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MULTIVARIATE QUALITY CONTROL PROCEDURES

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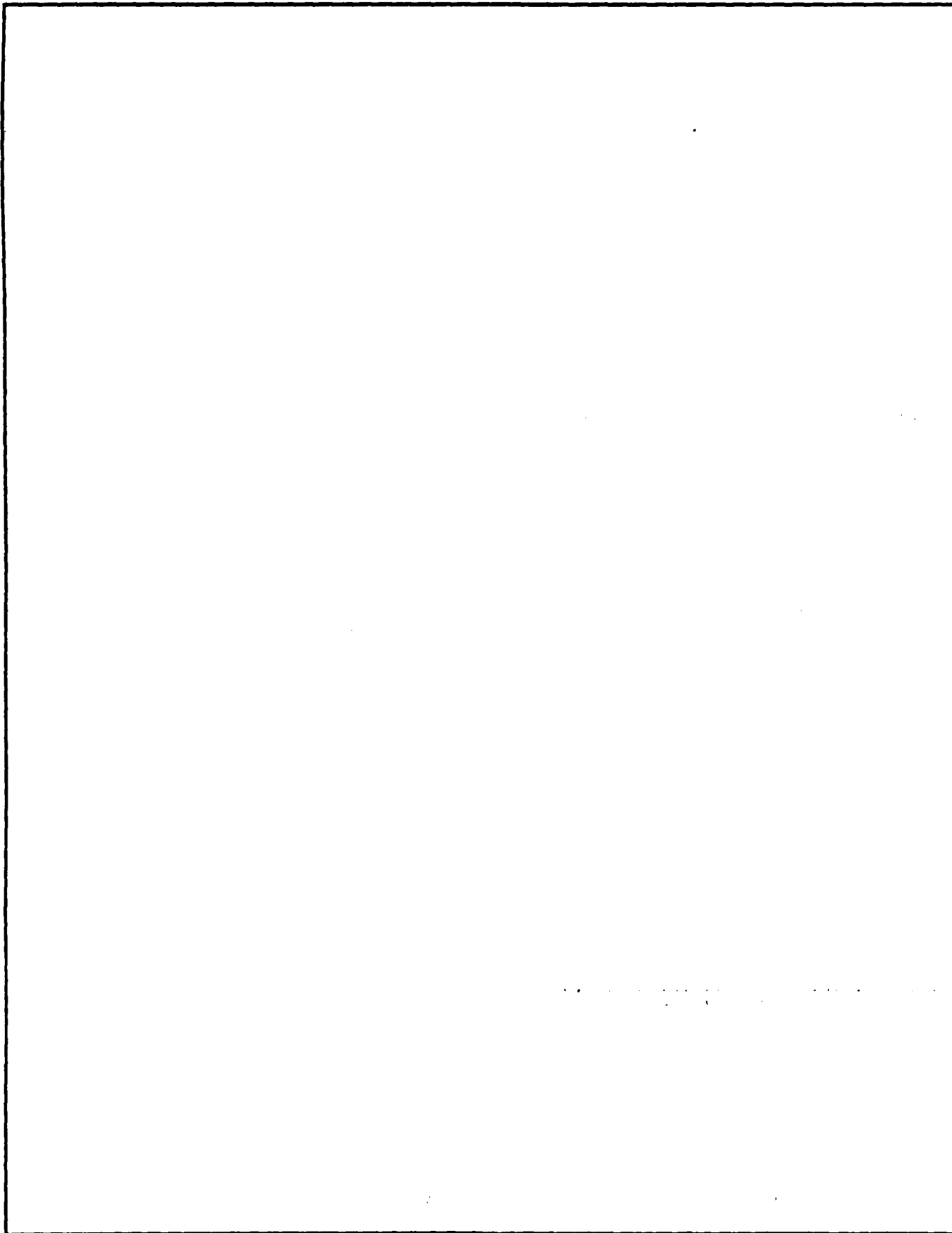
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PREFACE

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CONTENTS

	Page
1. INTRODUCTION	7
2. DESCRIPTION OF THE PROCEDURES	9
3. MULTIVARIATE SHEWHART CHARTS	11
4. CUMULATIVE SUM OF T-STATISTICS	11
5. MULTIVARIATE CUSUM SCHEMES	14
6. APPLICATIONS	26
7. SUMMARY AND CONCLUSIONS	28
LITERATURE CITED	29
APPENDIXES	
A. NUMERICAL METHODS	31
B. MATHEMATICAL PROOF	33
C. MARKOV CHAIN REPRESENTATION	37



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LIST OF FIGURES

Figure No.		Page
1.	ARL Curves for Multivariate Shewhart Charts with On-Target ARLs of 200	12
2.	ARL Curves for Multivariate Shewhart Charts with On-Target ARLs of 500	13
3.	ARL Curves for CUSUM of T Schemes with On-Target ARLs of 200	15
4.	ARL Curves for CUSUM of T Schemes with On-Target ARLs of 500	16
5.	ARL Curves for the COT Schemes of Figure 3 but with the Fast Initial Response Feature Implemented	17
6.	ARL Curves for the COT Schemes of Figure 4 but with the Fast Initial Response Feature Implemented	18
7.	ARL Curves for Multivariate CUSUM Schemes with On-Target ARLs of 200	20
8.	ARL Curves for Multivariate CUSUM Schemes with On-Target ARLs of 500	21
9.	ARL Curves for the Multivariate CUSUM Schemes of Figure 7 but with the Fast Initial Response Feature Implemented	23
10.	ARL Curves for the Multivariate CUSUM Schemes of Figure 8 but with the Fast Initial Response Feature Implemented	24

LIST OF TABLES

Table No.		Page
1.	Numerical Example of Bivariate Quality Control Schemes	10
2.	ARL Curves for Bivariate Schemes with $k = 0.5$, 1, and 1.5	19
3.	Comparison to the Woodall and Ncube Procedure on Principal Components: Bivariate Procedures with On-Target ARLs of 125	25

MULTIVARIATE QUALITY CONTROL PROCEDURES

1. INTRODUCTION

Cumulative sum (CUSUM) quality control schemes are used in industry to detect a change in the quality of a manufactured product. It is helpful to view CUSUM schemes as a sequence of sequential probability ratio tests. The most frequent application of CUSUM schemes is the detection of a change in the mean of a normally distributed variable. For this application, an algebraic rearrangement of the logarithm of the probability ratio yields a simple, recursive test statistic. There are two major problems that can arise in deriving CUSUM schemes from the theory of sequential tests. First, the theory requires specification of two simple hypotheses (as opposed to composite hypotheses)¹ to be tested; but, the most common application of quality control schemes requires testing the simple hypothesis that the mean is at its desired level versus the composite hypothesis that the mean has shifted from its target value. Second, the logarithm of the probability ratio may be too complex to yield a simple, practical scheme. Both of these problems have had an impact on the development of a multivariate CUSUM scheme.

The specification of both an aim or target value a and a specific alternative d for the mean vector u of a multivariate normal distribution with known covariance matrix V does yield a CUSUM scheme.² In many applications, however, there is no basis for selecting a specific point d for the alternative hypothesis. In the univariate case, this problem is not so severe: there are only two directions for the mean to shift, either higher or lower. The exact amount of shift is not a problem. To paraphrase Tukey,³ detecting a shift of five standard deviations is nearly trivial; whereas, detecting a shift of 0.05 standard deviation is nearly impossible. CUSUM schemes designed to detect a shift of one standard deviation are widely used and, of course, also quickly detect shifts of more than one standard deviation. The choice between detecting a shift to the high side and detecting a shift to the low side is resolved by operating two schemes simultaneously. The two schemes are considered to be a single two-sided CUSUM scheme, and the performance of the procedure is determined accordingly.

Woodall and Ncube⁴ suggest extending the univariate CUSUM procedure to the multivariate case: to detect a shift in the mean vector of a p -variate normal distribution, operate p one-sided or two-sided CUSUM schemes simultaneously, and evaluate the performance of the collection of schemes. The performance of CUSUM schemes is usually measured by the average run length (ARL), which is the average number of samples required for the scheme to signal that the mean has changed. In the univariate case, the ARL is often plotted as a function of

the standardized deviation of the mean from its target value; the graph is referred to as an ARL curve. The ARL of the Woodall and Ncube⁴ procedure depends on the direction that the mean vector shifts. The dependency of the ARL on the direction of the shift is lessened but not removed by using principal components rather than the original variables.

In contrast, the ARL of the multivariate Shewhart chart (due to Hotelling,⁵ and also known as a T-squared or chi-squared chart), depends on the mean vector μ and covariance matrix V only through the noncentrality parameter

$$d = [(\mu - a)' V^{-1} (\mu - a)]^{1/2} \quad (1)$$

Hence, it is possible to consider the ARL as a function of d and construct an ARL curve. The multivariate Shewhart chart signals that the mean has shifted at the first observation x such that

$$T_n = [(x_n - a)' V^{-1} (x_n - a)]^{1/2} > SCL \quad (2)$$

where SCL is the Shewhart control limit. Hotelling⁵ suggested plotting T-squared, rather than T , to avoid "the labor of extracting square roots." The positive square roots of quadratic forms will be used in this report to express the quantities on a more meaningful scale.

A natural method to develop a multivariate CUSUM procedure that has ARLs dependent only on the noncentrality parameter is to base the CUSUM on the noncentrality parameter itself, that is, test for a change in the noncentrality parameter of a chi-square distribution. Unfortunately, this test produces a mathematically intractable probability ratio, and it is not clear what the CUSUM test statistic should be. Transforming from the chi-square distribution to the chi distribution does not help because the Jacobian of the transformation appears in the numerator and denominator of the probability ratio, thus canceling out and yielding the same complex expression. Crosier⁶ proposes two heuristically derived multivariate CUSUM procedures that have ARLs depending only on the noncentrality parameter and hence are easily compared to multivariate Shewhart charts. Similar but distinct procedures have been developed independently by Pignatiello and Kasunic⁷ and by Pignatiello, Runger, and Koipela.⁸

The CUSUM schemes examined in this report are described in Section 2, which also gives a numerical example of their operation. Sections 3, 4, and 5 present the design procedures and ARLs of multivariate Shewhart charts, a CUSUM of T statistics scheme and a CUSUM vector scheme, respectively. Two applications of multivariate quality control schemes are examined in Section 6, and the results are summarized in Section 7. The methods used to calculate the ARLs of the schemes are given in Appendix A.

2. DESCRIPTION OF THE PROCEDURES

The most direct and obvious method of replacing the multivariate Shewhart chart by a CUSUM procedure is to form a CUSUM of the scalars T_n , $n = 1, 2, 3, \dots$. This will be referred to as a CUSUM of T (COT) scheme; the CUSUM is given by

$$S_n = \max(0, S_{n-1} + T_n - k), \quad (3)$$

where $S_0 > 0$ and $k > 0$. The COT scheme signals when $S_n > h$.

Although multivariate Shewhart charts based on T-squared and on T are equivalent, CUSUM schemes based on T-squared and on T are not. CUSUM of T statistics cumulate distance, whereas CUSUM of squared T statistics would cumulate squared distance. Healy² shows that a CUSUM of squared T statistics is the appropriate sequential theory test for an inflation (multiplication by a scalar constant) of the covariance matrix V.

A vector-valued CUSUM scheme can be "derived" by replacing the scalar quantities of a univariate CUSUM scheme by vectors. The univariate CUSUM scheme to detect an increase in the mean is $S_n = \max[0, S_{n-1} + (X_n - a) - ks]$, where a is the aim point or target value for the mean, s is the standard deviation of the X's, $k > 0$, and $S_0 > 0$. Replacing the scalars by vectors gives $s_n = \max[0, s_{n-1} + (x_n - a) - k]$. The problems are how to find k and how to interpret taking the maximum of a vector and the null vector. In the univariate case, the quantity $s_{n-1} + x_n - a$ is shrunk toward zero by k standard deviations. If this is to hold for the multivariate case, k must satisfy $k' V^{-1} k = k^2$, that is, k must be of length k , where length is defined using the covariance matrix V. If the subtraction of k is to shrink $s_{n-1} + x_n - a$ toward zero (the null vector 0), then k must be in the same direction as $s_{n-1} + x_n - a$. Hence, $k = (k/C_n)(s_{n-1} + x_n - a)$, where C_n is the length of $s_{n-1} + x_n - a$. The maximum with the null vector can be interpreted as setting $s_n = 0$, rather than subtracting k ; whenever the length of k is greater than the length of $s_{n-1} + x_n - a$, that is, whenever $k > C_n$. Rather than calculate the vector k and subtract it from $s_{n-1} + x_n - a$, it is simpler to just contract the vector $s_{n-1} + x_n - a$ by $(1 - k/C_n)$, provided that $k < C_n$. Hence, the multivariate CUSUM scheme may be expressed as follows:

$$\begin{aligned} \text{Let } C_n &= [s_{n-1} + x_n - a]' V^{-1} (s_{n-1} + x_n - a)]^{1/2} \\ \text{then } s_n &= 0 & \text{if } C_n < k \\ s_n &= (s_{n-1} + x_n - a)(1 - k/C_n) & \text{if } C_n > k, \end{aligned} \quad (4)$$

where $s_0 = 0$ and $k > 0$. Let

$$Y_n = (s_n' V^{-1} s_n)^{1/2} \quad (5)$$

The multivariate CUSUM scheme signals when $Y_n > h$.

Table 1 gives a numerical example of these schemes for a bivariate normal distribution with unit variances and correlation 0.5. The process mean is (0,0) for the first five observations and (1,2) for the last five observations. The first three columns of Table 1 give the sample number (n) and the observations of the random variables X_1 and X_2 . The columns headed S_1 and S_2 are the elements of the multivariate CUSUM vector (equation 4), and the last column is the multivariate CUSUM test statistic Y_n from equation 5. The k values for the CUSUM of T and multivariate CUSUM schemes are 1.41 and 0.5, respectively. These k values are optimal for detecting a shift of one generalized standard deviation (in the sense that the ARL at $d = 1$ is a minimum, given that the on-target ARL is held constant). The signal criteria (values of h and SCL) yield an on-target ARL of 200 for each scheme. When the multivariate CUSUM scheme signals, the CUSUM vector elements are both positive and approximately in the 1:2 ratio of the individual component means. This indicates the direction that the mean has shifted; it is not necessarily intended as a formal mechanism for estimating the process mean.

Table 1. Numerical Example of Bivariate Quality Control Schemes.

n	Observations			CUSUM OF T		CUSUM Vector		
	X_1	X_2	T^2	T	S	S_1	S_2	Y
1	-1.19	0.59	3.29	1.81	0.40	-0.86	0.43	1.31
2	0.12	0.90	0.96	0.98	0.00	-0.56	1.01	1.60
3	-1.69	0.40	4.92	2.22	0.81	-1.95	1.22	3.20
4	0.30	0.46	0.22	0.47	0.00	-1.40	1.43	2.83
5	0.89	-0.75	2.70	1.64	0.23	-0.30	0.39	0.69
6	0.82	0.98	1.11	1.05	0.00	0.33	0.88	0.89
7	-0.30	2.28	7.96	2.82	1.41	0.03	2.72	3.13
8	0.63	1.75	3.14	1.77	1.77	0.59	4.01	4.33
9	1.56	1.58	3.29	1.81	2.18	1.96	5.09	5.14
10	1.46	3.05	9.31	3.05	3.82	3.21	7.65	7.68*
Criteria for signal:				SCL	h	h		
				3.36	4.04	5.50		

*off-aim signal; the other two schemes have not yet signaled.

3. MULTIVARIATE SHEWHART CHARTS

Figures 1 and 2 give ARLs of Shewhart charts as a function of d for $p = 2, 5, 10$, and 20 variables. The SCLs are the 99.5 and 99.8 percentiles of the (central) chi distribution p degrees of freedom. This choice of SCLs gives on-target ARLs of 200 and 500, respectively. The off-target ($d > 0$) ARLs were found using the numerical approximations described in Appendix A. One characteristic of multivariate Shewhart charts is that the SCL must be increased as the number of variables increases to obtain the same on-target ARL. (Interpreting the multivariate Shewhart charts as multivariate CUSUM schemes with $h = 0$ and $k = \text{SCL}$ indicates that multivariate Shewhart charts are "designed" to detect larger shifts in the noncentrality parameter as p , the number of variables, increases.)

A practical problem with multivariate Shewhart charts is their lack of robustness. They are sensitive to multivariate outliers. Multivariate outliers are observations $\mathbf{x}$ that have large T statistics; however, no element of $\mathbf{x}$ would be considered an outlier by a univariate outlier test. Many of the multivariate outliers in industrial plant data are due to clerical or keypunching errors (the correct numbers are often found on the original data sheets). Further, when it does shift, the process mean often does so along the major axis of the multivariate probability ellipsoid. The presence of multivariate outliers suggests that robustness is a desirable feature for multivariate quality control schemes. Because typical process failures shift the mean in a particular direction, it may be helpful to have outlier criteria that are sensitive to the direction of the observation as well as its distance from the target value.

4. CUMULATIVE SUM OF T-STATISTICS

The COT schemes offer several advantages over multivariate Shewhart charts. First, COT schemes may be designed to detect a specific shift in the process mean (i.e., in the noncentrality parameter). Second, recent enhancements for CUSUM schemes may be applied to COT schemes. A robustness procedure, such as the two-in-a-row rule⁹ may be applied to the sequence of T statistics. The two-in-a-row rule states that outliers should be ignored (not used in the CUSUM calculations), but the occurrence of two outliers in succession is taken as an off-aim signal. The Fast Initial Response (FIR) feature for CUSUM schemes¹⁰ is easily extended to COT schemes. Quick detection of an initial off-aim condition is obtained by starting the scheme with $S_0 = h/2$ rather than zero. If the process is off-aim, the CUSUM will signal quickly due to the head start. If the process is on-target at start up, the head start will likely be removed by the subtraction of k at each observation. Finally, a combined multivariate Shewhart-COT scheme, analogous to the combined Shewhart-CUSUM schemes of Lucas¹¹ is readily obtained using the T statistics. A combined

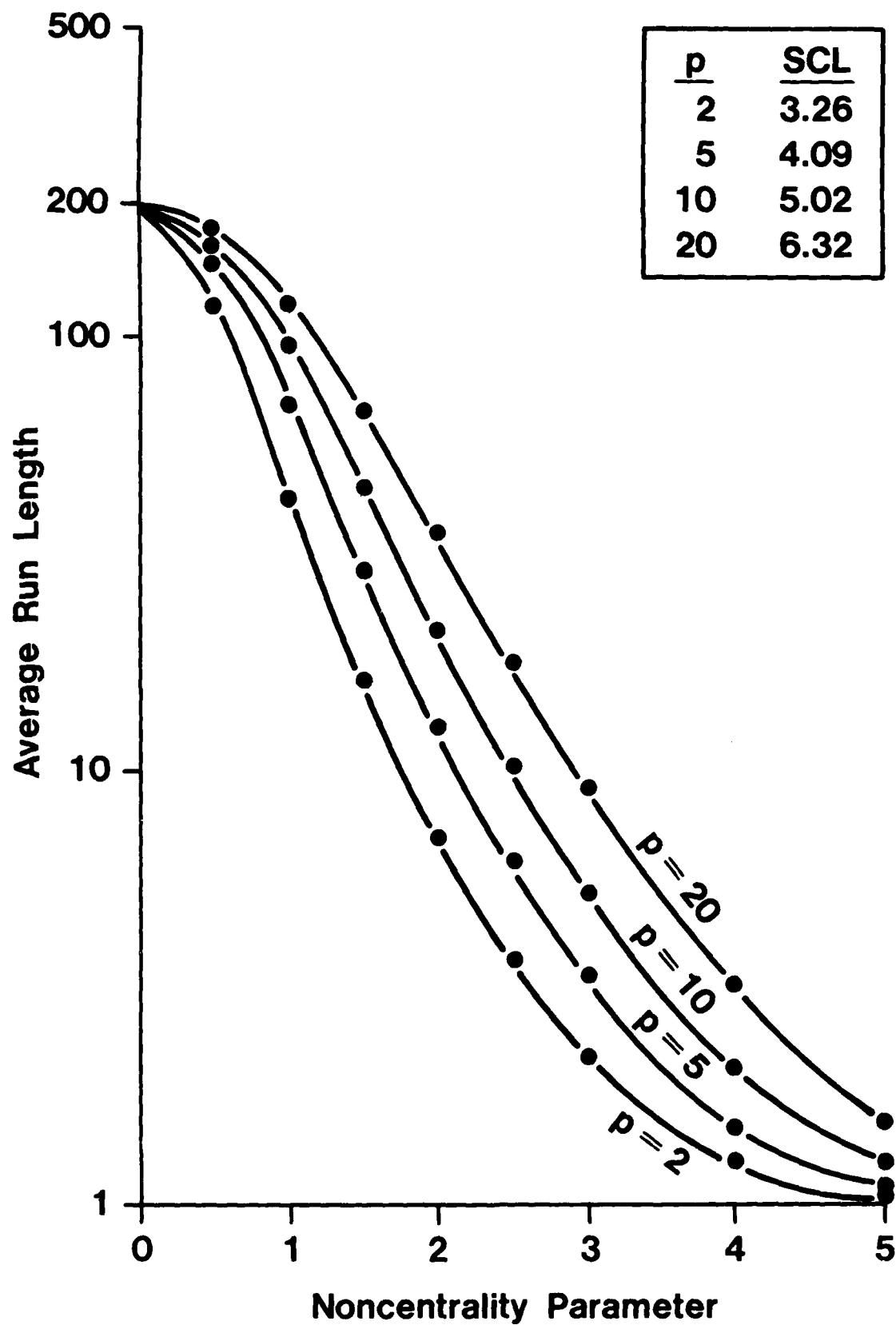


Figure 1. ARL Curves for Multivariate Shewhart Charts with On-Target ARLs of 200.

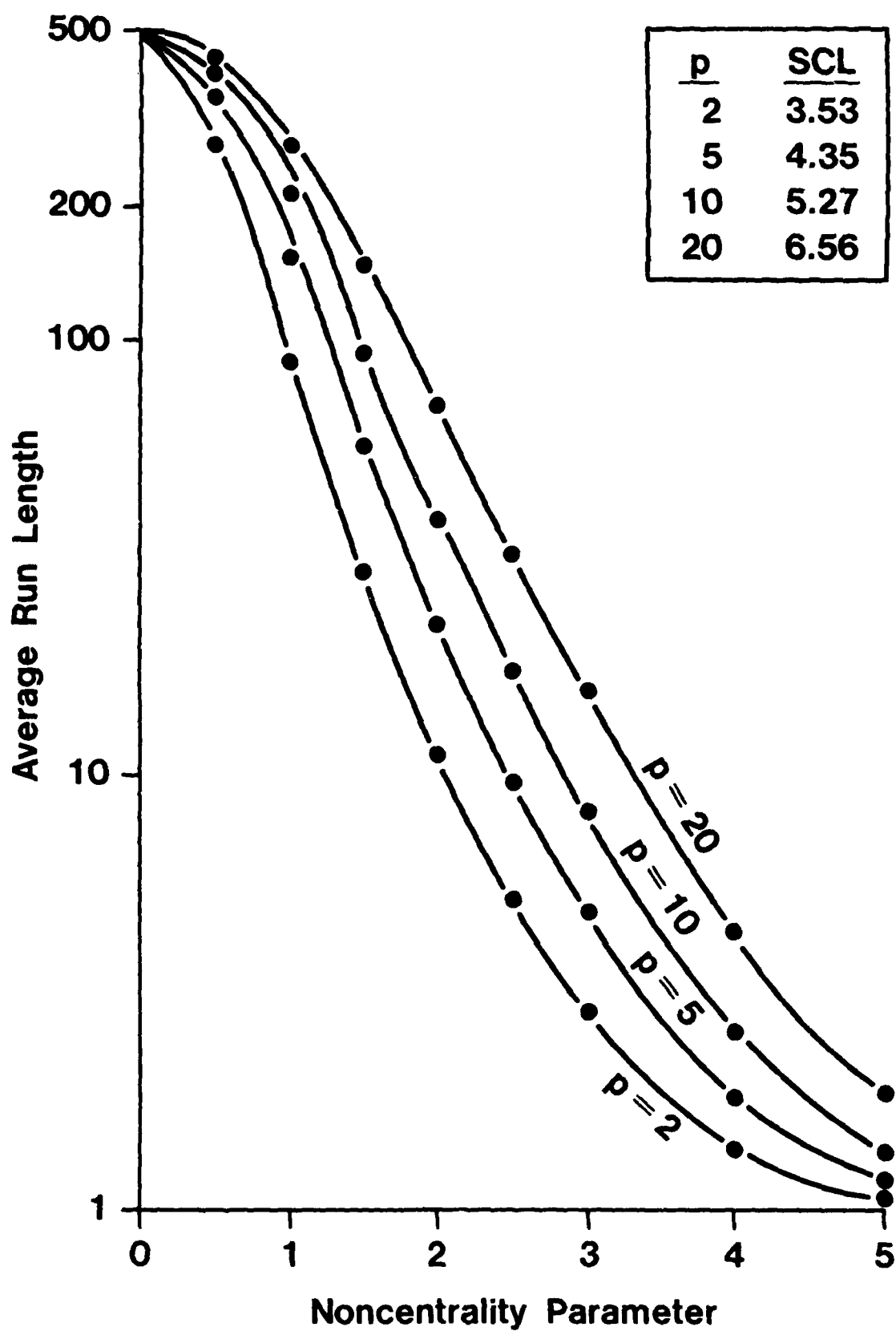


Figure 2. ARL Curves for Multivariate Shewhart Charts with On-Target ARLs of 500.

multivariate Shewhart-COT quality control scheme is implemented by operating a COT scheme and a multivariate Shewhart chart simultaneously; the combined scheme signals if either component scheme signals. Combined Shewhart-COT schemes lack robustness, but they may be used to monitor laboratory measurement error¹¹ where any extreme value must be examined.

Figures 3 and 4 present ARLs of COT schemes for $p = 2, 5, 10,$ and 20 variables. These schemes are designed to detect any shift in the mean vector yielding $d = 1$. The h values were chosen to provide an on-target ARL of 200 or 500. The ARL curves in Figures 3 and 4 indicate that COT schemes give improved detection of small shifts (e.g., $d = 1$) over multivariate Shewhart charts. ARL curves for the COT schemes of Figures 3 and 4 with the FIR feature implemented are given in Figures 5 and 6. The head start decreases the on-target ARL more for the larger rather than the smaller values of p . For COT schemes with an on-target ARL of 200, the FIR feature decreased the on-target ARL by 9% for the $p = 2$ case and by 15% for the $p = 20$ case. As the off-target ($d = 1$) ARLs decreased by 28% and 27%, respectively, the FIR feature is less advantageous at $p = 20$ than it is at $p = 2$.

A k value may be defined as optimal to detect a shift to $d = 1$ if the ARL at $d = 1$ is a minimum given that the on-target ARL is held constant. (For any value of k , the desired on-target ARL can be obtained by varying h .) A search for the optimal k produced a sequence that closely resembled the square root of the number of variables. Hence, the k 's used in Figures 3-6 were found, to about two and a half significant figures, by a simple search; the square root of the p sequence determined the last digit.

5. MULTIVARIATE CUSUM SCHEMES

The ARLs of multivariate Shewhart charts and COT schemes depend on the mean vector and covariance matrix only through the noncentrality parameter because these procedures are based on Hotelling's T statistic.⁵ It is not as clear that multivariate CUSUM schemes have this property, even though both parameters (h and k) are used to define ellipsoidal regions. Initially, the dependence of the ARL on only the noncentrality parameter was checked by using simulation results for the bivariate case. Dr. John Healy has provided a detailed proof of the dependence of the ARL on only the noncentrality parameter. The proof and some mathematical properties of the multivariate CUSUM procedure are discussed in Appendix B.

Multivariate CUSUM schemes, like COT schemes, offer the advantages of a CUSUM scheme over a Shewhart chart: ability to design the scheme to detect a specific shift in the mean vector and ability to implement recent enhancements for CUSUM schemes (e.g., the FIR feature). In addition, the directional nature of multivariate CUSUM offers some advantages over the directionless

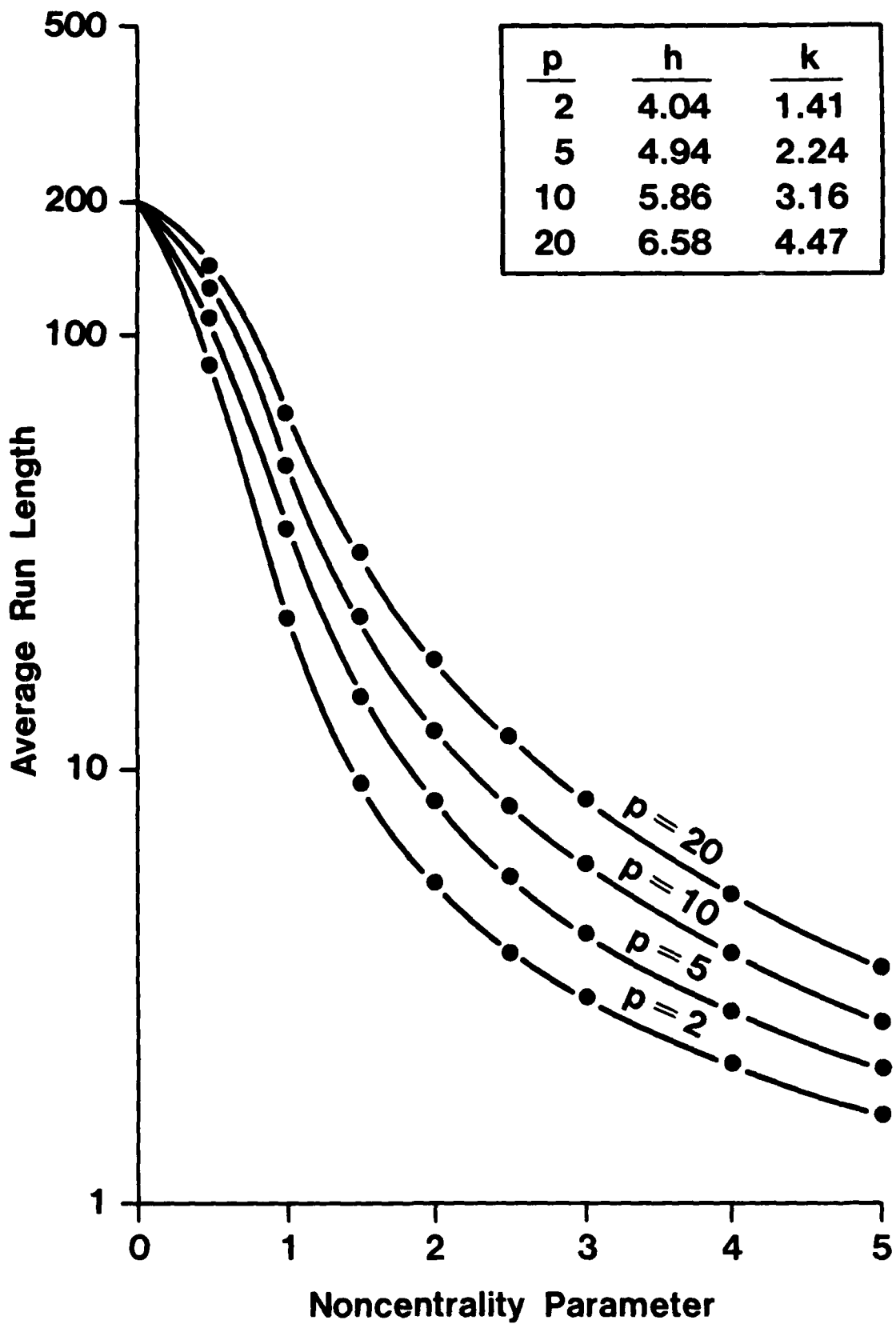


Figure 3. ARL Curves for CUSUM of T Schemes with On-Target ARLs of 200.

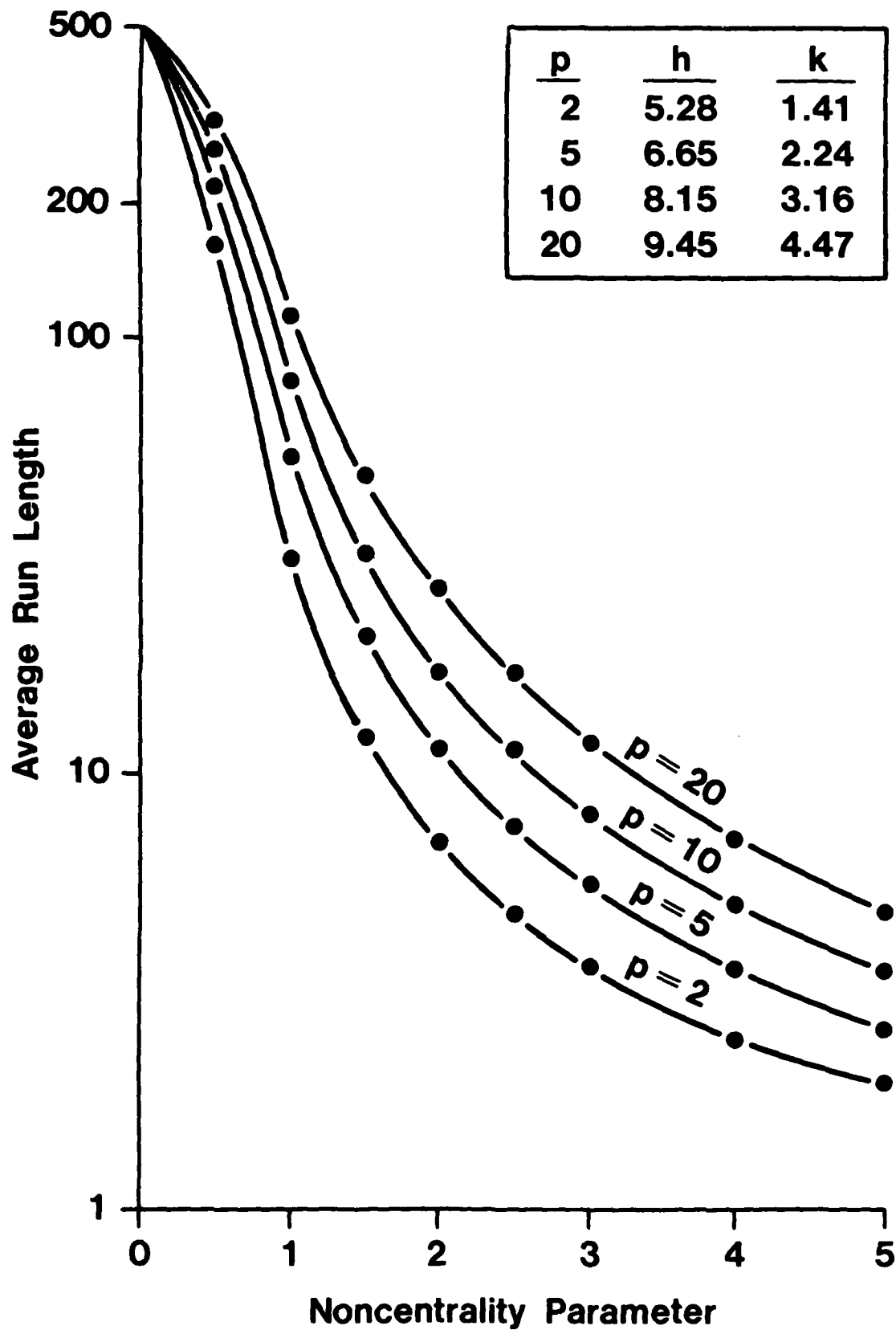


Figure 4. ARL Curves for CUSUM of T Schemes with On-Target ARLs of 500.

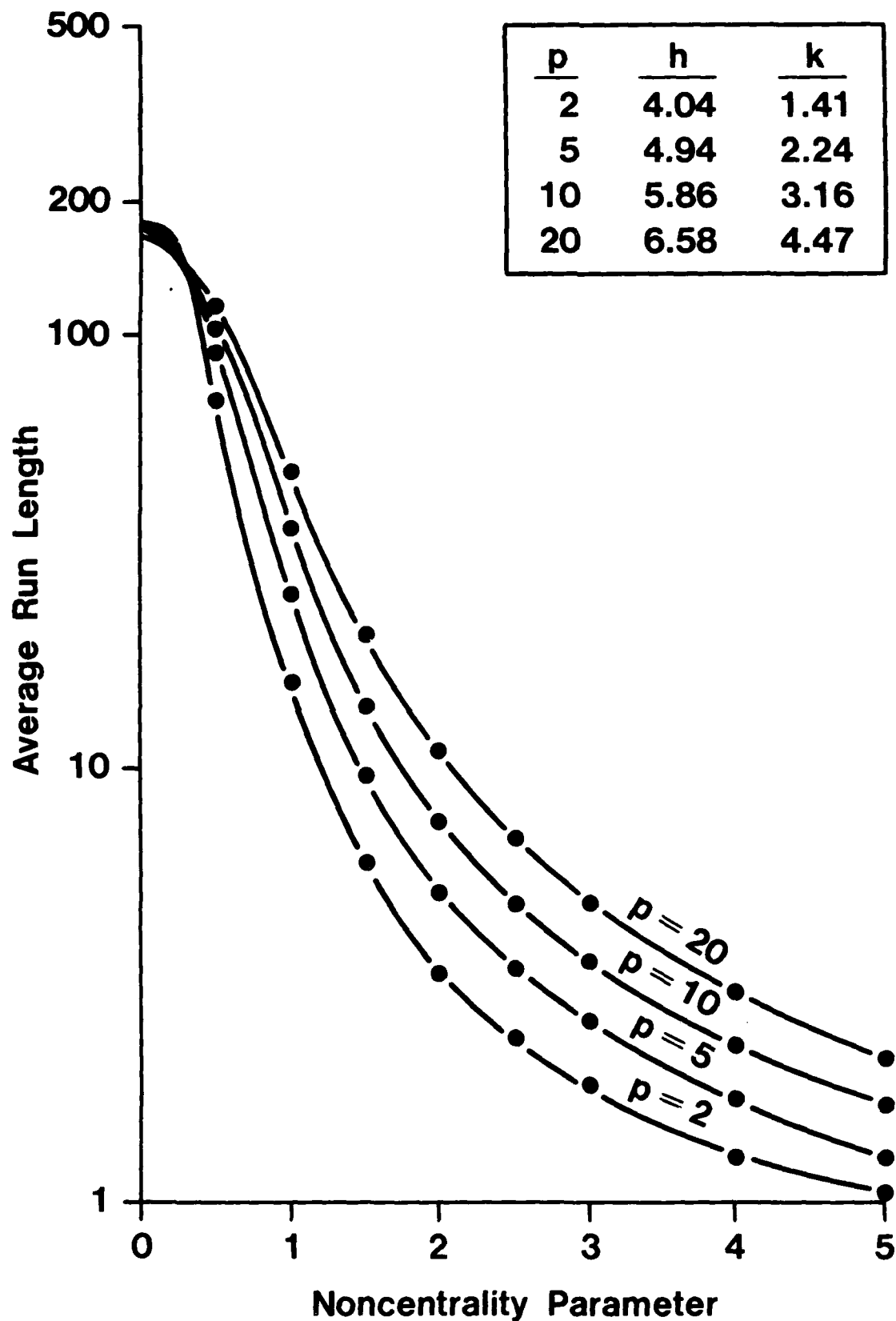


Figure 5. ARL Curves for the COT Schemes of Figure 3 but with the Fast Initial Response Feature Implemented.

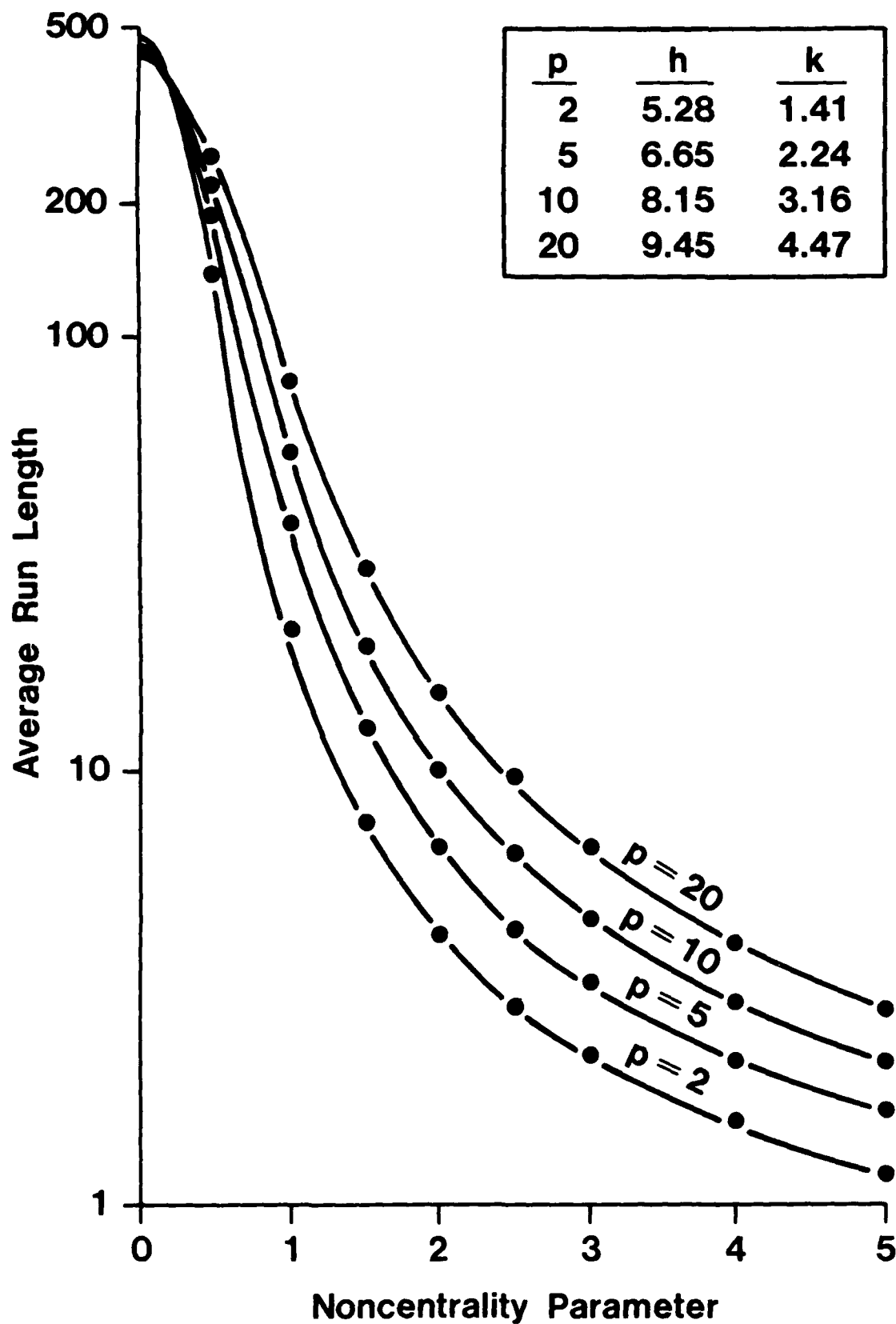


Figure 6. ARL Curves for the COT Schemes of Figure 4 but with the Fast Initial Response Feature Implemented.

COT schemes. Because multivariate CUSUM schemes allow observations opposite directions from the target value to cancel each other, one suspects that multivariate CUSUM schemes will have better ARL properties than COT schemes, that is, the cancellation will occur more often when the process mean is on target, thus raising the on-target ARL relative to the off-target ARL. Figures 7 and 8 give ARL curves for multivariate CUSUM schemes that can be compared to the ARL curves for multivariate Shewhart charts (Figures 1 and 2) and COT schemes (Figures 3 and 4). The ARL curves in Figures 7 and 8 show that multivariate CUSUM schemes give quicker detection of small shifts than multivariate Shewhart charts and COT schemes. Another advantage to the vector-valued CUSUM scheme is it provides at least some indication of where the mean has shifted when a signal is given.

The design procedure of multivariate CUSUM schemes is straightforward. To detect any shift in the mean vector μ , yielding noncentrality parameter d , choose $k = d/2$. Table 2 compares the ARLs of bivariate schemes with $k = 0.5$, $k = 1$, and $k = 1.5$. The choice of $k = d/2$ appears to minimize the ARL at d for a given on-target ARL. The decision interval h is chosen to provide an acceptable on-target ARL. Details of the method used to select the h values in Figures 7 and 8 are given in Appendix A. [A Markov chain approximation may be used to determine the on-target ARLs (Appendix C).]

Table 2. ARL Curves for Bivariate Schemes with $k = 0.5$, 1 , and 1.5 .

d	$h = 5.50$ $k = 0.5$	$h = 2.99$ $k = 1$	$h = 1.87$ $k = 1.5$
0.0	200.0	200.0	200.0
0.5	28.8	48.0	78.7
1.0	9.35	11.0	18.4
1.5	5.94	5.08	7.14
2.0	4.20	3.48	3.72
2.5	3.26	2.51	2.36
3.0	2.78	2.08	1.69

Development of a combined multivariate Shewhart-CUSUM quality control scheme is straightforward: a multivariate CUSUM scheme and a multivariate Shewhart chart are operated simultaneously; a signal by either scheme indicates that the process mean has shifted. Robustness for the multivariate CUSUM scheme may be obtained by applying the two-in-a-row rule to the T statistics for the observations. Special outlier criteria, rather than T statistics, could be used to tailor the robustness procedure to specific applications.

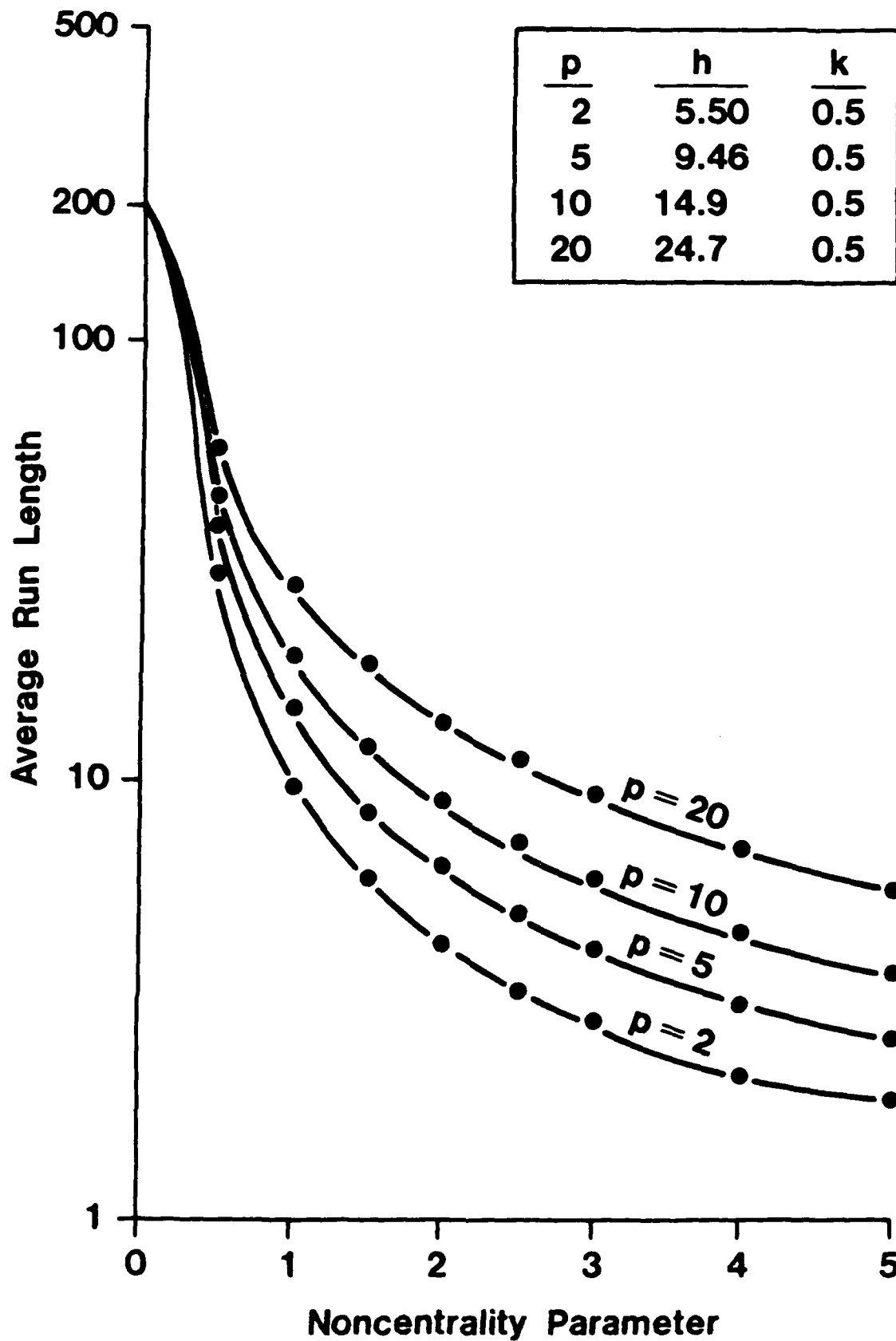


Figure 7. ARL Curves for Multivariate CUSUM Schemes with On-Target ARLs of 200.

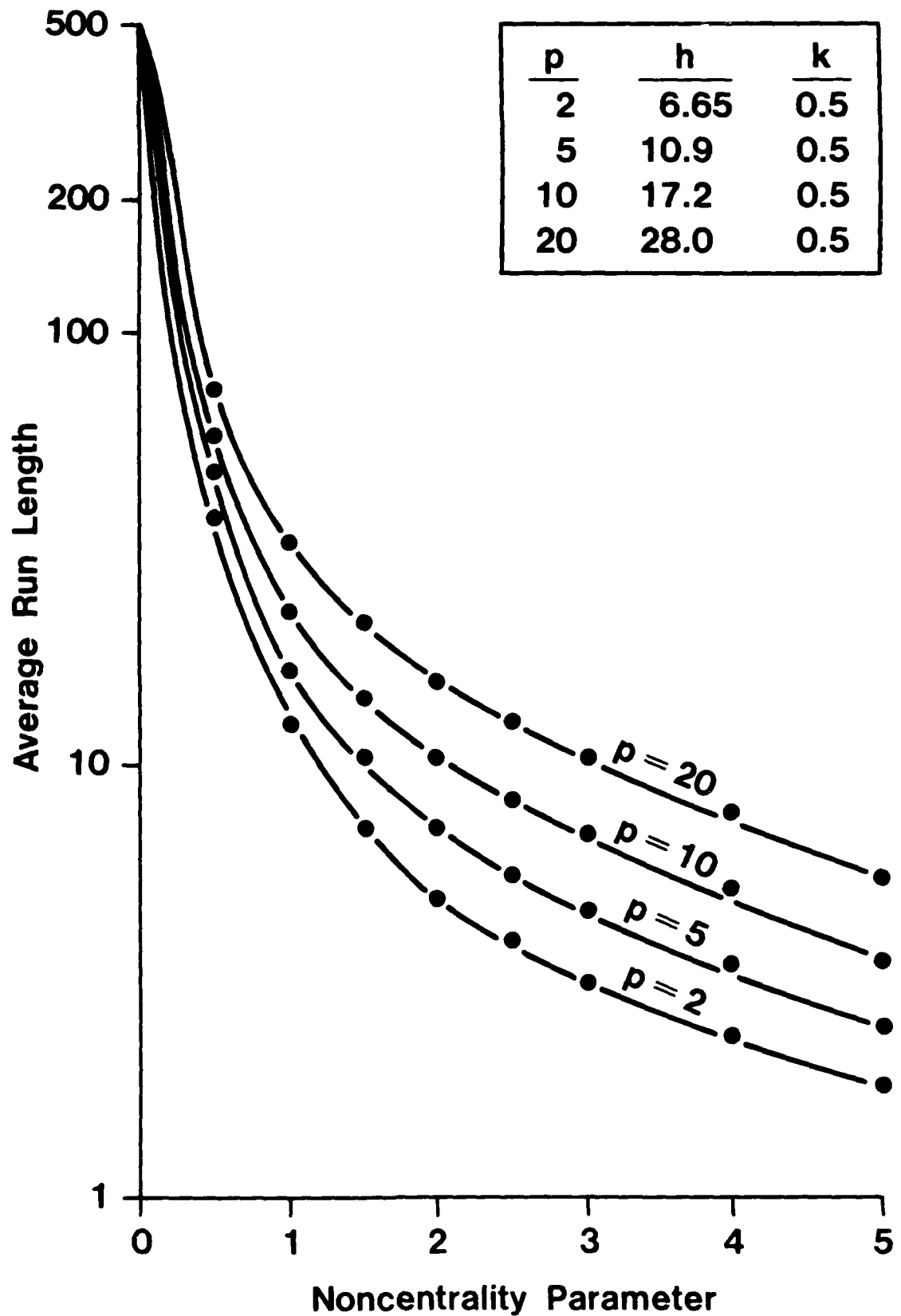


Figure 8. ARL Curves for Multivariate CUSUM Schemes with On-Target ARLs of 500.

The FIR feature for multivariate CUSUM schemes is implemented by changing the value of h at the start of the scheme.

Let $h_0 = h/2$

and $h_n = \min[h, h_{n-1} + \max(0, k^* - T_n)]$ for $n = 1, 2, 3, \dots$ (6)

where T_n is Hotelling's T statistic⁵ for the n th observation, and k^* is the k value for a COT scheme designed to detect the same deviation as the multivariate CUSUM scheme. Figures 9 and 10 give ARL curves of the multivariate CUSUM schemes in Figures 7 and 8 but with the FIR feature implemented. The FIR feature decreases the on-target ARLs more for larger p than it does for smaller p , but the effect is not as deleterious as it is for COT schemes because the off-target ($d = 1$) ARLs are also decreased more for larger p than they are for smaller p . For multivariate CUSUM schemes with an on-target ARL of 200, the FIR feature decreases the on-target ARL by 9% for $p = 2$ and by 22% for $p = 20$, but the off-target ($d = 1$) ARLs are decreased by 29% and 49%, respectively. The results for multivariate CUSUM schemes with an on-target ARL of 500 are very similar.

Multivariate CUSUM schemes compare favorably to the Woodall and Ncube⁴ procedure. Table 3 gives the ARLs for the Woodall and Ncube procedure applied to principal components (that are scaled to have variance 1) and the ARLs (with standard errors) of a comparable multivariate CUSUM scheme. (Notice that, for the same value of d , the ARLs of the Woodall and Ncube procedure⁴ are usually larger when the direction of the shift is along one of the original axes than when the direction of the shift is along one of the principal component axes.) In Table 3, the off-target ARLs of the multivariate CUSUM scheme are less than or equal to the ARLs of the Woodall and Ncube procedure.⁴ The difference between the ARLs of the two procedures is usually several times the standard error of the estimated ARL of the multivariate CUSUM scheme. However, there is another source of error that must be considered. The value of h required to give the multivariate CUSUM scheme an on-target ARL of 125 is an estimate obtained by the method given in Appendix A. This method requires regressing $\log(\text{ARL})$ on h , where the ARLs for different h 's are obtained by simulation. The estimated h for an on-target ARL of 125 is 4.95, the value used for Table 3. A 95% fiducial interval¹² for the value of h yielding an on-target ARL of 125 is (4.84, 5.09). Using an h value of 5.09, the ARLs of the multivariate CUSUM scheme, for $d = 0.5, 1, 2$, and 4 are 27.1, 9.3, 3.9, and 2.0 with standard errors of 0.95, 0.24, 0.06, and 0.02, respectively. Except for $d = 4$, where the ARLs of the two procedures are equal, these ARLs are still significantly smaller than the ARLs of the Woodall and Ncube procedure. (The Markov chain approach described in Appendix C gives an on-target ARL of 126 for the bivariate CUSUM scheme $h = 4.95, k = 0.5$.)

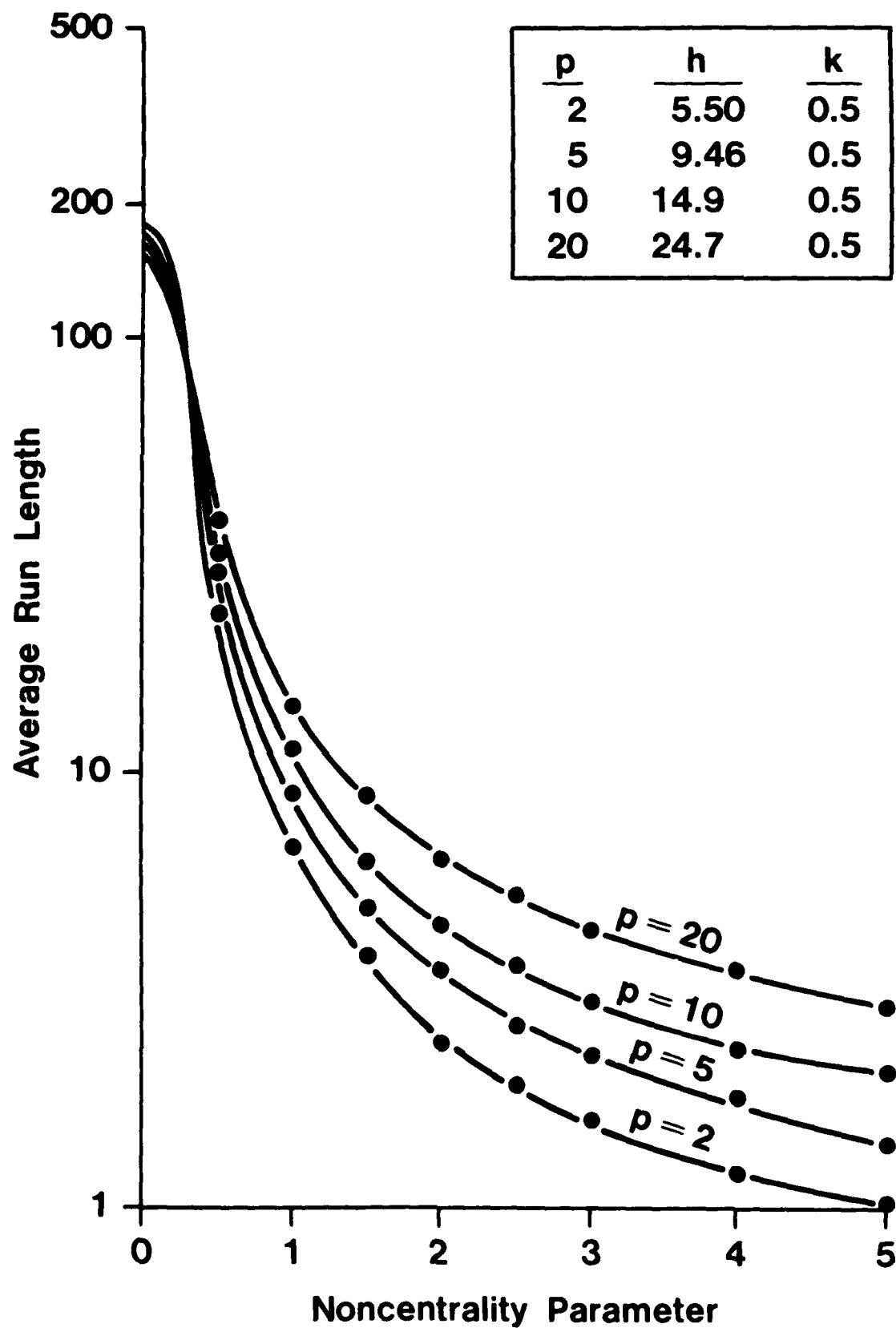


Figure 9. ARL Curves for the Multivariate CUSUM Schemes of Figure 7 but with the Fast Initial Response Feature Implemented.

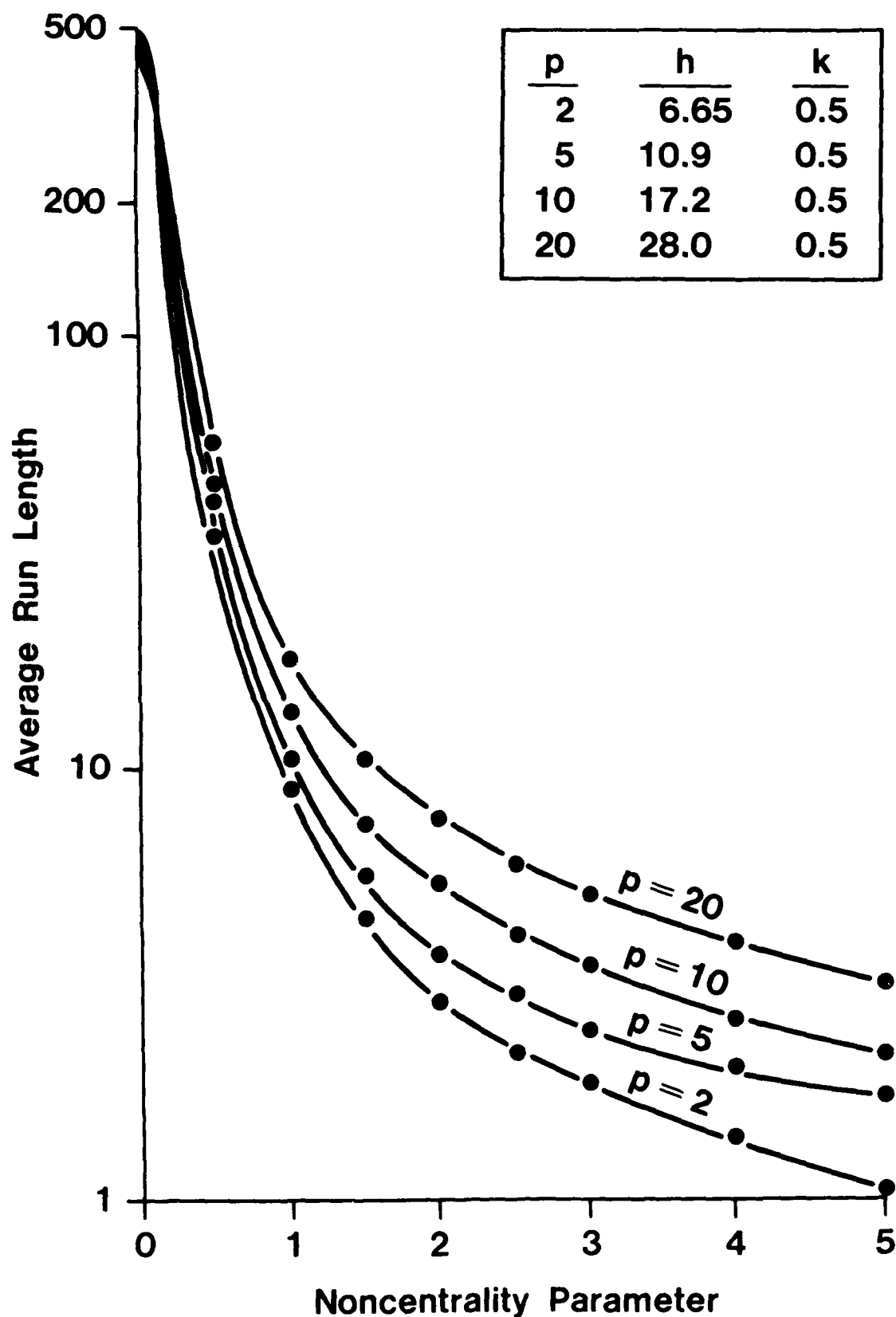


Figure 10. ARL Curves for the Multivariate CUSUM Schemes of Figure 8 but with the Fast Initial Response Feature Implemented.

Table 3. Comparison to the Woodall and Ncube Procedure on Principal Components: Bivariate Procedures with On-Target ARLs of 125.

r	u_1	u_2	d	Woodall and Ncube ARL	Section 5 ARL	SE
0.0	0.5	0.0	0.5	33.6	26.8	1.02
-0.5	0.5	0.0	0.58	28.7	20.7	0.76
-0.5	0.5	-0.5	0.58	26.7	20.6	0.79
0.5	0.5	0.0	0.58	28.7	18.9	0.62
0.5	0.5	0.5	0.58	26.7	19.3	0.68
0.0	1.0	0.0	1.0	10.9	8.9	0.22
-0.5	0.5	0.5	1.0	10.9	9.2	0.21
0.5	0.5	-0.5	1.0	10.9	9.1	0.23
-0.5	1.0	0.0	1.15	9.8	7.1	0.15
-0.5	1.0	-1.0	1.15	8.8	7.2	0.14
0.5	1.0	0.0	1.15	9.8	7.3	0.17
0.5	1.0	1.0	1.15	8.8	7.6	0.17
0.0	2.0	0.0	2.0	6.0	3.8	0.06
-0.5	1.0	1.0	2.0	4.1	3.8	0.06
0.5	1.0	-1.0	2.0	4.1	3.7	0.06
-0.5	2.0	0.0	2.31	3.9	3.2	0.05
-0.5	2.0	-2.0	2.31	3.5	3.3	0.05
0.5	2.0	0.0	2.31	3.9	3.3	0.05
0.5	2.0	2.0	2.31	3.5	3.2	0.05
-0.5	2.0	2.0	4.0	2.0	2.0	0.02
0.5	2.0	-2.0	4.0	2.0	2.0	0.02

NOTE: The Woodall and Ncube procedure has $h = 5$ and $k = 0.5$; the Section 5 CUSUM procedure has $h = 4.95$ and $k = 0.5$.

6. APPLICATIONS

In making synthetic yarn, the fibers are stretched as they are made.¹³ The stretching of the fiber orients the molecules and makes the fiber stronger and more brittle. A measure of this stretching is the draw ratio, which is defined as the stretched length divided by the original length. The finished fiber is tested for acceptable strength by a tensile machine that pulls a fiber until it breaks. The force required to break the fiber (break strength) and how far the fiber stretched while being pulled (elongation) are reported by the tensile machine. Break strength and elongation are positively correlated because the fibers are all made at the same draw ratio. Break strength and elongation show a negative relationship only when the draw ratio is varied. A multivariate quality control scheme for this example should be based on the positive correlation between break strength and elongation.

Lucas¹³ mentions that a multivariate Shewhart chart was used to obtain tighter control of this process than is possible using simultaneous univariate CUSUM schemes. Either a COT scheme or a multivariate CUSUM scheme could be used for even tighter control of the process. Univariate CUSUMs of the principal components would also be an excellent procedure for this application. First, a rectangle based on principal components fits around the tilted ellipsoidal region much more closely than a rectangle based on the original components. Second, the principal components are interpretable: the minor component corresponds to problems with the draw ratio, whereas the major component corresponds to the usual variation (perhaps due to temperature fluctuations) in the process. A multivariate Shewhart chart or a COT scheme will not indicate what the problem is when the scheme signals. However, a multivariate CUSUM scheme will provide an indication of the direction that the mean has shifted and identify the problem.

Principal components allow adoption of an outlier rule specific to this application. In testing synthetic fibers by a tensile machine, unusual values of the minor principal component are much more likely to indicate data errors than an actual process shift, whereas unusual values of the major principal component are much more likely to indicate a process shift than a data error. Hence, the minor principal component, rather than a T statistic, could be used to judge the acceptability of an observation. This outlier criterion could be used with any multivariate quality control procedure, not just CUSUMs of the principal components.

Philpot and Ranney* discuss the use of multivariate Shewhart charts for a rolling operation. A roller is used to control the thickness of a paper, plastic, or metal sheet product. If three measurements of thickness are made across the sheet (left side, middle, and right side), these measurements will be highly (positively) correlated. Two types of problems encountered in rolling operations are tilt of the roller, which makes the measurement on one side too high and the measurement on the other side too low, and buildup of material on the roller, which makes one measurement too low. Philpot and Ranney* demonstrate the superiority of the multivariate Shewhart chart over simultaneous univariate Shewhart charts to detect these problems in a rolling operation. These authors* also examine the individual components of the observation vector x to determine whether the problem is tilt or buildup on the roller. COT schemes and multivariate CUSUM schemes would give improved detection of these types of problems over multivariate Shewhart charts. The CUSUM vector of a multivariate CUSUM scheme could be examined to determine the nature of the process problem.

The covariance matrix of thickness measurement across a sheet product made by a rolling operation will have all diagonal elements equal and all off-diagonal elements equal. This assumes that the covariance matrix is estimated from data during a period of stable operation, that is, a period during which the process mean is constant. If buildup on the roller occurs during the period of data collection, the covariances in one particular row and column will be too low. An unstable tilt of the roller during data collection would make the covariances decrease with increasing distance between the measurements. Of course, even in a univariate case, one does not estimate the variance from data taken during a period of process instability. Sampling variability will prevent the estimated variances and covariances from being exactly equal; a constrained estimation procedure may be useful.

Rolling operations provide an example in which neither CUSUMs of the original variables nor CUSUMs of principal components are a satisfactory procedure. Only the first principal component of the equal-variance, equal-covariance matrix is uniquely defined,¹⁴ it is proportional to the sum of the measurements. A CUSUM of the first principal component would detect changes in the overall thickness of the sheet. A linear trend could be used for the second principal component and this would correspond to problems with the tilt of the roller. But the buildup problem cannot be reduced to $p-2$ meaningful principal components. The $p-2$ additional principal components do not indicate where the buildup has occurred, and there may be more than three measurements across the sheet, thus producing many such uninformative principal components.

*Philpot, J.W., and Ranney, G., Multivariate Control Charts in Action: Some Uses and Examples, unpublished data, 1985.

7. SUMMARY AND CONCLUSIONS

The first multivariate CUSUM quality control procedure reduces each observation to a scalar (Hotelling's T statistic)⁵ and forms a CUSUM of the T statistics. This procedure is referred to as COT. The second procedure, referred to as multivariate CUSUM, forms a CUSUM vector directly from the observations. Both procedures allow use of recent enhancements for CUSUM schemes (e.g., robustness and the FIR feature). Both these cumulative sum procedures reduce to multivariate Shewhart charts when the CUSUM scheme parameter h is zero. (The analogous relationship holds for univariate CUSUM schemes and Shewhart charts.) The ARL of the two multivariate CUSUM procedures depend on the mean vector and correlation structure of the data only through the noncentrality parameter d . This property also holds for multivariate Shewhart charts and allows the three multivariate quality control schemes to be compared easily. Multivariate CUSUM schemes and COT schemes give faster detection of small shifts in the mean vector than multivariate Shewhart charts with multivariate CUSUM schemes giving faster detection than COT schemes. Multivariate CUSUM schemes may also be referred to COT schemes because the CUSUM vector indicates the direction that the mean has shifted.

The nature of multivariate data is briefly discussed from an applied point of view. Robustness is practically required in a multivariate quality control scheme due to the presence of multivariate outliers. In some applications, the correlation structure of multivariate data may allow development of a unique outlier rule for the specific application.

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APPENDIX A

NUMERICAL METHODS

The calculation of ARLs for multivariate Shewhart charts is relatively straightforward: $ARL = 1/q$, where $q = \text{Prob}(T > SCL)$. In addition, the probability that T exceeds SCL is the probability that a chi-squared variable (central or noncentral) with p degrees of freedom exceeds the Shewhart control limit squared. These probabilities were found using the International Mathematical and Statistical Libraries, Incorporated (IMSL) routine MDCHN.*

The calculation of ARLs for COT schemes was based on the Markov chain approach of Brook and Evans.** Their development will not be repeated here except as necessary to document the procedures used for this work. The transition probabilities were found using the techniques given by Brook and Evans** but with the chi distribution (central or noncentral) replacing the Gaussian distribution. The cumulative distribution function of the chi distribution at a point x was obtained by squaring x and referring to the chi-square distribution calculated by the IMSL routine MDCHN. Thirty-two transient states were used in the Markov chain approximation; the ARL starting from the first state was used as the ARL when the continuous CUSUM scheme started at zero.** For the FIR feature, the ARL was calculated by quadratic interpolation (least squares fit) using the four states closest to the head start value $h/2$.

The ARLs for the multivariate CUSUM schemes were obtained by simulation. The only difficulty was finding the value of h (call it h') that gives the required on-target ARL. To find h' for an on-target of 200, an ARL was calculated from a simulation of 50 run lengths; if the ARL was less than 200, an increment of 0.25 was added to h but was subtracted from h if the ARL was greater than 200. Even with a close initial guess, eight iterations of this technique (400 run lengths) did not yield a good estimate of h' . Hence, the procedure was repeated using an increment of 0.1 and 20 iterations. All 28 ARLs (each based on 50 run lengths) were used in a linear regression of $\log(ARL)$ on h . The regression equation was used to estimate h' . The values of h for all other multivariate CUSUM schemes (those with on-target ARLs of 500 or 125, or with $k = 1$ or 1.5) were obtained by the same procedure but used only 20 iterations and an increment of 0.1. Therefore, on-target ARLs were assumed to be the required values. The ARLs for $d > 0$ were found from simulations of 400 run lengths.

*International Mathematical and Statistical Libraries, Inc., IMSL Library, 9th ed., Houston, TX, 1982.

**Brook, D., and Evans, D.A., "An Approach to the Probability Distribution of CUSUM Run Lengths," Biometrika Vol. 59, pp 539-549 (1972).

The ARLs for multivariate CUSUM schemes with the FIR feature were also obtained by simulation of 400 run lengths. However, the ARLs at $d = 0$ were quite variable and were smoothed by regressing $\log(\text{ARL})$ on p . The predicted ARLs from this regression were used in Figures 9 and 10 for the ARLs at $d = 0$.

APPENDIX B
MATHEMATICAL PROOF

This proof that the distribution of the multivariate CUSUM test statistic $Y(n)$ depends only on the value of the noncentrality parameter is based on the proof provided by Dr. John Healy.

Without loss of generality, assume that $a = 0$ and let $u = E(x)$. Then the multivariate CUSUM becomes

$$C_n = [(s_{n-1} + x_n)' V^{-1} (s_{n-1} + x_n)]^{1/2} \quad (B-1)$$

$$s_n = 0 \quad \text{if} \quad C_n \leq k$$

$$s_n = (s_{n-1} + x_n)(1 - k/C_n) \quad \text{if} \quad C_n > k. \quad (B-2)$$

Let $u' V^{-1} u$ denote the squared noncentrality parameter. If $u'_1 V^{-1} u_1 = u'_2 V^{-1} u_2$, then the distribution of Y_n is the same. First, some lemmas.

Lemma 1:

If M is a $p \times p$ full rank matrix and $x^* = Mx$, then the statistics $C(n)$ and $Y(n)$ have the same values when calculated from x^* as when calculated from x . In addition, s^* , the multivariate CUSUM vector for x^* , satisfies $s^* = Ms$.

Proof

The proof is by induction. Note that $E(x^*) = Mu$ and $\text{Var}(x^*) = MVM'$.

For $n = 1$,

$$\begin{aligned} C^*_1 &= [x^{*1}' (M'^{-1} V^{-1} M^{-1}) x^{*1}]^{1/2} = [x^1_1 M' (M'^{-1} V^{-1} M^{-1}) M x_1]^{1/2} \\ &= (x^1_1 V^{-1} x_1)^{1/2} = C_1 \end{aligned} \quad (B-3)$$

and

$$s^*_1 = x^*_1 (1 - k/C^*_1) = x^*_1 (1 - k/C_1) = Mx_1 (1 - k/C_1) = Ms_1. \quad (B-4)$$

Now assume for $n-1$ and prove for n :

$$\begin{aligned}
C_n^* &= [(s_{n-1}^* + x_n^*)'(M'^{-1}V^{-1}M^{-1})(s_{n-1}^* + x_n^*)]^{1/2} & (B-5) \\
&= [(Ms_{n-1} + Mx_n)'(M'^{-1}V^{-1}M^{-1})(Ms_{n-1} + Mx_n)]^{1/2} \\
&= [(s_{n-1} + x_n)'M'(M'^{-1}V^{-1}M^{-1})M(s_{n-1} + x_n)]^{1/2} \\
&= [(s_{n-1} + x_n)'V^{-1}(s_{n-1} + x_n)]^{1/2} \\
&= C_n
\end{aligned}$$

and

$$\begin{aligned}
s_n^* &= (s_{n-1}^* + x_n^*)(1 - k/C_n^*) & (B-6) \\
&= (s_{n-1}^* + x_n^*)(1 - k/C_n) \\
&= (Ms_{n-1} + Mx_n)(1 - k/C_n) \\
&= M(s_{n-1} + x_n)(1 - k/C_n) \\
&= Ms_n.
\end{aligned}$$

Therefore, $Y_n^* = [s_n^*(M'^{-1}V^{-1}M^{-1})s_n^*]^{1/2} = [s_n'M'(M'^{-1}V^{-1}M^{-1})Ms_n]^{1/2} = Y_n$. That is, the test statistic $Y(n)$ is identical when x^* is used instead of x .

Apply lemma 1 with $M = P$ where P is an orthogonal matrix ($P'P = PP' = I$) that diagonalizes V . The principal components are $w = Px$ and $PVP' = D$, a diagonal matrix of the eigenvalues of V . This shows that the multivariate CUSUM test statistics $Y(n)$ are identical when calculated from the principal components instead of from the original variables. Lemma 1 can then be applied with

$$M = D^{-1/2} \quad (B-7)$$

to show that principal components scaled to have variance one,

$$z = D^{-1/2}w, \quad (B-8)$$

also give the same test statistics.

Lemma 2:

If $x^* = Mx$ where M is a $p \times p$ matrix of full rank, then

$$x^{*'}(M'^{-1}V^{-1}M^{-1})x^* = x'M'(M'^{-1}V^{-1}M^{-1})Mx = x'V^{-1}x.$$

This lemma implies that the noncentrality parameter has the same value whether computed from the original dependent variables, principal components, or principal components scaled to have variance one.

Lemma 3:

If $u_1'V^{-1}u_1 = u_2'V^{-1}u_2$, a nonsingular matrix M exists such that $u_1 = Mu_2$.

Proof:

M can be found by the following procedure. Because it is a product of invertible matrices, it is nonsingular.

The first step is to transform x to z , the principal components scaled to have variance one. Let $E(z) = v$. By lemma 2, $v_1'v_1 = v_2'v_2$ where v_1 and v_2 are the images of u_1 and u_2 under the transformation from x to z . Note an orthogonal matrix Q exists such that $v_1 = Qv_2$.

The transformation defined by the matrix Q changes from one basis to another in a vector space. Orthogonal transformations preserve length in the sense that if $v_1 = Qv_2$, then $v_1'v_1 = v_2'Q'Qv_2 = v_2'v_2$. To find M , substitute $D^{-1/2}Pu$ for v in $v_1 = Qv_2$: $D^{-1/2}Pu_1 = Q(D^{-1/2}Pu_2)$, or $u_1 = P^{-1}D^{1/2}QD^{-1/2}Pu_2$ so that $M = P^{-1}D^{1/2}QD^{-1/2}P$.

Lemma 4:

$$Y_n = \max[0, C_n - k].$$

Proof:

By definition, $Y_n = +[s_n'V^{-1}s_n]^{1/2}$. Recall that

$$\begin{aligned} s_n &= 0 \text{ if } C_n \leq k \\ s_n &= (s_{n-1} + x_n)(1 - k/C_n) \text{ if } C_n > k. \end{aligned} \quad (B-9)$$

Therefore, for $C_n > k$,

$$\begin{aligned} Y_n^2 &= s_n'V^{-1}s_n = (s_{n-1} + x_n)'(1 - k/C_n)V^{-1}(s_{n-1} + x_n)(1 - k/C_n) \\ &= (1 - k/C_n)^2(s_{n-1} + x_n)'V^{-1}(s_{n-1} + x_n) \\ &= (1 - k/C_n)^2C_n^2 \\ &= (C_n - k)^2 \end{aligned} \quad (B-10)$$

or

$$Y_n = C_n - k$$

Let $f(C_n|E(x) = u_1)$ denote the distribution function of C_n calculated from the random variable x given $E(x) = u_1$.

Theorem

If $u_1'V^{-1}u_1 = u_2'V^{-1}u_2$, then $f[C_n|E(x) = u_1] = f[C_n|E(x) = u_2]$.

The theorem equates the distributions of $C(n)$ when the data vectors have one of two alternative probability densities. Let pdf1 refer to the density specified by $E(x) = u_1$, and pdf2 refer to the density specified by $E(x) = u_2$. To prove the theorem, express pdf2 in transformed variates $t = Mx$ where M is given in lemma 3. This gives

$E(t) = Mu_2 = u_1$ and $Var(t) = MVM' = V$. To show $Var(t) = V$, write out

$MVM' = P'D^{1/2}QD^{-1/2}PVP'D^{-1/2}Q'D^{1/2}P$. As $PVP' = D$, this becomes

$MVM' = P'D^{1/2}Q(D^{-1/2}DD^{-1/2})Q'D^{1/2}P = P'D^{1/2}(QQ')D^{1/2}P = P'DP$

Substituting $D = PVP'$ into $P'DP$ gives $MVM' = P'(PVP')P = V$. Hence, pdf2, expressed in the transformed coordinates t , is the same as pdf1 expressed in x coordinates. The value of $C(n)$ is invariant with respect to the transformation from x to t , so that

$$f[C_n|E(x) = u_2] = f[C_n|E(t) = Mu_2 = u_1]. \quad (B-11)$$

Because the data vectors for pdf1 (in x coordinates) and pdf2 (in t coordinates) have multivariate normal distributions with the same mean vector and covariance matrix,

$$f[C_n|E(x) = u_1] = f[C_n|E(t) = u_1]. \quad (B-12)$$

Combining equations B-11 and B-12 gives

$$f[C_n|E(x) = u_1] = f[C_n|E(x) = u_2].$$

By lemma 4, $y_n = \max(0, C_n - k)$ so that the distribution of y_n given u_1 is the same as the distribution of y_n given u_2 when $u_1'V^{-1}u_1 = u_2'V^{-1}u_2$.

APPENDIX C MARKOV CHAIN REPRESENTATION

For the on-aim case, the ARLs of the multivariate CUSUM procedure can be approximated by using a discrete Markov chain. Following Brook and Evans,* the possible values of Y are represented by $t + 1$ states. One state is an absorbing state representing $Y > h$. The t transient states are numbered $0, 1, 2, \dots, (t-1)$ and represent values of Y between 0 and h . It is helpful to think of the Markov chain in terms of a discrete random variable, call it Y' , that takes on values $0, w, 2w, \dots, tw$, where $w = 2h/(2t - 1)$. The transition probabilities among the transient states are needed to find the ARL. The transition probabilities are

$$\text{Prob}(Y'_n = jw | Y'_{n-1} = iw), \quad i, j \in [0, 1, 2, \dots, (t-1)]. \quad (\text{C-1})$$

To find the transition probabilities, note that $Y_n = \max(0, C_n - k)$

where $C_n = [(s_{n-1} + x_n - a)'V^{-1}(s_{n-1} + x_n - a)]^{1/2}$.

The transition probabilities are conditional probabilities, so that $s(n-1)$ is considered a constant rather than a random variable. Hence, for the on-aim case, $E[s(n-1) + x(n) - a] = s(n-1)$ and $\text{Var}[s(n-1) + x(n) - a] = V$. Under the assumption of a multivariate normal distribution for $x(n)$, $C(n)$ has a Chi distribution with noncentrality parameter

$$[s'_{n-1}V^{-1}s_{n-1}]^{1/2} = Y_{n-1}. \quad (\text{C-2})$$

Therefore,

$$\text{Prob}(Y'_n = 0 | Y'_{n-1} = iw) = \text{Prob}(C_n \leq k + w/2) \quad (\text{C-3})$$

and, for $j > 0$,

$$\begin{aligned} \text{Prob}(Y'_n = jw | Y'_{n-1} = iw) &= \text{Prob}[k + (j - 0.5)w < C_n \leq k \\ &\quad + (j + 0.5)w] \end{aligned} \quad (\text{C-4})$$

where $C(n)$ has a Chi distribution with noncentrality parameter iw . Brook and Evans suggest obtaining the ARL for several different size Markov chains and extrapolating to the continuous case by the formula

$$\text{ARL}(t) = \text{Asymptotic ARL} + B/t + C/t^2.$$

*Brooks, D., and Evans, D.A., "An Approach to the Probability Distribution of CUSUM Run Lengths," Biometrika Vol. 59, pp 539-549 (1972).

For most of the schemes discussed in this article, using $t = 12, 15, 18, 21$, and 24 was adequate to verify the on-aim ARLs. Larger values of t are needed for schemes with large values of h . For the scheme $p = 20$, $h = 28$, and $k = 0.5$, using $t = 12, 15, 18, 21$, and 24 gave an asymptotic ARL of 634, whereas the use of $t = 12, 24, 36, 48$, and 60 gave an asymptotic ARL of 505.