "Maximum Likelihood Estimation From Incomplete Data," *Biometrics,* 14, 174–194.

Hoyer, M. V., and Jones, J. R. (1983), "Factors Affecting the Relation Between Phosphorus and Chlorophyll *a* in Midwestern Reservoirs," *Canadian Journal of Fisheries and Aquatic Sciences,* 40, 192–199.

Jensen, A. L. (1988), "Modeling the Effect of Acidity on Mercury Uptake by Walleye in Acidic and Circumneutral Lakes," *Environmental Pollution,* 50, 285–294.

Jones, J. R., and Bachmann, R. W. (1976), "Prediction of Phosphorus and Chlorophyll Levels in Lakes," *Journal of the Water Pollution Control Federation,* 48, 2176–2182.

——— (1978), "Phosphorus Removal by Sedimentation in Some Iowa Reservoirs," *Verhandlungen Internationale Vereinigung Fur Theoretische und Angewandte Limnologie,* 20, 1576–1580.

Jones, J. R., Knowlton, M. F., and Swar, D. B. (1989), "Limnological Reconnaissance of Waterbodies in Central and Southern Nepal," *Hydrobiologia,* 184, 171–189.

Kaiser, M. S. (1990), "Statistical Models for Limiting Factors in Ecology," unpublished Ph.D. dissertation, University of Missouri-Columbia, Dept. of Statistics.

Knowlton, M. F., Hoyer, M. V., and Jones, J. R. (1984), "Sources of Variability in Phosphorus and Chlorophyll and Their Effects on Use of Lake Survey Data," *Water Resources Bulletin,* 20, 397–407.

Liebig, J. (1840), *Chemistry in its Application to Agriculture and Physiology,* London: Taylor and Walton.

Louis, T. A. (1982), "Finding the Observed Information Matrix When Using the EM Algorithm," *Journal of the Royal Statistical Society,* Ser. B, 44, 226–233.

Maller, R. A., deBoer, E. S., Joll, L. M., Anderson, D. A., and Hinde, J. P. (1983), "Determination of the Maximum Foregut Volume of Western Rock Lobsters (*Panulirus cygnus*) From Field Data," *Biometrics,* 39, 543–551.

Marten, G. G., and Polovina, J. J. (1982), "A Comparative Study of Fish Yields From Various Tropical Ecosystems," in *Theory and Management of Tropical Fisheries, Proceedings of the ICLARM/CSIRO Workshop on the Theory and Management of Tropical Multispecies Stocks,* eds. D. Pauly and G. I. Murphy, Cronulla, Australia: Commonwealth Scientific and Industrial Research Organization, pp. 255–285.

McCauley, E., Downing, J. A., and Watson, S. (1989), "Sigmoid Relationships between Nutrients and Chlorophyll among Lakes," *Canadian Journal of Fisheries and Aquatic Sciences,* 46, 1171–1175.

Morris, D. P., and Lewis, Jr., W. M. (1988), "Phytoplankton Nutrient Limitation in Colorado Mountain Lakes," *Freshwater Biology,* 20, 315–327.

Nelder, J. A., and Mead, R. (1965), "A Simple Method for Function Minimization," *The Computer Journal,* 7, 308–313.

Orchard, T., and Woodbury, M. A. (1972), "A Missing Information Principle: Theory and Applications," in *Proceedings of the Sixth Berkeley Symposium on Mathematical Statistics and Probability* (Vol. 1), eds. L. M. LeCam, J. Neyman, and E. L. Scott, Berkeley, CA: University of California Press, pp. 697–715.

Pianka, E. R. (1978), *Evolutionary Ecology* (2nd ed.), New York: Harper and Row.

Prairie, Y. T., Duarte, C. M., and Kalff, J. (1989), "Unifying Nutrient–Chlorophyll Relationships in Lakes," *Canadian Journal of Fisheries and Aquatic Sciences,* 46, 1176–1182.

Press, W. H., Flannery, B. P., Teukolsky, S. A., and Vetterling, W. T. (1986), *Numerical Recipes: The Art of Scientific Computing,* Cambridge, U.K.: Cambridge University Press.

Prepas, E. E., and Trew, D. O. (1983), "Evaluation of the Phosphorus–Chlorophyll Relationship for Lakes Off the Precambrian Shield in Western Canada," *Canadian Journal of Fisheries and Aquatic Sciences,* 40, 27–35.

Quesenberry, C. P. (1986), "Some Transformation Methods in Goodness-of-Fit," in *Goodness-of-Fit Techniques,* eds. R. B. D'Agostino and M. A. Stephens, New York: Marcel Dekker, pp. 235–277.

Raftery, A. E. (1984), "A Continuous Multivariate Exponential Distribution," *Communications in Statistics, Part A—Theory and Methods,* 13, 947–965.

Sakamoto, M. (1966), "Primary Production by Phytoplankton Community in Some Japanese Lakes and Its Dependence on Lake Depth," *Archives for Hydrobiologia,* 62, 1–28.

Schindler, D. W. (1977), "Evolution of Phosphorus Limitation in Lakes," *Science,* 195, 260–262.

Smith, V. H. (1979), "Nutrient Dependence of Primary Productivity in Lakes," *Limnology and Oceanography,* 24, 1051–1064.

——— (1982), "The Nitrogen and Phosphorus Dependence of Algal Biomass in Lakes: An Empirical and Theoretical Analysis," *Limnology and Oceanography,* 27, 1101–1112.

Smith, V. H., and Shapiro, J. (1981), "Chlorophyll–Phosphorus Relations in Individual Lakes: Their Importance to Lake Restoration Strategies," *Environmental Science and Technology,* 15, 444–451.

Trexler, J. C., McCulloch, C. E., and Travis, J. (1988), "How Can the Functional Response Best be Determined?," *Oecologia,* 76, 206–214.

Walker, W. W., Jr. (1986), "Empirical Methods for Predicting Eutrophication in Impoundments: Applications Manual," Technical Report E-81-9, U. S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

Walmsley, R. D. (1984), "A Chlorophyll_a Trophic Status Classification System for South African Impoundments," *Journal of Environmental Quality,* 13, 97–104.

Ward, L. K. (1982), "The Conservation of Juniper: Longevity and Old Age," *Journal of Applied Ecology,* 19, 917–928.

White, E. (1989), "Utility of Relationships Between Lake Phosphorus and Chlorophyll_a as Predictive Tools in Eutrophication Control Studies," *New Zealand Journal of Marine and Freshwater Research,* 23, 35–41.

Winkler, O. W. (1980), "On Triangular Correlation," in *Proceedings of the Business and Economic Statistics Section, American Statistical Association,* pp. 606–611.