Empirical Transform Estimation of Parameters in the Monomolecular Growth Model*

By DEVIN S. JOHNSON†, JENNIFER A. HOETING
Colorado State University
Fort Collins, USA

and RICHARD L. TWEEDIE
University of Minnesota
Minneapolis, USA

April 30, 2001

SUMMARY

In this paper we explore the use of empirical transform methodology to estimate growth curve parameters. We briefly describe empirical transform methodology for nonlinear stochastic models, such as growth models. A covariance matrix estimator is developed for monomolecular growth model parameter estimators using a Taylor's series approximation. Simulations show that the transform point estimators perform well in comparison with maximum likelihood estimators. We demonstrate the methodology by estimating growth curve parameters from Kemp's ridley sea turtle data.

Key Words: empirical transform, monomolecular growth model, robust estimation, weighted area estimation, covariance estimation

1 Introduction

Our goal in this paper is to study properties of empirical transform parameter estimators for the monomolecular growth model (von Bertanalffy, 1957), which has the form

$$\mathbb{E}[l_t] = f_M(t) = \lambda\{1 - e^{-\kappa(t-\tau)}\}, \qquad t \geq 0, \tag{1}$$

*Research supported in part by National Science Foundation grants DUE-0094514, DMS-9806243 and DMS-9803682

†*Address for correspondence*: Department of Statistics, Colorado State University, Ft. Collins, CO 80523; *E-mail*: johnson@stat.colostate.edu

where $\mathbb{E}[l_t]$ is the expected size of an organism at time t, λ represents the limiting size of the organism, κ is the growth rate constant, and τ is the zero time. The monomolecular model is a special case of the Richards growth model (Richards, 1959). The monomolecular model has no inflection point and the growth rate decreases linearly as size increases ($df_M/dt = \kappa\{\lambda - f_M(t)\}$) (Seber and Wild, 1989).

Parameters for the monomolecular model are traditionally estimated using non-linear least squares or maximum likelihood methodology (Seber and Wild, 1989). Empirical transform (ET) estimation was first used by Leedow and Tweedie (1983) for growth curve parameter estimation for the monomolecular growth model under the name "weighted area estimation," following Schuh and Tweedie (1979) who proposed the use of empirical transforms to estimate parameters in general time evolving models. Through a simulation study and fishery data examples, Leedow and Tweedie demonstrated that the ET estimator can be nearly as efficient as the maximum likelihood estimator (MLE) and also possesses useful robustness properties. Yao and Morgan (1999) expanded upon Leedow and Tweedie's work by proving that ET estimators for time indexed stochastic model parameters are asymptotically normal and consistent given a few sensible regularity conditions.

A major weakness with the ET estimators developed by Leedow and Tweedie is the lack of any parameter covariance estimator. The main contribution of this paper is the development of such a covariance estimator, which we carry out in Section 3 after constructing in Section 2 a variation on ET estimators using a slightly different approach suggested by Yao and Morgan (1999). We investigate behavior of the covariance estimator as well as behavior of the ET point estimators in Section 4. Our results indicate that the method compares favorably with maximum likelihood methods, generally providing reasonable covariance estimates and

confidence interval coverage for the parameters. In Section 5, ET methodology is used to estimate growth curve parameters as well as covariance estimates from Kemp's ridley sea turtle (*Lepidochelys kempii*) data.

2 Empirical transform estimators for time indexed models

2.1 General form

The models we consider are in a context where Y_{ik} is the observed response (size in the case of growth models) of the kth individual, and $k = 1, \ldots, n_i$ and $i = 1, \ldots, n$: that is, the number of individuals observed at time t_i equals n_i and the total number of unique times of observation equals n.

A common general form for time indexed stochastic models for such observations is

$$Y_{ik} = f(\boldsymbol{\theta}_0, t_i) + \sigma_i \epsilon_{ik}. \tag{2}$$

The $p \times 1$ parameter vector $\boldsymbol{\theta}_0 \in \Theta \subset \mathbb{R}^p$ is unknown and $f(\cdot, \cdot)$ is a known continuous function. The random variables $\{\epsilon_{ik}\}$ usually have common mean 0 and variance 1. The multiplier σ_i can either have the form $\sigma(\boldsymbol{\theta}_0, t_i)$, where $\sigma(\cdot, \cdot)$ is a function, or an unknown constant.

Theoretical and empirical transforms related to (2) are defined as follows. First, let $g(t, s)$ be a function chosen such that the transform

$$G(s, \boldsymbol{\theta}) = \int_0^\infty g(t, s) f(\boldsymbol{\theta}, t) dt \tag{3}$$

is a well defined continuous function on $\Theta \times S$, where $S \subset \mathbb{R}$. We shall use the Laplace transform with $g(t, s) = se^{-st}$, a common choice for the transform function. The function $G(s, \boldsymbol{\theta})$ is called the *theoretical transform* of $f(\boldsymbol{\theta}, t)$.

To develop the empirical transform for sampling times, $t_1, \ldots, t_n$, we partition $[0, \infty)$ using $c_1, \ldots, c_{n+1}$ such that $t_i \in (c_i, c_{i+1}]$ for $i = 1, \ldots, n$. For now we will let $c_1 = 0$ and $c_{n+1} = \infty$. Using the partition, $f(\boldsymbol{\theta}, t)$ can be approximated by

$$f(\boldsymbol{\theta}, t) \approx \begin{cases} f(\boldsymbol{\theta}, t_1), & \text{for } c_1 \le t < c_2 \\ f(\boldsymbol{\theta}, t_2), & \text{for } c_2 \le t < c_3 \\ \quad \vdots & \\ f(\boldsymbol{\theta}, t_{n-1}), & \text{for } c_{n-1} \le t < c_n \\ f(\boldsymbol{\theta}, t_n), & \text{for } c_n \le t < c_{n+1} \end{cases} . \tag{4}$$

The theoretical transform (3) can then be approximated by

$$G(s, \boldsymbol{\theta}) \approx \sum_{i=1}^{n} f(\boldsymbol{\theta}, t_i) \int_{c_i}^{c_{i+1}} g(t, s) dt. \tag{5}$$

Letting $\overline{Y}_i$ be the sample average of the observations at time t_i and using (5), a natural *empirical transform* is then

$$G_n(s) = \sum_{i=1}^{n} \overline{Y}_i \int_{c_i}^{c_{i+1}} g(t, s) dt,$$

since $\overline{Y}_i$ is an unbiased estimator of $f(\boldsymbol{\theta}_0, t_i)$ in (2).

In order to estimate $\boldsymbol{\theta}_0$ the approximate equality of the empirical and theoretical transforms will be used with a method of moments type argument. Given a set of "transform variables" $\{s_j : j = 1, \ldots, q\}$, the estimate of $\boldsymbol{\theta}_0$ is defined to be

$$\hat{\boldsymbol{\theta}}(\mathbf{s}) = \min_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} \left[\sum_{k=1}^{q} \{G(\boldsymbol{\theta}, s_k) - G_n(s_k)\}^2 \right], \tag{6}$$

where $\mathbf{s} = (s_1, \ldots, s_q)^{\mathrm{t}}$ (Yao and Morgan, 1999). In many cases, we would take $q \ge p$; but if $q = p$, then $\hat{\boldsymbol{\theta}}(\mathbf{s})$ becomes the solution to the p equations

$$G(s_j, \boldsymbol{\theta}) = G_n(s_j) \qquad j = 1, \ldots, p, \tag{7}$$

provided a solution exists. This is the approach of Leedow and Tweedie (1983) who show that it leads to explicit estimators for the monomolecular model, as discussed in Section 2.2 below.

Note that the solution to (6) does not involve assumptions about the error term in (2). Given some natural regularity conditions, Yao and Morgan (1999) have shown that the solution to (6) is a consistent and asymptotically normal estimator of $\boldsymbol{\theta}_0$, and in what follows we shall use this in constructing confidence intervals for $\boldsymbol{\theta}_0$, once we have the appropriate covariance structure.

One of the more interesting features of the ET method, observed by Leedow and Tweedie (1983) and elaborated on by Yao and Morgan (1999), is that the optimal choice of the transform variables s_j appears to occur by taking the values all close to one particular s (and then choosing that s in some optimal manner). Yao and Morgan suggest formalizing this approach to obtaining an ET estimator by letting $s_j \to s_1$ $(j = 2, \ldots, q)$ in the estimator resulting from (7). These methods require selection of only a single transform variable value, and we will pursue this in the monomolecular examples below.

2.2 Empirical transforms and the monomolecular model

We now develop the ET estimators for the monomolecular model (1). Let $s \in \mathbb{R}$, where $s > 0$, and $g(s,t) = se^{-st}$. Choose the $c_{i+1} = (t_i + t_{i+1})/2$, $i = 1, \ldots, n-1$, $c_1 = t_1$ and $c_{n+1} = t_n$. Following Leedow and Tweedie (1983), we define the *end corrected theoretical transform* as

$$\begin{aligned} G_c(s, \boldsymbol{\theta}) &= \int_{t_1}^{t_n} \lambda\{1 - e^{-\kappa(t-\tau)}\} se^{-st} dt \\ &= \frac{\lambda\kappa}{s+\kappa}(e^{-st_1} - e^{-st_n}) + \frac{s}{s+\kappa}\left\{ f_M(t_1)e^{-st_1} - f_M(t_n)e^{-st_n} \right\}. \end{aligned} \tag{8}$$

The end-corrected empirical transform is given by

$$G_{n,c}(s) = \sum_{i=1}^{n} \bar{l}_i \int_{c_i}^{c_{i+1}} se^{-st} dt = \sum_{i=1}^{n} w_i \bar{l}_i,$$

where $\bar{l}_i, i = 1, \ldots, n$ is the mean size of all organisms observed at time t_i and $w_i = \int_{c_i}^{c_{i+1}} se^{-st}dt = e^{-sc_{i+1}} - e^{-sc_i}$. The end-corrected form is used because, typically, the initial and last time points t_1, t_n are far from $0, \infty$ and as a consequence the uncorrected empirical form is not a good estimator of the uncorrected theoretical form.

In order to solve for the parameters in terms of the empirical transforms, a new transform will be defined from (8). Let

$$\begin{aligned} F(s,\boldsymbol{\theta}) &= \frac{G_c(s,\boldsymbol{\theta})}{e^{-st_1} - e^{-st_n}} \\ &= \frac{\lambda\kappa}{s+\kappa} + \frac{s}{s+\kappa}\left\{\frac{f_M(t_1)e^{-st_1} - f_M(t_n)e^{-st_n}}{e^{-st_1} - e^{-st_n}}\right\} \\ &= \frac{\lambda\kappa}{s+\kappa} + \frac{s}{s+\kappa}D(s,\boldsymbol{\theta}). \end{aligned} \tag{9}$$

The empirical version of (9) is

$$\begin{aligned} F_n(s) &= \frac{G_{n,c}(s)}{e^{-st_1} - e^{-st_n}} \\ &= \sum_{i=1}^{n} \frac{e^{-sc_i} - e^{-sc_{i+1}}}{e^{-st_1} - e^{-st_n}}\bar{l}_i \\ &= \sum_{i=1}^{n} p_i\bar{l}_i, \qquad \text{say.} \end{aligned}$$

Now, by choosing two values s_1 and s_2, and setting $F_n(s_1) = F(s_1,\boldsymbol{\theta})$ and $F_n(s_2) = F(s_2,\boldsymbol{\theta})$, one can solve for the population parameters. These estimators will be functions of $D(s,\boldsymbol{\theta})$, which is also a function of the parameters. Therefore, $D(s,\boldsymbol{\theta})$ will be replaced in the parameter estimators by its unbiased estimator,

$$D_n(s) = \frac{e^{-st_1}\bar{l}_1 - e^{-st_n}\bar{l}_n}{e^{-st_1} - e^{-st_n}}.$$

The resulting ET estimators are then

$$\hat{\kappa} = \frac{s_1\{D_n(s_1) - F_n(s_1)\} - s_2\{D_n(s_2) - F_n(s_2)\}}{F_n(s_1) - F_n(s_2)}, \tag{10}$$

$$\hat{\lambda} = \frac{s_1 F_n(s_2)\{D_n(s_1) - F_n(s_1)\} - s_2 F_n(s_1)\{D_n(s_2) - F_n(s_2)\}}{s_1\{D_n(s_1) - F_n(s_1)\} - s_2\{D_n(s_2) - F_n(s_2)\}}, \tag{11}$$

and

$$\hat{\tau} = \frac{1}{\hat{\kappa}} \log\left(1 - \frac{\bar{l}_1}{\hat{\lambda}}\right) + t_1. \tag{12}$$

Note that the ET estimator for τ does not result from the solution to the equations $F_n(s_i) = F(s_i, \boldsymbol{\theta})$, since τ is no longer present in the equations due to the substitution of $D_n(s)$ for $D(s, \boldsymbol{\theta})$ in $F(s, \boldsymbol{\theta})$. Therefore, in order to derive an ET estimator for τ, Leedow and Tweedie used the third equation $\bar{l}_1 = \lambda\left[1 - e^{-\kappa(t_1 - \tau)}\right]$, and solved for τ.

The estimators above depend on s_1, s_2, and we now derive another set of estimators requiring only one choice for the value of the transform variable, using the observation that the optimal choice of s_1, s_2 is typically at values close together. Letting $s_2 \to s_1 = s$ in (10), (11), and (12) gives the single transform variable estimators

$$\tilde{\kappa} = \lim_{s_2 \to s_1 = s} \hat{\kappa} = \frac{\{D_n(s) - F_n(s)\} + s\{D_n'(s) - F_n'(s)\}}{F_n'(s)}, \tag{13}$$

$$\tilde{\lambda} = \lim_{s_2 \to s_1 = s} \hat{\lambda} = \frac{F_n(s)\{D_n(s) - F_n(s)\} + s\{F_n(s) D_n'(s) - F_n'(s) D_n(s)\}}{\{D_n(s) - F_n(s)\} + s\{D_n'(s) - F_n'(s)\}}, \tag{14}$$

and

$$\tilde{\tau} = \lim_{s_2 \to s_1 = s} \hat{\tau} = \frac{1}{\tilde{\kappa}} \log\left(1 - \frac{\bar{l}_1}{\tilde{\lambda}}\right) + t_1. \tag{15}$$

Now we have that

$$F_n'(s) = \sum_{i=1}^{n} \frac{\partial}{\partial s} p_i \bar{l}_i = \sum_{i=1}^{n} p_i' \bar{l}_i,$$

where

$$p_i' = \frac{(c_i - c_{n+1}) e^{-s(c_i + c_{n+1})} + (c_{i+1} - c_1) e^{-s(c_{i+1} + c_1)}}{\left(e^{-sc_1} - e^{-sc_{n+1}}\right)^2} + \frac{(c_1 + c_i) e^{-s(c_1 + c_i)} + (c_{n+1} - c_{i+1}) e^{-s(c_{n+1} + c_{i+1})}}{\left(e^{-sc_1} - e^{-sc_{n+1}}\right)^2}.$$

If we formally write

$$D_n(s) = \sum_{i=1}^{n} q_i \bar{l}_i,$$

where

$$q_i = \begin{cases} e^{-sc_1}/(e^{-sc_1} - e^{-sc_{n+1}}), & \text{for } i = 1 \\ 0, & \text{for } i = 2, \ldots, n-1 \\ -e^{-sc_{n+1}}/(e^{-sc_1} - e^{-sc_{n+1}}), & \text{for } i = n \end{cases},$$

then we similarly have

$$D'_n(s) \quad = \quad \sum_{i=1}^{n} \frac{\partial}{\partial s} q_i \bar{l}_i = \sum_{i=1}^{n} q'_i \bar{l}_i,$$

where

$$q'_i = \begin{cases} \frac{(c_1 - c_{n+1})e^{-s(c_1+c_{n+1})}}{(e^{-sc_1} - e^{-sc_{n+1}})^2}, & \text{for } i = 1 \\ 0, & \text{for } i = 2, \ldots, n-1 \\ \frac{(c_{n+1} - c_1)e^{-s(c_1+c_{n+1})}}{(e^{-sc_1} - e^{-sc_{n+1}})^2}, & \text{for } i = n \end{cases}.$$

2.3 ET covariance estimator

In order to facilitate the derivation of an approximate covariance matrix, the empirical transforms will be denoted by their matrix forms;

$$\begin{aligned} D_n(s) = \sum_{i=1}^{n} q_i \bar{l}_i = \mathbf{q}^{\mathrm{t}}\mathbf{l}, \qquad & D'_n(s) = \sum_{i=1}^{n} q'_i \bar{l}_i = \mathbf{u}^{\mathrm{t}}\mathbf{l} \\ F_n(s) = \sum_{i=1}^{n} p_i \bar{l}_i = \mathbf{p}^{\mathrm{t}}\mathbf{l}, \qquad & F'_n(s) = \sum_{i=1}^{n} p'_i \bar{l}_i = \mathbf{v}^{\mathrm{t}}\mathbf{l} \\ \bar{l}_1 \quad = \quad & \sum_{i=1}^{n} z_i \bar{l}_i = \mathbf{z}^{\mathrm{t}}\mathbf{l}, \end{aligned}$$

where $\mathbf{z}$ is a vector with a 1 in the first position and 0's everywhere else. From the previous section, the two vectors

$$\hat{\boldsymbol{\theta}} = \begin{bmatrix} \hat{\kappa} \\ \hat{\lambda} \\ \hat{\tau} \end{bmatrix} \tag{16}$$

and

$$\tilde{\boldsymbol{\theta}} = \begin{bmatrix} \tilde{\kappa} \\ \tilde{\lambda} \\ \tilde{\tau} \end{bmatrix}$$

will be used to estimate the parameter vector $\boldsymbol{\theta}_0$.

First, we will develop an approximate covariance matrix for $\hat{\boldsymbol{\theta}}$ and then use the same argument to develop an approximate covariance matrix for $\tilde{\boldsymbol{\theta}}$. To begin, let $D_n(s_1) = \mathbf{q}_1^{\mathrm{t}}\mathbf{l}$, $D_n(s_2) = \mathbf{q}_2^{\mathrm{t}}\mathbf{l}$, $F_n(s_1) = \mathbf{p}_1^{\mathrm{t}}\mathbf{l}$, and $F_n(s_2) = \mathbf{p}_2^{\mathrm{t}}\mathbf{l}$. Then the empirical transform vector is defined by

$$\mathbf{G} = \begin{bmatrix} D_n(s_1) \\ D_n(s_2) \\ F_n(s_1) \\ F_n(s_2) \\ \bar{l}_1 \end{bmatrix} = \mathbf{T}^{\mathrm{t}}\mathbf{l}, \tag{17}$$

where

$$\mathbf{T} = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \mathbf{p}_1 & \mathbf{p}_2 & \mathbf{z} \end{bmatrix}.$$

The expectation and variance of $\mathbf{G}$ are easily calculated from (17):

$$\mathbb{E}[\mathbf{G}] = \boldsymbol{\gamma} = \begin{bmatrix} \delta_1 \\ \delta_2 \\ \phi_1 \\ \phi_2 \\ f_M(t_1) \end{bmatrix} = \mathbf{T}^{\mathrm{t}}\boldsymbol{\mu}, \tag{18}$$

and

$$\mathrm{Var}[\mathbf{G}] = \mathbf{T}^{\mathrm{t}}\boldsymbol{\Sigma}\mathbf{T}, \tag{19}$$

where $\boldsymbol{\mu} = (f_M(t_1), \ldots, f_M(t_n))^{\mathrm{t}}$ and $\boldsymbol{\Sigma}$ is the $n \times n$ covariance matrix of $\mathbf{l}$. The elements in the vector (18) and matrix (19) are, of course, functions of the transform variables s_1 and s_2.

We will now consider (16) as a vector valued function $\mathbf{h}(\mathbf{G})$, where $h_1(\mathbf{G}) = \hat{\kappa}$, $h_2(\mathbf{G}) = \hat{\lambda}$, $h_3(\mathbf{G}) = \hat{\tau}$. Using the Taylor's series expansion (Casella and Berger, 1990) of $\mathbf{h}(\mathbf{G})$, an

approximate covariance matrix for (16) is

$$\mathrm{Var}[\hat{\boldsymbol{\theta}}] \approx \frac{\partial \mathbf{h}(\boldsymbol{\gamma})}{\partial \boldsymbol{\gamma}^{\mathrm{t}}} \mathbf{T}^{\mathrm{t}} \boldsymbol{\Sigma} \mathbf{T} \frac{\partial \mathbf{h}^{\mathrm{t}}(\boldsymbol{\gamma})}{\partial \boldsymbol{\gamma}}. \tag{20}$$

The matrix $\partial \mathbf{h}(\boldsymbol{\gamma})/\partial \boldsymbol{\gamma}^{\mathrm{t}}$ is a 3×5 matrix defined as follows:

$$\frac{\partial \mathbf{h}(\boldsymbol{\gamma})}{\partial \boldsymbol{\gamma}^{\mathrm{t}}} = \begin{bmatrix} \partial h_1(\boldsymbol{\gamma})/\partial \boldsymbol{\gamma}^{\mathrm{t}} \\ \partial h_2(\boldsymbol{\gamma})/\partial \boldsymbol{\gamma}^{\mathrm{t}} \\ \partial h_3(\boldsymbol{\gamma})/\partial \boldsymbol{\gamma}^{\mathrm{t}} \end{bmatrix},$$

where

$$\begin{aligned}
\frac{\partial h_1(\boldsymbol{\gamma})}{\partial \delta_1} &= \frac{s_1}{\phi_1 - \phi_2}, \\
\frac{\partial h_1(\boldsymbol{\gamma})}{\partial \delta_2} &= \frac{-s_2}{\phi_1 - \phi_2}, \\
\frac{\partial h_1(\boldsymbol{\gamma})}{\partial \phi_1} &= \frac{-s_1(\delta_1 - \phi_2) + s_2(\delta_2 - \phi_2)}{(\phi_1 - \phi_2)^2}, \\
\frac{\partial h_1(\boldsymbol{\gamma})}{\partial \phi_2} &= \frac{s_1(\delta_1 - \phi_1) - s_2(\delta_2 - \phi_1)}{(\phi_1 - \phi_2)^2}, \\
\frac{\partial h_1(\boldsymbol{\gamma})}{\partial f_M(t_1)} &= 0,
\end{aligned}$$

$$\begin{aligned}
\frac{\partial h_2(\boldsymbol{\gamma})}{\partial \delta_1} &= \frac{s_1 s_2(\phi_2 - \delta_2)(\phi_2 - \phi_1)}{\{s_1(\delta_1 - \phi_1) - s_2(\delta_2 - \phi_2)\}^2}, \\
\frac{\partial h_2(\boldsymbol{\gamma})}{\partial \delta_2} &= \frac{s_1 s_2(\phi_1 - \delta_1)(\phi_1 - \phi_2)}{\{s_1(\delta_1 - \phi_1) - s_2(\delta_2 - \phi_2)\}^2}, \\
\frac{\partial h_2(\boldsymbol{\gamma})}{\partial \phi_1} &= \frac{s_2^2(\delta_2 - \phi_2)^2 - s_1 s_2(\delta_1 - \phi_2)(\delta_2 - \phi_2)}{\{s_1(\delta_1 - \phi_1) - s_2(\delta_2 - \phi_2)\}^2}, \\
\frac{\partial h_2(\boldsymbol{\gamma})}{\partial \phi_2} &= \frac{s_1^2(\delta_1 - \phi_1)^2 - s_1 s_2(\delta_2 - \phi_1)(\delta_1 - \phi_1)}{\{s_1(\delta_1 - \phi_1) - s_2(\delta_2 - \phi_2)\}^2}, \\
\frac{\partial h_2(\boldsymbol{\gamma})}{\partial f_M(t_1)} &= 0.
\end{aligned}$$

If ξ is the expected value of any transform in $\hat{\kappa}$ or $\hat{\lambda}$, then

$$\begin{aligned}
\frac{\partial h_3(\boldsymbol{\gamma})}{\partial \xi} &= h_1^{-1}(\boldsymbol{\gamma}) \frac{\partial h_2(\boldsymbol{\gamma})}{\partial \xi} \left[\frac{f_M(t_1)}{h_2(\boldsymbol{\gamma})\{h_2(\boldsymbol{\gamma}) - f_M(t_1)\}} \right] \\
&\qquad - h_1^{-1}(\boldsymbol{\gamma}) \frac{\partial h_1(\boldsymbol{\gamma})}{\partial \xi} \{h_3(\boldsymbol{\gamma}) - t_1\}, \qquad (21) \\
\frac{\partial h_3(\boldsymbol{\gamma})}{\partial f_M(t_1)} &= -h_1^{-1}(\boldsymbol{\gamma}) \left\{ \frac{1}{h_2(\boldsymbol{\gamma}) - f_M(t_1)} \right\}.
\end{aligned}$$

In order to estimate Var$[\hat{\boldsymbol{\theta}}]$ as in (20) from data, we will replace $\boldsymbol{\gamma}$ by $\hat{\boldsymbol{\gamma}}$ and $\boldsymbol{\Sigma}$ by the estimate $\widehat{\boldsymbol{\Sigma}}$. The predicted values from $\hat{f}_M(t)$ will be used to estimate $\boldsymbol{\gamma}$;

$$\hat{\boldsymbol{\gamma}} = \mathbf{T}^{\mathrm{t}} \begin{bmatrix} \hat{\lambda}(1 - e^{-\hat{\kappa}(t_1 - \hat{\tau})}) \\ \hat{\lambda}(1 - e^{-\hat{\kappa}(t_2 - \hat{\tau})}) \\ \vdots \\ \hat{\lambda}(1 - e^{-\hat{\kappa}(t_n - \hat{\tau})}) \end{bmatrix}$$

When estimating $\boldsymbol{\Sigma}$, we will only consider the case where the $\bar{l}_i$ are independent. This is a reasonable assumption for many growth model problems, although it is not required for the validity of (20). Let $\widehat{\boldsymbol{\Sigma}}$ be an $n \times n$ matrix with elements described by:

$$\hat{\sigma}_{i,j} = \begin{cases} \frac{1}{n_i^2} \sum_{k=1}^{n_i} \{l_{i,k} - \hat{f}(t_i)\}^2, & \text{for } i = j \\ 0, & \text{for } i \neq j \end{cases}, \tag{22}$$

where n_i is the number of organisms observed at time t_i. Now, letting

$$\mathbf{B} = \frac{\partial \mathbf{h}^{\mathrm{t}}(\hat{\boldsymbol{\gamma}})}{\partial \hat{\boldsymbol{\gamma}}}$$

and replacing $\boldsymbol{\Sigma}$ with $\widehat{\boldsymbol{\Sigma}}$, an estimator of Var$[\hat{\boldsymbol{\theta}}]$ is

$$\widehat{\mathrm{Var}}[\hat{\boldsymbol{\theta}}] = \mathbf{B}^{\mathrm{t}} \mathbf{T}^{\mathrm{t}} \widehat{\boldsymbol{\Sigma}} \mathbf{T} \mathbf{B}.$$

In order to develop an approximate covariance matrix for the single transform variable estimator $\tilde{\boldsymbol{\theta}}$, we simply change the weighting matrix, $\mathbf{T}$ in (17) to

$$\mathbf{T}_{\mathrm{d}} = \begin{bmatrix} \mathbf{q} & \mathbf{u} & \mathbf{p} & \mathbf{v} & \mathbf{z} \end{bmatrix},$$

and follow the same steps presented previously for deriving the approximate covariance matrix associated with the double transform estimator $\hat{\boldsymbol{\theta}}$. Details including all relevant derivatives are given in Johnson (2000).

3 Simulation experiment

3.1 Details

Our simulation study of the estimators is similar to that performed by Leedow and Tweedie (1983). In each of five simulations, 1000 datasets were generated.

In the first three simulations we chose sampling times $\{t_i = i : i = 1, \ldots, 20\}$. At each sampling time we generated 10 independent sample observations from

$$l_{i,k} = \lambda\{1 - e^{-\kappa(t_i - \tau)}\} + Z_{i,k}\sigma; \qquad k = 1, \ldots, 10,\ i = 1, \ldots, 20,$$

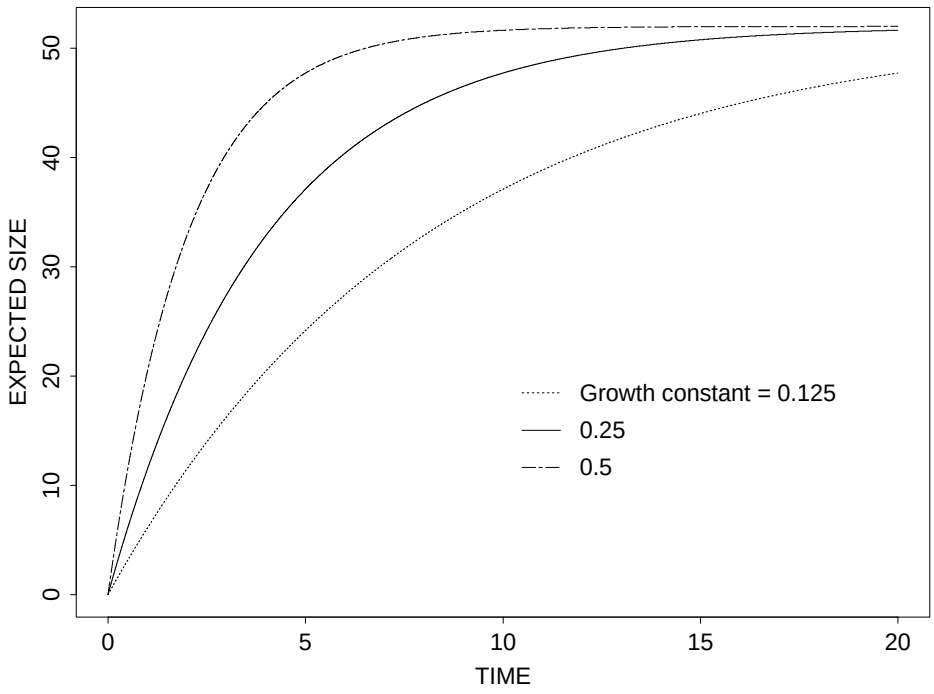
where $Z_{i,k} \sim N(0, 1)$. We chose $\lambda = 52$, $\tau = 0$, and $\sigma = 2.5$ for all three simulations. Each simulation, however, was performed with a different value for κ, namely 0.125, 0.25, and 0.5. Holding λ and τ constant is appropriate since it is the growth rate constant κ which determines the shape of the curve (Figure 1).

To assess the effect of the end-correction in a somewhat more realistic situation, a fourth simulation was conducted with sample times $\{t_i = i : i = 5, \ldots, 16\}$, $\lambda = 52$, $\kappa = 0.25$, $\tau = 0$, $\sigma = 5$, and $\kappa = 0.25$.

In the fifth simulation we generated data using exponential random variables, in order to investigate the effect of heavier tailed distributions on the method. For each of the sampling times $\{t_i = i : i = 1, \ldots, 20\}$ we generated 10 independent observations from an exponential distribution with mean $f_M(t_i)$, where $f_M(t_i)$ is given by equation (1).

Point estimators and their estimated covariances for the ET estimators were calculated in each experiment according to the formulae developed in Sections 2.2 and 2.3. For the double transform variable estimators, (10)-(12), we set the transform space to be $s_1 > 1 \times 10^{-9}$ and $s_2 = s_1 + 0.005$, as in Leedow and Tweedie (1983). For the single transform variable

Figure 1: Monomolecular growth curve shape for three different growth rate constant (κ) values. For all three plots $\lambda = 52$ and $\tau = 0$.



estimators, (13)-(15), we set the transform space to be $s > 1 \times 10^{-9}$. The lower bound 1×10^{-9} was chosen because the ET estimators are undefined at $s = 0$. In the calculations for a given sample we chose the value of the transform variable(s) that minimized the residual sum of squares (Leedow and Tweedie, 1983).

For each simulation we computed the mean and variance of each point estimator, and the mean of the Taylor approximation covariance matrix estimator over the 1000 runs. We use the term "mean estimate" to refer to the average of the 1000 estimator realizations of both the point estimator and the covariance matrix estimator. The effectiveness of the covariance approximations, and in particular of the variance estimates associated with each parameter,

are assessed by comparing them to the covariance of the 1000 realizations (the "simulated" covariance). We compare the ET estimators with the maximum likelihood estimators which were based on the distribution used to generate the data. In the normal simulations, the S-plus function `nls` was used to calculate maximum likelihood estimates and `vcov` was used to produce maximum likelihood covariance estimates. In the exponential simulation, the S-plus function `nlminb` was used to maximize the likelihood and the inverse information matrix was used for maximum likelihood covariance estimation.

The confidence interval

$$\text{estimate} \pm 1.96\sqrt{\widehat{\text{Var}}(\text{estimate})}$$

was also calculated on each data set, where $\widehat{\text{Var}}$ is from the Taylor approximation, since the point estimates are asymptotically normal (Yao and Morgan, 1999). The confidence interval coverage percentages were then also calculated.

3.2 Results

3.2.1 Normal error simulations

Point estimate results for the ET estimators in the normal simulations agreed with the double transform variable results given in Leedow and Tweedie (1983). The single s version gives almost the same results throughout as the version using two close values of s, as one might expect.

For the organism limiting size parameter, λ, bias of the transform estimator was the largest for $\kappa = 0.125$ (Table 1). This is reasonable since the mean size at $t = 20$, $\bar{l}_{20}$, is likely to be farther from the asymptotic size when the growth rate constant, κ, is small, as Leedow

and Tweedie note. As κ increased, however, bias of the ET λ estimators decreased becoming nearly equivalent to the MLE estimator (Tables 2 and 3).

Conversely, bias of the ET estimators of κ was largest when $\kappa = 0.5$ (Table 3). This also seems reasonable since the majority of growth is happening in a short amount of time (Figure 1), and so the step function used to estimate the theoretic transform, (4), may not be a good approximation in the time interval in which growth is occurring. Including more sampling times during periods of steep growth should eliminate this problem in real applications.

The ET method does appear to slightly underestimate the value of τ, but in general by an immaterial amount.

Table 4 shows that, as one should expect, for the truncated sampling times simulation, the ET estimators did not perform as well as in the full range simulations due to truncated sampling time and higher variance. The standard error estimates calculated still seemed to be of the same order of accuracy, when compared to the real (simulated) values.

When comparing the ET estimators to the MLE, however, the λ and κ estimators performed competitively, with relative efficiency ranging from 48-91% on the full data sets, and 73-82% on the truncated data sets.

Using the variance estimators developed in Section 2 led to over-estimation of the standard errors in each simulation (Tables 1-4), as judged by the simulated standard errors. As κ became larger, however, standard error estimation improved. For a small number of replications, the ET covariance estimators produced very large over-estimates of parameter standard error. These few large over-estimates influenced the mean. For this reason, the median standard error estimate is also given in Tables 1 through 4. Examining the median ET standard error estimates indicates the over-estimation is typically slight.

Table 1: *Parameter and variance estimation for simulation 1,* $\kappa = 0.125$, $\lambda = 52$, *and* $\tau = 0$.

	Parameter[a]								
	κ			λ			τ		
	SS	S	MLE	SS	S	MLE	SS	S	MLE
POINT ESTIMATION									
mean estimate	0.124	0.124	0.125	52.19	52.19	52.04	-0.013	-0.013	-0.004
relative efficiency[b]	48%	48%	–	53%	53%	–	47%	47%	–
VAR. ESTIMATION									
simulated SE	0.0058	0.0058	0.0040	0.77	0.77	0.56	0.12	0.12	0.08
median SE est.	0.0060	0.0060	0.0040	0.95	0.96	0.56	0.11	0.11	0.08
mean SE est.	0.0071	0.0072	0.0040	1.17	1.19	0.56	0.11	0.11	0.08
CI COVERAGE[c]	95.5%	95.6%	94.3%	97.3%	97.3%	94.4%	91.8%	91.8%	95.3%

[a] SS denotes double transform variable estimator (10)-(12), S denotes single transform variable estimator (13)-(15).
[b] Relative efficiency = variance of MLE estimator / variance of ET estimator
[c] The target CI coverage is 95%.

Table 2: *Parameter and variance estimation for simulation 2,* $\kappa = 0.25$, $\lambda = 52$, *and* $\tau = 0$.

	Parameter[a]								
	κ			λ			τ		
	SS	S	MLE	SS	S	MLE	SS	S	MLE
POINT ESTIMATION									
mean estimate	0.247	0.248	0.250	52.07	52.07	52.00	-0.015	-0.015	-0.002
relative efficiency[b]	64%	65%	–	69%	69%	–	59%	59%	–
VAR. ESTIMATION									
simulated SE	0.0074	0.0074	0.0059	0.27	0.27	0.23	0.073	0.073	0.056
median SE est.	0.0075	0.0076	0.0060	0.31	0.31	0.22	0.067	0.068	0.056
mean SE est.	0.0079	0.0079	0.0060	0.34	0.34	0.22	0.068	0.068	0.056
CI COVERAGE[c]	92.9%	93.3%	95.1%	95.9%	95.9%	94.3%	91.4%	91.6%	95.6%

[a] SS denotes double transform variable estimator (10)-(12), S denotes single transform variable estimator (13)-(15).
[b] Relative efficiency = variance of MLE estimator / variance of ET estimator
[c] The target CI coverage is 95%.

Table 3: *Parameter and variance estimation for simulation 3,* $\kappa = 0.5$, $\lambda = 52$, *and* $\tau = 0$.

	Parameter[a]								
	κ			λ			τ		
	SS	S	MLE	SS	S	MLE	SS	S	MLE
POINT ESTIMATION									
mean estimate	0.49	0.49	0.50	52.02	52.02	52.00	-0.027	-0.027	-0.000
relative efficiency[b]	91%	91%	–	75%	75%	–	86%	86%	–
VAR. ESTIMATION									
simulated SE	0.016	0.016	0.015	0.17	0.17	0.15	0.055	0.055	0.051
median SE est.	0.016	0.016	0.014	0.17	0.17	0.15	0.055	0.055	0.051
mean SE est.	0.016	0.016	0.014	0.18	0.18	0.15	0.066	0.055	0.051
CI COVERAGE[c]	86.7%	86.8%	95.1%	94.9%	94.9%	94.9%	92.8%	92.9%	94.9%

[a] SS denotes double transform variable estimator (10)-(12), S denotes single transform variable estimator (13)-(15).
[b] Relative efficiency = variance of MLE estimator / variance of ET estimator
[c] The target CI coverage is 95%.

Table 4: *Parameter and variance estimation for simulation 4,* $\kappa = 0.25$, $\tau = 0$, $\lambda = 52$, $\tau = 0$, *time range is 5-16, and* $\sigma(t_i) = 5$.

	Parameter[a]								
	κ			λ			τ		
	SS	S	MLE	SS	S	MLE	SS	S	MLE
POINT ESTIMATION									
mean estimate	0.245	0.245	0.251	52.25	52.25	52.14	-0.19	-0.19	-0.05
relative efficiency[b]	82%	82%	–	73%	73%	–	69%	69%	–
VAR. ESTIMATION									
simulated SE	0.041	0.041	0.037	0.97	0.96	0.83	0.91	0.91	0.75
median SE est.	0.045	0.045	0.037	1.12	1.12	0.77	0.95	0.95	0.72
mean SE est.	0.047	0.047	0.037	1.26	1.26	0.81	1.03	1.03	0.75
CI COVERAGE[c]	96.6%	96.6%	95.9%	98.1%	98.1%	95.2%	97.4%	97.4%	95.2%

[a] SS denotes double transform variable estimator (10)-(12), S denotes single transform variable estimator (13)-(15).
[b] Relative efficiency = variance of MLE estimator / variance of ET estimator
[c] The target CI coverage is 95%.

The over-estimation of variances led to confidence interval coverage that was greater than 95% in some cases. As κ increased, however, and variance estimation improved, confidence interval coverage fell below 90% for the κ estimators due to the bias of the estimator (Table 3).

Even though covariance estimates are usually not as useful as standard error estimates, the Taylor's series covariance estimates performed well. Table 5 illustrates the performance of the correlation estimators for $\kappa = 0.25$. For each replication, parameter correlation was calculated by dividing the covariance estimate by the product of the standard error estimates. Correlations involving the λ estimator were slightly over-estimated in magnitude, while $\rho(\tau, \kappa)$ was slightly under-estimated. Correlation estimation also improved slightly, in terms of bias, as κ increased as well.

Table 5: *Correlation estimation for simulation 2,* $\kappa = 0.25$, $\lambda = 52$, *and* $\tau = 0$.

	Estimator[a]	
Parameter	SS	S
$\rho(\lambda, \kappa)$		
simulated	-0.79	-0.79
median estimate	-0.82	-0.82
mean estimate	-0.83	-0.83
$\rho(\lambda, \tau)$		
simulated	-0.45	-0.48
median estimate	-0.47	-0.47
mean estimate	-0.51	-0.52
$\rho(\tau, \kappa)$		
simulated	0.84	0.84
median estimate	0.82	0.82
mean estimate	0.82	0.82

[a] SS denotes double transform variable estimator (10)-(12), S denotes single transform variable estimator (13)-(15).

3.2.2 Exponential error simulations

When the observations are exponentially distributed, the ET point estimators performed well in comparison with the maximum likelihood estimators (Table 6). The ET estimators of λ and τ performed similarly in terms of bias and relative efficiency as compared to the maximum likelihood estimators. The ET estimator of κ was actually more efficient than the MLE estimator and slightly less biased as well.

Standard error estimation for the ET estimators of κ was very accurate (Table 6). For the ET estimators of both λ and τ, standard errors were typically under-estimated. In 3 of the 1000 simulation replications the Taylor's series variance approximations greatly over-estimated the standard errors of λ and τ. This is reflected in the large mean of the standard error estimates. A similar problem occurred with the maximum likelihood estimates; the information matrix was occasionally singular when evaluated at the MLE. So, as a whole, standard error estimation was roughly equivalent for the ET estimators and the MLE's.

Table 6: *Parameter and variance estimation for simulation 5 with exponentially distributed observations,* $\kappa = 0.25$, $\lambda = 52$, *and* $\tau = 0$.

	Parameter[a]								
	κ			λ			τ		
	SS	S	MLE	SS	S	MLE	SS	S	MLE
POINT ESTIMATION									
mean estimate	0.27	0.27	0.28	55.23	55.26	54.80	-0.19	-0.19	-0.15
relative efficiency[b]	130%	130%	–	93%	90%	–	87%	87%	–
VAR. ESTIMATION									
simulated SE	0.14	0.14	0.16	13.29	13.48	12.79	0.91	0.91	0.85
median SE est.	0.14	0.14	0.12	7.50	7.50	6.40	0.57	0.58	0.57
mean SE est.	0.15	0.15	0.15	141.86	135.93	11.49	0.95	3.45	0.79
CI COVERAGE[c]	97.0%	96.6%	94.1%	95.2%	95.3%	93.8%	87.2%	87.3%	87.3%

[a] SS denotes double transform variable estimator (10)-(12), S denotes single transform variable estimator (13)-(15).
[b] Relative efficiency = variance of MLE estimator / variance of ET estimator
[c] The target CI coverage is 95%.

Confidence interval coverage was close to nominal for both λ and κ ET estimators. The actual coverage for the τ ET estimator was slightly low at 87%, however, the MLE confidence level was also about 87%. Quantile-quantile plots for all of the estimators in simulation 5 indicated the distribution to be skewed as compared to the normal distribution. Therefore, using the normal based confidence interval may have affected the realized confidence levels for this simulation.

3.2.3 Comments

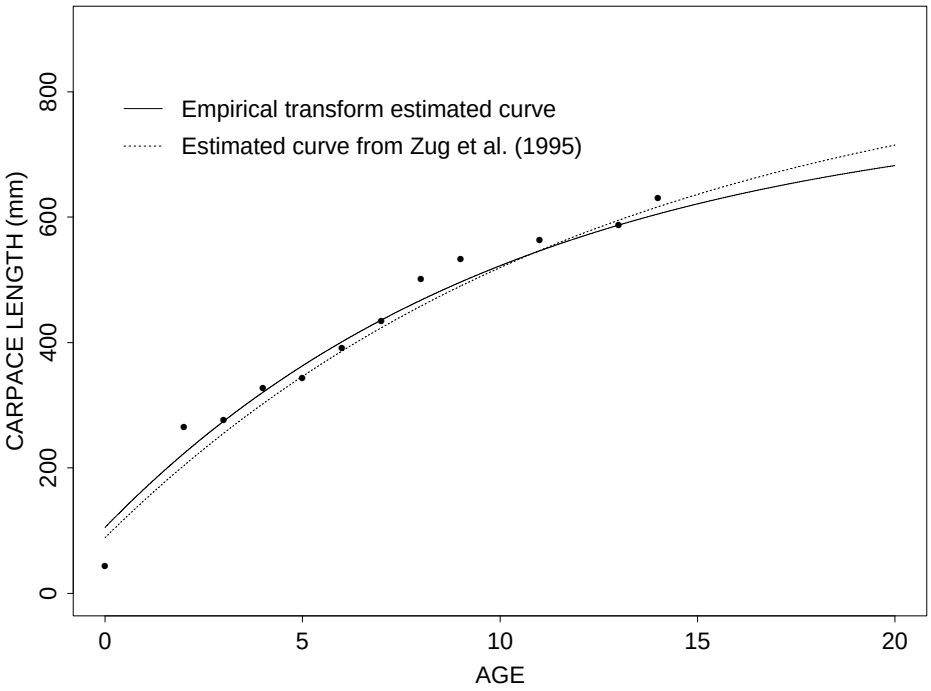
The simulation results suggest both the ET estimates and the associated standard error estimates work quite well in a variety of situations. In our simulations the ET estimators and variance estimators did not perform as well as the MLE as a whole, although this is rather a harsh comparison in that the MLE makes use of the correct (known) error distribution. Considering, however, that the empirical ET estimation method makes no assumptions about error structure, performance of the ET point and variance estimators is perhaps surprisingly good.

4 Modeling sea turtle growth

We apply the ET methods to model the growth pattern of Kemp's ridley sea turtles (*Lepidochelys kempii*), using data taken from Zug, Kalb, and Luzar (1995), hereafter ZKL.

During the time periods 1979-1981 and 1988-1990, stranded sea turtles were collected off the coast of Long Island, Virginia, and Georgia. Age estimates were made using skeletochonology and size was measured by carapace length. ZKL determined that a three parameter monomolecular model was a better fit to the data than a logistic or Gompertz model. ZKL

Figure 2: Estimated growth curve for Kemp's ridley sea turtle.



do not provide estimates of variability, but using the methods developed here we are able to provide confidence intervals for the transform estimates. Since the difference between single and double transform variable estimators was minimal in all simulations, we will only use the single transform estimator.

Preliminary analysis indicated that the arbitrary choice of using the first sampling time and its associated mean observation in the transform estimator of τ (15) was not appropriate for these data. If the initial mean observation is far from the trend of the remaining data, in terms of a "residual", the fit of the transform estimated curve can be very poor when t_1 is used in the transform estimator of τ. This was not a factor in the simulations since the mean at the first sampling time did not have a larger residual than the rest of the data.

For the sea turtle data, however, the first observation was collected as part of another study and is far from the trend of the remaining data (Figure 2). We will use a slight modification to (15) that involves choosing the sampling time and associated mean that produces an estimated curve with the lowest residual sum of squares. Therefore, the subscript "1" in (12) and (15) should be replaced by the subscript "i^*", representing the sampling time that produces the curve with the lowest sum of squares. The optimal choice of the transform variable s also changes with the sampling time used, and so the analysis is repeated for each of the n sampling times to identify i^*.

Since ZKL do not give the full data set, but only means at each age and variances for those means, we will use the sample variances given for the diagonal elements of the $\widehat{\mathbf{\Sigma}}$ matrix in equation (22) instead of the estimators given previously.

ZKL use a different parameterization of the monomolecular model than we have used in this paper. Their model is given by

$$f_M(t) = \lambda(1 - \xi e^{-\kappa t}).$$

The relation between our version and this version (1) is $\xi = e^{\kappa\tau}$. An empirical transform estimator for ξ follows by using $\bar{l}_i \approx \lambda[1 - \xi e^{-\kappa t_i}]$ in the same manner as in the derivation of the τ estimators, giving

$$\hat{\xi} = e^{\hat{\kappa} t_{i*}} \left(1 - \frac{\bar{l}_{i*}}{\hat{\lambda}}\right), \tag{23}$$

where again we use the value of $i^* \in \{1, \ldots, n\}$ which produces a curve with the lowest residual sum of squares. Although we will calculate an estimate for ξ, for comparison with ZKL, we have not calculated a variance estimate for this parameterization. We have, however, calculated point estimates and confidence intervals for λ, κ, and τ in the version used in this

paper.

Although ZKL do not explicitly state what method of parameter estimation they used, we assumed that they used standard homogeneous variance, normal maximum likelihood estimators. ZKL give the parameter estimates:

$$\lambda = 877.3, \qquad \kappa = 0.079, \qquad \xi = 0.899.$$

The empirical transform methodology with end corrections gives the estimates

$$\tilde{\lambda} = 781.3, \qquad \tilde{\kappa} = 0.096, \qquad \tilde{\tau} = -1.503$$

with corresponding 95% confidence intervals (69.0, 1493.6), (0.061, 0.132), and (-17.731, 14.726). The sampling time that produced the best fitting curve is at $t_{i*} = t_{11}$ (age = 13 years). Using (23), we calculated an estimate of 0.865 for ξ, comparable to that of ZKL. The residual sum of squares based on the means at each sample time for the ZKL curve is 11,447.06, while the RSS for the ET curve is 9,668.77.

Figure 2 illustrates the empirical transform estimated curve as well as the curve estimated by ZKL. Note that both curves fit the growth pattern over the range of the data, but the implications of the point estimators are rather different. In particular, the ET method implies that the maximum carapace length of the sea turtle (λ) is 781.3 mm, which is much shorter than the 877.3 mm predicted by ZKL, and which is well past the range of the sighted turtles; and similarly predicts shorter carapace lengths for all ages above the 15 years sighted.

References

Casella, G. and Berger, R. L. (1990). *Statistical Inference*. Wadsworth, California.

Johnson, D. S. (2000). Empirical transform estimation of growth curve parameters. Master's thesis, Colorado State University.

Leedow, M. I. and Tweedie, R. L. (1983). Weighted area techniques for the estimation of the parameters of a gowth curve. *Australian Journal of Statistics*, 25:310–320.

Richards, F. J. (1959). A flexible growth function for empirical use. *Journal of Experimental Botany*, 10:290–300.

Schuh, H. and Tweedie, R. L. (1979). Parameter estimation using transform estimation in time evolving models. *Mathematical Biosciences*, 45:37–67.

Seber, G. A. F. and Wild, C. J. (1989). *Nonlinear Regression*. John Wiley & Sons, Inc, New York.

von Bertanalffy, L. (1957). Quantitative laws in metabolism and growth. *Quarterly Review of Biology*, 32:217–231.

Yao, Q. and Morgan, B. J. T. (1999). Empirical transform estimation for indexed stochastic models. *Journal of the Royal Statistical Society - Series B*, 61:127–141.

Zug, G. R., Kalb, H. J., and Luzar, S. J. (1995). Age and growth in wild Kemp's ridley seaturtles *lepidochelys kempii* from skeletochronological data. *Biological Conservation*, 80:261–268.

List of Figures

List of Tables