BINOMIAL AND HYPERGEOMETRIC GROUP-TESTING*

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In binomial and hypergeometric group-testing the basic problem is to classify each of a fixed number N of units as satisfactory or defective. Corresponding to each unit we assign a random variable with the values zero or one according as the unit is satisfactory or defective, and we assume that these random variables are all independent and identically distributed. We shall distinguish problems (using the symbols B and H) according as our a priori knowledge gives us the value of the probability p of a unit being defective or the actual number of defectives D present among the N units at the outset. In each individual test we can include any number x of units ($1 \leq x \leq N$) but we also distinguish problems according to the type of results obtained by a single test. In the B-type the individual test informs us that either all x are good or at least one of the x is defective (but we don't know which ones or how many); in the H-type it tells us the exact number of defectives d_x present among the x units (but we don't know which ones they are, unless $d_x = x$). Thus we obtain four problems which we denote by BB, HB, BH and HH, where the first symbol refers to the a priori knowledge and the second refers to the type of results on a single test; we shall also refer to them as problems 1, 2, 3, 4, respectively. Problem BB has been considered by Sobel and Groll [7] and by Sobel [8] and is included in the present paper only for the purpose of making comparisons. We shall show that all these problems can be handled by a common technique which we call procedure R_1 and we shall be interested in the interrelations between these problems. For example, using the appropriate procedure R_1 (defined below) the expected number of tests required for problem BB is an upper bound for the expected number of tests for both problems HB and BH; and similarly

HH provides a lower bound. Problem BH is closely related to HH since, if we perform a single test at the outset on all N units, we can determine the number D of defectives; the knowledge of p then becomes superfluous and the problem reduces to an HH problem from that point on. Problems BH and HH can be regarded as coin weighing problems in which all the defective coins weigh the same (too heavy or too light) provided the scale used is an ordinary weighing scale and not a two-arm balance. (For the HH problem with a two-arm balance see Cairns [2] and Bellman and Gluss [1].)

It is also possible to replace the a priori information by a (weaker) a priori distribution or by no information at all. Letting B* denote the former and a blank the latter, this gives problems B*B, B, B*H and H. Problems B*B and B were considered by Sobel and Groll [10]. An information-theoretic analysis of problem H (without the assumption of independent, identically distributed random variables) has been under active investigation by several workers as indicated in the remark at the end of the paper by Erdos and Renyi [3]. None of these authors appear to have considered any explicit procedures for carrying out the classification. Lindstrom [5] has shown that for this problem H

$$\lim_{n \to \infty} \frac{A(n|H)\log_2 n}{n} = 2 \tag{1.1}$$

where $A(n|H)$ is the expected number of tests using the optimal procedure. We shall be interested in making some numerical comparisons with (1.1). The close relation between H and HH stems from the fact that under H we could test all the units on the first test and hence

$$A(n|HH) \leq A(n|H) \leq A(n|HH) + 1. \tag{1.2}$$

The question of optimality of the procedure R_1 will also be considered. In particular, it is conjectured that for problem HB this procedure is optimal for any starting value of N; this is unlike the results for BB in [7] (see also [8] and [9]) where it is shown that the procedure R_1 is not optimal for all values of p. This conjecture is based on the fact that the expected number of tests under procedure R_1 for problem HB is equal to the Huffman lower bound (for any group-testing procedure) for an infinite sequence of N-values.

In some sense the problems BB (where p is known) and HH (where D is known) have an interesting relationship; the remarks that follow also apply to B and H (where p and D are, respectively, unknown). In some applications the result of an individual test is such that the model falls between the BB-model and the HH-model. For example, if the individual test told us that either (i) $d_x = 0$ or (ii) $1 \leq d_x \leq 2$ or (iii) $3 \leq d_x \leq x$ then we are neither in the BB-model nor the HH-model but somewhere in-between. The BB and HH-models give upper and lower bounds, respectively, for the expected number of tests required by such a model if the corresponding R_1 procedure is used.

We assume throughout that tests are conducted one at a time and that the results of any test are available before any subsequent test is started.

The major contribution of this paper will be toward the problem HB and hence the notation and the procedure R_1 for this problem is introduced first below.

2. Notation and Preliminaries for Problem HB

The total number N of units to be classified, the number D of defectives among them and hence the number $S = N - D$ of satisfactory units at the outset are all given. At any stage of the procedure let n, d, s, with $n = d + s$, denote respectively the number of units not yet classified, the number of defectives among the n and the number of satisfactory units among the n.

The procedure R_1 is implicitly defined by two recursion formulas and some trivial boundary conditions. It has the property that at any stage all the relevant information about previous tests is retained by merely separating the n units not yet classified into at most 2 sets. If there are 2 sets present then one of these sets of size m (where $2 \leq m \leq s$) is known to contain at least one defective unit and we refer to this set as the defective set; the other set of size n - m will then be called the remainder set if $d > 1$, since we do not know at this point whether it contains defectives or not. The terminology H-situation when there is only 1 set present ($m = 0$) and G-situation when there are 2 sets present ($m \geq 2$) is a carryover from the BB problem in [7].

In an H-situation with parameters n, d, s the probability $Q_H(x|d,s)$ that a sample of size x (chosen at random from the n units) contains no defectives is

$$(2.1) \qquad Q_H(x|d,s) = \binom{s}{x}/\binom{n}{x} = \binom{n-x}{d}/\binom{n}{d}$$

and the probability $P_H(x|d,s)$ that it contains at least 1 defective is simply $1-Q_H(x|d,s)$.

In a G-situation with parameters m,d,s let Y denote the number of defectives in the defective set and let X denote the number of defectives in a sample of size x drawn (at random) from the defective set. Then

$$(2.2) \qquad P\{X \geq 1|Y \geq 1\} = \frac{P\{X \geq 1\}}{P\{Y \geq 1\}} = \frac{1-[\binom{s}{x}/\binom{n}{x}]}{1-[\binom{s}{m}/\binom{n}{m}]} = \frac{\binom{s+d}{d}-\binom{s+d-x}{d}}{\binom{s+d}{d}-\binom{s+d-m}{d}}$$

$$= P_G(x|m,d,s)$$

and

$$(2.3) \qquad P\{X = 0|Y \geq 1\} = \frac{[\binom{s}{x}/\binom{n}{x}]-[\binom{s}{m}/\binom{n}{m}]}{1-[\binom{s}{m}/\binom{n}{m}]} = \frac{\binom{s+d-x}{d}-\binom{s+d-m}{d}}{\binom{s+d}{d}-\binom{s+d-m}{d}}$$

$$= Q_G(x|m,d,s).$$

Let $G(m;d,s) = G(m;d,s|R_1,HB)$ denote the expected number of tests required under procedure R_1 if we start with a G-situation with parameters m,d,s and let $H(d,s) = H(d,s|R_1,HB)$ denote the same quantity for an H-situation with parameters d and s.

Procedure R_1 for Problem HB

The recursion formulas defining procedure R_1 are for $d \geq 1$ and $s \geq 1$

(2.4) $$H(d,s) = 1 + \min_{1\leq x\leq s} [Q_H(x|d,s)H(d,s-x) + P_H(x|d,s)G(x;d,s)]$$

and for $m \geq 2$, $d \geq 2$, $s \geq 1$

(2.5) $$G(m;d,s) = 1 + \min_{1\leq x\leq m-1} [Q_G(x|m,d,s)G(m-x;d,s-x)+P_G(x|m,d,s)G(x;d,s)]$$

where Q_H, $P_H = 1-Q_H$, P_G and Q_G are given by (2.1), (2.2) and (2.3).

The boundary conditions for this recursion are

(2.6) $$H(0,s) = H(d,0) = 0 \quad \text{for all } d \geq 0,\ s \geq 0.$$

(2.7) $$G(1;d,s) = H(d-1,s) \quad \text{for all } d \geq 2,\ s \geq 0.$$

(2.8) $$G(m;1,s) = H(1,m-1) \quad \text{for all } s + 1 \geq m \geq 1.$$

In particular, the boundary conditions take care of the cases in which $m = 1$ or where there is a change in the value of d.

Remark 1: In writing (2.5) it is assumed that in a G-situation all the x units are taken from the defective set of size m without mixing, i.e., without combining units from the two sets. This assumption characterizes the procedure R_1. In the BB problem this assumption was responsible for the lack of optimality; we shall be interested below in seeing whether it also causes a lack of optimality in the HB problem.

Remark 2: If at any stage in the HB problem we reach a situation with $d = 1$ then we have only H-situations from that point on and every test identifies good units. From that point on it is also an HH-problem with $D = 1$ and, as mentioned earlier, it is known that the so-called "halving procedure" is optimal for this case; we show below that the procedure R_1 is the halving procedure as soon as we get d equal to 1. Assuming this result we can then rewrite (2.4) for $d = 1$ in this problem (and also for the HH-problem with $D = 1$) in the following simpler form. If s is odd (say, $s = 2t-1$ where $t \geq 1$)

$$H(1, 2t-1) = 1 + H(1, t-1) \tag{2.9}$$

and if s is even (say, $s = 2t$ where $t \geq 1$)

$$H(1, 2t) = 1 + \frac{t}{2t+1} H(1, t-1) + \frac{t+1}{2t+1} H(1,t) \tag{2.10}$$

and the boundary condition is $H(1,0) = 0$. An explicit expression for $H(1,s)$ is given in (2.22) below.

Remark 3: In writing $G(x;d,s)$ at the end of (2.5) we used the following result. If x units taken (at random) from a defective set of size m contain at least one defective then the m-x remaining units can be combined with the remainder set of size s+d-m without any "loss of information." In other words, the a posteriori distribution is such that we again have a G-situation with only two sets to keep track of. A general proof of this without using the hypergeometric distribution will be given below. This process of combining the m-x and s+d-m units will be called recombination.

For any $s \geq 1$ we let $s' = s+1$ and define the integers $b = b(s')$ and $c = c(s')$ by

$$s' = 2^b + c \quad (0 \leq c < 2^b). \tag{2.11}$$

Consider the explicit nonnegative function

$$h_1(s') = bs' + 2c = (b+2)s' - 2^{b+1} \tag{2.12}$$

which is clearly an increasing function of s; we define $h_1(1)$ to be 0.

If we set d = 1 in (2.4), use (2.1), (2.2) and (2.3) for Q_H, P_H, Q_G and P_G, and set $xH(1,x-1) = h(x)$ then we obtain for $s' \geq 2$

$$h(s') = s' + \min_{1 \leq x \leq s'-1} [h(x) + h(s'-x)] \tag{2.13}$$

with boundary condition $h(1) = 0$. We now wish to show

Lemma 1: The function $h(s')$ in (2.13) with $h(1) = 0$ is identical with $h_1(s')$ given by (2.12) with $h_1(1) = 0$. For $s' \geq 1$ the set of x values that minimize the right hand side of (2.13) include the integer (or integers) closest to $s'/2$.

Proof: We will show that $h_1(s')$ satisfies (2.13) and since the boundary condition is the same and (2.13) then determines $h(s')$ for all integers $s' > 1$ the result will follow. Suppose first that $h(x) + h(s'-x)$ is minimized by taking x as close as possible to $s'/2$. Then for even $s' \geq 2$ we put $h_1(s'/2)$ on the right side of (2.13) and obtain for $x = s'/2$

$$s'+2[(b-1)\frac{s'}{2} + 2(\frac{s'}{2} - 2^{b-1})] = bs'+2(s'-2^b) = h_1(s'), \tag{2.14}$$

so that (2.13) is satisfied for $h(s') = h_1(s')$ for s' even. For odd $s' \geq 3$ we take $x = (s'-1)/2$ and it is easy to verify that $b(x) = b-1$ and if $s' \neq 2^{b+1}-1$ then $b(s'-x) = b((s'+1)/2) = b-1$. Then the right side of (2.13) gives

$$s'+(b-1)(\frac{s}{2})+2(\frac{s}{2} - 2^{b-1})+[(b-1)(\frac{s'+1}{2})+2(\frac{s'+1}{2} -2^{b-1})] \tag{2.15}$$

$$= bs'+2(s'-2^b) = h_1(s').$$

If $s' = 2^{b+1}-1$ then the bracketed part B of (2.15) becomes

$$(\frac{s'+1}{2})b+2(\frac{s'+1}{2} -2^b) = (b-1)(\frac{s'+1}{2})+2(\frac{s'+1}{2} -2^{b-1}) = B \tag{2.16}$$

and thus we obtain $h_1(s')$ again. Hence $h_1(s')$ satisfies the recursion (2.13) with $x = s'/2$ and if our above supposition is true it follows that $h_1(s') = h(s')$ for all $s' \geqq 1$.

We now show that the values of x closest to $s'/2$ minimize

$$(2.17) \qquad h_2(x;s') = h_1(x)+h_1(s'-x) \quad (1 \leqq x \leqq s),$$

where $h_1(x)$ is given by (2.12). Clearly, for any $s' \geqq 1$, $h_2(x;s')$ is symmetric about $x = s'/2$. Hence it suffices to show that $h_2(x;s')$ is convex on the domain of integers x where $1 \leqq x \leqq s'/2$. For this convexity it is sufficient to show that $h_1(x)$ is convex for $x \geqq 2$, i.e., that for any 3 consecutive integers x-1, x, x+1 with $x \geqq 2$ the second difference $\Delta^2 h_1(x) = h_1(x+1)-2h_1(x)+h_1(x-1) \geqq 0$. For $x \geqq 2$ three cases arise according as for some $z \geqq 0$

$$(2.18) \qquad \text{(i)} \ x = 2^z; \ \text{(ii)} \ x = 2^z-1; \ \text{(iii)} \ 2^{z-1} < x < 2^z-1.$$

For case (i) we obtain

$$(2.19) \ \Delta^2 h_1(x) = z(2^z+1)+(2(2^z+1-2^z)-2[z2^z+2(2^z-2^z)]+(z-1)(2^z-1)+2(2^z-1-2^{z-1})=1$$

Similarly for cases (ii) and (iii), respectively, we obtain

$$(2.20) \qquad \Delta^2 h_1(x) = 0 \text{ and } \Delta^2 h_1(x) = 6x > 0 \text{ for } x \geq 2.$$

This proves the convexity of $h_1(x)$ for $1 \leqq x \leqq s$ and hence $h_1(x)$ assumes its minimum at the integer (s) closest to $s'/2$.

To complete the proof of lemma 1 we use induction and assume that $h(x) = h_1(x)$ for all integers $x < s'$. Then by (2.13)

$$(2.21) \qquad h(s') - s' = \min_{1 \leqq x \leqq s} [h(x)+h(s'-x)] = \min_{1 \leqq x \leqq s} [h_1(x)+h_1(s'-x)] = h_1(s')$$

Since $h(1) = h_1(1) = 0$, this proves the lemma.

In terms of the original notation the above lemma tells us that for $s \geq 1$ (and also for $s = 0$)

$$(2.22) \qquad H(1,s) = b + \frac{2(s+1-2^b)}{s+1} = b+2- \frac{2^{b+1}}{s+1}$$

where b and c are defined by (2.11) with $s' = s+1$.

3. A Characterization of Procedure R_1 for the HB-Problem

In this section we define a procedure R_0 in an explicit manner and it is claimed that procedure R_0 is precisely the same as the above procedure R_1 defined by the recursion formulas (2.4) and (2.5) with boundary conditions (2.6), (2.7) and (2.8); since this result has not been proved this claim is to be regarded as a conjecture. We shall consider here only the case $D = 2$ with general S. The procedure R_1 has already been characterized for $d = 1$ and, by definition, R_0 is the "halving procedure"for $d = 1$; hence we only need to define R_0 for $d = 2$. For more generality we consider any H-situation and replace the initial S by s.

For $s' = s+1 \geq 2$ let $b = b(s')$ and $c = c(s')$ be nonnegative integers defined exactly as in (2.11). Using (3.1) we define $x(s)= x_H(2,s)$ by setting $x(0) = 0$, $x(1) = 1$ and for $s \geq 2$ by

$$(3.1) \qquad x(s) = \begin{cases} [2^{b-2}+ \frac{c+1}{2}] & \text{for } 2^b \leq s' < 3.2^{b-1} \\ 2^{b-1} & \text{for } 3.2^{b-1} \leq s' < 2^{b+1} , \end{cases}$$

where [y] is the largest integer less than or equal to y. It is easy to verify that x(s) is a nondecreasing function of s (in particular, it is the same for $s' = 3.2^{r-1}-1$ and $s' = 3.2^{r-1}$), that x(s) is the minimum of the two expressions in (3.1) and finally that for all $s \geq 1$

$$(3.2) \qquad \frac{s+1}{4} \leq x(s) \leq \frac{s+2}{3} = \frac{n}{3} .$$

Under the proposed procedure R_0 the sample size x(s) for the H-situation with $d = 2$ and $n = 2+s$ is given by (3.1).

To describe the procedure R_0 for the G-situation with $d = 2$ and general m, s with $s \geqq m \geqq 2$ we first note that a non-trivial G-situation, i.e., with $m \geqq 2$, can only arise from an H-situation with $s \geqq 4$; this is so because $x_H(2,s) = 1$ for $s < 4$. Define the integers $p = p(m)$ and $r = r(m)$ for $m \geqq 2$ by

$$m = 2^p - r \qquad 0 \leqq r < 2^p; \tag{3.3}$$

for $m = 1$ we can write $p = r = 0$ or $p = r = 1$. For $m \geqq 1$ (and hence $s \geqq 1$) we define the vector $\vec{v}_m = \vec{v}(m;2) = (v_1, v_2, \ldots, v_m)$ by setting

$$v_\alpha = \begin{cases} p-1 & \text{for } \alpha = 1,2,\ldots,r \\ p & \text{for } \alpha = r+1, r+2, \ldots, m. \end{cases} \tag{3.4}$$

We note that this definition of $\vec{v}_m$ does not depend on s except possibly for $s \leqq 3$ when $m = 1$. Every such vector $\vec{v}_m$ has the property that

$$\sum_{\alpha=1}^{m} 2^{-v_\alpha} = \frac{r}{2^{p-1}} + \frac{m-r}{2^p} = 1 \tag{3.5}$$

and we shall call this sum the value of the vector $\vec{v}_m$.

It is clear from (3.5) and the above that for $m \geqq 2$ we can always subdivide $\vec{v}_m$ into subvectors $\vec{v}_j$ consisting of the first j components and $\vec{v}_{m-j}$ consisting of the last $m-j$ components so that each has the value 1/2. This process can be repeated on any subvector that has at least 2 components and the smallest possible value is clearly 2^{-p}.

We now complete the explicit description of procedure R_0 for the G-situation in terms of these subdivisions. In the G-situation i.e., after a test on x_i units has failed and we set $m = x_i$, we test j units from the defective set of size m where j is defined above; let $\vec{v}_j$ and $\vec{v}_{m-j}$ be the left and right subvectors formed. If the test on j units succeeds then these are classified and we consider only $\vec{v}_{m-j}$ for subsequent tests; if it fails then we label these j units as a new defective set and we consider $\vec{v}_j$ for the next test since the $m-j$ units in $\vec{v}_{m-j}$ are now eligible for recombination with all the unclassified units outside the new defective set. In either case the procedure R_0 is to continue subdividing the newly formed subvectors until the subvector to be considered for subsequent tests contains only one component. We then continue this process further (testing a single unit at a time) until a defective unit is found, either by a direct test or by inference. This part of the procedure always leads to the classification of exactly one defective unit.

After a defective unit is found we are back in an H-situation and the whole process (including the determination of x values from the new s-value) starts all over again with the number of defectives reduced by one and the number of satisfactory units reduced by a random integer.

4. Explicit Formulas for R_0

Although we are interested in evaluating R_0 for all values of s, we shall be particularly interested in a sequence s_j of s values in which $s_1 = 1$, $s_2 = 2$ and s_j for $j \geq 3$ is defined recursively by

$$s_{j+2} = \begin{cases} 2s_j+1 & \text{for } j = 4i+1 \text{ and } 4i+2 \\ 2s_j+2 & \text{for } j = 4i+3 \text{ and } 4i+4 \end{cases} \tag{4.1}$$

by letting $i = 0,1,2,\ldots$. If we break up the sequence into groups of 4 and write each subgroup vertically, then some numerical values of the s_j after $s_0 = 0$ are

$$\begin{array}{rrrrrl} 1, & 8, & 36, & 148, & 596, & \ldots \\ 2, & 12, & 52, & 212, & 852, & \ldots \\ 3, & 17, & 73, & 297, & 1193, & \ldots \\ 5, & 25, & 105, & 425, & 1705, & \ldots . \end{array} \tag{4.2}$$

Using (4.1) it is easy to obtain explicit expressions for s_j for each of the 4 types of j-values above; for odd and even j, respectively, these can be written fc

$$
(4.3)\qquad s_j = \begin{cases} 2^{(j+1)/2} + \left[\dfrac{2^{(j-1)/2}-4}{3}\right] & \text{for odd } j \geq 1 \\ 2^{j/2} + \left[\dfrac{2^{(j+2)/2}-4}{3}\right] & \text{for even } j \geq 0, \end{cases}
$$

where $[x]$ was already defined in (3.1). For $j = 4i+1$ and $4i+2$ the bracket signs in (4.3) can be removed without any change and for $j = 4i+3$ and $4i+4$ the bracket signs can be removed if we replace the "4" by a "5." For $j \geq 1$, the expression in (4.3) gives the correct b and c-values (say, b_j and c_j) for $s'_j = s_j+1$ as defined in (2.11). In particular, we note that $b_j = b(s'_j) = [(j+1)/2]$ for $j \geq 0$. It is easily verified that for $s_j \geq 1$ (or $j \geq 1$)

$$
(4.4)\qquad \begin{aligned} s'_j &< 3.2^{(j-1)/2} && \text{for } j \text{ odd} \\ s'_j &\geq 3.2^{(j-2)/2} && \text{for } j \text{ even} \end{aligned}
$$

and hence $x(s_j)$ takes its value from the first line of (3.1) when j is odd and from the second line in (3.1) when j is even. Using (3.1) and (4.3) we then obtain for $j \geq 2$

$$
(4.5)\qquad x(s_j) = \begin{cases} 2^{(j-1)/2} - \left[\dfrac{2^{(j-1)/2}+1}{3}\right] & \text{for odd } j \\ 2^{(j-1)/2} & \text{for even } j \end{cases}
$$

and we note that the same expression holds for $j = 1$.

We wish to establish 3 properties of the numbers s_j; these properties will help to characterize the procedure R_0 (and hence also R_1 if R_1 is identical with R_0).

<u>Property 1</u>: For every $j \geq 1$

$$
(4.6)\qquad s_j - x(s_j) = s_{j-1} .
$$

Proof: For odd $j = 4i+1$ we get from (4.3) and (4.5) for the left side of

(4.7) $$2^{(j-1)/2}+[\frac{2^{(j-1)/2}-4}{3}] + [\frac{2^{(j-1)/2}+1}{3}] = 2^{(j-1)/2}+ (\frac{2^{(j+1)/2}-5}{3}),$$

subtracting 2/3 to make the 2^{nd} square bracket an integer; this is the same as the result for s_{j-1} for even (j-1) in (4.3). For odd $j = 4i+3$ we subtract 1/3 from the first square bracket argument (and 0 from the second) so that 1/3 is added to the last expression in (4.7); this gives the expression for s_{j-1} in (4.3) for even j-1. For even $j \geqq 2$ we obtain for the left side of (4.6)

$$2^{(j-2)/2}+[\frac{4.2^{(j-2)/2}-4}{3}] = 2^{(j-1)/2}+[\frac{2^{(j-2)/2}-4}{3}] = s_{j-1}.$$

<u>Property 2</u>: For every $j \geqq 0$

(4.8) $$2^j \leqq \binom{s_j+2}{2} < 2^{j+1},$$

i.e., the b-value for $\binom{s_j+2}{2}$ is j.

<u>Proof</u>: For odd j, using (4.3), the inequalities (4.8) reduce to

(4.9) $$2^j \leqq \frac{98y_1^2 \pm 7y_1-1}{9} < 2^{j+1}$$

where the + and - correspond to $j = 4i+1$ and $4i+3$, respectively, and $y_1 = 2^{(j-3)/2}$. Using the + sign with the upper inequality in (4.9), dropping the -1 yields

$$7y_1 < 46y_1^2 \text{ or } y_1 > 7/46,$$

which holds for all odd $j \geqq 1$. Using the negative sign with the lower inequality in (4.9) yields

$$30y_1^2 - 7y_1 - 1 \geqq 0 \text{ or } y_1 \geqq 1/3,$$

which holds for all odd $j \geqq 1$.

For even j the inequalities (4.8) reduce to

(4.10) $$2^j \leqq \frac{25.2^{j-1} \pm 5.2^{(j-2)/2}-1}{9} < 2^{j+1}$$

where the + and - sign correspond to $j = 4i+2$ and $4i+4$, respectively.

Letting $y_2 = 2^{(j-2)/2}$ we obtain as above for the upper and lower inequalities in (4.10), respectively

$$y_2 > \frac{5}{22} \quad \text{and} \quad 14y_2^2 - 5y_2 - 1 \geq 0 \text{ or } y_2 \geq 1/2,$$

both of which hold for all even $j \geq 0$. In fact, we note that equality is attained only for $j = 0$.

<u>Property 3</u>: For $j \geq 2$

$$(4.11) \qquad 2^{j-1} \leq \binom{s_j+2}{2} - \binom{s_{j-1}+2}{2} < 2^j.$$

<u>Proof</u>: Letting M_j denote the middle expression in (4.11) and using the above notation, we have

$$(4.12) \qquad M_j = \begin{cases} \dfrac{y_3^2 \pm y_3}{3} & \text{for odd } j \\ \dfrac{34y_4^2 \pm y_4}{3} & \text{for even } j, \end{cases}$$

where $y_3 = 2^{(j+1)/2}$ and $y_4 = 2^{(j-4)/2}$. Using (4.12) it is easy to verify that for odd j we need $j \geq 3$ to satisfy (4.11) and for even j we need $j \geq 2$ to satisfy (4.11). In fact the equality in (4.11) holds only for $j = 3$.

From the description of procedure R_0 in section 3 we now obtain explicit formulas for the test group size $x_G = x_G(m;2,s)$ for any G-situation. Then we obtain explicit formulas for $G_0(m;2,s)$ and for $H_0(2,s)$ under the procedure R_0. With the help of the above 3 properties we then show that the formula for $H_0(2,s)$ simplifies for $s = s_j$ in the infinite sequence (4.1).

Consider the vector $\vec{v}_m$ defined in terms of m in (3.4). If $r/_2p\text{-}1 \geq 1/2$ (or $m \leq 3.2^{p-2}$) then by procedure R_0 the next test-group size x is the root of

$$\frac{x}{2^{p-1}} = 1/2 \quad \text{or } x = 2^{p-2}.$$

If $r/_2p\text{-}1 \leq 1/2$ (or $m \geq 3.2^{p-2}$) then by procedure R_0 the next test group size x is the root of

$$\frac{m-x}{2^p} = 1/2 \text{ or } x = m - 2^{p-1} > 0.$$

Thus we can write for procedure R_0

$$(4.13) \qquad x_G(m;2,s) = \begin{cases} 2^{p-2} & \text{for } 2^{p-1} \le m < 3.2^{p-2} \\ m - 2^{p-1} & \text{for } 3.2^{p-2} \le m < 2^p, \end{cases}$$

and we denote it by $x_G(m;2)$ since it does not depend on s. From (4.13) we note that

$$(4.14) \qquad \frac{m}{3} \le x_G(m;2) \le \frac{m}{2}$$

and moreover

$$(4.15) \qquad \begin{aligned} 2^{p-2} &\le m-x < 2^{p-1} \text{ when } x = 2^{p-2}, \\ 2^{p-2} &\le x < 2^{p-1} \text{ when } m-x = 2^{p-1}, \end{aligned}$$

so that the largest powers of 2 contained in x and m-x are p-1 and p-2.

After some preliminaries we now develop an explicit expression for $H_0(2,s)$ under procedure R_0 for any $s = s_j$ in the infinite sequence (4.1). Let $m_j = x_H(2,s_j)$ and let $b_j = b(s_j+1)$ as defined in (3.1) and (2.11). Let $\vec{v}_j = \vec{v}(m_j;2,s_j) = (v_{1j}, v_{2j}, \ldots, v_{m_j j})$; we need to discuss the significance of the components v_{ij} in the procedure R_0. The component $v_{\alpha j}$ of $\vec{v}_j$ corresponds to the α^{th} unit ($\alpha=1,2,\ldots, m_j$), after the units have been randomized and put in an arbitrary fixed order. If the first defective is in position α then from the description of R_0 it will take exactly $v_{\alpha j}$ tests, starting with the G-situation denoted by $G(m_j;2,s_j)$, to discover this defective unit and thus get back to an H-situation. The probability that the first defective is in the α^{th} position is easily seen to be $(s_j+2-\alpha)f_j^{-1}$ where $f_j = \binom{s_j+2}{2}$. Hence using (4.6) we can write for $i \ge 4$

$$(4.16) \qquad f_i H_0(2,s_i) = f_i + (f_{i-1}H_0(2,s_{i-1}) + \sum_{\alpha=1}^{m_i} (s_i+2-\alpha)\{v_{\alpha i}+H_0(1,s_i+1-\alpha)\}).$$

Actually (4.16) also holds for i = 1, 2 and 3 if we define $v_{1i} = 0$ for $1 \leq i \leq 3$; this is reasonable since $m_i = s(s_i) = 1$ for these i-values. If we now iterate (4.16) on i (i=1,2,...,j) then, using the definition of h(x) in (2.13), we have for $j \geq 1$

$$(4.17) \qquad f_j H_0(2,s_j) = \sum_{i=1}^{j} f_i + \sum_{i=1}^{j} \sum_{\alpha=1}^{m_i} (s_\alpha+2-i)\, v_{\alpha i} + \sum_{\beta=1}^{s_j} h(\beta+1).$$

Similarly, using the fact that $v_{\alpha i} = p_i - 1$ for $\alpha = 1,2,\ldots, r_i$ and $v_{\alpha i} = p_i$ for the remaining $m_i - r_i$ values of i, we can combine the first single sum and the double sum in (4.16) to obtain for any $j \geq 1$

$$(4.18) \qquad f_j H_0(2,s_j) = \sum_{\alpha=1}^{j} \binom{t_\alpha+2}{2} + \sum_{\beta=1}^{s_j} h(\beta+1) + \sum_{i=1}^{j} p_i(f_i - f_{i-1})$$

where $t_\alpha = s_\alpha - r_\alpha$, $s_0 = p_1 = p_2 = 0$ and $p_3 = 1$. Comparing (4.3) and (4.5) we note that $p_i = b_i - 1$ for $i \geq 4$ and we define $p_1 = p_2 = 0$ and $p_3 = 1$ so that this relation also holds for i=1,2 and 3. We note from (4.3) or (4.5) that p_i increases by one when (and only when) i changes from even to odd and that $t_\alpha = s_\alpha$ for even α; hence (4.18) can be written as

$$(4.19) \qquad f_j H_0(2,s_j) = p_j f_j + \sum_{\alpha=1}^{j} \binom{t_\alpha+2}{2} - \sum_{\alpha=1}^{[\frac{j-1}{2}]} f_{2\alpha} + \sum_{\beta=1}^{s_j} h(\beta+1)$$

$$= [\tfrac{j}{2}]\, f_j + \sum_{\alpha=1}^{[\frac{(j+1)}{2}]} \binom{t_{2\alpha-1}+2}{2} + \sum_{\beta=1}^{s_j} h(\beta+1).$$

By (4.3) we find that

$$(4.20) \qquad t_{2\alpha-1} = \begin{cases} 2^\alpha - 1 & \text{for } \alpha \text{ odd} \\ 2^\alpha - 2 & \text{for } \alpha \text{ even} \end{cases}$$

and hence the first sum F_j in the last expression in (4.19) becomes for odd $j \geq 1$

$$(4.21) \qquad F_j = \frac{2^{j+2} \pm 2^{\frac{j+1}{2}} - 1}{3}$$

where the + sign holds for $j = 4i+1$ and the - sign holds for $j = 4i+3$. For even j we use (4.21) with j replaced by j-1, applying the above "sign rule" to j-1.

Using (2.12) we find after some straightforward summation of series that

$$(4.22)\qquad \sum_{\beta=1}^{s_j} h(\beta+1) = (b_j+2)\, f_j + \frac{2^{2b_j+1}+1}{3} - (2s_j+3)\, 2^{b_j} \quad (j \geq 1).$$

We now insert this result in (4.19); using (4.3) to substitute for s_j and b_j in terms of j we obtain

$$(4.23)\qquad f_j H_0(2,s_j) = \begin{cases} (j+2)f_j + F_j - \left(\frac{2^{j+3}-1}{3}\right) - 2^{(j+1)/2}\left[\frac{2^{(j+1)/2}+1}{3}\right] & \text{for } j \text{ odd} \\ (j+2)f_j + F_{j-1} - \left(\frac{2^{j+2}-1}{3}\right) - 2^{j/2}\left[\frac{2^{(j+4)/2}+1}{3}\right] & \text{for } j \text{ even.} \end{cases}$$

If we now consider the 4 cases for j and substitute for F_j from (4.21) then we obtain for $j \geq 1$ in all 4 cases the same simple result

$$(4.24)\qquad H_0(2,s_j) = j + 2 - \frac{2^{j+1}}{f_j}\ .$$

We note from property 2 in (4.8) that 2^j is the largest power of 2 contained in f_j and hence by (4.24)

$$(4.25)\qquad j = [\log_2 f_j] \leq H_0(2,s_j) < 1 + [\log_2 f_j] = j + 1.$$

Using the monotonicity of $H_0(2,s)$ as a function of s we have

$$(4.26)\qquad \lim_{j\to\infty} H_0(2,s_j) = \lim_{s\to\infty} H_0(2,s) \approx 2\log_2 s.$$

<u>Remark:</u> Suppose that $F(x,s) = \binom{s+2}{2} - \binom{s+2-x}{2}$ and $F(m-x,s-x)$, the numerators of P_G and Q_G in (2.2) and (2.3), respectively, have the same highest power of 2, say β-1, contained in them. If the formula

$$(4.27)\qquad G_0(m_1,2,s_1) = q + 2 - \frac{2^{q+1}}{F(m_1,s_1)}\ ,$$

which is analogous to (4.24), holds for $s_1 < s$ and all $m_1 (2 \leq m_1 \leq s_1)$ with $q = [\log_2 F(m_1,s_1)]$, then, using the fact that $F(m,s) = F(x,s) + F(m-x,s-x)$ so that $2^\beta \leq F(m,s) < 2^{\beta+1}$, we have from (2.5)

(4.28) $$G_0(m;2,s) = 1 + \frac{F(m-x,s-x)}{F(m,s)}\left(\beta+1 - \frac{2^\beta}{F(m-x,s-x)}\right) + \frac{F(x,s)}{F(m,s)}\left(\beta+1 - \frac{2^\beta}{F(x,s)}\right)$$
$$= \beta+2 - \frac{2^{\beta+1}}{F(m,s)} .$$

If $[\log_2 F(x,s)] = \beta_1 < \beta_2 = [\log_2 F(m-x,s-x)]$ then $\beta = [\log_2 F(m,s)] = \beta_2$ and the result in (4.28) becomes

(4.29) $$\beta+2 - \frac{2^{\beta+1}}{F(m,s)} + \frac{F(m-x,s-x)-2^{\beta+1}-F(x,s)(\beta_2-\beta_1-1)}{F(m,s)}$$
$$> \beta+2 - \frac{2^{\beta+1}}{F(m,s)} + \frac{\{2^{\beta_2-\beta_1-1}-(\beta_2-\beta_1)\}2^{\beta_1+1}}{F(m,s)}$$

where the last term is nonnegative since $x \leq 2^{x-1}$ for any integer $x \geq 1$. Moreover $F(m-x,s-x) = (m-x)(2s+3-m-x)/2$ cannot be a power of 2 since the 2 factors have different parity and hence the inequality in (4.29) is strict. It follows that the result in (4.28) is a lower bound under R_0 for any m,s. Similarly we find from (2.4) and (2.8) that for any s

(4.30) $$H_0(2,s) \geq \beta+2 - \frac{2^{\beta+1}}{f}$$

where $f = \binom{s+2}{2}$ and $\beta = [\log_2 f]$; strict inequality holds in (4.30) if $[\log_2 \binom{s+2-x}{2}] \neq [\log_2 F(x,s)]$ where x is the next group test size. Comparing with (4.24), we note that procedure R_0 meets this lower bound (4.30) for every s_j in the infinite sequence (4.1).

From the explicit results obtained in section 5 below for $G_0(m;2,s)$ for any pair (m,s) it can be verified that (4.28) holds for $s = s_j$ and $m = m_j$ for any j. It follows that (4.28) must hold for any G-situation that is attainable if we start with an H-situation with $s = s_j$ in the infinite sequence (4.1) and a similar result holds for (4.30). In fact equality in (4.28) and (4.30) appears to hold if and only if we start with an H-situation with $s = s_j$, but this has not been shown.

On the other hand neither (4.28) nor (4.30) hold with equality in general. For example, they do not hold for $G_0(3;2,9)$ and $H_0(2,4)$.

5. Optimality of Procedures R_0 and R_1

In this section we investigate lower bounds for the expected number of tests for any group testing procedure for the HB problem. In particular, we show that for $n = d+s_j$ with $d = 2$ and s_j in the infinite sequence (4.1), the result for $H_0(2,s)$ in (4.24) is equal to the lower bound and hence the procedure R_0 must be optimal for $s = s_j$ for any j.

The main technique used is the Huffman encoding scheme [4] which was originally devised to find an optimal code, i.e., a code that used the smallest expected number of letters in the encoding alphabet. In our application the encoding alphabet is binary (say, zeros and ones) since each test has 2 possible outcomes. Each sequence of test results (or zeros and ones) leading to a decision about the true state of nature is a code word. If the probabilities of the various possible states of nature are given then the Huffman scheme gives us a plan for finding the true state of nature with a minimum expected number of tests. This plan may or may not correspond to an "allowable procedure," i.e., in our case to a group-testing procedure.

It is well known that the Huffman scheme consists of (i) ordering the known probabilities (say, $p_1, p_2, \ldots, p_t$) associated with the t states of nature (we shall refer to these as "old" or"original" numbers), (ii) adding the two smallest and replacing them by their sum (which is the first "new" number), (iii) reordering the set of t-1 numbers and (iv) repeating the first three steps until a single "new" number equal to 1 remains. It is also well known that the sum of the "new" numbers, say $H^*(p_1, p_2, \ldots, p_t)$, is the required Huffman expected value for the optimal code or in our case the Huffman lower bound to the expected number of group tests for any group-testing procedure. Since the Huffman scheme may not yield a group-testing procedure this lower bound may not be attainable. It has been shown in [9] that for the BB problem the Huffman scheme in general does not yield a group-testing procedure and that the Huffman lower bound is in general not attainable.

It has also been pointed out, e.g., by C. Picard in [6] that any scheme of adding the p_i's two at a time can be regarded as a questionnaire for finding the true state of nature and that the sum of the probabilities associated with each question (or the sum of the "new" numbers) is its expected value. Hence we can regard the Huffman lower bound $H^*(p_1, p_2, \ldots,$ as the minimum value over all such "combining procedures" for the given vector $\vec{p} = (p_1, p_2, \ldots, p_t)$. It is slightly more convenient to drop the condition that the arguments be probabilities and consider the set of schemes for combining any set of nonnegative numbers $a_1, a_2, \ldots, a_t$ two at a time. Then $H^*(a_1, a_2, \ldots, a_t)$ is the sum of the new numbers for the Huffman scheme and gives the minimum sum over all such procedures since for any $A > 0$

$$(5.1) \qquad \frac{1}{A}H(a_1, a_2, \ldots, a_t) = H(\frac{a_1}{A}, \frac{a_2}{A}, \ldots, \frac{a_t}{A})$$

and, in particular, (5.1) holds for $A = a_1+a_2+\ldots+a_t$.

In our problem we shall be concerned with two Huffman lower bounds whi[ch] we denote as HLB(2,s) and $L_H(2,s)$ for $d = 2$. The former is the usual lower bound over those procedures which search out the defectives in a cert[ain] pattern. In the latter case the $L_H(2,s)$ is found as the sum of 2 quantiti[es] $L_H' + L_H''$, after assuming without any loss of generality that the units have been ordered. L_H' is the HLB for the initial subproblem of finding the position of the first defective and L_H'' is the expected value of the conditional HLB for finding the second defective given the position of the first defective. The value of L_H'' reduces to the usual HLB(d,s) with $d = 1$.

For our problem with $d = 1$ the value of t above is the same as the number of units remaining n and the (a posteriori) probabilities p_i are all equal to $1/n$. In this case the Huffman procedure is a group-testing procedure; namely, it is the halving procedure (as well as R_0 and R_1). It follows that $H^*(\frac{1}{n}, \frac{1}{n}, \ldots, \frac{1}{n}) = H_0(1,n-1) = H_1(1,n-1)$ (which we write as

H(1,n-1)) as given in (2.22) and, using (5.1) and the definition of h(n) in (2.13), we can write this as

$$H^*(1,1,\ldots,1) = H(n) \tag{5.2}$$

where n is the number of components on the left side of (5.2). For any d we have $f_d = \binom{n}{d}$ states of nature with equal probabilities $1/f_d$ for each and hence, writing f for f_2,

$$HLB(2,s) = H^*(\frac{1}{f}, \frac{1}{f}, \ldots, \frac{1}{f}) = \frac{h(f)}{f} . \tag{5.3}$$

We now can prove a main result of this paper as

<u>Theorem 1</u>: For any integer $j \geq 0$ the procedure R_0 for d = 2 and $s = s_j$ is optimal.

<u>Proof</u>: By property 2 in (4.8) the b-value for $f_j = \binom{s_j+2}{2}$ is j and hence, using (2.12) and (5.3),

$$HLB(2,s_j) = j+2 - \frac{2^{j+1}}{f_j} = H_0(2,s_j). \tag{5.4}$$

Since the HLB(2,s) is the "absolute" minimum it follows that for any integer s

$$HLB(2,s) \leq L_H(2,s) = L_H'(2,s) + L_H''(2,s). \tag{5.5}$$

We shall be interested to see whether equality holds in (5.5) for any s and to study the relation between HLB(2,s) and $H_0(2,s)$. To derive $L_H(2,s)$ we note that the probability that the first defective is in the i^{th} position is (s'+1-i)/f where $f = \binom{s'+1}{2}$ and hence

$$L_H(2,s) = H^*(\frac{1}{f}, \frac{2}{f}, \ldots, \frac{s'}{f}) + \sum_{i=1}^{s'} (\frac{s'+1-i}{f})H(1,s'-i) \tag{5.6}$$

$$= \frac{1}{f} \{H^*(1,2,\ldots,s') + \sum_{\alpha=2}^{s'} h(\alpha)\}$$

since h(1) = 0 and s' = s+1.

We now consider two lemmas for evaluating $H^*(1,2,\ldots,s')$ for any integer s'.

Lemmas 1: For $s' \equiv 0$ or $-1 \pmod 3$

$$(5.7) \qquad H^*(1,2,\ldots,s') = \frac{3}{2}\left[\frac{2s'}{3}\right]\left(\left[\frac{2s'}{3}\right]+1\right) + H^*\left(3\left[\frac{s'}{3}\right]+3, 3\left[\frac{s'}{3}\right]+6, \ldots, 3\left[\frac{2s'}{3}\right]\right)$$

and for $s' \equiv -2 \pmod 3$

$$(5.8) \qquad H^*(1,2,\ldots,s') = \frac{(s'-1)(2s'+1)}{3} + H^*(s', s'+2, s'+5, \ldots, 2s'-2);$$

here (5.8) agrees with (5.7) except for the "extra" component s' in the last term in (5.8).

Proof: Using induction it is easy to show that the "new" numbers up to 2s' form the arithmetic progression $3,6,9,\ldots, 3[\frac{2s'}{3}]$. In fact, if this were true for $s'_0 = 3r_0$ then on the next step we would add $(s'_0+1) + (s'_0+2) = 2s'_0+3 = 3[\frac{2s'}{3}] + 3$ and on the following step we would add an "old" s'_0+3 plus a "new" s'_0+3 giving $2s'_0+6$, which adds two "new" numbers to the same progression. Since this holds for $r_0 = 1$, yielding the new numbers 3 and 6, it holds for all $r_0 \geq 1$. For $s'_0 = 3r_0-1$ and $3r_0+1$ it is easy to see that essentially the same proof holds but in the former case the last number s'_0 is "used up," i.e., combined with another, whereas in the latter case the last number s'_0 is not "used up" and has to be included in subsequent combinations.

In (5.7) and (5.8) the first term represents the sum of the arithmetic progression from 3 to $3[\frac{2s'}{3}]$ and the last term represents the subsequent combinations. From the discussion above the subsequent combinations start with $3[\frac{s'}{3}]+3$ for the cases in (5.7) and with s' in the case of (5.8), using these numbers up to $[\frac{2s'}{3}]$ as originals. This proves lemma

Lemma 2: If $a_1, a_2, \ldots, a_u$ form an increasing arithmetic progression between any positive number and its double then

$$H^*(a_1, a_2, \ldots, a_u) = (v + 1)(a_1+\ldots+a_{2w}) + v(a_{2w+1}+\ldots+a_u) \tag{5.9}$$

where v and w are defined by

$$u = 2^v+w, \quad 0 \leq w < 2^v. \tag{5.10}$$

Proof: In this case the combining procedure forms a regular pattern and we can arrange the "new" sums in columns, starting a new column for each "new" sum containing a_1. If u is a power of 2 then every a_i appears exactly v times and (5.9) is clear. If it is not a power of 2 then we obtain v+1 columns and the number of sums in the c^{th} column is $[u/2^c]$ for $c = 1,2,\ldots,v$ and one sum equal to $\sum_{i=1}^{t} a_i$ in the last column.

In the first column a_u is "eligible" for omission (it is omitted if and only if u is odd). If it is omitted then it combines with a_1 in the second column and appears in each subsequent column, and the "new" sum $a_{u-2}+ a_{u-1}$ becomes eligible for omission in the second column. If a_u is not omitted in the first column then it combines with a_{u-1} and the "new" sum $a_{u-1}+ a_u$ is eligible for omission in the second column. In general, if any "new" sum with 2^{c-1} consecutive terms is omitted in the c^{th} column then in the next column it combines with a_1 and appears in each subsequent column; either this "new" sum terminates with a_t or all subsequent terms have been omitted in previous columns (and are now combined with a_1).

It follows from the above that

i) No a_i can be omitted in more than one column.

ii) The set of a_i that are omitted exactly once must form a "tail interval" of the form $a_i, a_{i+1}, \ldots, a_u$.

To complete the proof of the lemma we have to show that the number of a's omitted is u-2w where w is given by (5.10). The number of a's included in the "new" sums or in $H^*(a_1, a_2, \dots, a_u)$ is precisely $h(u) = H^*(1,1,\dots,1)$ with u components, which equals uv+2w. If we subtract this from u(v+1) we get the desired result. This completes the proof of lemma 2.

<u>Corollary 2</u>: If $\Delta > 0$ is the common difference of successive a's of lemma 2 and $0 \leqq \epsilon \leqq \Delta$ then

$$H^*(a_1 + \epsilon, a_2, a_3, \dots, a_t) = (v+1)\epsilon + H^*(a_1, a_2, \dots, a_t). \tag{5.11}$$

<u>Proof</u>: Since $E \leqq \Delta$ the pattern will not be affected and since E has to appear exactly the same number of times as a_1, thus proving the corollary.

We are now ready to apply these results to the three cases in lemma 1. We replace t by s' and use the symbols b and c defined in (2.11) by writing $s' = 2^b + c$. Let u_i denote the value of u if $s' \equiv i \pmod 3$ for i = 0, -1, -2 and define v_i and w_i similarly. Then

$$u_i = [\frac{s'+2}{3}] = \frac{s'-i}{3} \quad \text{and} \quad v_i = \begin{cases} b-2 & \text{if } s < 3.2^{b-1}+i \\ b-1 & \text{if } s' \geqq 3.2^{b-1}+i \end{cases} \tag{5.12}$$

and, of course, $w_i + 2^{v_i} = (s'-i)/3$.

It is clear that the arithmetic progression on the right side of (5.7) satisfies the conditions of lemma 2 since $t \leqq 3[\frac{t}{3}] + 3$ and $3[\frac{2t}{3}] \leqq 2t$; also the progression on the right side of (5.8) satisfies the condition in corollary 2 with $\epsilon = 1$. Substituting these sequences for $a_1, a_2, \dots, a_u$ in (5.9), we now compute the last term in (5.7) and (5.8) or $H^*(a_1, a_2, \dots, a_{u_i}) = H_i^*$(say) for i = 0, -1, -2 using (5.9), (5.11) and (5.12). For $2^b \leqq s' < 3.2^{b-2} + i$ we obtain for the last term in (5.7) and (5.8)

$$H_i^* = (b-1)\binom{s'+1}{2} + 3.2^{2b-3} - 3(2s'+1)2^{b-2} + \frac{(s'-i)(5s'+3+i)}{6} \tag{5.13}$$

and for $3.2^{b-2} + i \leqq s' < 2^{b+1}$ we similarly obtain

$$(5.14) \qquad H_i^* = b\binom{s'+1}{2} + 3.2^{2b-2} - (5s'+1)\, 2^{b-1} + \frac{(s'-i)(5s'+3+i)}{6}$$

with (5.13) and (5.14) giving equal results at $s' = 3.2^{b-2} + i$. If we now complete the evaluation of $H^*(1,2,\ldots,s')$ in (5.7) and (5.8) by adding on the first term then we obtain for each i the same result which we now state as

Theorem 2: For any integer $s' \geq 2$

$$(5.15) \qquad H^*(1,2,\ldots,s') = \begin{cases} (b+2)f + 3.2^{2b-3} - 3.2^{b-2}(2s'+1) & \text{for } 2^b \leq s' < 3.2^{b-1} \\ (b+3)f + 3.2^{2b-1} - 3.2^{b-1}(2s'+1) & \text{for } 3.2^{b-1} \leq s' < 2^{b+1} \end{cases}$$

where $f = \binom{s'+1}{2}$ and $b = b(s')$ is defined by (2.11).

Corollary: Using the result (5.15) it can be verified that for any integer $t \geq 2$

$$(5.16) \qquad H^*(1,2,\ldots,t) - H^*(1,2,\ldots,t-1) = h(t) + x_G(t;2)$$

and hence summing on t from 2 to s' gives

$$(5.17) \qquad H^*(1,2,\ldots,s') = \sum_{\beta=1}^{s} h(\beta+1) + \sum_{m=2}^{s'} x_G(m;2).$$

The proof of (5.17) is omitted.

In the rest of this section we shall prove that $L_H(2,s)$ in (5.6) with $H^*(1,2,\ldots,s')$ given by (5.15) is equal to $H_0(2,s)$; simultaneously we show that another expression $L_G(m;2,s)$, which we define below, is equal to $G_0(m;2,s)$. A by-product of this will be another main result that procedures R_0 and R_1 are identical.

Consider a subclass of group-testing procedures which give preference in any G-situation to partitioning the defective set and testing nested subsets in the defective set until a defective unit is found. We shall call these "non-mixing procedures" and denote the set of such procedures by $\mathcal{N}$, since they never mix units from a defective set and a remainder set. For example, the procedures R_1 and R_0 are both in $\mathcal{N}$.

The quantity $L_H(2,s)$ computed in (5.6) is a lower bound for any procedure in $\mathcal{R}$ if we start with an H-situation. Let $L_G(m;2,s)$ denote the corresponding lower bound if we start with a G-situation with parameters $(m;2,s)$. We again write $L_G(m;2,s)$ as the sum of two quantities, $L'_G(m;2,s) + L''_G(m;2,s)$ where the former is the lower bound for the subproblem of finding the first defective in the defective set and the latter is the expected value of the conditional lower bound for finding the second defective given the position of the first defective. For a G-situation the probability that the first defective is in the i^{th} position $(i=1,2,\ldots,m)$ is $(n-i)/F_m$ where $F_m = \binom{n}{2} - \binom{n-m}{2}$ and hence

$$(5.18)\qquad L_G(m;2,s) = H^*\left(\frac{n-m}{F_m}, \frac{n-m+1}{F_m}, \ldots, \frac{n-1}{F_m}\right) + \sum_{i=1}^{m} \left(\frac{n-i}{F_m}\right) H(1,n-i-1)$$

$$= \frac{1}{F_m}\left\{H^*(n-m,n-m+1,\ldots,n-1) + \sum_{\alpha=s'-m+1}^{s'} h(\alpha)\right\}.$$

If the condition of lemma 2 is satisfied then we obtain

$$(5.19)\qquad H^*(n-m,n-m+1,\ldots,n-1) = (v+1)\sum_{\alpha=1}^{2w} (s'-m+\alpha) + v \sum_{\alpha=2w+1}^{m} (s'-m+\alpha)$$

$$= \frac{mv}{2}(2s'+1-m) + (m-2^v)(2s'+1-2^{v+1})$$

where v is defined by writing $m = 2^v + w$ and $0 \leq w < 2^v$.

We now wish to show that the procedure R_0 satisfies both (5.6) and (5.18) and we do this by showing that $L_H(2,s)$ and $L_G(m;2,s)$ satisfy the basic recursion formulas (2.4) and (2.5) with x_H and x_G given by (3.1) and (4.13), respectively, as well as the boundary conditions (2.6), (2.7) and (2.8). With $b = b(s')$ defined as in (2.11), the right side of (2.4) gives

$$(5.20)\qquad 1 + \frac{\binom{n-x}{2}}{\binom{n}{2}} \frac{\{H^*(1,2,\ldots,s'-x) + \sum_{\alpha=2}^{s'-x} h(x)\}}{\binom{n-x}{2}} + \frac{F_x}{\binom{n}{2}} \frac{\{H^*(n-x,n-x+1,\ldots,s') + \sum_{\alpha=s'-x\ldots}^{s'} h(\ldots}{F_x}$$

$$= \frac{1}{\binom{n}{2}} \{H^*(1,2,\ldots,s'-x) + H^*(s'+1-x, s'+2-x,\ldots,s') + \binom{n}{2} + \sum_{\alpha=2}^{s'} h(\alpha)\},$$

where we have used the fact that the condition of lemma 2 is satisfied for the second term above. Suppose first that $3.2^{b-1} \leq s' < 2^{b+1}$ so that $x_H = 2^{b-1}$ and hence $2^b \leq s'-x_H < 3.2^{b-1}$. Then, using the top expression in (5.15) with s' replaced by s'-x and (5.19) with m replaced by x, we obtain for the sum of the first three terms in the last expression in (5.20)

$$\frac{1}{\binom{n}{2}} \{(b+2)\binom{s'+1-x}{2} + 3.2^{2b-3} - 3.2^{b-2}(2s'+1-2^b) + 2^{b-2}(b-1)(2s'+1-2^{b-1}) + \binom{n}{2}\}$$

$$= \frac{1}{\binom{n}{2}} \{(b+3)\binom{s'+1}{2} + 3.2^{2b-1} - 3.2^{b-1}(2s'+1)\} = \frac{H^*(1,2,\ldots,s')}{\binom{n}{2}}$$

which agrees with the left side of (2.4) using the 2nd expression for s' in (5.15). Similarly, if $2^b \leq s' < 3.2^{b-1}$ and $b \geq 2$ then $2^{b-2} \leq x_H = [\frac{s'+1}{2}] - 2^{b-2} < 2^{b-1}$ and $s'-x_H = [\frac{s'}{2}] + 2^{b-2}$; hence $3.2^{b-2} \leq s'-x_H < 2^b$, so that the b-value for $s'-x_H$ is b-1 and the v-value for x_H is b-2. The algebra is quite similar to the above (we omit the details) except that we consider two cases according as s' is odd or even; in both cases we get agreement with the upper value in (5.15).

To check (2.5) we note that the right side of (2.5) gives

$$(5.21) \qquad 1 + \left(\frac{F_m - F_x}{F_m}\right) \frac{\{H^*(s'-m+1, s'-m+2,\ldots, s'-x) + \sum_{\alpha=s'-m+1}^{s'-x} h(\alpha)\}}{F_m - F_x} + \frac{F_x}{F_m} \frac{\{H^*(s'-x+1, s'-x+2,\ldots, s') + \sum_{\alpha=s'-x+1}^{s'} h(\alpha)\}}{F_x}$$

and clearly we have only to show that

$$(5.22) \qquad H^*(s'-m+1,\ldots, s'-x) + H^*(s'-x+1,\ldots, s') + F_m = H^*(s'-m+1,\ldots, s')$$

for $x = x_G(m;2,s)$ given by (4.13). It is easily verified that the condition of lemma 2 is satisfied in all three terms above.

Suppose first that $2^{p-1} \leq m < 3.2^{p-2}$ so that $x_G = 2^{p-2}$ and $2^{p-2} \leq m-x_G < 2^{p-1}$, so that the v-value of $m-x_G$ is p-2. Then, applying (5.19) in (5.22) gives

$$F_m + \frac{(p-2)}{2}(m-2^{p-2})(2s'+1-m-2^{p-1})+(m-2^{p-1})(2s'+1-2^p)+2^{p-3}(p-2)(2s'+1-2^{p-2})$$

$$= \frac{m(p-1)}{2}(2s'+1-m) + (m-2^{p-1})(2s'+1-2^p),$$

which agrees with the right side of (5.19). In the second case $3.2^{p-2} \leq m < 2^p$ so that $x_G = m-2^{p-1}$. Hence $2^{p-2} \leq x_G < 2^{p-1}$. The algebra is again similar and is omitted.

To check the boundary conditions we find that (2.6) is trivially satisfied, (2.7) gives $h(s')/s'$ on both sides for d=2 by the definition of h(x) in (2.13), and (2.8) is concerned with the case d=1 where R_0 is known to be optimal. This completes the proof of

Theorem 3: Procedure R_0 is an optimal procedure in the subclass and $H_0(2,s)$ and $G_0(m;2,s)$ are given by (5.6) and (5.18), respectively for all allowable values of m and s.

By the definition of procedure R_1 in terms of recursion formulas and minimizing over the x-integers, it follows that R_1 must be the optimal procedure in the class η. The only assumption that could prevent R_1 from being optimal is that it is a non-mixing procedure. Hence, since procedure R_0 was shown to be optimal in η, it follows that the same result must hold for R_1, i.e., we obtain our final major result

Theorem 4: Procedure R_1 is equivalent to procedure R_0 if we start with an H-situation in the sense that they have the same expected number of tests and, if the x-values are unique, then they are identical.

Remark: We could not conclude the identity of procedures R_1 and R_0 in theorem 4 because the x_G and x_H-values under R_1 have not been shown to be unique. It is conjectured that they will always be unique if we start with an H-situation (or with any situation attainable from an H-situation). However it should be pointed out that for some unattainable G-situations the x_H-values under R_1 may not be unique and may even be different from that given by R_0 in (4.13). For example, we find under R_1 that $x_G(7;2,7) =$

$x_G(7;2,8) = 2$ and $x_G(7;2,9) = 2$ or 3 but under R_0 we have $x_G(7;2,8) = x_G(7) = 3$. These situation are unattainable if we start with an H-situation since by (3.2) we always have $m \leq (s+2)/4$.

6. Description of Tables

Table I gives the values for $H_1(d,s)$ for $d = 2$ and $s = 1(1)25$. Fractional values as well as their decimal equivalents are included here. The column headed min, max gives the minimum and maximum number of tests required by R_1. It would be of interest to prove that these values never differ by more than d (for any d) but this has not been shown. The fact that they never differ by more than 2 in Table I also indicates that the variance of the number of tests required by R_1 will be small. The lower bound HLB is also included.

Table II gives some similar information for d = 3, 4, and 5. We note that equalities between $H_1(d,s)$ and HLB(d,s) do not occur in this table for $s = 1(1)30$ as they did for $d = 2$ in Table I.

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Table I: Binomial and Hypergeometric Group Testing--The HB-problem

The Procedure# R_1, its Min, Max and Expected Number of tests and Lower Bounds to the Expected Number for any group-testing procedure.

(The number of defectives is 2 and the number of satisfactory units is s.)

H-SITUATION INFORMATION				LOWER BOUND INFORMATION	
s	Test Sizes† $x_H(2,s)$	Number of Tests Required: Min, Max	Number of Tests Required: Expected Value $H_1(2,s)$	Huffman Lower Bound HLB(2,s)	$H_1(2,s)$-HLB(2,s)
1*	1	1,2	5/3 = 1.667	5/3 = 1.667	0
2*	1	2,3	8/3 = 2.667	8/3 = 2.667	0
3*	1	3,4	17/5 = 3.400	17/5 = 3.400	0
4	2	3,5	4 = 4.000	59/15 = 3.933	1/15 = 0.067
5*	2	4,5	94/21 = 4.476	94/21 = 4.476	0
6	2	4,6	137/28 = 4.893	34/7 = 4.857	1/28 = 0.036
7	2	4,6	21/4 = 5.250	47/9 = 5.222	1/36 = 0.028
8*	3	5,6	251/45 = 5.578	251/45 = 5.578	0
9	3	5,7	323/55 = 5.873	321/55 = 5.836	2/55 = 0.037
10	4	5,7	135/22 = 6.136	200/33 = 6.061	5/66 = 0.075
11	4	5,7	497/78 = 6.372	248/39 = 6.359	1/78 = 0.013
12*	4	6,7	600/91 = 6.593	600/91 = 6.593	0
13	4	6,8	714/105 = 6.800	712/105 = 6.781	2/105 = 0.019
14	4	6,8	839/120 = 6.992	104/15 = 6.933	7/120 = 0.059
15	4	6,8	975/136 = 7.169	121/17 = 7.118	7/136 = 0.051
16	5	6,8	1123/153 = 7.340	1121/153 = 7.327	2/153 = 0.013
17*	5	7,8	1283/171 = 7.503	1283/171 = 7.503	0
18	6	7,9	1455/190 = 7.658	1454/190 = 7.653	1/190 = 0.005
19	6	7,9	1639/210 = 7.805	1634/210 = 7.781	1/42 = 0.024
20	7	7,9	1835/231 = 7.944	1823/231 = 7.892	4/77 = 0.052
21	7	7,9	2043/253 = 8.075	2021/253 = 7.988	2/23 = 0.087
22	8	7,9	2263/276 = 8.199	2248/276 = 8.145	5/92 = 0.054
23	8	7,9	2495/300 = 8.317	2488/300 = 8.293	7/300 = 0.023
24	8	7,9	2740/325 = 8.431	2738/325 = 8.425	2/325 = 0.006
25*	8	8,9	2998/351 = 8.541	2998/351 = 8.541	0

G-Situation Test Sizes†

m	1	2	3	4	5	6	7	8
$x_G(2;m)$	--	1	1	2	2	2	3	3

The results for procedure R_0 are the same as for procedure R_1.

† The values shown are all unique and they satisfy (3.1) and (4.13), respectively.

* Starred s-values are those in the infinite sequence (4.1).

Table II: Binomial and Hypergeometric Group Testing--The HB Problem

The Procedure R_1, its Expected Value

$H_1(d,s)$ and a Lower Bound HLB.

H-SITUATION INFORMATION

d = 3			d = 4			d = 5		
x_H	$H_1(d,s)$	HLB	x_H	$H_1(d,s)$	HLB	x_H	$H_1(d,s)$	HLB
1	2.2500	2.0000	1	2.8000	2.4000	1	3.3333	2.6667
1	3.5000	3.4000	1	4.2667	3.9333	1	5.0000	4.4762
1	4.4500	4.4000	1	5.3714	5.1715	1	6.2321	5.8571
1	5.2571	5.1714	1	6.3143	6.1714	1	7.2778	6.9841
1	5.9643	5.8571	1	7.1587	6.9841	1	8.2183	7.9841
2	6.5238	6.4762	1	7.9048	7.7810	1	9.0758	8.8918
2	7.0333	6.9333	2	8.5697	8.4485	1	9.8649	9.7071
2	7.4788	7.4485	2	9.1273	8.9657	1	10.5812	10.4087
2	7.9000	7.8364	2	9.6503	9.5678	2	11.2103	10.9770
2	8.2832	8.2098	2	10.1219	9.9770	2	11.7779	11.6360
3	8.6346	8.5934	2	10.5692	10.4996	2	12.3022	12.1246
3	8.9538	8.8747	2	10.9824	10.8747	2	12.7920	12.6761
3	9.2554	9.1714	2	11.3777	11.2790	2	13.2553	13.0878
4	9.5397	9.4941	3	11.7454	11.6614	2	13.6950	13.5910
4	9.7929	9.7451	3	12.0797	11.9432	2	14.1107	13.9433
4	10.0330	9.9432	3	12.4014	12.3092	2	14.5079	14.3897
4	10.2658	10.2035	3	12.7071	12.6312	3	14.8843	14.7557
4	10.4910	10.4601	3	12.9955	12.8801	3	15.2336	15.0524
4	10.7006	10.6701	4	13.2683	13.1497	3	15.5699	15.4581
4	10.9029	10.8436	4	13.5250	13.4581	3	15.8918	15.7665
4	11.1003	10.9881	4	13.7739	13.7048	3	16.1970	16.0074
5	11.2861	11.2192	4	14.0130	13.9041	3	16.4929	16.3764
5	11.4650	11.4246	4	14.2435	14.1329	4	16.7790	16.6663
5	11.6356	11.5997	4	14.4644	14.3996	4	17.0452	16.8963
6	11.8013	11.7497	4	14.6796	14.6204	4	17.3023	17.1605
6	11.9570	11.8790	4	14.8880	14.8043	4	17.5535	17.4572
6	12.1106	11.9911	4	15.0905	14.9586	4	17.7988	17.6982
6	12.2585	12.1776	5	15.2840	15.1775	4	18.0326	17.8955
7	12.3988	12.3484	5	15.4697	15.3984	4	18.2598	18.1158
7	12.5348	12.4986	5	15.6513	15.5869	4	18.4822	18.3850

G-Situation Test Sizes $x_G = x_G(m;d,s)$

d↓ \ m →	1	2	3	4	5	6	7
3	--	1	1	2	2	2	3
4	--	1	1	2	2		
5	--	1	1	2			

REFERENCES

[1] Bellman, R. E. and Gluss, B. (1961). On various versions of the defective coin problem. Information and Control 4 118-131.

[2] Cairns, S. S. (1963). Balance scale sorting. Amer. Math. Monthly 70 136-148.

[3] Erdos, Paul and Renyi, Alfred (1963). On two problems of information theory. Math. Inst. of Hung. Acad. Sci. 8 (Series A, Fasc. 1,2) 229-243.

[4] Huffman, D. A. (1952). A method for the construction of minimum redundancy codes. Proceedings I. R. E. 9 1098-1101.

[5] Lindstrom, B. (1965). On a combinatorial problem in number theory. Canad. Math. Bull. 8 477-490.

[6] Picard, Claude (1965). Theorie des Questionnaires. Gauthiers-Villars, Paris.

[7] Sobel, M. and Groll, P. A. (1959). Group testing to eliminate efficiently all defectives in a binomial sample. Bell System Tech. Journal 38 1179-1252.

[8] Sobel, M. (1960). Group testing to classify all defectives in a binomial sample. A chapter in Information and Decision Processes. 127-161. McGraw Hill, New York.

[9] Sobel, M. (1964). Optimal group testing. Stanford University Technical Report No. 72 1-57.

[10] Sobel, M. and Groll, P. A. (1966). Binomial group-testing with an unknown proportion of defectives. Accepted for publication in Technometrics.