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Summary

We review some of the statistical methods associated with change-point models, that is models which incorporate parameter shifts in sequences of random measurements. The application of bootstrap techniques is illustrated for some numerical examples. A subject-coded bibliography is provided.

Key Words: Bayesian Methods; Bootstrap; Change-point; CUSUM Techniques; Parameter Shift; Sequential Detection; Switching Regression; Two-phase Regression.

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0. Introduction: Scope and Outline

Change-point models are used to describe discontinuous behavior in stochastic phenomena. During the last twenty years there has developed a large body of statistical theory and methods specifically devoted to such models, divided between the topics of testing for presence of such discontinuities, and estimation of the discontinuity point -- the change-point. The subject matter overlaps with that of quality control and of piecewise curve fitting.

The present paper was prepared in conjunction with a presentation at the 13th European Meeting of Statisticians, which had invited a talk on the topic of change-point models. It seemed to be useful and timely to attempt a review of this topic, rather than to add to the vast body of theory. This review was undertaken with a critical eye for applicability of the theory, and focussed to some extent on the real applications of change-point methodology. The end result is rather unsatisfactory as a review of the literature, since the paper is rather selective in the topics discussed. However, a very extensive bibliography has been compiled, containing over 120 entries, coded by topic.

The paper looks mainly at two models: mean-shift models (Section 1) and intersecting two-phase regression models (Section 2). We review tests for the "no-shift" hypothesis in each context, both with and without specific change-point models as alternative hypotheses. Then we discuss estimation of the parameters in change-point models. In Section 3 we introduce the bootstrap techniques, and show by example how they might be used to aid statistical analysis of some change-point problems.

1. DISCONTINUOUS SHIFT PROBLEMS

1.1 Models and Examples

We shall restrict attention to models with at most one parameter shift. One wide class of change-point models assumes that $x_j = x(t_j)$, $j = 1,2,\ldots$ $(t_1 \le t_2 \le \ldots)$ are observations of independent random variables $X(t_j)$ such that

$$\mathrm{pr}(X(t) \le x) = \begin{cases} F(x|\theta_0) & t \le \gamma \\ F(x|\theta_1) & t > \gamma \end{cases} . \qquad (1.1)$$

The form of F is usually assumed known, but θ_0 and/or θ_1 would usually be unknown. The parameter γ, called the change-point, is often of primary interest. In many applications (1.1) is a specific alternative to the "no-shift" or homogeneity hypothesis.

The most common special cases of (1.1) are:

(a) F normal, θ_0 = mean θ_0, variance σ_0^2
θ_1 = mean θ_1, variance σ_1^2;

(a') same as (a) but with σ_0^2 and σ_1^2 equal;

(b) F binomial, with θ_0 and θ_1 the Bernoulli probabilities;

(c) F gamma, with θ_0 and θ_1 the scale parameters.

Particular useful variants of (a) or (a') include (i) serial correlation between the X_j and (ii) more general mean functions $\theta_0(t)$, $\theta_1(t)$ such as $\theta_i(t) = \alpha_i + \beta_i(t)$ $(i = 0,1)$ [with a break, $\theta_0(\gamma) \ne \theta_1(\gamma)$]. Although these variants will not be discussed further, they are included in the bibliography at the end of the paper.

We focus our attention now on (1.1a'), the normal mean-shift model, which seems to be by far the most important in application. Two examples that we shall refer to are illustrated in Figures 1.1 and 1.2. The first example is annual river discharge data, where estimation of the change-point γ is of interest. The second example is menstrual cycle basal body temperature (BBT) data, where rapid sequential detection of the mean shift is of major interest. In each case the normal mean-shift model seems to be a good assumption.

1.2 Tests for Deviation in Mean

A standard quality-control problem is to detect deviation in mean from an initial control level μ_0. In this context the problem is sequential, necessitating a decision procedure which involves some action with each new observation. For the normal case, consideration of the mean-shift model led to the now-standard cumulative sum, or CUSUM, procedure. The procedure for detection of a positive shift operates as follows: determine a positive mean shift $\mu_1 - \mu_0 = \delta\sigma$ which it is desired to detect quickly. Then compute truncated sequential sums

$$S_0 = 0,\ S_j = \max(0,\ S_{j-1} + x_j - \mu_0 - \tfrac{1}{2}\delta\sigma), \qquad j = 1,2,\ldots \tag{1.2}$$

and decide that an upward mean shift has occurred as soon as S_j exceeds the critical value h. Choice of the critical value h is based on tables of ARL = average run length = $E\{\inf(J : S_J \geq h)\}$ for various values of (δ,h). Note that a large value of ARL is desirable when no shift occurs, whereas

Figure 1.1 Annual Discharge Volume of the Nile River as Aswan (Source: Cobb, 1978)

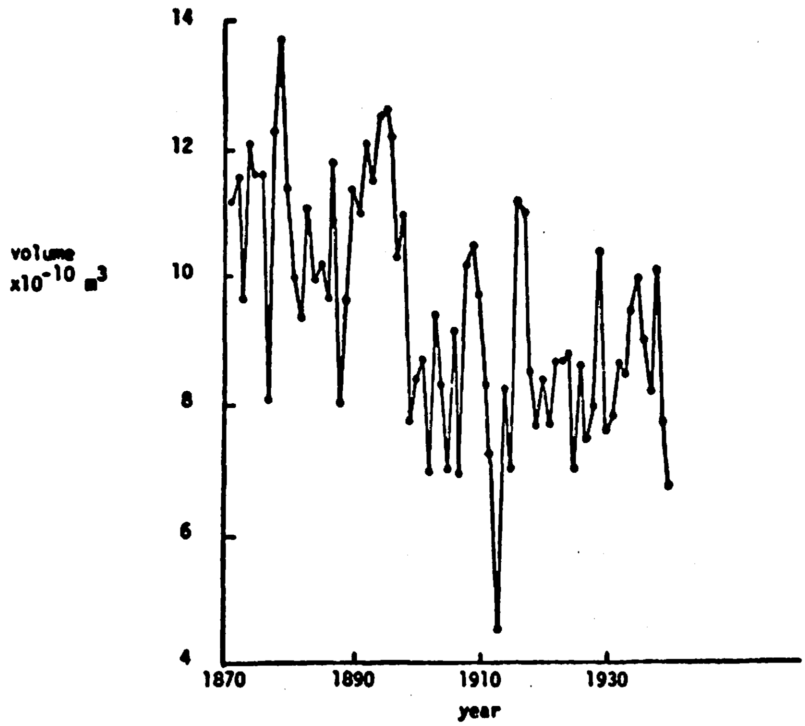
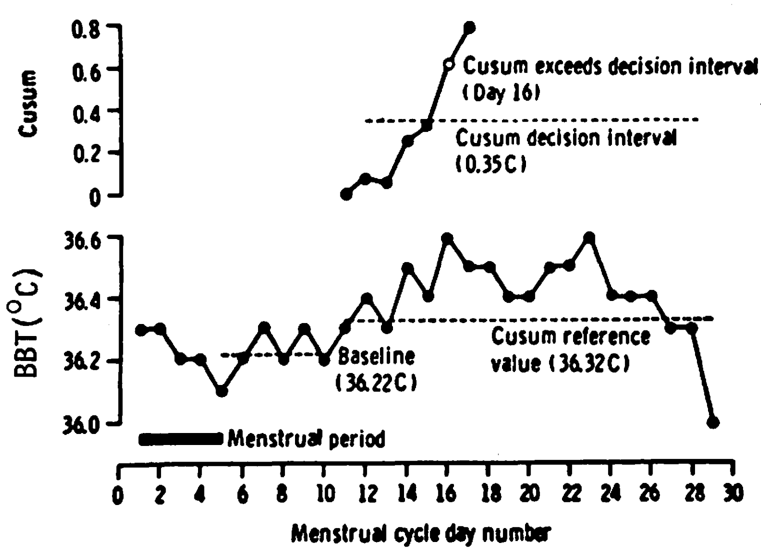


Figure 1.2 A Basal Body Temperature (BBT) Chart. (Source: Royston & Abrams, 1980)



a small value is desirable when a shift does occur -- the quantity of interest is then ARL - γ. The upper part of Figure 1.2 illustrates the CUSUM procedure in action with the BBT data shown in the lower part of the figure.

A similar, but more complicated procedure operates when μ_0 is unknown. Theoretical properties of CUSUM procedures involve application of random walk theory, and approximate Brownian motion theory. Among the standard references are books by van Dobben de Bruyn and Woodward & Goldsmith; see also the references in Section 2.2. Corresponding Bayesian procedures have been studied, notably by Bather (1967) and Shiryaev (1963, 1965).

A somewhat different testing problem obtains when a complete fixed sample is available and a retrospective test is required. Here one might propose model (1.1a') as the specific alternative against which to test the "no-shift" hypothesis. Proposed tests include backward (reverse time) CUSUM charts, normal-theory likelihood ratio tests, non-parametric rank significance tests, and tests based on Bayesian formulations. Particular mention should be made of the papers by Bhattacharya (1980) and Sen & Srivastava (1975b), which give partial reviews, comparisons of various tests and distributions of test statistics; see also Section 2.2.

One of the so-called Bayesian approaches averages out the possible change-point, giving a simple regression model as the alternative hypothesis, and thence arrives at the test statistic $\Sigma j(x_j - \bar{x}_{1,n})$, where $\bar{x}_{a,b} = \text{ave}(x_a,\ldots,x_b)$. Likelihood ratio tests are more complicated. For example, if σ^2 and μ_0 are known, then the likelihood ratio test statistic for the positive-shift alternative $(\mu_1 > \mu_0)$ is

$$\sup_{1 \leq r < n} \{(n - r)^{\frac{1}{2}}(\bar{x}_{r+1,n} - \mu_0)\}/\sigma, \tag{1.3}$$

whose approximate null distribution for large n can be related to Browian motion with shifting drift. Since the distributional problems for statistics like (1.3) are so complicated, the bootstrap technique discussed in Section 3.4 may be useful. Statistics such as (1.3) tend to be preferable to "smooth" statistics such as $\Sigma j(x_j - \bar{x}_{1,n})$ when model (1.1a') holds with γ or $n - \gamma$ quite small.

1.3 Particular Sequential Detection Scheme

For the application illustrated in Figure 1.2, a CUSUM technique has been advocated for detection of the upward mean shift in BBT. The CUSUM method is said to give good results, and is obviously very easy to use. Potential disadvantages are that the decision procedure requires careful choice of h, and that the actual significance of the end result is hard to measure. It is, then, of some interest to consider alternative methods which are more closely tied to the model and to the available data. There are several background points to note:

- (i) t = 1 corresponds to the last day of a menstrual period;
- (ii) the normal mean-shift model (1.1a') is a reasonable assumption, although the x_j are discretized;
- (iii) sample size n is approximately 25;
- (iv) the change-point γ is bounded below by 5;
- (v) for a given subject there is cycle-to-cycle variation of μ_0, μ_1 and possibly γ.

One direct approach to the detection problem involves sequential computations of $pr(\gamma < t | x_1, \ldots, x_t)$, using Bayes's Theorem together with existing empirical priors for μ_0, μ_1 and γ. To see how this might work, we suppose that σ^2 is known, that a priori distributions for μ_0 and μ_1 are respectively $N(\xi_0, \tau_0^2)$ and $N(\xi_1, \tau_1^2)$, and that a priori $pr(\gamma = j) = \pi_j$ $(j = 1, \ldots)$. Then a rather routine calculation shows that

$$pr(\gamma < t) = \frac{\sum_{j=1}^{t-1} \pi_j q_0(j, \bar{x}_{1,j}, SS_{1,j}) q_1(t-j, \bar{x}_{j+1,t}, SS_{j+1,t})}{\text{numerator} + (\sum_t^{\infty} \pi_j) q_0(t, \bar{x}_{1,t}, SS_{1,t})}, \qquad (1.4)$$

where

$$q_i(k, \bar{x}, SS) = (1 + k\pi_i^2/\sigma^2)^{-\frac{1}{2}} \exp\left[-\tfrac{1}{2}\left\{\frac{k(\bar{x} - \xi_i)^2}{k\tau_i^2 + \sigma^2} + \frac{SS}{\sigma^2}\right\}\right] \qquad (i = 0,1)$$

and

$$\bar{x}_{a,b} = (b - a + 1)^{-1} \sum_{j=a}^{b} x_j, \qquad SS_{a,b} = \sum_a^b (x_j - \bar{x}_{a,b})^2.$$

The special case $\tau_0^2 = \tau_1^2 = 0$ gives the posterior odds ratio formula

$$\frac{pr(\gamma < t)}{pr(\gamma \geq t)} = \sum_{j=1}^{t-1} \pi_j \exp\left[\frac{(\xi_1 - \xi_2)}{\sigma^2}\right] \sum_{k=j+1}^{t} \{x_k - \tfrac{1}{2}(\xi_0 + \xi_1)\} \div \sum_{j=t}^{\infty} \pi_j, \qquad (1.5)$$

which should be a reasonable approximation for small values of τ_0^2/σ^2 and τ_1^2/σ^2.

By way of illustration, consider the data in Figure 1.2. For this subject we assume $\sigma^2 = .04$, $\tau_0^2 = \tau_1^2 = \frac{1}{4}\sigma^2$, $\xi_0 = 36.2$, $\xi_1 = 36.5$ The non-zero prior probabilities for the change-point are

$$\pi_5 = \pi_6 = \pi_7 = \pi_{14} = \pi_{15} = \pi_{16} = 0.015,$$

$$\pi_8 = \pi_{13} = 0.055, \qquad \pi_9 = \pi_{10} = \pi_{11} = \pi_{12} = 0.2. \qquad (1.6)$$

These assumptions are loosely based on information in the article by Royston & Abrams (1980). With $t = 1$ corresponding to Day 5 of the cycle, formulae (1.4) and (1.5) then give the values for $pr(\gamma < t|x_1,\ldots,x_y)$ in Table 1.1.

Evidently at $t = 12$ it is nearly certain that $t = \gamma$ has been passed. The CUSUM procedure detects the shift at $t = 12$. In this particular data set the data and the prior agree quite closely. When a fairly flat prior is taken for γ, the posterior probabilities do not change appreciably.

Table 1.1 Bayes Sequential Detection Probabilities for BBT Data

t =	6	7	8	9	10	11	12	13	14	15	16	17
exact $pr(\gamma < t\|x_1,\ldots,x_t)$ using (1.4) =	0.02	0.03	0.09	0.25	0.55	0.73	0.95	0.98	0.99	0.99	1.00	1.00
approximation (1.5) =	0.01	0.03	0.10	0.26	0.61	0.80	0.97	0.99	1.00	1.00	1.00	1.00
prior probability =	0.03	0.05	0.10	0.30	0.50	0.70	0.90	0.96	0.99	1.00	1.00	1.00

The Bayesian procedure is certainly complicated, but is easily implemented in a calculator-assisted application. What would be of interest is an empirical comparison with the CUSUM procedure (see Section 3.3).

In this particular application one is not interested in testing the no-shift hypothesis given the whole cycle data $x_1,\ldots,x_n$. If one were, the statistic $\sum_{j=1}^{n} j(x_j - \bar{x}_{1,n})/\sigma$ could safely be used since $\gamma \doteq \frac{1}{2}n$, in which case the complicated likelihood ratio test is not noticeably superior.

1.4 Estimation of the Change-Point

The simplest case to consider is model (1.1) with θ_0 and θ_1 both known: for large values of γ, $n - \gamma$ the approximate distribution theory discussed below applies also when θ_0 and θ_1 are efficiently estimated. Much of the literature arbitrarily proposes maximum likelihood estimation for γ, which turns out to be sensible for a reason mentioned below. The log likelihood function $\ell(\gamma)$ of γ may be represented as

$$\ell(\gamma + d) = \begin{cases} \ell(\gamma) + \sum_{j=1}^{d} \log\{f(x_{\gamma+j}|\theta_0)/f(x_{\gamma+j}|\theta_1)\} & d \geq 1 \\ \ell(\gamma) + \sum_{j=d}^{-1} \log\{f(x_{\gamma+j}|\theta_1)/f(x_{\gamma+j}|\theta_0)\} & d \leq -1. \end{cases}$$

This clearly defines two random walks, so that the distribution of $\hat{\gamma} - \gamma$ is determined by the results related to times of suprema of random walks with negative drift; for dense sampling and small $||\theta_0 - \theta_1||$ one can use Wiener process results. See Hinkley (1970, 1972) and Bhattacharya (1980) for some of the relevant theory.

Unfortunately the distribution theory just described is unconditional and hence often inappropriate, in the sense that there exists an ancillary statistic which determines a conditional inference solution. This resolution was pointed out by Cobb (1978), who showed that the <u>shape</u> of the likelihood function is ancillary, and that the conditional distribution of $\hat{\gamma} - \gamma$ is

$$\mathrm{pr}(\hat{\gamma} - \gamma = d|\text{shape}) \sim \exp\{\ell(\hat{\gamma}_{obs} - d)\}/\sum_{c=1}^{n} \exp\{\ell(c)\}, \qquad (1.7)$$

for large values of γ and $n - \gamma$. The likelihood shape and $\hat{\gamma}$ are jointly sufficient. Equation (1.7) corresponds to the posterior distribution for

$\hat{\gamma} - \gamma$ when γ has invariant prior.

Although the conditional solution (1.7) is preferable for analysis of a single data set, the unconditional result would be of use in a situation such as the BBT application of Section 1.2, where the unconditional variation of $\hat{\gamma} - \gamma$ can be used together with empirical data from several cycles to approximate a frequency prior for γ.

Cobb (1978) illustrates the unconditional and conditional distributions of $\hat{\gamma} - \gamma$ using the data in Figure 1.1. These distributions are given in Table 3.1; Section 3.2 discusses the application of the bootstrap to this problem.

1.5 Other Topics

Very little work has been done on sensitivity of change-point inference to model misspecification (correlation, aberrant data values, etc.). The bibliography does include some references to non-parametric estimation and testing.

When there is clear evidence for a mean shift, as in the BBT data of Figure 1.2, it may not be entirely clear that the shift to a new constant level is abrupt rather than gradual. In many cases sampling may not be frequent enough to allow distinction between abrupt and gradual changes, although the distinction may be resolved on scientific grounds. If the distinction were of interest it might be difficult to obtain a good statistical test because the relevant models are not identified and nested. For example, if we wished to test a simple linear trend model against the mean-shift model (1.1a'), then the likelihood ratio statistic would have non-standard sampling properties. In such a situation one can make use of bootstrap techniques, as outlined in Section 3.

2. CONTINUOUS SHIFT MODELS: TWO-PHASE REGRESSION

2.1 Models and Examples

The major class of continuous shift models is that of piecewise continuous regression models. We consider only two-phase regression models of the form

$$x(t_j) = \begin{cases} \alpha + \beta_0(t_j - \gamma) + e_j, & t_j \leq \gamma \\ \alpha + \beta_1(t_j - \gamma) + e_j, & t_j > \gamma \end{cases}, \qquad (2.1)$$

where for convenience we assume the e_j to be $N(0,\sigma^2)$ random errors. Much of the theoretical literature considers more general linear models and non-linear models, but (2.1) is convenient for discussing the main points and is the most applicable case.

In many applications (2.1) will be the specific alternative to a simple linear regression, i.e., "no-shift", hypothesis, although many tests of the latter hypothesis are more general.

Figures 2.1, 2.2, 2.3, and 2.4 illustrate a few published applications of model (2.1). In at least one case the model is of dubious relevance. One of the main reasons for using two-phase regression is that the change-point γ may be easy to interpret, or may be a useful focus for comparison of data sets, even though a smoother model might be slightly more appropriate. This would probably be the case in Figure 2.2. The two-phase model is particularly prevalent in biological applications, where uncontrolled variation often precludes careful model definition.

Figure 2.1 Relation Between Phosphate and Oxygen Concentration in a Nutrient Redistribution Study (Source: Webb and D'Elia, 1980).

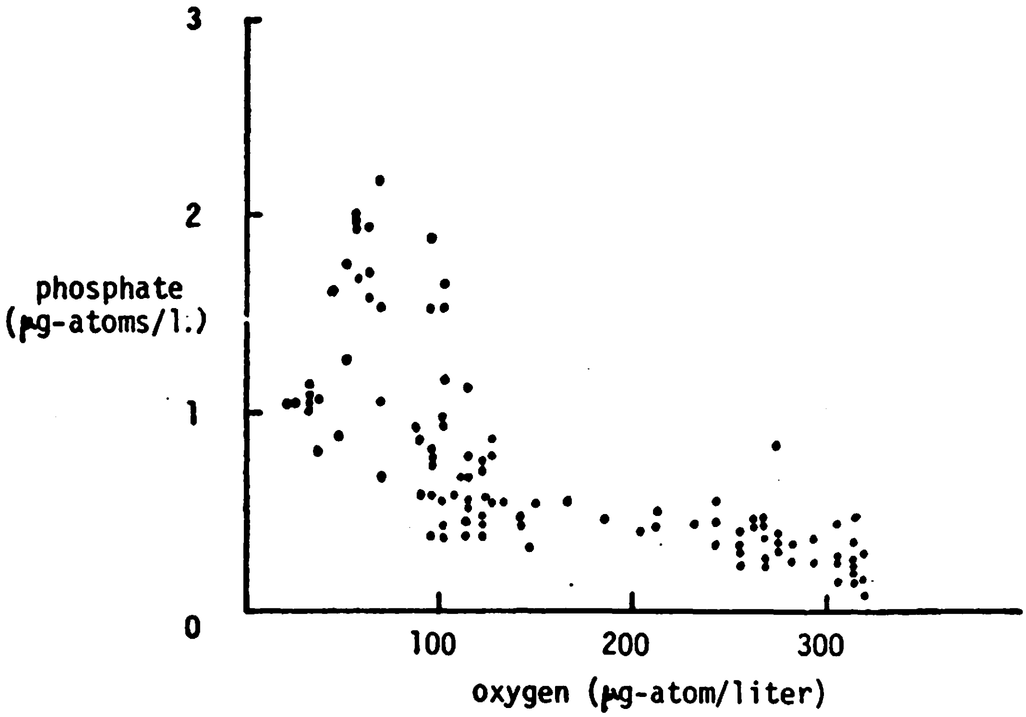


Figure 2.2 Relationship Between Egg Production and Methionine Intake (Source: Curnow, 1973)

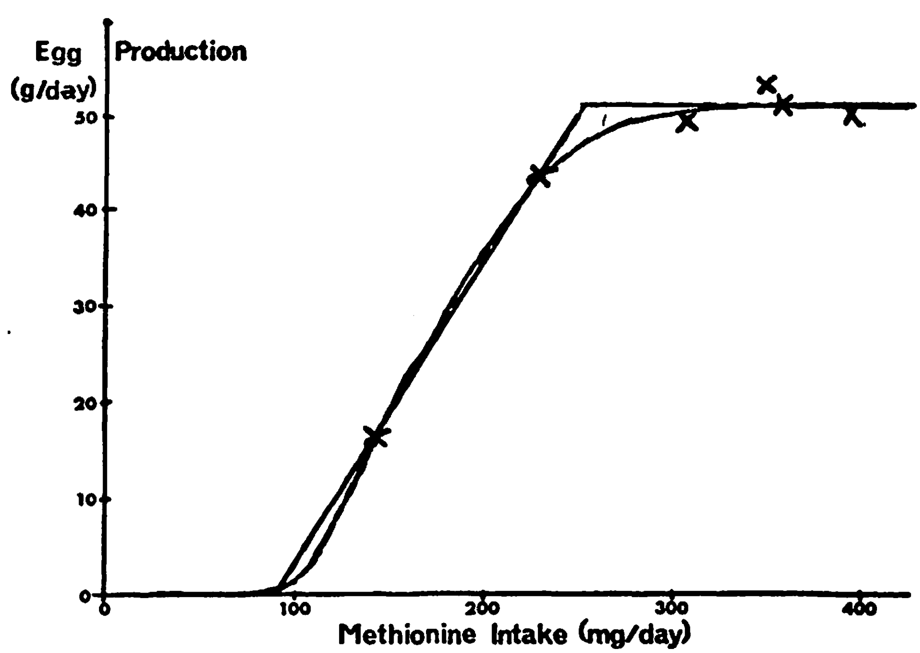


Figure 2.3 Relationship Between Alfalfa Plant Yield and Soil pH

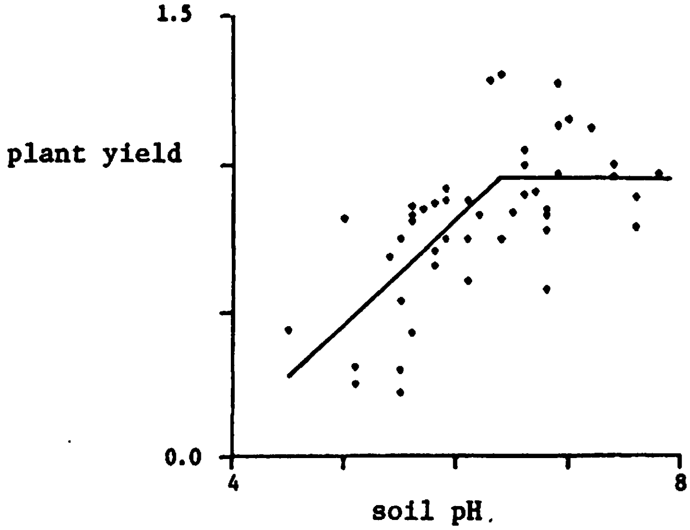
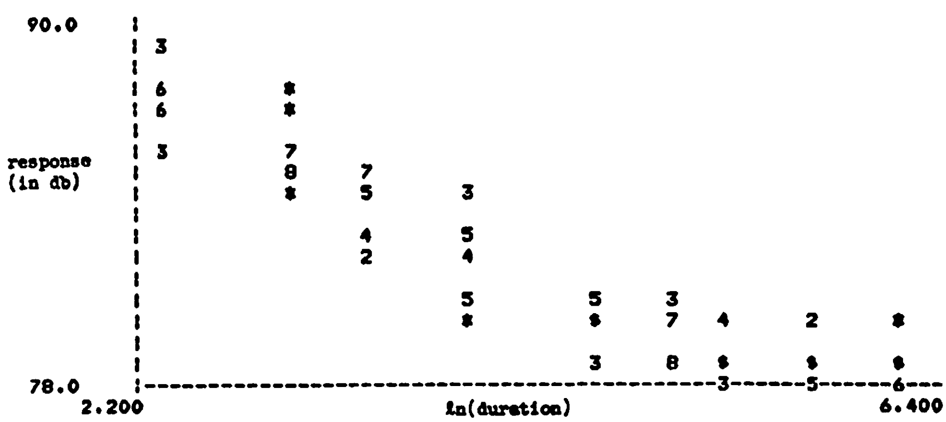


Figure 2.4 Response in Decibels vs. Logarithms of Duration for Target Signal (Source: Faith, 1980) [Displayed Numbers Indicate Multiplicities of Points].



2.2 Tests for Regression Shift

The procedures described briefly in Section 1.2 have their counterparts here. A particularly good survey, with examples, is given by Brown, Durbin & Evans (1975). Various analogs of the CUSUM techniques are based on standardized recursive residuals, defined as follows. Assume a simple linear regression model

$$x(t_j) = \alpha + \beta t_j + e_j, \qquad j = 1,\ldots,n, \tag{2.2}$$

and denote the least squares estimates of α and β given $(t_1,x_1),\ldots,(t_r,x_r)$ by $\tilde{\alpha}_r$ and $\tilde{\beta}_r$. Then the standardized recursive residuals are

$$w_r = \frac{y_r - (\tilde{\alpha}_{r-1} + \tilde{\beta}_{r-1} t_r)}{\sqrt{\left\{1 + \dfrac{(t_r - \bar{t}_{1,r-1})^2}{\sum_1^{r-1} (t_j - \bar{t}_{1,r-1})^2}\right\}}} \qquad (r = 3,4,\ldots),$$

which have zero mean, constant variance and zero correlation under the no-shift normal error hypothesis. CUSUM tests based on the forward sums $\sum_3^r w_j$ $(r = 3,4,\ldots)$ and $\sum_3^r w_j^2$ $(r = 3,4,\ldots)$ are then used for one- and two-sided tests respectively. Distribution theory for Σw_j is based on a Browian motion approximation, while the distribution of Σw_j^2 is related to that for the Kolmogorov-Smirnov statistic. In the non-sequential case, CUSUM schemes can be run backwards from the end of the data, and Schweder (1976) argues that this is preferable. A useful recent reference to the theory is Deshayes & Picard (1980).

For non-squential tests with model (2.1) as the specific alternative, the likelihood ratio statistic compares the maximum log likelihood $\ell(\hat{\gamma}, \hat{\alpha}, \hat{\beta}_0, \hat{\beta}_1)$ under (2.1) to the maximum log likelihood $\ell_0(\hat{\alpha}, \hat{\beta})$ under (2.2). The standard type of χ_2^2 approximation does not hold for the statistic

$$+ 2\{\ell(\hat{\gamma}, \hat{\alpha}, \hat{\beta}_0, \hat{\beta}_1) - \ell_0(\hat{\alpha}, \hat{\beta})\}, \tag{2.3}$$

since (2.2) does not define a linear subspace of the model (2.1). An elegant discussion of the problem may be found in Feder (1975b), where we read that "the asymptotic distribution is the distribution of the maximum of a large number of correlated $\chi_1{}^2$ and $\chi_2{}^2$ random variables... presumably different limiting distributions would result from different spacings of the independent variable." See Section 3.4.

One relatively simple test is obtained by averaging the model with respect to a uniform prior for γ and then deriving a locally most powerful test -- giving essentially a test for presence of an additional quadratic term in (2.1). This test is likely not to be very good if γ is near to either end of the sample range of t.

Various tests have been proposed which have a discontinuous shift alternative to (2.2). None of these tests seem to have tractable null distribution properties; see Beckman & Cook (1979) for related discussion.

2.3 Estimation of Change-Point Models

The unusual feature of estimation for the model (2.1) is that the likelihood (or residual sum of squares) is not a smooth function of γ:

its derivative is discontinuous at $\gamma = t_j$ $(j = 1,\ldots,n)$. Some algorithms for computation of the m.l.e. $\hat{\gamma}$ start by fitting unconstrained two-phase models, while other algorithms are efficient non-linear optimization procedures. See Lerman (1980) for a recent account.

The slight irregularity of the likelihood function causes a technical problem in verifying that standard asymptotic theory applies, but Feder (1975a) provides an ingenious proof. It is probable that standard normal approximations based on the Fisher information are not very accurate for small samples, and on general grounds one should probably use the likelihood surface to obtain confidence intervals. It therefore seems generally advisable to plot the marginal log likelihood $\sup_{\alpha,\beta_0,\beta_1} \ell(\gamma,\alpha,\beta_0,\beta_1)$ in applications. Since the change-point model is non-linear, it might be worth studying the relevance of recent work by Bates & Watts (1980).

2.4 Tests of Fit for Two-Phase Regression

In any one of the situations illustrated in Figures 2.1-2.4 one might question whether the shift from one regression to the other is abrupt. Watts and Bacon (1974) consider more general models with a smooth transition, model (2.1) being a special (boundary) case. This seems particularly appropriate in low-error industrial experiments where detailed study of the regression relation is possible. With an additional parameter δ, representing curvature of the regression function at $t = \gamma$, one can examine the plausibility of abrupt shift $(\delta = 0)$ via a likelihood contour plot in the (γ,δ) plane.

A formal test of the abrupt-shift hypothesis ($\delta = 0$) requires special study, since the hypothesis is a boundary point of the parameter space. An alternative ad hoc method is to split the data into three sections corresponding to $t < \hat{\gamma} - d_1$, $\hat{\gamma} - d_1 \leq t \leq \hat{\gamma} + d_2$ and $\hat{\gamma} + d_2 \quad t$, say; then fit linear regressions to the first and third sections; then test whether or not the middle section of data fits the predictions from the first and third sections.

3. BOOTSTRAP TECHNIQUES

3.1 General Remarks

Many of the distributional problems associated with change-point methods are difficult to solve theoretically, even when special assumptions are made (such as normality of errors). In more regular statistical estimation problems there are two useful alternatives: (i) use the jackknife technique to obtain standard errors and bias corrections, (ii) generate computer simulated properties of estimates using assumed probability models. A general set of techniques including these two has been discussed by Efron (1979, 1980) under the name "Bootstrap". The basic idea here is to simulate statistical procedures and their properties using the sample data to help generate similar samples. In the next three short subsections we show how bootstrap techniques can be used in connection with some change-point problems.

3.2 Estimation of Mean-Shift Change-Point

For the simple mean-shift model (1.1a'), we express the fitted model as

$$\begin{aligned} x_j &= \hat{\mu}_0 + e_j \qquad j = 1,\ldots,\hat{\gamma} \\ x_j &= \hat{\mu}_1 + e_j \qquad j = \hat{\gamma}+1,\ldots,n \,. \end{aligned} \tag{3.1}$$

If we are content to assume homogeneity of errors, but make no further assumption about them, then the obvious estimate of the error distribution function is the sample c.d.f.

$$\hat{F}_n(e) = n^{-1} \sum_{j=1}^{n} I(e - \hat{e}_j) \quad ,$$

Next we simulate artificial samples

$$x_j^* = \begin{cases} \hat{\mu}_0 + e_j^* & j = 1,\ldots,\hat{\gamma} \\ \hat{\mu}_1 + e_j^* & j = \hat{\gamma}+1,\ldots,n \end{cases} \tag{3.2}$$

by randomly sampling e_j^* from $\hat{F}_n(e)$, that is by sampling with replacement from $\{\hat{e}_j\}$. Each such sample gives estimates $\hat{\mu}_0^*, \hat{\mu}_1^*$, γ^*, and σ^*. The empirical distributions of $\hat{\gamma}^* - \hat{\gamma}$, etc. then estimate the sampling distributions of $\hat{\gamma} - \gamma$, etc. Typically several hundred samples would be used, with fairly minimal computing cost.

To illustrate the procedure, we have applied it to the Nile data in Figure 1.1. Actually several types of bootstrap were applied, two of which will be discussed here. The first bootstrap simulation (B1) used m.l. estimation for γ from $\{x_j^*\}$ defined by (3.2), assuming $\mu_0 = \hat{\mu}_0$ and $\mu_1 = \hat{\mu}_1$ known. The second bootstrap (B2) used separate pre- and post-shift error distributions, and assumed different means and variances all unknown in the m.l. estimation from generated data. Table 3.1 shows resulting empirical distributions of $\hat{\gamma}^* - \hat{\gamma}$ from 1000 samples, together with asymptotic normal-theory distributions of $\hat{\gamma} - \gamma$ (unconditional and conditional (1.7)).

Table 3.1 Bootstrap* and Theoretical Distributions for $\hat{\gamma} - \gamma$ for Nile Data

	Theoretical Probabilities		Bootstrap Empirical Probabilities	
$\hat{\gamma} - \gamma$	Conditional	Unconditional	B1	B2
$\geq$ 6+	0	0.003	0.005	0.012
5	0.000	0.003	0.005	0.006
4	0.000	0.007	0.011	0.015
3	0.001	0.015	0.010	0.021
2	0.045	0.038	0.049	0.042
1	0.109	0.113	0.122	0.108
0	0.808	0.641	0.618	0.598
-1	0.032	0.113	0.102	0.112
-2	0.004	0.038	0.039	0.039
-3	0.001	0.015	0.022	0.014
-4	0.000	0.007	0.008	0.010
-5	0.000	0.003	0.003	0.008
$\leq$ -6	0	0.003	0.006	0.015

*1000 samples.

The table clearly illustrates the pronounced effect of conditioning, the similarity of bootstrap to unconditional distributions, and the effect of having to estimate mean and variance parameters. Of course the conditional distribution is only trustworthy if our original model assumption of $N(0,\sigma^2)$ errors is correct -- which it seems to be here. The bootstrap analysis clearly approximates an unconditional analysis, as is generally true.

3.3 Sequential Detection of Mean-Shift

In Section 1.2 we discussed sequential detection of shift in the context of the BBT data illustrated by Figure 1.2. One could boostrap both the CUSUM procedure and the Bayes procedure in a fairly obvious manner, for example using (3.2) to generate data. Further, one could incorporate in the bootstrap various peculiarities of the applications, such as discretization of measurements. Given a series of cycles for one particular subject, one could also simulate pre- and post-shift mean levels of BBT from the empirical distributions of $\hat{\mu}_i$. Presumably the major characteristics of interest would include

$$p = \text{chance of false (early) detection of shift} \qquad (3.3)$$

$$m = \text{average value of (decision time} - \gamma). \qquad (3.4)$$

As a preliminary indication of what can be done, we bootstrapped the Bayes decision procedure, or rather its main ingredient $P_t = \{pr(\gamma < t|x_1,\ldots,x_t), t = 6,7,\ldots\}$, using only the data plotted in Figure 1.2. Model (3.1) was fitted to the data and 1000 bootstrap samples were generated according to (3.2). In addition to simulating the sequence of posterior probabilities,

P_t, we simulated the CUSUM procedure outlined in Section 1.2, here with h = 0.35 and $\delta\sigma$ = 0.2, 0.3 (h = 0.35 and $\delta\sigma$ = 0.2 were recommended by Royston & Abrams).

Figure 3.1 shows histograms of $P_t^* = \text{pr}(\gamma < t | x_1^*, \ldots, x_t^*)$ for t = 8(1)12 for two prior distributions on γ, first the one in (1.6) and second the more diffuse prior

$$\pi_1 = \ldots = \pi_5 = 0, \qquad \pi_6 = \ldots = \pi_{10} = .05,$$

$$\pi_{16} = \ldots = \pi_{20} = 0.05, \qquad \pi_{11} = \ldots = \pi_{15} = 0.1. \qquad (3.5)$$

From Figure 3.1 we can estimate the performance of any decision procedure determined by a cut-off value of P_t. To take a specific example, suppose $P_t = 0.8$ is the cut-off: if $P_t \geq 0.8$, then we decide that $\gamma < t$. The bootstrap frequencies of

$$T = \text{decision time } t - \gamma$$

are given in Table 3.2, which includes for comparison the corresponding frequencies for the two CUSUM procedures. (Note that T = 0 corresponds to premature detection.) Evidently the Bayesian procedure can give slightly lower values of p and m, defined in (3.3) and (3.4), than the CUSUM procedures. A more thorough practical analysis of this problem would require also bootstrapping the within-subject cycle-to-cycle variation and the between-subject variation.

Figure 3.1(a) Bootstrap Distribution of $P_t^* = pr(\gamma < t | x_1^*,\ldots,x_t^*)$ Using Prior of Example in Section 1.2. 1000 Samples.

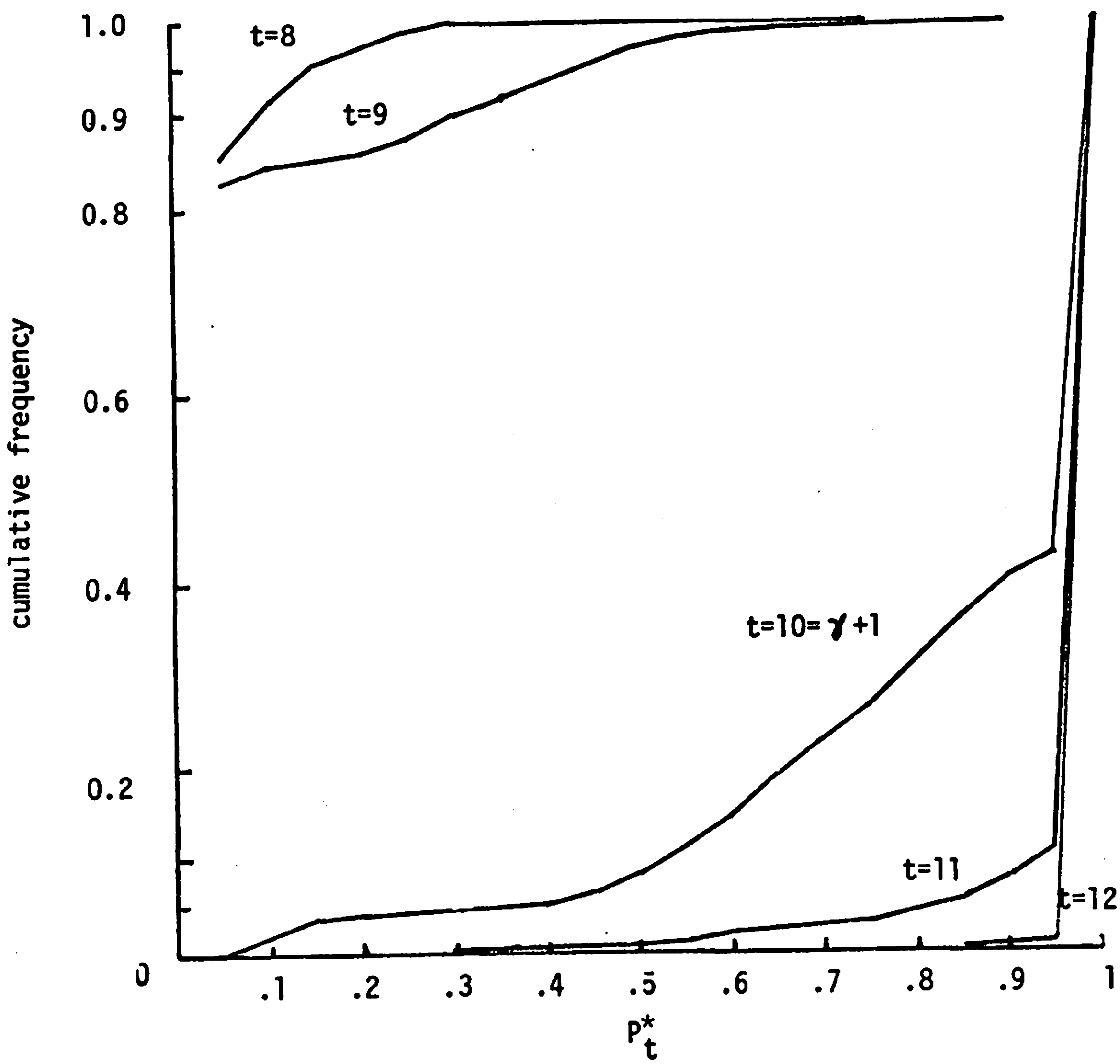


Figure 3.1(b) As in (a) But With Flatter Prior (3.5) Instead of (1.6)

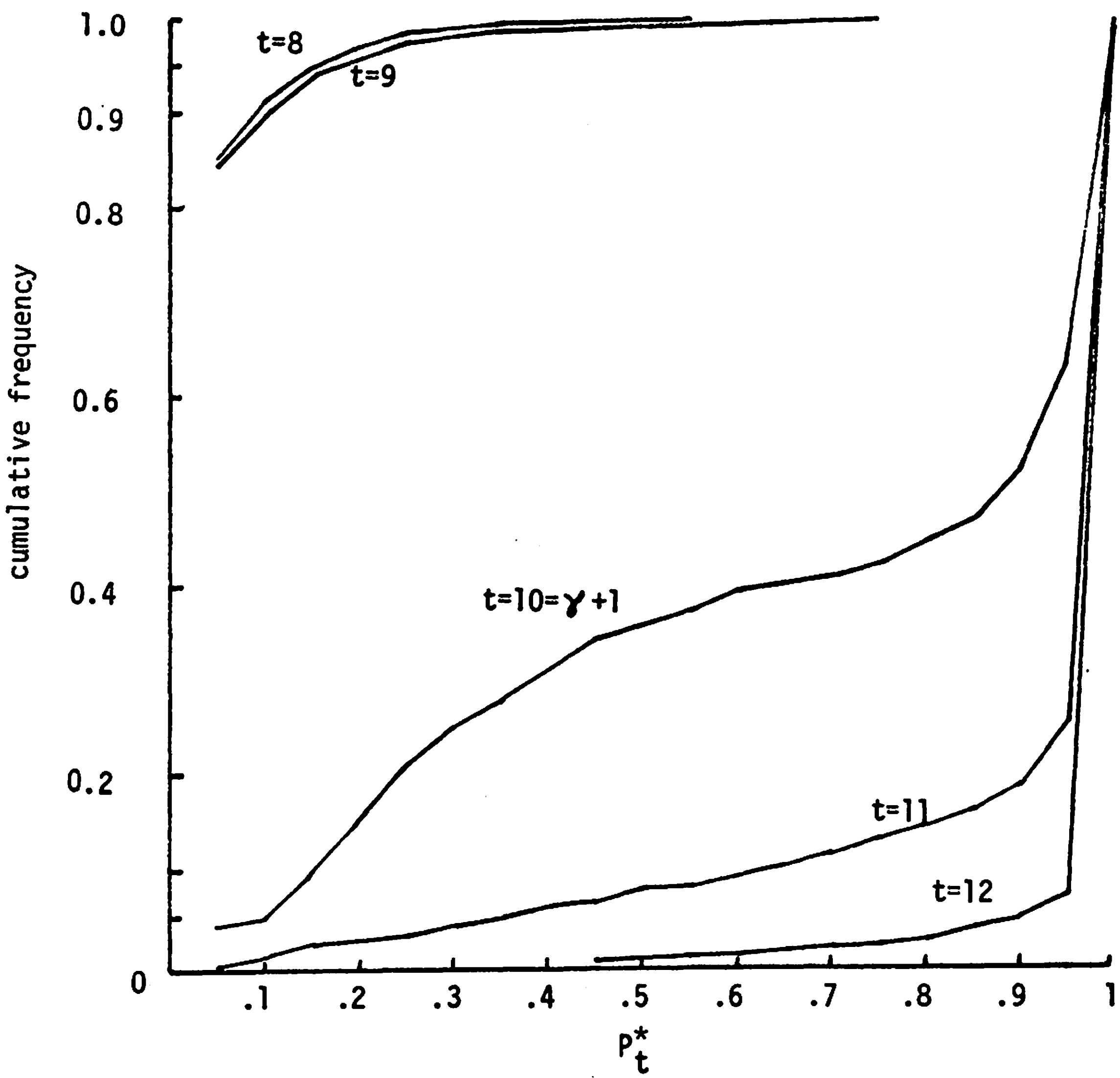


Table 3.2 Bootstrap Frequencies for T = Decision Time - γ, Based on Data in Figure 1.2.

		T = -2	-1	0	1	2	3	4	5+
CUSUM Procedure	$h = 0.35$, $\delta\sigma = 0.2$	0.013	0.028	0.025	0.662	0.198	0.055	0.014	0.005
	$h = 0.35$, $\delta\sigma = 0.3$	0.001	0.002	0.004	0.533	0.257	0.105	0.054	0.044
Bayes Procedure Cut-off $P_t = 0.8$	prior (1.6)	0	0	0.020	0.669	0.268	0.041	0.001	0.001
	prior (3.5)	0	0	0	0.554	0.298	0.116	0.025	0.007

3.4 Test of Simple Versus Two-Phase Linear Regression

Suppose that model (2.1) is viewed as a probable model, except that there may actually be no shift. Then we are interested in testing the adequacy of the simple model

$$x_j = \alpha + \beta t_j + e_j, \qquad (j = 1,\ldots,n) \qquad (3.6)$$

with (2.1) as alternative. For a particular test statistic T, perhaps one of those mentioned in Section 2.2, the following simple bootstrap method would give an approximate level of significance.

First, fit the model (2.1) by least squares and obtain the residuals $\hat{e}_1,\ldots,\hat{e}_n$. Next fit (3.6) by least squares to obtain $\hat{\alpha}$ and $\hat{\beta}$. Then generate bootstrap samples

$$x_j^* = \hat{\alpha} + \hat{\beta} t_j + e_j^*, \qquad (j = 1,\ldots,n)$$

where the e_j^* are sampled without replacement from $\{\hat{e}_j\}$. For each bootstrap sample compute the value T* of the test statistic, and thence obtain the empirical null hypothesis distribution of T*. The approximate significance of the observed value T_{obs} is then the proportion of T*'s exceeding T_{obs}, assuming large values of T are indicative of (2.1).

Note that the sample c.d.f. of e is not obtained using residuals from (2.1), since these would be inflated by systematic effects if (2.1) were true. Of course the estimation method need not be simple least squares if a more appropriate method is available.

To illustrate the procedure we have taken part of the data set graphed in Figure 2.4. There were six observations at each of nine values of t (the latter being natural logarithms of 10, 20, 30, 50, 100, 150, 200, 300, 500), but because the six were not genuine replicates we simply took the response x to be the average of the six observations in each group. The nine averages were

$$87.8\dot{3},\ 86.50,\ 84.8\dot{3},\ 83.50,\ 80.1\dot{6},\ 79.50,\ 79.1\dot{6},\ 78.6\dot{6},\ 78.6\dot{6}.$$

We then generated 1000 bootstrap samples, following the procedure described above, and took T to be the log likelihood ratio statistic (2.3), which is

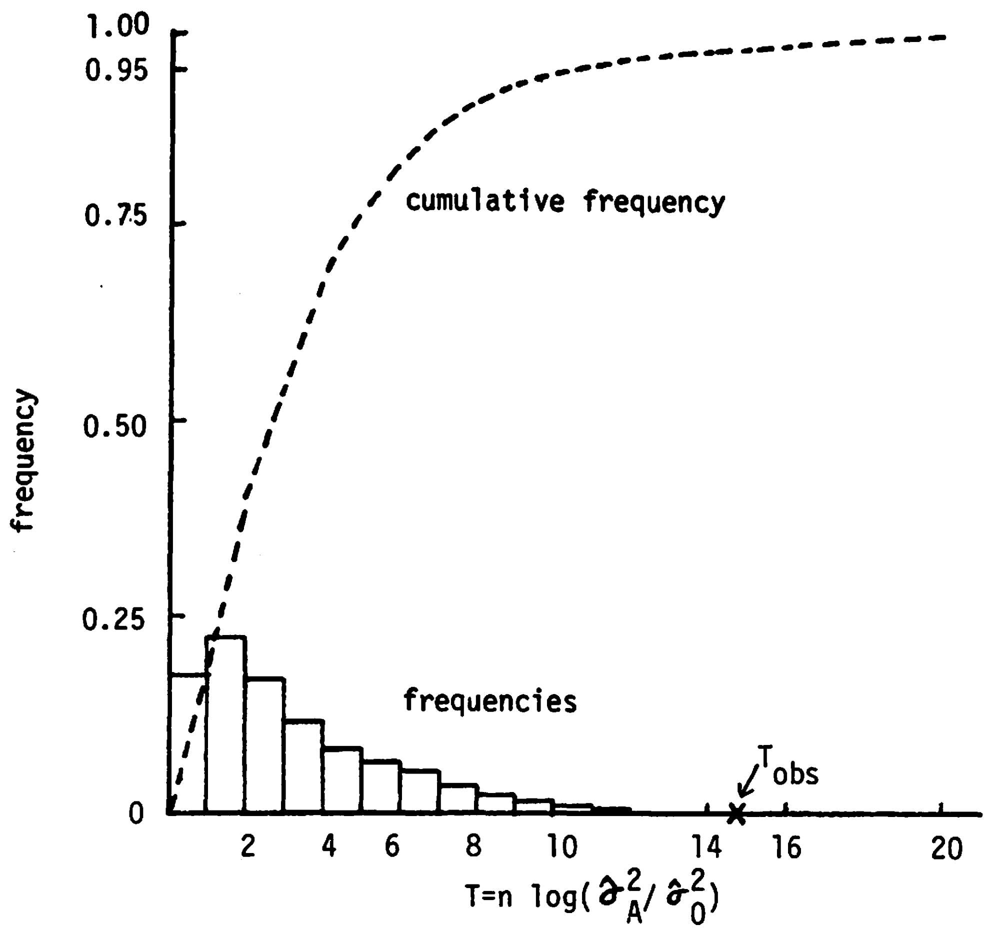
$$T = n \log(\hat{\sigma}_0^2/\hat{\sigma}_A^2),$$

where subscripts 0 and A refer to null and alternative models, (3.6) and (2.1), respectively. The data statistics are $\hat{\gamma}_{obs} = 5.088$, $T_{obs} = 14.74$. Figure 3.2 shows the bootstrap null hypothesis frequencies of T*, from which we conclude that T_{obs} is significant at about the 2% level.

Notice that the bootstrap distribution of T^* is not close to the χ_2^2 distribution which a naive application of standard theory would suggest.

A corresponding bootstrap simulation of the two-phase model (2.1) yields an estimate of the distribution of $\hat{\gamma} - \gamma$ which is in close agreement with the normal approximation described by Hinkley (1971).

Table 3.2 Bootstrap Frequencies and Cumulative Frequencies for Log Likelihood Ratio Test of No-Shift Hypothesis in Regression, i.e., Model (2.1) Versus Model (3.6), for Subset of Data in Figure 2.4.



4. CONCLUDING REMARKS

This all-too-brief review of change-point model analysis suggests, among other things, that much of the related distribution theory is non-standard and complicated. One practical option that seems to have some merit is the use of Bootstrap techniques, although these seem to be incapable of providing conditional distributions in general (since models are required to define relevant subsets of the sample space).

Change-point models are open to scientific criticism, and more attention might be paid to comparisons with smoother models. Nevertheless, from a practical viewpoint the notions of change-point and threshold are undoubtedly often useful.

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APPENDIX: BIBLIOGRAPHY OF ARTICLES ON CHANGE-POINTS

The following bibliography contains more than 100 entries, yet cannot be treated as complete. For example, there are substantial literatures on: spline regression fitting, CUSUM quality control procedures, and economic switching regression models. Only a few papers from these areas are included in the bibliography, although hopefully the few are among the major references.

Nearly all articles have been coded using four classifications: model specification; statistical objectives; type of theory developed or used; presence of examples. The categories within each classification, with codes, are as follows.

MODEL SPECIFICATION

RL	Regression, Linear
RLC	Regression, Linear Continuous
RLD	Regression, Linear Discontinuous
RNC	Regression, Nonlinear Continuous
RND	Regression, Nonlinear Discontinuous
RLSp	Regression, Linear Spline fitting
RNSp	Regression, Nonlinear Spline fitting
TMI	Time series, Mean shift, Independent variables
RVI	Time series, Variance shift, Independent variables
TGI	Time series, General shift, Independent variables
TMD	Time series, Mean shift, Dependent variables
TVD	Time series, Variance shift, Dependent variables
TGD	Time series, General shift, Dependent variables

Notes: (a) time series is used to describe processes that are stationary in mean (and other characteristics) on either side of the change-point -- as opposed to regression models where the mean function is nonstationary, depending upon explanatory variables.

(b) TGI includes both general distributions and specific distributions such as Binomial and Gamma.

(c) TGD includes models with shifting autoregressive parameters.

STATISTICAL OBJECTIVES

TS	Test of no-shift hypothesis, Sequential
TN	Test of no-shift hypothesis, Non-sequential
E	Estimation of change-point and/or other model parameters, assuming a shift
G	Test for Goodness-of-fit of the change-point model

THEORY DEVELOPED OR USED

P	Parametric
NP	NonParametric
B	Bayesian
D	Distributions of statistics
O	Optimality of procedures
NU	NUmerical analysis

EXAMPLES

A	Application to real data set
D	Data set given in the paper
G	Graph given in the paper

Notes: (a) artificial data do not count,

(b) relatively few sources for examples are given in the bibliography, but many may be found by checking references in articles coded A.

For a particular classification, especially the last one, a blank (---) indicates "not in the article", whereas a question mark (?) indicates uncertainty about the category.

Corrections and additions to the bibliography are welcome.

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