Maximizing Irregularity and the Golomb Ruler Problem

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April 25, 1997

Abstract

The problem of attempting to construct radar signals whose ambiguity functions are sharply peaked in both time and frequency gives rise to a quantitative concept of the *irregularity* of a distribution of points. The problem of maximizing the irregularity of N points distributed on a bounded closed interval is here examined. A discrete mathematical tool for studying the irregularity function is developed — Pascal-like triangles constructed from non-negative integers obeying a particular addition rule. These triangles make explicit the structure of the irregularity function; all questions about the (continuous) irregularity function become questions about this integral construction, many of which can be answered easily and elegantly. One important question about the integral construction has been previously studied under the name of the *Golomb Ruler Problem*. It turns out that maximizing irregularity and constructing Golomb rulers are closely related problems, each providing a interesting new perspective from which to study the other.

1 Introduction

Quite recently, A. Grossmann introduced a canonical way of defining a continuous function that can be used to describe the "degree of irregularity" of a distribution of N points [1]. Such functions occur naturally in the search for radar or sonar signals with "optimal" autocorrelation properties. In this context, the N points naturally live in (some compact subset of) the 2-dimensional phase space. More generally, however, the problem of maximizing irregularity can be formulated as a point placement problem on any D-dimensional surface — subject to certain topological and group theoretic restrictions [1].

In the present work, we treat the simplest case of N points distributed on a bounded closed (1-dimensional) interval. In this case, one can define the "degree of irregularity" of a distribution of N points to be simply the *minimum difference of differences* attained among those N points. The result is a continuous function on the N-dimensional hypercube which, despite its deceptively simple definition, is surprisingly rich in structure. Exploring this structure by using the idea of "rulers", or representations of integers by differences is the unifying theme.

Reference [1] should be regarded as a companion paper to the present work. Although independent, that work contains two things which are of particular relevance. First, it contains the more general group-theoretic definition of *irregularity*, of which the present treatment is a special case. Secondly, it gives a detailed description of how the concept of irregularity arises naturally in radar theory, and can be used to construct signals with *ambiguity functions* which are sharply peaked in phase space. As this second item provides the primary motivation for the present work, we will provide a very brief summary. A clear introductory treatment of radar theory, which has more detailed explanations of the terminology and concepts used below, is given in reference [2].

Let $f \in L^2(\mathbb{R})$. The (narrowband) *ambiguity function* of f is defined to be the inner product of f with a copy of itself which has been shifted in both time and frequency. We define an operator which effects this time-frequency shift by

$$[E_{\tau,\omega} f](t) \equiv f(t-\tau)e^{-i\omega t}. \tag{1}$$

The ambiguity function of f is then

$$\begin{aligned} A_f(\tau,\omega) &\equiv (f, E_{\tau,\omega} f) \\ &= \int_{-\infty}^{\infty} dt\, f^*(t) f(t-\tau) e^{-i\omega t}. \end{aligned} \tag{2}$$

This function can be used to characterize the performance of the waveform $f(t)$ in radar and sonar applications. In particular, the shape of $A_f(\tau,\omega)$ near the origin determines the accuracy of time and frequency shift measurements using the waveform $f(t)$, and its ability to resolve closely spaced targets; therefore, we would like $A_f(\tau,\omega)$ to be as sharply "peaked" as possible. Due to the close relationship it bears with the Fourier transform, many simple properties of the ambiguity function can easily be proved [2]. For our purposes, the following two are most relevant:

$$|A_f(\tau,\omega)| \leq |A_f(0,0)|; \tag{3}$$

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\omega\, |A_f(\tau,\omega)|^2 = |A_f(0,0)|^2. \tag{4}$$

The first property says that the maximum value of $|A_f(\tau,\omega)|$ is attained at the origin. The second property says that the total volume under $|A_f(\tau,\omega)|^2$ is proportional to the square of this maximum value. Taken together, these two properties say roughly that any attempt to make the main lobe narrower must result in an increase of $|A_f(\tau,\omega)|$ somewhere else. This is a consequence of the Heisenberg uncertainty principle.

In an attempt to overcome the above constraint (in as much as this is possible), the following idea has been proposed. Suppose the signal f is actually a superposition of time and frequency shifted copies of some more basic function f_0; i.e.,

$$f = \sum_j E_{\tau_j,\omega_j} f_0. \tag{5}$$

The function f_0 may be, for example, a Gaussian.[1] We wish to express $A_f(\tau,\omega)$ in terms of $A_{f_0}(\tau,\omega)$. This is a straighforward calculation which uses the following two easily-proved properties of $E_{\tau,\omega}$:

$$\begin{aligned} E^*_{\tau,\omega} &= e^{i\omega\tau} E_{-\tau,-\omega}; & (6)\\ E_{\tau,\omega} E_{\tau',\omega'} &= e^{i\omega'\tau} E_{\tau+\tau',\omega+\omega'}. & (7) \end{aligned}$$

The result is

$$\begin{aligned} A_f(\tau,\omega) = \quad & A_{f_0}(\tau,\omega) \sum_j e^{i(\omega_j\tau-\omega\tau_j)} \\ + \quad & \sum_{j\neq k} e^{i(\omega_j\tau_j+\omega_k\tau-\omega\tau_j-\omega_k\tau_j)} A_{f_0}(\tau+\tau_k-\tau_j, \omega+\omega_k-\omega_j). \end{aligned} \tag{8}$$

The first term represents the main lobe, and is peaked at the origin as dictated by (3). The second term represents the sum of the sidelobes. These sidelobes are located at the *differences* of the original time and frequency shifts; i.e., whenever $(\tau,\omega) = (\tau_j - \tau_k, \omega_j - \omega_k)$. The idea is to assure that these sidelobes do not reinforce one another so that the ambiguity function $A_f(\tau,\omega)$ is, in effect, sharply peaked. This is achieved by choosing the time and frequency shifts (τ_j,ω_j) so as to minimize the overlap between the sidelobes. In other words, we wish to choose these coordinates in in such a way as to maximize the *minimum difference of differences*.[2] This is precisely our definition of *irregularity*. In accepting this discussion as our motivation for studying 1-dimensional irregularity, we ignore two important issues — the effect of the phase factors in equation (8) and the relationship between the 1-dimensional and 2-dimensional problems. These questions are addressed in the companion paper [1].

The *Golomb Ruler Problem*, simply stated, is to find the shortest possible "ruler" with n integral tick marks, which has the property that the distances measured between each pair of tick marks are distinct [3]. An excellent survey treatment of this problem is given in reference [4]. More generally, the problem falls under the study of *difference bases*; i.e., the representation of a set of numbers by differences of other numbers [5]. Golomb rulers and their generalizations are applicable in numerous and diverse areas of mathematics, physics, and electrical engineering — including graph theory, x-ray crystallography, radar pulse codes, and the efficient layout of electronic circuits [5, 6]. Despite this applicability, however, the amount of published literature on the subject is surprisingly small. Consequently, Golomb rulers seem to be periodically rediscovered [3], as happened in the case of the present work. As anyone who has "discovered" the first few Golomb rulers can

[1] It is easy to show that if f_0 is a Gaussian then $|A_{f_0}(\tau,\omega)|$ is a (2-dimensional) Gaussian.

[2] The maximum allowable values of τ_j and ω_j are determined by the constraint that the signal be physically realizable.

attest, the problem is intriguing independently of its potential for application. It is simply stated, easily explored, and possesses an inherent mathematical beauty [4].

Even from the qualitative definitions given above, it is clear that maximizing irregularity and finding Golomb rulers are closely related problems. This work explores the relationship between these two problems in detail. In the process of the exploration, it will become clear that Golomb rulers are an important tool for studying the continuous irregularity function. On the other hand, one may also regard the study of irregularity as a continuous analogue of the Golomb Ruler Problem. In this spirit, we postulate that the results developed herein will stimulate further progress in the search for new Golomb rulers.

We conclude this introduction by providing a road map through the rather lengthy discourse which is to follow. In Section 2, we formally define the N-point irregularity function in one dimension, discuss its symmetries and other structural properties, and explicitly compute it for the cases $N = 1$ and $N = 2$. It will become evident that, for larger values of N, an alternative approach to studying irregularity is needed. With this in mind, in Section 3, we formally map the study of the continuous irregularity function onto the study of integral "difference triangles", such as are used in studying Golomb rulers. In Section 4, we restate the Golomb Ruler Problem in terminology suitable for the subsequent analysis, and conjecture that maximizing irregularity and finding Golomb rulers are actually equivalent problems. We then turn our attention to interpreting and proving this equivalence conjecture. Section 5 details exactly what we mean by saying that maximizing irregularity and finding Golomb rulers are equivalent problems. In Section 6, we digress in order to study some properties of "difference triangles" which will be needed in the subsequent analysis.

Sections 7 and 8 are the focal point of the paper. Here, we develop the theory of local maxima of the irregularity function by using various ideas from convex analysis and the theory of integer linear programming. This will allow us to see under exactly which situations the two problems are equivalent or almost equivalent. This technical material is followed, in Section 9, by two illustrative examples.

In Section 10, we study a recursion relation obeyed by the irregularity function and note its consequences for both the continuous and discrete problems. Finally, for completeness, Section 11 discusses some simple bounds and algorithms closely related to the Golomb Ruler Problem. This section is important primarily in the application of irregularity to constructing sharply peaked ambiguity functions, as discussed in reference [4].

2 Irregularity in One Dimension

2.1 Definition and Symmetries

Motivated by the preceding discussion and following Grossmann [1], we begin by attaching a precise definition to the intuitive concept of *irregularity*. The basic idea is to place N points on a line in such a way as to maximize the minimum difference of differences. Clearly this problem can only have a solution if the points are confined to a bounded interval; therefore, we proceed as follows. Let $x \in [0,1]^N$ and put $x_0 = 0$ and $x_{N+1} = 1$. We wish to consider the set of differences between any two distinct components of x or endpoints, and enumerate the set of functions measuring the difference between any two distinct elements of this set; i.e., the set of functions measuring the difference of differences.

This set of functions is simply

$$f_{i,j,k,l}(x) \equiv \Big| |x_i - x_j| - |x_k - x_l| \Big|; \qquad i \neq j,\ k \neq l,\ (i,j) \neq (k,l); \tag{9}$$

where $0 \leq i, j, k, l \leq N+1$. Intuitively, one would expect the *irregularity* of a distribution of points to be large provided that none of the functions defined by equation (9) is too small. Accordingly, the N-point irregularity function $F_N(x)$ is defined to measure the worst case scenario; i.e.,

$$F_N(x) \equiv \min f_{i,j,k,l}(x), \tag{10}$$

the minimum being taken over the set of all functions $f_{i,j,k,l}(x)$ in equation (9). The N-point irregularity function $F_N(x)$ is therefore a continuous piecewise-linear function on the N-dimensional hypercube. The fundamental problem which is to be addressed is to maximize $F_N(x)$. We state this problem formally as

Problem 1 *For a given N, find all global maxima of the N-point irregularity function $F_N(x)$.*

It will be seen that what makes this problem interesting and nontrivial is the extremely rapid rate at which the number of local maxima of $F_N(x)$ grows with N.

The N-point irregularity function has two simple symmetries. First, the definition of $F_N(x)$ is manifestly symmetric under the interchange of any two components of x. This invariance will be referred to as the *permutation symmetry.* In light of this symmetry, it is sufficient to study the behavior of $F_N(x)$ on the restricted domain

$$\Big\{ x \in [0,1]^N \ \Big|\ x_1 \leq \ldots \leq x_N \Big\}. \tag{11}$$

This defines an N-dimensional simplex which will be called the *ordered-x simplex.*

Secondly, it is intuitively obvious that the "mirror image" of a distribution of points should have the same irregularity as the distribution itself. In order to make this more precise, for any point x in the ordered-x simplex define x^* by

$$(x_1,\ \ldots,\ x_N)^* \equiv (1 - x_N,\ \ldots,\ 1 - x_1). \tag{12}$$

It is then easy to see that x^* is also in the ordered-x simplex and that $F_N(x) = F_N(x^*)$. We will call x^* the *conjugate* of x (since, for example, $x^{**} = x$) and the associated invariance the *conjugate symmetry.* If $x_1 \leq 1 - x_N$ then trivially $x_1^* \geq 1 - x_N^*$, thus the conjugate symmetry can be eliminated by enforcing the former inequality. It is therefore sufficient to study the behavior of $F_N(x)$ on the additionally restricted domain

$$\Big\{ x \in [0,1]^N \ \Big|\ x_1 \leq \ldots \leq x_N \leq 1 - x_1 \Big\}. \tag{13}$$

This is again an N-dimensional simplex and will be referred to as the *conjugate-free* ordered-x simplex. The full N-dimensional hypercube is composed of $2 \cdot N!$ copies of this simplex, on each of which $F_N(x)$ exhibits the exact same behavior.

2.2 Counting Component Functions

Having restricted the domain of $F_N(x)$ as much as possible, it is natural to ask how many of the component functions $f_{i,j,k,l}(x)$ actually contribute to $F_N(x)$ on the resulting simplexes. In other words, we wish to enumerate a minimal set of functions $f_{i,j,k,l}(x)$ which are sufficient to construct $F_N(x)$. An obvious practical benefit of this enumeration is that it will allow one to calculate $F_N(x)$ efficiently. In the present section, this problem will be solved somewhat heuristically (but nonetheless correctly). The justification for the assertions made herein will be a consequence of the analysis contained in subsequent sections.

The number of component functions which contribute to $F_N(x)$ can be counted by using elementary combinatorics together with the following two observations, which are direct consequences of equation (10). Firstly, if a component function is dominated by some other component function on the entire domain of consideration, the dominating function certainly does not contribute to $F_N(x)$. Secondly, if a particular component function vanishes on some subset of the domain of consideration, then (roughly speaking) this component function determines $F_N(x)$ near these zero sets. With these two observations in mind, we first consider the ordered-x simplex. On this domain, the set of functions defined by equation (9) reduces immediately to

$$f_{i,j,k,l}(x) = |x_i - x_j - x_k + x_l|; \qquad i > j,\ k > l,\ (i,j) \neq (k,l). \tag{14}$$

There are then three mutually exclusive and exhaustive possibilities.

The first possibility is that some component of x inside the absolute value in equation (14) is repeated with the opposite sign. This gives rise to $\binom{N+2}{2}$ distinct component functions corresponding to the choice of the remaining two points. However, by the first observation above, the minimum in equation (10) can only be attained by one of the $N+1$ elementary differences

$$x_i - x_{i-1}, \qquad 1 \leq i \leq N+1. \tag{15}$$

These $N+1$ component functions are significant in that setting each one to zero determines a *facet* [7] of the ordered-x simplex. This means that the N-point irregularity function $F_N(x)$ vanishes on the boundary of the ordered-x simplex, which in turn implies (by the second observation above) that sufficiently close to one of the facets, the minimum in equation (10) is determined by the corresponding component function (15).

The second possibility is that some component of x inside the absolute value in equation (14) is repeated with the same sign. This gives rise to $\binom{N+2}{3}$ distinct component functions which can be enumerated as

$$|x_i - 2x_j + x_l|, \qquad 0 \leq l < j < i \leq N+1. \tag{16}$$

It is not difficult to see that the zero set of each of these component functions intersects the interior of the ordered-x simplex; and therefore, each function contributes to $F_N(x)$.

The third and final possibility is that all four components of x inside the absolute value in equation (14) are distinct. This gives rise to $\binom{N+2}{4}$ distinct component functions which can be enumerated as

$$|x_i - x_j - x_k + x_l|, \qquad 0 \leq l < k < j < i \leq N+1. \tag{17}$$

As before (by the second observation above), each of these functions must contribute to $F_N(x)$. The third possibility also forces one to consider component functions of the form

$$|x_i - x_j + x_k - x_l|, \qquad 0 \leq l < k < j < i \leq N+1. \tag{18}$$

However,

$$\begin{aligned} |x_i - x_j + x_k - x_l| &= |x_i - x_j| + |x_k - x_l| \\ &\geq \big||x_i - x_j| - |x_k - x_l|\big| \\ &= |x_i - x_j - x_k + x_l|; \end{aligned} \tag{19}$$

therefore, the first observation implies that these functions cannot contribute to $F_N(x)$.

Summarizing, in addition to the $N+1$ "facet functions" given by (15), there are

$$\binom{N+2}{3} + \binom{N+2}{4} = \binom{N+3}{4} \tag{20}$$

component functions given by equations (16) and (17) which contribute to $F_N(x)$ on the ordered-x simplex. With this in mind, one can now ask how this set of component functions is further reduced when one restricts x to the *conjugate-free* ordered-x simplex; i.e., when the condition $x_1 \leq 1 - x_N$ is enforced. In this case,

$$|1 - x_N - x_1| = 1 - x_N - x_1 \leq 1 - x_N, \tag{21}$$

which means that $|1 - x_N - x_1|$ (given by equation (17) with $i = N+1$, $j = N$, $k = 1$, and $l = 0$) becomes a facet function replacing $1 - x_N$ (given by equation (15) with $i = N+1$), thus reducing the total number of component functions by one. This implies that $F_N(x)$ vanishes on the boundary of the conjugate-free ordered-x simplex as well. In addition, we have

$$0 \leq 1 - x_N - x_1 \leq 1 - x_j - x_1 = |1 - x_j - x_1|, \qquad 1 \leq j \leq N-1; \tag{22}$$

which results in a further reduction of $N-1$ component functions, making the total reduction N relative to the previous count. Each of the remaining component functions has a zero set which intersects the interior of the conjugate-free ordered-x simplex; and therefore, each contributes to $F_N(x)$ on this domain.

2.3 The Cases $N = 1$ and $N = 2$

The concepts and terminology presented in the previous section will now be elucidated. First, the simplest two cases, $N = 1$ and $N = 2$, will be treated more or less completely. Secondly, the cases $N = 3$ and $N = 6$ will be briefly examined in order to illustrate how rapidly the complexity of the problem increases with N. Again, the present treatment is heuristic and intuitive; the more formal treatment is presented in the following sections.

We begin with the case $N = 1$. As x has only one component, the ordered-x simplex is the entire interval $[0, 1]$. According to the arguments in the preceding section, there are $N+1 = 2$ facet functions and $\binom{N+3}{4} = 1$ additional component function which contribute to $F_1(x)$. These are easily determined from equations (15) and (16) so that the 1-point irregularity function is just

$$F_1(x) = \min \left\{ \begin{array}{c} x \\ 1 - x \\ |1 - 2x| \end{array} \right\}. \tag{23}$$

The graph of this function is shown in Figure 1. The three points where $F_1(x) = 0$ (two of which determine the facets of the ordered-x simplex) are just the zeros of the three component functions. It is trivial to show (and evident from Figure 1) that there are two solutions to Problem 1: $x = 1/3$ or $x = 2/3$. These two solutions are conjugates of one another. The conjugate-free ordered-x simplex is obtained by enforcing the condition $x \leq 1 - x$; i.e., $x \leq 1/2$. In this interval, the irregularity function is simply

$$F_1(x) = \min \left\{ \begin{array}{c} x \\ 1 - 2x \end{array} \right\} \tag{24}$$

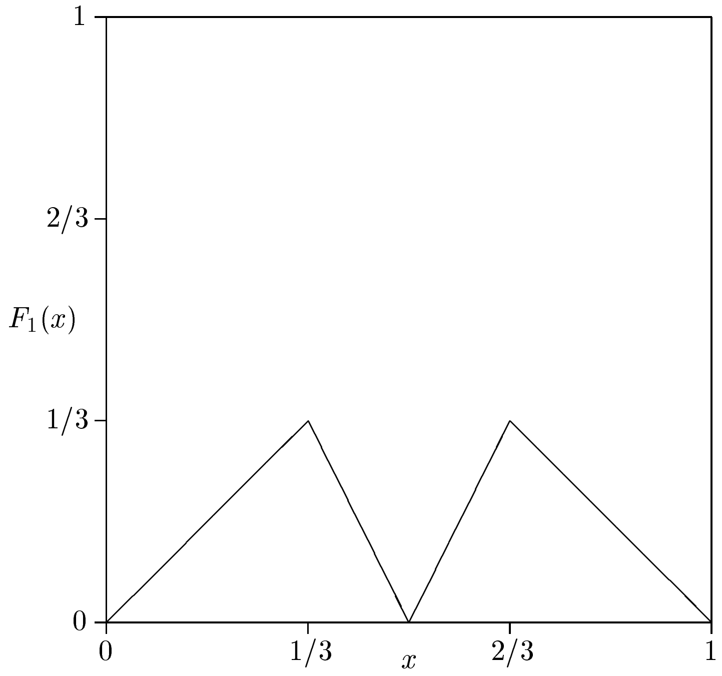

Figure 1: $N = 1$ Irregularity Function

and the solution to Problem 1 is unique.

For $N = 2$, the irregularity function starts to become interesting; the graph of $F_2(x)$ on $[0,1] \times [0,1]$ is shown in Figure 2. The ordered-x simplex is the triangular region $0 \le x_1 \le x_2 \le 1$. According to the arguments in the preceding section, there are $N+1 = 3$ facet functions and $\binom{N+3}{4} = 5$ additional component function which contribute to $F_2(x)$ on the ordered-x simplex. By using equations (15), (16), and (17) to determine these functions, the 2-point irregularity function can be written as

$$F_2(x) = \min \left\{ \begin{array}{l} x_1 \\ x_2 - x_1 \\ 1 - x_2 \\ |x_2 - 2x_1| \\ |1 - 2x_1| \\ |1 - 2x_2| \\ |1 - 2x_2 + x_1| \\ |1 - x_2 - x_1| \end{array} \right\}. \tag{25}$$

The zero sets of the first three component functions (those with no absolute-value sign) are just the three boundary lines of the ordered-x simplex. The zero sets of the remaining five component functions coincide with the five white lines which can be seen intersecting the interior of the ordered-x simplex in Figure 2. The conjugate-free ordered-x simplex is the lower half of the ordered-x simplex; i.e., the triangular region $0 \le x_1 \le x_2 \le 1 - x_1$.

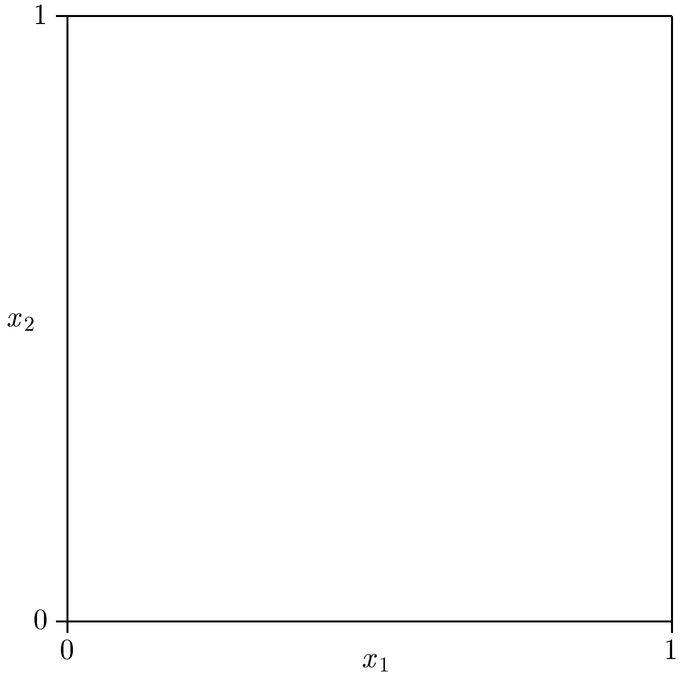

Figure 2: $N = 2$ Irregularity Function

According to the above analysis, $F_2(x)$ restricted to this domain simplifies to

$$F_2(x) = \min \left\{ \begin{array}{l} x_1 \\ x_2 - x_1 \\ 1 - x_2 - x_1 \\ |x_2 - 2x_1| \\ |1 - 2x_2| \\ |1 - 2x_2 + x_1| \end{array} \right\}. \tag{26}$$

As in the previous case, the zero set of each of these component functions is a line — which either determines a boundary or intersects the interior of the simplex under consideration. Again, this correspondence can easily be seen from Figure 2. By using this minimal set of six component functions (and with the help of Figure 2), the existence of five local maxima of $F_2(x)$ in the conjugate-free ordered-x simplex can be verified and their values can be calculated and compared. The largest of these (determined by the intersection of x_1, $1-x_2-x_1$, and $-1+2x_2-x_1$) occurs at $x = (1/6, 2/3)$ where the irregularity function takes on a value of $1/6$. This is the solution to Problem 1 for the case $N = 2$. Like the case $N = 1$, the solution is unique on the conjugate-free ordered-x simplex.

For $N \geq 3$, the brute-force procedure used above for solving Problem 1 is no longer practical. A slice of the graph of $F_3(x)$ with x_3 fixed is shown in Figure 3. The value of x_3 was chosen so that four global maxima are visible. We here state without justification that, within the conjugate-free ordered-x simplex alone, $F_3(x)$ possesses sixty-one local maxima and *two* distinct global maxima, so the solution to Problem 1 is no longer unique. These two global maxima occur at $x = (1/11, 4/11, 9/11)$ and $(2/11, 7/11, 8/11)$ where the irregularity function takes on a value of $1/11$. The two darkest "pyramids" in the region $x_1 \leq x_2$ of Figure 3 depict the global maxima occurring at $x = (1/11, 4/11, 9/11)$

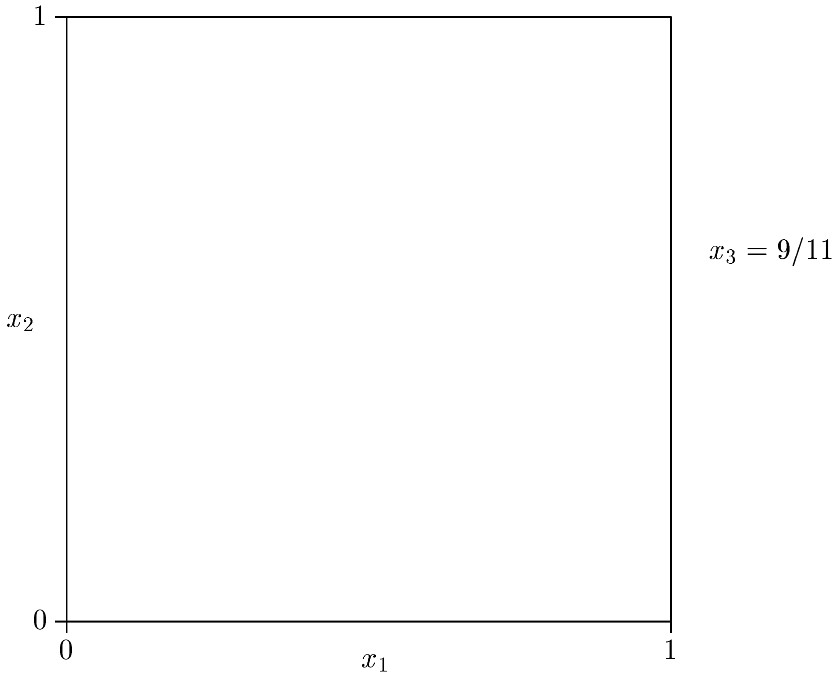

Figure 3: $N = 3$ Irregularity Function

and $(3/11, 4/11, 9/11)$, the conjugate of the second point above. This example illustrates the tremendous difference in complexity between the $N = 2$ and the $N = 3$ irregularity functions.

As N continues to increase, the number of local maxima of the N-point irregularity function $F_N(x)$ grows extremely rapidly. As a final example, a slice of the graph of $F_6(x)$ with x_3, x_4, x_5, and x_6 fixed is shown in Figure 4. In this case, Problem 1 again has a unique solution on the conjugate-free ordered-x simplex (which can be seen in Figure 4); however, the number of local maxima is not yet known.

From these examples, the need for an alternative approach to studying irregularity is evident. This alternative approach is developed in the remainder of the paper.

3 The N-Triangle Bijection

Because $F_N(x)$ is piecewise linear, all local maxima (as well as all other points at which the behavior of $F_N(x)$ is "interesting") occur at the intersection of at least $N + 1$ hyperplanes (of dimension N). The components of x at all such points of intersection must be rational, as the coefficient of each x_i in the equation defining each intersecting hyperplane can only be 0, ± 1, or ± 2. More formally, we will see that the *hypograph* [8] of $F_N(x)$ is the union of suitably defined, manifestly rational polyhedra; so that the points at which the behavior of $F_N(x)$ is "interesting" are precisely the vertices of these polyhedra. Consequently, it is sufficient to study the behavior of $F_N(x)$ on the *rational* ordered-x simplex, which will be denoted by X_N; i.e.,

$$X_N \equiv \Big\{ x \in \mathbb{Q}^N \;\Big|\; 0 \le x_1 \ldots \le x_N \le 1 \Big\}. \tag{27}$$

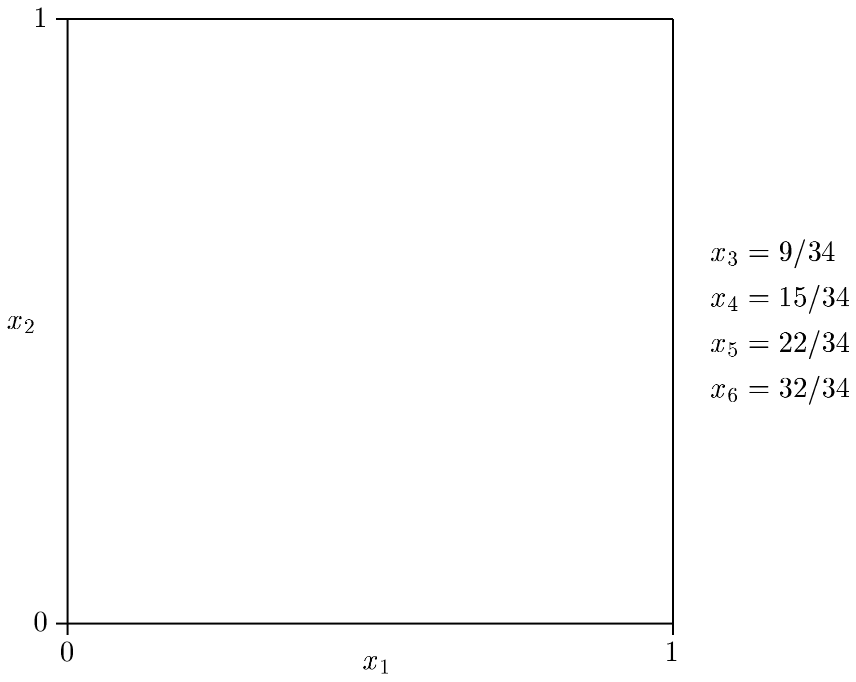

Figure 4: $N = 6$ Irregularity Function

Suppose $x \in X_N$. There are $\binom{N+2}{2}$ distinct positive differences $x_i - x_j$ (including the trivial difference $x_{N+1} - x_0 = 1$). These are conveniently tabulated in a triangular format as shown in Figure 5. Note that each entry in the triangle is the sum of adjacent elementary differences in the first column. For example,

$$x_3 = x_1 + (x_2 - x_1) + (x_3 - x_2). \tag{28}$$

When the differences are displayed in this format, $F_N(x)$ is (by definition) just the minimum positive difference between any two entries in the triangle. Thus, instead of studying the behavior of $F_N(x)$ on X_N, one can study the properties of this triangular construction.

We take this idea one step further. As all of the entries in the triangle of Figure 5 are rational, they can be normalized to integers by multiplying through by the least common denominator. Therefore, with proper bookkeeping, it is sufficient to restrict the study of the above construction to those triangles with integral entries. Accordingly, we define a space of integral vectors corresponding to the integer-normalized elementary differences and denote this space by P_N; i.e.,

$$P_N \equiv \left\{ p \in \Big[\{0\} \cup \mathbb{N}\Big]^{N+1} \,\Big|\, p \neq 0 \right\}. \tag{29}$$

If $p \in P_N$, we will call p an *N-triangle generator* or simply a *generator*. For a given generator p, we define its *N-triangle expansion* by

$$p_{i,j} \equiv \sum_{k=i}^{j} p_k, \qquad 0 \leq i \leq j \leq N. \tag{30}$$

This expansion is shown explicitly in Figure 6. Loosely, we will refer to either an N-

$$
\begin{array}{llllll}
x_1 & & & & & \\
 & x_2 & & & & \\
x_2 - x_1 & & x_3 & & & \\
 & x_3 - x_1 & & & & \\
x_3 - x_2 & & & & & \\
 & & & & x_N & \\
\vdots & \vdots & \vdots & \cdots & & 1 \\
 & & & & 1 - x_1 & \\
x_{N-1} - x_{N-2} & & & & & \\
 & x_N - x_{N-2} & & & & \\
x_N - x_{N-1} & & 1 - x_{N-2} & & & \\
 & 1 - x_{N-1} & & & & \\
1 - x_N & & & & &
\end{array}
$$

Figure 5: Differences Displayed in Triangular Format

triangle generator p or its N-triangle expansion $p_{i,j}$ as simply an *N-triangle.* The addition law (30) can be written in a "local" form provided that $p_{i,j}$ is taken to be zero when $i > j$, namely

$$p_{i,j} = p_{i,j-1} + p_{i+1,j} - p_{i+1,j-1}, \qquad 0 \le i < j \le N. \tag{31}$$

This version will sometimes be more convenient.

The correspondence between the spaces X_N and P_N will be exploited throughout the remainder of the paper, thus it will now be made explicit. Proceeding formally, we define a mapping $T : X_N \to P_N$ by

$$p_j = C_x(x_{j+1} - x_j), \qquad 0 \le j \le N; \tag{32}$$

where

$$C_x = \text{LCD } (x_1, \dots, x_N). \tag{33}$$

We will call T the *N-triangle bijection*; the name will be justified by Theorem 3.1. From the definition of T it follows that, if $x \in X_N$ and $p = T(x)$, the components of p are relatively prime. Therefore, in order for T to be surjective, it will be necessary to regard all N-triangles which differ only in normalization as being equivalent.

Definition 3.1 *Let $p, q \in P_N$. Then p and q are said to be equivalent (written as $p \approx q$) whenever $\exists m, n \in \mathbb{N} \mid mp = nq$.*

With this definition, it is easy to see that there is a unique member of each $\approx$-equivalence class whose components are relatively prime. However, dealing with $\approx$-equivalence classes rather than these canonical representatives will eliminate the cumbersome task of checking for relative primeness. This is illustrated by the following theorem, which is also of fundamental importance.

Theorem 3.1 *The mapping T is a bijection from X_N onto $\approx$-equivalence classes of P_N.*

Proof

We first prove injectivity. Let $x, y \in X_N$ and suppose $T(x) \approx T(y)$. According to equation (32) and Definition 3.1, this implies that $\exists m, n \in \mathbb{N}$ such that

$$mC_x(x_{j+1} - x_j) = nC_y(y_{j+1} - y_j), \qquad 0 \le j \le N. \tag{34}$$

$$
\begin{array}{cccccc}
p_{0,0} & & & & & \\
 & p_{0,1} & & & & \\
p_{1,1} & & p_{0,2} & & & \\
 & p_{1,2} & & & & \\
p_{2,2} & & & & & \\
 & & & & p_{0,N-1} & \\
\vdots & \vdots & \vdots & \cdots & & p_{0,N} \\
 & & & & p_{1,N} & \\
p_{N-2,N-2} & & & & & \\
 & p_{N-2,N-1} & & & & \\
p_{N-1,N-1} & & p_{N-2,N} & & & \\
 & p_{N-1,N} & & & & \\
p_{N,N} & & & & &
\end{array}
$$

Figure 6: N-triangle expansion of p

Summing both sides of this equation for $0 \le j \le i-1$ yields

$$mC_x x_i = nC_y y_i, \qquad 1 \le i \le N+1. \tag{35}$$

Putting $i = N+1$ then implies $mC_x = nC_y$, which in turn implies $x = y$.

The proof of surjectivity is equally simple. Let $p \in P_N$ and define

$$x_i = p_{0,i-1} \,/\, p_{0,N}, \qquad 1 \le i \le N. \tag{36}$$

Note that this defines the same $x \in X_N$ for all members of a particular equivalence class. Substituting into equation (32) yields

$$[T(x)]_j = C_x \frac{p_{0,j} - p_{0,j-1}}{p_{0,N}} = C_x \frac{p_j}{p_{0,N}}. \tag{37}$$

Therefore $p_{0,N}\, T(x) = C_x\, p$ which, by Definition 3.1, implies $T(x) \approx p$. Both parts of the proof make use of the fact that equation (36) is an explicit formula for the mapping $T^{-1} : P_N \to X_N$.

$\square$

We remark that if x^* is the conjugate of x and $p^* = T(x^*)$ then

$$p^*_{i,j} = p_{N-j,N-i} \tag{38}$$

so that a given N-triangle can be regarded as representing both x and x^*.

Theorem 3.1 allows one to study subsets of X_N on which $F_N(x)$ possesses some property of interest by studying the corresponding subsets of P_N. With Problem 1 in mind, we define the following subsets of X_N:

$$X'_N \equiv \left\{ x \in X_N \;\middle|\; F_N(x) > 0 \right\} \tag{39}$$

$$X''_N \equiv \left\{ x \in X_N \;\middle|\; x \text{ is a local maximum of } F_N(x) \right\} \tag{40}$$

$$X'''_N \equiv \left\{ x \in X_N \;\middle|\; x \text{ is a global maximum of } F_N(x) \right\} \tag{41}$$

and remark that $X_N \supset X'_N \supset X''_N \supset X'''_N$. We then seek a concise description of the image of each of these subsets under the N-triangle bijection T. The first of these, as given by the following definitions and theorem, is trivial.

Definition 3.2 *Let $p \in P_N$. Then p is said to be <u>Good</u> whenever*

$$p_{i,j} = p_{k,l} \Longleftrightarrow (i,j) = (k,l); \qquad \forall i,j,k,l.$$

In other words, p is Good if and only if all of the elements in its N-triangle expansion are distinct. We capitalize "Good" in order to distinguish the technical meaning from the everyday usage, and will use this convention with other adjectives as well. Define

$$P'_N \equiv \left\{ p \in P_N \;\middle|\; p \text{ is Good} \right\}. \tag{42}$$

We then have the following theorem.

Theorem 3.2 *The mapping T restricted to X'_N is a bijection from X'_N onto $\approx$-equivalence classes of P'_N.*

<u>Proof</u>

As previously mentioned, $F_N(x)$ is (by definition) just the minimum positive difference between any two entries in the triangle of Figure 5. Thus $F_N(x) > 0$ if and only if all of these entries are distinct. On the other hand, $p = T(x)$ is Good if and only if all of the entries in its N-triangle expansion (shown in Figure 6) are distinct. Since these two triangles differ only in normalization, the theorem follows immediately.

□

This theorem may be abbreviated as $T(X'_N) \approx P'_N$ while keeping in mind that injectivity is inherited from the injectivity of T on the larger domain X_N. In the following sections, statements similar to Theorem 3.2 will be abbreviated in this way.

4 The Perfect N-Triangle Problem

Our primary objective is to solve Problem 1. In this section, we propose (without formal justification) a solution to this problem and examine some of its consequences. Beginning in the next section, we consider the issues involved in actually proving that our solution is valid. As a by-product of these considerations, we will gain a rather detailed understanding of the irregularity function $F_N(x)$.

In light of Theorem 3.1, solving Problem 1 is equivalent to calculating $T(X'''_N)$ as a subset of P_N. Since $X'''_N \subset X'_N$, Theorem 3.2 implies that $T(X'''_N)$ should actually be a subset of the class of Good N-triangles P'_N.

Let $p \in P_N$ and $x = T^{-1}(p)$. With reference to the discussion following equation (27), note that $F_N(x)$ can be calculated by first dividing each element of the N-triangle by $p_{0,N}$, and then calculating the minimum positive difference between any two entries in the resulting triangular array. This array is just the differences $x_i - x_j$ displayed in triangular format, as shown in Figure 5. Evidently, the N-triangle element $p_{0,N}$ is of particular importance; therefore, for any $p \in P_N$, we define its *trace* to be

$$\operatorname{Tr} p \equiv \sum_{k=0}^{N} p_k \ (= p_{0,N}). \tag{43}$$

The terminology is appropriate, since $\operatorname{Tr} p$ is the sum of the "diagonal" ($i = j$) elements of the N-triangle expansion $p_{i,j}$. If p is Good then, loosely speaking, the smaller $\operatorname{Tr} p$ is, the larger $F_N(x)$ will be. It is therefore natural to ask how small of a trace can be attained subject to the constraint that p must be Good. We will denote this minimal value of the trace by D_N, and those Good N-triangles which satisfy $\operatorname{Tr} p = D_N$ will be called *Perfect* N-triangles. We formalize this concept with the following definition.

Definition 4.1 *Let $p \in P'_N$. Then p is said to be* <u>*Perfect*</u> *whenever*

$$\operatorname{Tr} p \leq \operatorname{Tr} q, \qquad \forall q \in P'_N.$$

Thus D_N is the common trace of all Perfect N-triangles. Define

$$P'''_N \equiv \left\{ p \in P_N \;\middle|\; p \text{ is Perfect} \right\}. \tag{44}$$

As the number of partitions of D_N is finite, so must be the cardinality of P'''_N. The problem of actually computing the elements of P'''_N will be formally called the Perfect N-Triangle Problem.

Problem 2 *For a given N, find all Perfect N-triangles.*

In contrast to Problem 1, this problem is purely combinatorial. Nevertheless, the main proposition of the present work is that these two problems are, in fact, equivalent. More precisely, we propose the following conjecture.

Conjecture 1

$$T(X'''_N) \approx P'''_N.$$

This assertion turns out to be trivial for $N = 1$ and $N = 2$ and can been proved by brute force for $N = 3$ and $N = 4$ (see Appendix B). The majority of the remainder of this work is devoted to the development of ideas pertaining to the proof for arbitrary N.

Assume for the moment that Conjecture 1 is true. Then Problem 1 is equivalent to the purely combinatorial Problem 2. Indeed, given a Perfect N-triangle p, one can simply read off the corresponding value of x (at which $F_N(x)$ attains a global maximum) from its upper diagonal according to equation (36). The strength of this statement can be appreciated by considering the first few values of N.

Appendix A lists all Perfect N-triangles (modulo conjugacy) for $N \leq 9$. Even without the assistance of a computer, this list can be verified for $N = 1$, 2, 3, 4, and perhaps $N = 5$. The cases $N = 1$ and $N = 2$ are quite trivial; it requires only a few seconds thought to write down a solution to Problem 2 and verify its uniqueness. This should be contrasted with the (relatively) complicated analysis of Section 2.3.

For $N = 3$, the difference in the amount of work involved is even more dramatic. It is easy to verify that if the generator p is any permutation of $\{1, 2, 3, 4\}$, the N-triangle is not Good.[3] The next best possibility is a permutation of $\{1, 2, 3, 5\}$; there are two such permutations (modulo conjugacy) which yield Perfect N-triangles. Thus $F_3(x)$ possesses two distinct global maxima within the conjugate-free ordered-x simplex, in accordance

[3] Clearly, the 1 cannot be adjacent to the 2 or 3; therefore, the 1 must be at the end of the generator and adjacent to the 4. But then the N-triangle expansion contains two 5's.

with the discussion of Figure 3. The proof of this fact by direct analysis of the irregularity function $F_3(x)$ would require determining which hyperplanes intersect to form each of the 61 local maxima, calculating each point of intersection and the corresponding value of $F_3(x)$, and comparing these values to determine which are the global maxima — a formidable task in comparison to the Perfect N-triangle approach.

Problem 2 has been previously studied under the name of the *Golomb Ruler Problem* [3, 4]; a Golomb ruler with $N+2$ tick marks is exactly the same thing as a Perfect N-triangle. As of 1985, all Golomb rulers with fewer than 13 tick marks ($N \leq 11$) were known [3, 4]. Since then, a few more values of N have undoubtedly been conquered. Beyond this, however, the results are only speculative, as the number of possibilities which need to be checked has essentially collided with the capabilities of modern computing.

Finding Perfect N-triangles (or constructing Golomb rulers) is *not* the emphasis of the present work; rather, we concentrate on proving the equivalence of Problem 1 and Problem 2 by exploiting the correspondence between the continuous and N-triangle formulations. For this purpose, the notation and terminology of N-triangles will be maintained. Some other aspects of the previous work on Golomb rulers will be mentioned at the point at which they become relevant.

5 Globally Maximal N-Triangles

In order to understand what is involved in proving Conjecture 1, we must first introduce another important characteristic of N-triangles. Let $p \in P_N$ and $x = T^{-1}(p)$. Again with reference to the discussion following equation (27), note that $F_N(x)$ can just as well be calculated by *first* calculating the minimum positive difference between any two entries in the N-triangle, and then dividing by $\operatorname{Tr} p$. Accordingly, for any $p \in P_N$, we define its *index* to be

$$\operatorname{In} p \equiv \min |p_{i,j} - p_{k,l}|, \qquad (i,j) \neq (k,l). \tag{45}$$

It follows that

$$F_N(x) = \frac{\operatorname{In} p}{\operatorname{Tr} p}. \tag{46}$$

This equation is really the fundamental fact underlying the usefulness of N-triangles in studying the continuous irregularity function $F_N(x)$; it enables all questions about the latter to be translated into questions about the former. As a result of this equality, it is natural to call the quantity on the right-hand side of equation (46) the *irregularity* of the N-triangle p. In the same spirit, we can use equation (46) to define the concept of a *globally maximal* N-triangle in such a way that p is globally maximal if and only if $p \in T(X_N''')$ (the image of the set of points at which $F_N(x)$ attains a global maximum).

Definition 5.1 *Let $p \in P_N$. Then p is said to be globally maximal whenever*

$$\frac{\operatorname{In} p}{\operatorname{Tr} p} \geq \frac{\operatorname{In} q}{\operatorname{Tr} q}, \qquad \forall q \in P_N.$$

This completely characterizes $T(X_N''')$ as a subset of P_N. As previously remarked, $T(X_N''')$ is actually a subset of P_N', the set of Good N-triangles. Moreover, $q \in P_N \setminus P_N'$ if and only if $\operatorname{In} q = 0$. Consequently, both occurrences of P_N in Definition 5.1 can be replaced by P_N' without changing its meaning.

Conjecture 1 says that Perfect and globally maximal N-triangles are the same thing, modulo $\approx$-equivalence. In order to see exactly what this means, one must compare the two definitions. In doing so, one observes that, mechanically, Definition 5.1 can be transformed into Definition 4.1 by replacing P_N by P'_N and both $\mathrm{In}\, p$ and $\mathrm{In}\, q$ by 1. Very roughly speaking, this observation suggests that Conjecture 1 will be true if all the "important" N-triangles have unit index. In order to make this precise, let A_N denote the class of N-triangles which have unit index; i.e.,

$$A_N \equiv \Big\{ p \in P_N \;\Big|\; \mathrm{In}\, p = 1 \Big\}. \tag{47}$$

We then seek to understand the set-theoretic relations between A_N, P'''_N, and $T(X'''_N)$.

A highly intuitive (but not quite obvious) fact is that $P'''_N \subset A_N$. Indeed, a larger value of $\mathrm{In}\, p$ should force $\mathrm{Tr}\, p$ to be larger (this intuition will be justified by Theorem 5.7). Therefore, since Perfect N-triangles are precisely those Good N-triangles with minimal trace, one would expect their index to be as small as allowable for Good N-triangles.

Theorem 5.1 *If p is Perfect then $\mathrm{In}\, p = 1$ ($P'''_N \subset A_N$).*

<u>Proof</u>

Let $p \in P_N$ and suppose $\mathrm{In}\, p \geq 2$. This certainly implies that no element $p_{i,j}$ of the N-triangle expansion can equal 1. Let p' denote the N-triangle obtained by replacing p_0 by 1. Except when $i = 0$, $p'_{i,j} = p_{i,j}$, so this subset of the elements of the N-triangle p' are all distinct. In addition, when $j \geq 1$, $p'_{0,j} = p'_{0,0} + p'_{1,j} = 1 + p_{1,j}$, so these elements are also distinct. Thus if two elements of the N-triangle p' are identical, they must be of the form $p'_{k,l} = p'_{0,j}$ with $j, k \geq 1$. But this is the same as $p_{k,l} - p_{1,j} = 1$, which is impossible since $\mathrm{In}\, p \geq 2$. Therefore p' is Good and $\mathrm{Tr}\, p' < \mathrm{Tr}\, p$, which implies that p cannot be Perfect.

□

A trivial but important consequence is that

Corollary 5.2 *All Perfect N-triangles have irregularity D_N^{-1}.*

This corollary, in turn, implies that

Corollary 5.3 *If $T(X'''_N) \cap P'''_N \neq \emptyset$ then $P'''_N \subset T(X'''_N)$.*

In other words, if one Perfect N-triangle is globally maximal then all must be globally maximal.

By using Theorem 5.1 and comparing Definitions 4.1 and 5.1, one concludes that Perfect N-triangles have maximal irregularity among all those N-triangles in the class A_N. It follows that, in order for Conjecture 1 to be true, it is necessary and sufficient that every globally maximal N-triangle be $\approx$-equivalent to some N-triangle in the class A_N. This assertion is proved as part of Theorem 5.6. However, one can still partially characterize the relationship between P'''_N and $T(X'''_N)$ without knowing the relationship between A_N and $T(X'''_N)$. This is the content of the following theorem, which is similar to Corollary 5.3, but stronger.

Theorem 5.4 *If $T(X'''_N) \cap A_N \neq \emptyset$ then $P'''_N = T(X'''_N) \cap A_N$.*

<u>Proof</u>

Assume $T(X'''_N) \cap A_N \neq \emptyset$ and let $p \in T(X'''_N) \cap A_N$. Since p is globally maximal and $\mathrm{In}\, p = 1$, Definition 5.1 implies

$$\frac{1}{\mathrm{Tr}\, p} = \frac{\mathrm{In}\, p}{\mathrm{Tr}\, p} \geq \frac{\mathrm{In}\, q}{\mathrm{Tr}\, q} \geq \frac{1}{\mathrm{Tr}\, q}; \qquad \forall q \in P'_N. \tag{48}$$

Thus, by Definition 4.1, $p \in P_N'''$. This proves $P_N''' \supset T(X_N''') \cap A_N$. Since $p \in T(X_N''') \cap P_N'''$, Corollary 5.3 implies $P_N''' \subset T(X_N''')$. By Theorem 5.1, $P_N''' \subset A_N$; therefore, $P_N''' \subset T(X_N''') \cap A_N$.

□

Our immediate goal is to use Theorem 5.4 (along with Theorem 5.1 and its corollaries) to give a less abstract (but equivalent) formulation of Conjecture 1. First, however, it is necessary to note the consequences of multiplying an N-triangle generator by a positive integer.

Theorem 5.5 *Let $q \in P_N$, $k \in \mathbb{N}$, and $p = kq$. Then $p \in P_N$, $\operatorname{In} p = k \operatorname{In} q$, and $\operatorname{Tr} p = k \operatorname{Tr} q$.*

Proof

If $p = kq$ then $p_{i,j} = kq_{i,j}$ for all i, j satisfying $0 \leq i \leq j \leq N$; i.e., every element in the N-triangle expansion is multiplied by k. All three assertions then follow trivially.

□

Thus, if $p = kq$ then p and q have the same irregularity. We now can give two equivalent formulations of Conjecture 1.

Theorem 5.6 *The following three propositions are equivalent:*

1. *$T(X_N''') \approx P_N'''$ (Conjecture 1).*
2. *For every $p \in P_N$, p is globally maximal if and only if $p = kq$, where $k \in \mathbb{N}$ and q is Perfect.*
3. *For every $p \in P_N$, if p is locally maximal then p is divisible by $\operatorname{In} p$.*

Proof

Propositions 1 and 2 are essentially the same thing written in different notations. To see this, recall that $p \approx q$ means that $\exists m, n \in \mathbb{N} \mid mp = nq$ (Definition 3.1), which implies $m \operatorname{In} p = n \operatorname{In} q$ (Theorem 5.5). If q is Perfect then $\operatorname{In} q = 1$ (Theorem 5.1), which implies that n is divisible by m. Let $k = n/m = \operatorname{In} p$. The equivalence of propositions 1 and 2 follows. Proposition 3, in turn, is a direct corollary of proposition 2. We will complete the proof of the theorem by arguing that proposition 3 implies proposition 2.

Assume proposition 3 is true and suppose p is globally maximal. Then p is divisible by $\operatorname{In} p$, which means precisely that $p = kq$ with $\operatorname{In} p = k$ and $\operatorname{In} q = 1$. By Theorem 5.5, q has the same irregularity as p, hence q is globally maximal. Therefore, by Theorem 5.4, q is Perfect. This proves the forward implication in proposition 2. On the other hand, Corollary 5.2 together with Theorem 5.5 implies that any multiple of a Perfect N-triangle must have the same irregularity as q; therefore, any multiple of a Perfect N-triangle must be globally maximal. This proves the reverse implication in proposition 2.

□

As a result of this theorem, we will henceforth refer to any or all of the above propositions as Conjecture 1.

In Appendix B, we will prove Conjecture 1 directly for the first few values of N. From the proof, it will become evident that the generalization of this direct approach to arbitrary

N is difficult or impossible to carry out. Our strategy, then, will be to approach the proof indirectly by developing the theory of *locally* maximal N-triangles (corresponding to local maxima of the continuous irregularity function). This is the subject of Section 7.

We conclude this section by proving that, for fixed index, the trace is bounded below (or, for fixed trace, the index is bounded above). First, define

$$C_N \equiv \binom{N+2}{2} = \frac{(N+2)(N+1)}{2}. \tag{49}$$

This quantity plays a fundamental role in the following theorem and corollaries.

Theorem 5.7 *Let $p \in P_N$. Then*

$$\mathrm{Tr}\, p \geq \mathrm{In}\, p\, C_N. \tag{50}$$

Proof

Let $p \in P_N$ and put $k = \mathrm{In}\, p$. Clearly, the smallest component of the N-triangle generator p must be at least k; otherwise, there will be two N-triangle elements which differ by less than k. Similarly, the second smallest component of p must be at least $2k$; otherwise, it will differ from the smallest component by less than k. Continuing in this manner, the largest component of p must be at least $(N+1)k$. Therefore,

$$\mathrm{Tr}\, p \geq k \sum_{i=1}^{N+1} i = k\, C_N. \tag{51}$$

Since $k = \mathrm{In}\, p$, the theorem is proved.

□

According to equation (46), this theorem provides a simple upper bound on the continuous irregularity function $F_N(x)$.

Corollary 5.8

$$F_N(x) \leq C_N^{-1}. \tag{52}$$

On the other hand, if p is Perfect then Theorem 5.1 and Theorem 5.7 imply

Corollary 5.9

$$D_N \geq C_N. \tag{53}$$

With reference to Appendix A, we remark that this bound is actually attained for $N = 1$ ($D_1 = C_1 = 3$) and $N = 2$ ($D_2 = C_2 = 6$). For $N \geq 3$, it is not difficult to show that the lower bound C_N is never attained [4]. In connection with the Golomb Ruler Problem, much effort has been directed towards improving this lower bound on D_N for the purpose of making the computer search for Golomb rulers more efficient [3]. These more sophisticated bounds will not be needed in the present work; the simple lower bound C_N will be sufficient. The quantity C_N will appear frequently in the following sections because of its dual significance as both the number of elements in an N-triangle expansion and a lower bound on D_N.

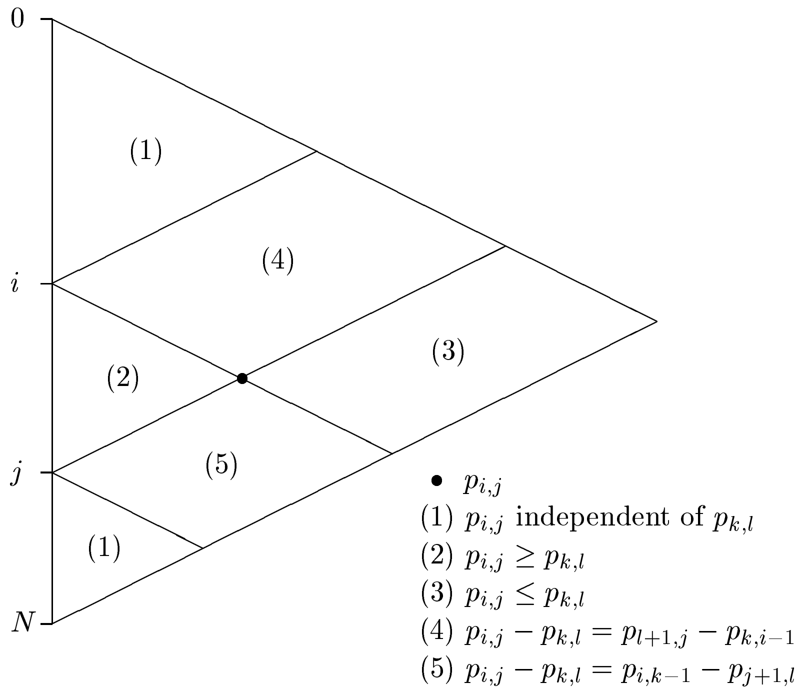

Figure 7: Schematic N-triangle Showing Element Interdependence

6 Independent N-Triangle Elements

In calculating the index of an N-triangle using equation (45), it is clearly not necessary to consider every possible choice of two elements. For example, if $i < k \leq j < l$ then

$$\begin{aligned} p_{i,j} - p_{k,l} &= (p_{i,k-1} + p_{k,j}) - (p_{k,j} + p_{j+1,l}) \\ &= p_{i,k-1} - p_{j+1,l}. \end{aligned} \tag{54}$$

It is therefore natural to ask how many of the possible choices of two N-triangle elements actually do need to be considered. A moment's reflection convinces one that this is equivalent to recounting the number of component functions which contribute to $F_N(x)$ on the ordered-x simplex, as done in Section 2.2. Here, the answer to this question will be recalculated using N-triangle arguments, as the treatment is more formal and the combinatorics are different. In order to single out the sort of "overlap" in the above example, we introduce the following concept.

Definition 6.1 *Two elements of a N-triangle are said to be* <u>independent</u> *if they share no generator component as a common summand; i.e., $p_{i,j}$ and $p_{k,l}$ are independent if either $j < k$ or $l < i$.*

Note that the independence of two N-triangle elements $p_{i,j}$ and $p_{k,l}$ is not a function of p, but of (i,j) and (k,l). The various interdependence possibilities that can arise are summarized schematically in Figure 7. With reference to this figure, each of these possibilities will now be considered.

We first consider the case of independent elements. According to the definition, the set of N-triangle elements which are independent of $p_{i,j}$ are precisely those elements which

$$
\begin{array}{cccccc}
\cdots & 10 & & & & \\
 & & 6 & & & \\
 & 7 & & 3 & & \\
 & & 4 & & 1 & \\
\cdots & 6 & & 2 & & 0 \\
 & & 4 & & 1 & \\
 & 7 & & 3 & & \\
 & & 6 & & & \\
\cdots & 10 & & & &
\end{array}
$$

Figure 8: Values of $t_{i,j}$ Displayed in Triangular Format

lie in the two triangular regions labeled (1). Define $t_{i,j}$ to be the total number of such elements. Because there are i generator components which are summands for the upper triangular region and $N-j$ generator components which are summands for the lower triangular region, it follows that

$$t_{i,j} = \frac{i(i+1)+(N-j)(N-j+1)}{2}.$$

These values of $t_{i,j}$ can be displayed in the familiar triangular format, as shown in Figure 8. Note that the right-most portion of this triangle does not change with N; i.e., for each successive value of N, a new column of numbers is appended to the left side of the triangle. Of course $t_{i,j}$ itself is not an N-triangle expansion, although its elements do obey a local addition law analogous to equation (31). The number of ways to choose two independent elements from a N-triangle (without regard to order) is just the sum of all of the $t_{i,j}$'s divided by two. By brute force calculation or induction on N, it is straight forward to show that

$$\frac{1}{2}\sum_{i=0}^{N}\sum_{j=i}^{N} t_{i,j} = \binom{N+3}{4}. \tag{55}$$

According to equation (20), this is precisely the number of non-facet component functions which contribute to $F_N(x)$ on the ordered-x simplex.

If $p_{k,l}$ lies in region (2) of Figure 7, it is the sum of a proper subset of the (non-negative) generator components which make up $p_{i,j}$; therefore, $p_{i,j} \geq p_{k,l}$. Similarly, if $p_{k,l}$ lies in region (3), $p_{i,j}$ is the sum of a proper subset of the (non-negative) generator components which make up $p_{k,l}$; and therefore, $p_{i,j} \leq p_{k,l}$. In both cases, strict inequality will hold if there are no zeros in the generator. For $p_{k,l}$ in region (2) or (3), each difference $|p_{i,j} - p_{k,l}|$ is equal to the sum of either one or two other N-triangle elements. Among the possibilities is that this difference is equal to one of the generator components. Since these are necessarily less than or equal to all other N-triangle elements, these differences are the only ones which need be considered when calculating the minimum. The $N+1$ generator components correspond to the $N+1$ facet functions which contribute to $F_N(x)$ on the ordered-x simplex.

Finally, if $p_{k,l}$ lies in region (4) of Figure 7, then $p_{i,j} - p_{k,l}$ must be equal to the difference of two independent N-triangle elements, one from the upper part of region (1) and one from region (2). Likewise, if $p_{k,l}$ lies in region (5), then $p_{i,j} - p_{k,l}$ is equal to the difference of one N-triangle element from the lower part of region (1) and one from region (2). This is the case in the example of equation (54).

We recap the results of this section in the form of the following simple theorem and corollary.

Theorem 6.1 *The index of an N-triangle p is equal to the minimum element in the set consisting of 1) the $\binom{N+3}{4}$ positive differences between each choice of two independent N-triangle elements and 2) the $N+1$ generator components.*

Corollary 6.2 *An N-triangle p is Good if and only if 1) each choice of two independent N-triangle elements produces two unequal numbers and 2) each generator component is nonzero.*

7 Superb and Locally Maximal N-Triangles

In this section, we develop the theory of local maxima. Much of the formalism will be analogous to that developed for global maxima in the preceding sections. The motivation for treating local maxima stems from both the continuous and N-triangle problems.

The reason that Problem 1 is not easily handled by conventional optimization algorithms (except for very small values of N) is that $F_N(x)$ possesses a very large number of local maxima (recall, for example, Figure 4). On the other hand, if one restricts oneself to the immediate vicinity of one of these local maxima, $F_N(x)$ is quite simple. In fact, when restricted to certain polyhedral subsets of X_N, $F_N(x)$ is a *polyhedral function* [8]; and as such, it is trivial to find its local maxima.[4] The reason for this is that standard results from convex analysis and the theory of linear programming can be applied. By using these results to study the local maxima of $F_N(x)$, we can gain a better understanding of the global maxima.

A parallel problem is encountered in the proof of Conjecture 1 in Appendix B. Because of the proliferation in the number of cases which need to be checked, the proof technique becomes impractical after $N=4$. We therefore would like to formulate a localized version of Conjecture 1 which is simpler to analyze. In order to do this, we will first need to develop the local analogue of Perfect N-triangles, which will be called *Superb* N-triangles. In contrast to solving Problem 2 (which essentially requires a brute force computer search), we will be able to construct Superb N-triangles algorithmically (see Section 9).

Many of the results in this section are simple convexity statements about the continuous irregularity function $F_N(x)$ disguised in the language of N-triangles. Although these results may be more naturally motivated in the continuous domain, the results themselves are more transparent when written as facts about N-triangles. For this reason, we will concentrate on the N-triangle formulation more or less exclusively. The more important implications of these results for the continuous problem will be discussed in Section 8.

7.1 Definitions and Convexity Results

We first address the question of how to characterize the subsets of X_N on which (the restriction of) $F_N(x)$ is polyhedral. These subsets must themselves be polyhedra. According to the analysis in Section 2.2, X_N is intersected by a number of $(N-1)$-dimensional hyperplanes of the form $f_{i,j,k,l}(x)=0$. As a polyhedron is, by definition, an intersection of affine half-spaces, these intersecting hyperplanes partition X_N into a number of N-dimensional polyhedra. From equation (10), it follows that $F_N(x)=0$ if and only if $f_{i,j,k,l}(x)=0$ for

[4]This observation is in accordance with the low dimensional cases shown in Figures 1–4.

some i, j, k, l; therefore, the interiors of these polyhedra are just the connected components of (the disconnected set) X'_N; i.e., on each interior $F_N(x) > 0$. This partitioning of X_N can be seen clearly for the $N = 2$ case of Figure 2.

It is not difficult to see that, restricted to each of these regions, $F_N(x)$ is polyhedral; i.e., the corresponding component of the *hypograph* of $F_N(x)$ is a $(N+1)$-dimensional polyhedron.[5] The polyhedral components of X_N should not be confused with the corresponding polyhedral components of the hypograph.

We may now ask how to characterize the polyhedral components of X_N in the language of N-triangles. A moment's reflection leads one to the conclusion that, if the relative order of any two N-triangle elements is reversed, the component function corresponding to the difference between those two elements must pass through a zero somewhere in between the values of x corresponding to the two N-triangles. Thus, all N-triangles whose elements have the same relative ordering correspond to values of x which lie in the same connected component of X'_N. This motivates the following definition.

Definition 7.1 *Let $p, q \in P'_N$. Then p and q are said to have the same structure (written as $p \sim q$) whenever*

$$p_{i,j} > p_{k,l} \Longleftrightarrow q_{i,j} > q_{k,l}; \qquad \forall i, j, k, l.$$

This is also an equivalence relation, but it is weaker than $\approx$-equivalence; i.e., if $p, q \in P'_N$ then

$$p \approx q \Longrightarrow p \sim q. \tag{56}$$

Also note that the concept of structure is only defined for Good N-triangles; therefore, the set of $\sim$-equivalence classes form a partition of P'_N. Definition 7.1 allows us to define a localized analogue of Perfect N-triangles.

Definition 7.2 *Let $p \in P'_N$. Then p is said to be Superb whenever*

$$\operatorname{Tr} p \leq \operatorname{Tr} q, \qquad \forall q \mid q \sim p.$$

The adjectives have been chosen so that Perfect $\Longrightarrow$ Superb $\Longrightarrow$ Good, naturally. In analogy with equation (44), define

$$P''_N \equiv \left\{ p \in P_N \;\middle|\; p \text{ is Superb} \right\} \tag{57}$$

so that $P'''_N \subset P''_N \subset P'_N \subset P_N$.

Thus far, we have not defined precisely what we mean by a local maximum of $F_N(x)$, having instead relied on the intuitive or technical concept. We now remedy this situation by first defining the concept of a *locally maximal* N-triangle in analogy with Definition 5.1.

Definition 7.3 *Let $p \in P'_N$. Then p is said to be locally maximal whenever*

$$\frac{\operatorname{In} p}{\operatorname{Tr} p} \geq \frac{\operatorname{In} q}{\operatorname{Tr} q}, \qquad \forall q \mid q \sim p.$$

[5] The hypograph of $F_N(x)$ is the set $\{(x, z) \mid 0 \leq z \leq F_N(x)\}$.

We then say that $F_N(x)$ attains a local maximum at some point x (i.e., $x \in X''_N$) if and only if $p = T(x)$ is locally maximal. That this definition agrees with the usual definition of local maxima follows from the fact that, when restricted to the corresponding polyhedral subset of X_N, $F_N(x)$ is polyhedral and hence concave. This point will be elucidated in Section 8.

According to Theorem 5.6, Conjecture 1 is true if and only if every globally maximal N-triangle is divisible by its index. It is a much stronger statement to assert that every *locally* maximal N-triangle is divisible by its index. In other words, the property in question arises from the local maximality of p, not the global maximality. If this is true, then Superb and locally maximal N-triangles are related in the same way as Perfect and globally maximal N-triangles. We conjecture that this is indeed the case.

Conjecture 2

$$T(X''_N) \approx P''_N$$

Even though this is much stronger than Conjecture 1, by using convex analysis, we will be able to obtain a much deeper understanding of its content.

To conclude this section, we briefly develop a sort of special convex analysis for the integral space P_N. This is really just standard convex analysis for the space X_N translated into the language of N-triangles. We exploit this fact in choosing the terminology, but do not attempt to formalize it until Section 8. In the next section, these convexity results will be used to prove some basic facts about Superb and locally maximal N-triangles.

Let $p, q \in P_N$ and define the *open segment* spanned by p and q according to

$$(p, q) \equiv \{r \mid r = mp + nq; \quad m, n \in \mathbb{N}\}. \tag{58}$$

It is trivial fact that $(p, q) \subset P_N$; i.e., with respect to this definition of "open segment", the space P_N is "convex". In the same sense, each structure equivalence class is also convex.

Theorem 7.1 *Let $p, q \in P'_N$. Then*

$$p \sim q \Longrightarrow \forall r \in (p, q),\ r \sim p.$$

Proof

Let $m, n \in \mathbb{N}$ and put $r = mp + nq$. Suppose $p_{i,j} > p_{k,l}$. Then since $p \sim q$, $q_{i,j} > q_{k,l}$. Consequently, $mp_{i,j} + nq_{i,j} > mp_{k,l} + nq_{k,l}$, or $r_{i,j} > r_{k,l}$. The same trivial argument applies for "$<$"; therefore, $r \sim p$.

□

Continuing in the same spirit, we can prove that the index (viewed as a function on some fixed structure equivalence class) is a concave function.

Theorem 7.2 *Let $p, q \in P'_N$. Then*

$$p \sim q \Longrightarrow \forall r \in (p, q),\ \operatorname{In} r \geq m \operatorname{In} p + n \operatorname{In} q.$$

Proof

Let $m, n \in \mathbb{N}$ and put $r = mp + nq$. Define $(p)_k$ to be the k^{th} smallest element of the N-triangle p so that $(p)_1 < (p)_2 < \cdots < (p)_{C_N}$. With analogous definitions for $(q)_k$ and $(r)_k$, Theorem 7.1 implies that $(r)_k = m(p)_k + n(q)_k$. Using this notation, we have

$$\begin{aligned} \operatorname{In} p &= \min_k \{(p)_{k+1} - (p)_k\} \\ \operatorname{In} q &= \min_k \{(q)_{k+1} - (q)_k\} \\ \operatorname{In} r &= \min_k \{m[(p)_{k+1} - (p)_k] + n[(q)_{k+1} - (q)_k]\}. \end{aligned} \tag{59}$$

It follows that $\operatorname{In} r \geq m \operatorname{In} p + n \operatorname{In} q$.

$\square$

Finally, the above two theorems allow us to give an alternative definition of *structure*.

Theorem 7.3 *Let $p, q \in P'_N$. Then*

$$p \sim q \Longleftrightarrow \forall r \in (p, q),\ \operatorname{In} r > 0.$$

Proof

The "$\Longrightarrow$" part of the implication follows from Theorem 7.2. To prove "$\Longleftarrow$", suppose $p \not\sim q$. Then $\exists i, j, k, l \mid p_{i,j} > p_{k,l}$ and $q_{i,j} < q_{k,l}$. Set $n = p_{i,j} - p_{k,l}$, $m = q_{k,l} - q_{i,j}$, and put $r = mp + nq$. Then

$$\begin{aligned} r_{i,j} - r_{k,l} &= m(p_{i,j} - p_{k,l}) + n(q_{i,j} - q_{k,l}) \\ &= mn - mn = 0. \end{aligned} \tag{60}$$

So $\operatorname{In} r = 0$, which completes the proof.

$\square$

7.2 The Index Reduction Property

We will now use the convexity results developed in the previous section to prove some facts concerning Superb and locally maximal N-triangles. Unlike the convexity results themselves, these facts do not translate directly into useful statements about the continuous irregularity function; rather, the results are offered as heuristic evidence in favor of Conjecture 2. The main result is that Superb and locally maximal N-triangles both possess a distinctive property which we will call the *index reduction property.* A few of the intermediate results will also be of importance.

We first prove a simple lemma which says that if any one component of an N-triangle generator is changed by an amount k, the index cannot change by more than k.

Lemma 7.4 *Let $p \in P_N$ and let l and k be integers satisfying $0 \leq l \leq N$ and $k \leq p_l$. Define q by $q_j = p_j - k\,\delta_{j,l}$ so that $q \in P_N$. Then*

$$\operatorname{In} p - |k| \leq \operatorname{In} q \leq \operatorname{In} p + |k|. \tag{61}$$

Proof

For each choice of two elements from the N-triangle q, either

$$\begin{aligned} |q_{i,j} - q_{i',j'}| &= |p_{i,j} - p_{i',j'}| \\ &\geq \operatorname{In} p \end{aligned} \tag{62}$$

or

$$\begin{aligned} |q_{i,j} - q_{i',j'}| &= |p_{i,j} - p_{i',j'} \pm k| \\ &\geq |p_{i,j} - p_{i',j'}| - |k| \\ &\geq \operatorname{In} p - |k|. \end{aligned} \tag{63}$$

It follows that $\operatorname{In} q \geq \operatorname{In} p - |k|$. Since $p_j = q_j + k\,\delta_{j,l}$, the same argument can be applied with the roles of p and q reversed. Therefore, it is also true that $\operatorname{In} p \geq \operatorname{In} q - |k|$, which completes the proof.

□

Of course, changing one component of an N-triangle generator by an amount k will not, in general, preserve the structure of the N-triangle. However, if $|k|$ is no larger than the index, the structure will be preserved provided that the perturbed N-triangle is Good. Otherwise, the perturbed N-triangle lies on the "boundary" of the structure equivalence class of the original N-triangle. Nevertheless, the conclusion of Theorem 7.2 still holds. Basically, this last assertion is true because of the *Accessibility Lemma for Polyhedra* [8]. We prove these assertions as the following theorem.

Theorem 7.5 *Let $p \in P'_N$ and let l and k be integers satisfying $0 \leq l \leq N$ and $|k| \leq \operatorname{In} p$. Define q by $q_j = p_j - k\,\delta_{j,l}$ so that $q \in P_N$. Then:*

1. *$\forall r \in (p, q)$, $\operatorname{In} r \geq m \operatorname{In} p + n \operatorname{In} q$.*
2. *$\operatorname{In} q > 0 \Longrightarrow q \sim p$.*

Proof

Let $m, n \in \mathbb{N}$ and put $r = mp + nq$ so that $r_j = (m+n)\,p_j - nk\,\delta_{j,l}$. Applying the previous lemma with the replacements $q \to r$, $p \to (m+n)\,p$, and $k \to nk$ yields

$$\begin{aligned} \operatorname{In} r &\geq (m+n) \operatorname{In} p - n|k| \\ &= m \operatorname{In} p + n(\operatorname{In} p - |k|) \\ &\geq m \operatorname{In} p > 0. \end{aligned} \tag{64}$$

If $\operatorname{In} q = 0$ then this proves the first assertion and the second assertion is vacuous. If $\operatorname{In} q > 0$ then this result together with Theorem 7.3 implies $q \sim p$, which proves the second assertion. The first assertion then follows from Theorem 7.2.

□

As a corollary to Theorem 7.5, we have the following fundamental result.

Corollary 7.6 *If p is Superb then $\operatorname{In} p = 1$ ($P''_N \subset A_N$).*

Proof

Let $p \in P_N$ and suppose $\operatorname{In} p \neq 1$. As $P''_N \subset P'_N$, we may assume $\operatorname{In} p \geq 2$. With reference to the notation of Theorem 7.5, define q by putting $k = 1$ and choosing any integer l satisfying $0 \leq l \leq N$. Then according to Lemma 7.4, $\operatorname{In} q \geq \operatorname{In} p - 1 \geq 1$. Theorem 7.5 then implies that $q \sim p$. On the other hand, $\operatorname{Tr} q = \operatorname{Tr} p - 1$; therefore, p cannot be Superb.

□

Thus, Corollary 7.6 implies Theorem 5.1. The complete picture is

$$P_N''' \subset P_N'' \subset A_N \subset P_N' \subset P_N. \tag{65}$$

It is interesting to note that the above argument is not just a single proof that Superb N-triangles have index equal to unity, but actually $N+1$ "linearly independent" proofs of this fact — one corresponding to each choice of generator component.

If some component of an N-triangle generator is reduced by the index, the perturbed N-triangle may or may not be Good. If *every* choice of generator component yields an N-triangle which is *not* Good, then, roughly speaking, the N-triangle elements are tightly packed together (relative to the index). Intuitively, we would expect this to be true if the N-triangle is either Superb or locally maximal. We formally define this property as follows.

Definition 7.4 *Let $p \in P_N'$. With reference to the notation of Theorem 7.5, put $k = \operatorname{In} p$ and suppose that, for each integer l satisfying $0 \le l \le N$, $\operatorname{In} q = 0$. We then say that p has the <u>index reduction property</u>.*

All the examples of N-triangles in Section 11, as well as the Perfect N-triangles tabulated in Appendix A, have the index reduction property. More generally, we have the following two theorems.

Theorem 7.7 *If p is Superb then p has the index reduction property.*

<u>Proof</u>

Let $p \in P_N'$ and suppose p does *not* have the index reduction property. As $P_N'' \subset A_N$, we may assume $\operatorname{In} p = 1$. With reference to the notation of Theorem 7.5, define q by putting $k = 1$ and choosing an integer l satisfying $0 \le l \le N$ which yields $\operatorname{In} q > 0$. Such an l must exist since p does not have the index reduction property. Theorem 7.5 then implies that $q \sim p$. On the other hand, $\operatorname{Tr} q = \operatorname{Tr} p - 1$; therefore, p cannot be Superb.

□

Theorem 7.8 *If p is locally maximal then p has the index reduction property.*

<u>Proof</u>

Let p be locally maximal and let l and k be integers satisfying $0 \le l \le N$ and $1 \le k \le \operatorname{In} p$. We again rely on the notation of Theorem 7.5, but regard l as fixed while making explicit the dependence of q on k; i.e., define q^k by $q_j^k = p_j - k\,\delta_{j,l}$ so that $q^k \in P_N$. We can now prove the theorem by induction on k.

First consider $k = 1$. According to Lemma 7.4, $\operatorname{In} q^1 \ge \operatorname{In} p - 1$. If $\operatorname{In} q^1 = 0$ then it must be true that $\operatorname{In} p = 1$ and we are finished. Otherwise Theorem 7.5 implies that $q^1 \sim p$. In this case, by using Definition 7.3 and $\operatorname{Tr} q^1 = \operatorname{Tr} p - 1$, the local maximality of p implies that

$$\operatorname{In} q^1 \le (1 - 1/\operatorname{Tr} p) \operatorname{In} p < \operatorname{In} p. \tag{66}$$

It follows that $\operatorname{In} q^1 = \operatorname{In} p - 1$.

We now assume that

$$\operatorname{In} q^{k-1} = \operatorname{In} p - (k-1). \tag{67}$$

According to Lemma 7.4, $\operatorname{In} q^k \geq \operatorname{In} p - k$; thus, in order to complete the proof by induction, we must show the reverse inequality. We make use of the simple algebraic fact

$$kq^{k-1} = p + (k-1)q^k. \tag{68}$$

According to equation (58), this implies that $kq^{k-1} \in R(p, q^k)$ (with $m = 1$ and $n = k-1$). Theorem 7.5 then implies that

$$k \operatorname{In} q^{k-1} \geq \operatorname{In} p + (k-1) \operatorname{In} q^k. \tag{69}$$

provided that $k \leq \operatorname{In} p$. By substituting equation (67), this is algebraically equivalent to $\operatorname{In} q^k \leq \operatorname{In} p - k$. It follows that $\operatorname{In} q^k = \operatorname{In} p - k$, which completes the proof.

□

The reverse implication is not true in either case. In order to see this, consider the N-triangle shown in Figure 9. It is easy to verify that this N-triangle has the index

$$\begin{array}{cccc}
1 & & & \\
 & 7 & & \\
6 & & 12 & \\
 & 11 & & 15 \\
5 & & 14 & \\
 & 8 & & \\
3 & & &
\end{array}$$

Figure 9: Example of an N-triangle with the Index Reduction Property

reduction property; i.e., reducing any of the generators by 1 yields an N-triangle which is not Good. However, the N-triangle in Figure 9 is neither Superb nor locally maximal, as simultaneously reducing the 5 and 6 by 1 yields a Good N-triangle with the same structure, smaller trace, and larger irregularity. The reason for this situation is that the N-triangle in Figure 9 lacks another crucial property closely related to Superbness and local maximality — the *vertex property*. This property will be discussed in Section 7.5.

We conclude this section with the following theorem, which is really a comment on the proof of Theorem 7.8. In effect, it says that proving $\operatorname{In} q = \operatorname{In} p - k$ by *reverse* induction on k is trivial, even with no special assumptions on p.

Theorem 7.9 *Let $p \in P_N$. With reference to the notation of Theorem 7.5, suppose that for some choice of integers l and k satisfying $0 \leq l \leq N$ and $k \leq p_l$, it is true that $\operatorname{In} q = \operatorname{In} p - k$. Then*

$$\operatorname{In} q' = \operatorname{In} p - k', \qquad \forall k' \mid 0 \leq k' \leq k; \tag{70}$$

where q' is defined by $q'_j = p_j - k' \, \delta_{j,l}$.

Proof

Define q and q' as above and assume $\operatorname{In} q = \operatorname{In} p - k$. According to Lemma 7.4, we have $\operatorname{In} q' \geq \operatorname{In} p - k'$. Assume strict inequality holds. Write q as $q_j = q'_j - (k-k') \, \delta_{j,l}$ and apply Lemma 7.4 again to yield

$$\begin{aligned}
\operatorname{In} q &\geq \operatorname{In} q' - (k - k') \\
&> (\operatorname{In} p - k') - (k - k') \\
&= \operatorname{In} p - k.
\end{aligned} \tag{71}$$

This contradicts the main assumption on q; therefore, $\operatorname{In} q' = \operatorname{In} p - k'$.

□

7.3 Counting Structure Equivalence Classes

As previously mentioned, the relation "$\sim$" is an equivalence relation on P'_N; therefore, P'_N is the disjoint union of $\sim$-equivalence classes. In light of Definition 7.1, the number of $\sim$-equivalence classes is trivially bounded by the number of permutations of C_N objects, and therefore finite. We will denote the number of $\sim$-equivalence classes by $2S_N$, the factor of two being an explicit acknowledgement of the conjugate symmetry. Loosely speaking, $2S_N$ is the number of ways of ordering the C_N elements of the N-triangle subject to the constraint that these orderings must respect the N-triangle addition law. In terms of the continuous irregularity function $F_N(x)$, $2S_N$ is the number of connected components of the disconnected set X'_N (with respect to the Euclidean metric). The closure of each of these connected components is a polyhedron whose faces are determined by the intersections of the zero hyperplanes of $F_N(x)$.

For the case $N = 1$, it easy to see that there are only two possible structures for Good N-triangles and that they are conjugates of one another. For $N = 2$, it can likewise be verified (by brute force) that there are ten. In light of Theorem 7.3, the values of $2S_1$ and $2S_2$ can also be determined by simply counting the number of polyhedrons which make up the ordered-x simplex in Figures 1 and 2.

For $N \geq 3$, both of the above methods for determining S_N become impractical or impossible. Instead of directly counting the number of N-triangles with distinct structures, we introduce a class of objects called *structure triangles* which will be easier to count. Intuitively, a structure triangle is just an ordering of the C_N elements of the N-triangle which "respects the N-triangle addition law". The following definition formalizes this idea.

Definition 7.5 *A* <u>*structure triangle*</u> *is a bijective mapping*

$$s : \{(i,j) \mid 0 \leq i \leq j \leq N\} \to \{1, 2, \ldots, C_N\} \tag{72}$$

which satisfies the following two criteria:

1. *$\forall i, j$ with $0 \leq i < j \leq N$,*

$$s_{i,j} > s_{i,j-1} \qquad \text{and} \qquad s_{i,j} > s_{i+1,j}. \tag{73}$$

2. *$\forall i, j, k, l$ with $0 \leq i < k \leq j < l \leq N$,*

$$s_{i,j} > s_{k,l} \Longleftrightarrow s_{i,k-1} > s_{j+1,l}. \tag{74}$$

Thus a structure triangle is an object with the same "data structure" as an ordinary N-triangle, but it does not (necessarily) obey the addition law of equation (30). It serves only to indicate an admissible ordering of the C_N elements for some Good N-triangle. For each Good N-triangle there exists a unique structure triangle satisfying

$$p_{i,j} > p_{k,l} \Longleftrightarrow s_{i,j} > s_{k,l}; \qquad \forall i, j, k, l. \tag{75}$$

In this situation, we will say that s is the structure triangle of p.

The two criteria in the above definition can be understood by again referring to Figure 7. First, assuming p is Good, $p_{i,j}$ must be strictly greater than all elements in region (2)

N	S_N
1	1
2	5
3	61
4	1642

Table 1: Number of Structure Equivalence Classes

and strictly less than all elements in region (3). By using equation (75), this condition transforms directly into an analogous condition on $s_{i,j}$. Moreover, it is easy to see that this is true if and only if each $s_{i,j}$ (with $i < j$) is strictly greater than its two closest neighbors to the left, $s_{i,j-1}$ and $s_{i+1,j}$. The second criteria is closely related to the concept of *independence* introduced by Definition 6.1. Again assuming p is Good, $p_{i,j}$ is either strictly greater than or strictly less than each element $p_{k,l}$ which lies in region (5). Therefore, after subtracting off the common summands, $p_{i,k-1}$ must satisfy the same inequality with $p_{j+1,l}$. This again transforms directly into an analogous condition on $s_{i,j}$ and $s_{k,l}$. The case where $p_{k,l}$ lies in region (4) is covered by the same criteria, as the roles of (i,j) and (k,l) can be interchanged.

It follows from the preceding discussion that the two criteria in Definition 7.5 are *necessary* in order that there actually exist a Good N-triangle with a particular ordering. On the other hand, that these criteria are also *sufficient* is not obvious. Although the proof is probably not difficult, we state this assertion as a conjecture.

Conjecture 3 *For each structure triangle s there exists a Good N-triangle p such that s is the structure triangle of p.*

Assuming this is true, S_N can be calculated by simply counting the number of structure triangles (modulo conjugacy). The results of this calculation for $N \leq 4$ are summarized in Table 1. Determining S_N for larger values of N and/or its asymptotic behavior is an interesting combinatorial problem in itself, independent of the Perfect N-Triangle Problem.

7.4 Structure Matrices

Possibly the most useful way to characterize structure equivalence classes is in terms of suitably defined polyhedra on P'_N. The fact that P'_N is an integral space makes the situation particularly interesting and brings the problem into the realm of *integer programming.* This consideration aside, the assertion that structure equivalence classes can be described by polyhedra follows almost immediately from Definition 7.1. Indeed, a structure equivalence class is just an ordering of the N-triangle elements, each of which is a sum of certain components of the generator p; therefore, one should be able to describe this ordering by a suitable set of inequalities involving the components of p. This is made explicit by the following theorem.

Theorem 7.10 *Let s be a structure equivalence class of P'_N. Then for some integer M satisfying $N+1 \leq M \leq C_N$, there exists a matrix A_s of order $M \times (N+1)$ consisting only of the elements 0 and ± 1 such that*

$$s = \{p \in P'_N \mid A_s p \geq 1\}. \tag{76}$$

The "1" appearing in equation (76) is an abbreviation for the M-dimensional column vector whose components are all equal to one. We will prove this theorem by defining an explicit canonical form for the matrix A_s. The following terminology will facilitate this definition.

Definition 7.6 *Let $p \in P'_N$ and let $p_{i,j}$ and $p_{i',j'}$ be two elements of the N-triangle expansion of p satisfying $p_{i,j} > p_{i',j'}$. Then $p_{i,j}$ and $p_{i',j'}$ are said to be* <u>*consecutive*</u> *if there are no other elements of the N-triangle expansion of p which fall between them; i.e., there is no $p_{k,l}$ satisfying $p_{i,j} > p_{k,l} > p_{i',j'}$.*

Let s be a structure equivalence class of P'_N and consider the matrix A_s defined as follows. Choose p to be any representative of s. Define the first row of A_s by placing a 1 in the column corresponding to the smallest component of the generator p (which is also necessarily the smallest element in the N-triangle expansion of p) and zeros in the remaining columns. Define the second row of A_s as follows. Let $p_{i,j}$ and $p_{i',j'}$ be the smallest pair of elements satisfying $p_{i,j} > p_{i',j'}$ which are *both consecutive and independent.* Place a 1 in columns i through j, a -1 in columns i' through j', and zeros in the remaining columns. Define the third row of A_s in the same way by considering the second smallest pair of elements which are both consecutive and independent. Continue until all such pairs have been exhausted.

The matrix A_s defined by this procedure will be called the *structure matrix* of p. For simplicity, we will sometimes write A instead of A_s when s can be regarded as fixed. Clearly A_s depends only on the structure equivalence class s, not on the chosen representative p. In fact, rather than applying the above procedure to the N-triangle expansion $p_{i,j}$ of a particular representative of s, it can equally well be applied to the structure triangle $s_{i,j}$ introduced in Definition 7.5 — the same matrix A_s results.

Returning to the proof of Theorem 7.10, equation (76) follows immediately provided that A_s is taken to be the structure matrix defined according to the above procedure. In this case, M (the row order of A_s) is one greater than the number of pairs of N-triangle elements which are both consecutive and independent. This number must be at least $N+1$; otherwise A_s could not even contain sufficient information for ordering the $N+1$ components of the generator. On the other hand, M is certainly less than or equal to C_N, the total number of elements in an N-triangle expansion. We remark that, whereas the lower bound on M is attainable (and therefore optimal), the upper bound is admittedly not very good. This suggests the question "What is the maximum number of consecutive independent pairs that can actually be attained in a Good N-triangle?" This (presently unknown) number is the best possible upper bound on M.

The primary importance of structure matrices is that they will allow us to characterize structure equivalence classes as polyhedra, thereby transforming questions involving N-triangles into standard linear and integer programming terminology. This is the subject of the following section. Another property which will also be important is that the structure matrix provides a simple formula for the index of an N-triangle in terms of the components of the generator, namely

$$\operatorname{In} p = \min_i \left\{ \sum_{j=0}^{N} A_{i,j}\, p_j \right\}. \tag{77}$$

This formula follows from the definition of the structure matrix, together with the observation that the index must be attained between N-triangle elements which are both independent and consecutive. Of course p must be a member of the structure equivalence class defined by A in order for equation (77) to be valid.

Because of their importance, it would be useful to have a simple procedure for generating the entire set of structure matrices for fixed N. Assuming Conjecture 3 is true, this can be done by first generating the set of structure *triangles* according to Definition 7.5, and then applying the above procedure for generating structure matrices to each one. It would be more useful, however, to have explicit necessary and sufficient conditions for determining directly if a given $(0, \pm 1)$-matrix is a structure matrix. Although some further properties characterizing structure matrices are noted below, this complete characterization is still an open question.

7.5 Structure Polyhedra and the Vertex Property

Let A be a structure matrix and define $\wp \subset \mathbb{R}^{N+1}$ according to

$$\wp = \{p \in \mathbb{R}^{N+1} \mid Ap \geq 1\}. \tag{78}$$

By definition, $\wp$ is a (convex) polyhedron [7]. Polyhedra which are defined by structure matrices according to equation (78) will be called *structure polyhedra.* The relationship between structure polyhedra and equation (76) depends on the simple observation that, if $p \in \wp$ and p is integral, the set of inequalities $Ap \geq 1$ forces p to belong to P'_N. In other words,

$$\begin{aligned} \{p \in \wp \mid p \text{ integral}\} &= \{p \in \mathbb{R}^{N+1} \mid Ap \geq 1;\ p \text{ integral}\} \\ &= \{p \in P'_N \mid Ap \geq 1\}. \end{aligned} \tag{79}$$

Hence, the set of all N-triangles with a given structure matrix A is precisely the set of all integral vectors in the corresponding structure polyhedron (78).

The following theorem lists some trivial properties of structure polyhedra using the standard terminology of convex analysis [7, 8].

Theorem 7.11 *Let $\wp$ be a structure polyhedron. Then $\wp$ is nonvacuous, rational, unbounded, and pointed.*

<u>Proof</u>

Let A denote the structure matrix which defines $\wp$. The assertion that $\wp$ is nonvacuous follows trivially from the definition of A. The assertion that $\wp$ is rational is a consequence of the fact that the system of inequalities $Ap \geq 1$ is rational. (In fact, the only coefficients are 0 and ± 1.) To see that $\wp$ is unbounded, let $p \in P'_N$, $k \in \mathbb{N}$, and put $q = kp$. Clearly $q \sim p$. It follows that $\wp$ is unbounded. Finally, a polyhedron is pointed if and only if it contains no line [8]. If $p \in \wp$ then all of the components of p must be positive (again by the definition of A). Therefore $\wp$ cannot contain a line and therefore must be pointed.

$\square$

A polyhedron is pointed if and only if it has vertices. If a pointed polyhedron is rational, the coordinates of its vertices will be rational. Thus a structure polyhedron $\wp$ always possesses rational vertices. Each rational vertex of $\wp$ is determined by $N+1$ linearly independent equations from the system $Ap = 1$ [7]. We do not know a priori if these vertices are necessarily *integral*, and hence belong to P'_N. This question will be of fundamental importance. However, even if some vertex of $\wp$ is not integral, it can be made so by multiplication by an appropriate integer. Thus all vertices of $\wp$ are "represented" by some $p \in P'_N$. This motivates the following definition.

Definition 7.7 *Let $p \in P'_N$, $k = \operatorname{In} p$, and $\wp$ be the structure polyhedron of p. If p/k is a vertex of $\wp$, we say p has the* vertex property.

The use of $k = \operatorname{In} p$ is justified by equation (77) and the preceding discussion. Loosely speaking, p has the vertex property if and only if there are $N+1$ independent occurrences of the index in the N-triangle expansion of p. All the examples of N-triangles in Section 11, as well as the Perfect N-triangles tabulated in Appendix A, have the vertex property. In fact, all these N-triangles are actually vertices of structure polyhedra, since all have $\operatorname{In} p = 1$.

We now seek to establish a connection between N-triangles which have the vertex property and N-triangles which are Superb and/or locally maximal. This is possible because the latter two properties can be formulated in terms of solutions to certain integer linear or linear programs [7], respectively. To this end, we have the following two theorems.

Theorem 7.12 *Let $p \in P'_N$ and A be the structure matrix of p. Then p is Superb if and only if p is a solution to the integer linear program*

$$\min\left\{\operatorname{Tr} p \;\middle|\; Ap \geq 1;\; p \text{ integral}\right\}. \tag{80}$$

Proof

This follows immediately from Definition 7.2.

□

Theorem 7.13 *Let $p \in P'_N$ and A be the structure matrix of p. Then p is locally maximal if and only if $p = k\rho$, where $k \in \mathbb{N}$ and ρ is a rational solution to the linear program*

$$\min\left\{\sum_{j=0}^{N} \rho_j \;\middle|\; A\rho \geq 1\right\}. \tag{81}$$

Proof

Suppose p is locally maximal and η is a rational solution to the above linear program. Set $k = \operatorname{In} p$, $\rho = p/k$, $l = \operatorname{LCD}(\eta_0, \ldots, \eta_N)$, and $q = l\eta$. Equation (77) implies that $Ap \geq k$, hence $A\rho \geq 1$. Furthermore,

$$\min_i \left\{\sum_j A_{i,j}\,\eta_j\right\} = 1, \tag{82}$$

since otherwise one could divide through by the minimum difference thereby reducing the objective function; hence, $\operatorname{In} q = l$. It follows that

$$\frac{\operatorname{Tr} p}{\operatorname{In} p} = \sum_{j=0}^{N} \rho_j \qquad \text{and} \qquad \frac{\operatorname{Tr} q}{\operatorname{In} q} = \sum_{j=0}^{N} \eta_j. \tag{83}$$

The fact that p is locally maximal implies that the quantities in the first equation are less than or equal to the quantities in the second; whereas, the fact that η solves the linear program implies that the quantities in the second equation are less than or equal to the quantities in the first. Therefore, all four quantities are equal, which implies that q is locally maximal and ρ is a rational solution to the linear program.

□

In this proof, it has been assumed that a rational solution to the linear program (81) exists. A comment on this assumption is in order. Firstly, if a linear function is bounded below on a nonvacuous polyhedron, the function attains a minimum on that polyhedron [8]. In the linear program (81), the objective function is bounded below by C_N. Secondly, it is a fundamental fact of linear programming theory that, if a solution to a linear program exists, it can be taken to be a vertex of the underlying polyhedron (provided that the polyhedron is pointed). Since structure polyhedra are pointed and rational, it follows that the linear program (81) possesses a rational solution.

We can now characterize the relationship between Superb and locally maximal N-triangles more or less completely. The main point underlying this relationship is that the linear program (81) is the *LP-relaxation* [7] of the integer linear program (80); in other words, it is exactly the same problem with the integrality constraint removed. However, the situation is complicated by the fact that we do not know if the solution to the linear program (81) is unique. The best possible scenario is summarized by the following theorem, which is analogous to Theorem 5.6.

Theorem 7.14 *The following four propositions are equivalent:*

1. $T(X''_N) \approx P''_N$ *(Conjecture 2).*
2. *For every* $p \in P_N$*,* p *is locally maximal if and only if* $p = kq$*, where* $k \in \mathbb{N}$ *and* q *is Superb.*
3. *For every* $p \in P_N$*, if* p *is locally maximal then* p *is divisible by* $\mathrm{In}\, p$*.*
4. *For every structure matrix* A*, the solution to the linear program (81) is unique and integral.*

Proof

The proof of the equivalence of the first three propositions is exactly parallel to the proof of Theorem 5.6. We will complete the proof of the theorem by arguing that proposition 4 implies proposition 2, and that the negation of proposition 4 implies the negation of proposition 3.

Assume proposition 4 is true and denote the unique integral solution to the linear program (81) by q. Then q is also the unique solution to the integer linear program (80); hence, q is the unique Superb N-triangle with structure matrix A. Then, according to Theorem 7.13, p is locally maximal if and only if $p = kq$, where $k \in \mathbb{N}$. This is just proposition 2.

Now assume proposition 4 is false. This means that (for some structure matrix A) the solution to the linear program (81) is either non-unique or non-integral. Since any convex combination of solutions to a linear program must also be a solution, an entirely integral solution set consisting of more than one point is impossible. Consequently, we may assume that there exists a rational non-integral solution to the linear program (81). Denote this solution by ρ and choose k so that $p = k\rho$ is integral. By Theorem 7.13, p is locally maximal. On the other hand, $k = \mathrm{In}\, p$, so p is not divisible by $\mathrm{In}\, p$. This is the negation of proposition 3.

□

As a result of this theorem, we will henceforth refer to any or all of the above propositions as Conjecture 2. As previously stated, if Conjecture 2 is true then Conjecture 1 is also true; i.e., Problem 1 is equivalent to Problem 2, the Perfect N-triangle (Golomb Ruler) Problem. All available evidence supports this desirable state of affairs. In contrast, the worst possible scenario is the following alternative to Conjecture 2.

Alternative 0 *For some structure matrix A, the linear program (81) possesses only non-integral solutions.*

If this were the case, there would be (in general) no correspondence between Superb and locally maximal N-triangles, regardless of the question of uniqueness. There are many possible intermediate situations, two of which we briefly discuss.

The first intermediate situation is the following weaker alternative to Conjecture 2.

Alternative 1 *For every structure matrix A, there exists an integral solution to the linear program (81).*

Assume for the moment that Alternative 1 is true and denote the integral solution by q. Then q is also a solution to the integer linear program (80); hence, q is Superb. If any other Superb N-triangles (with the same structure) exist, they must have the same irregularity as q; therefore, one can again conclude that all Superb N-triangles are locally maximal. However, in order to distinguish Alternative 1 from the analogous proposition in Theorem 7.14, one may assume that (for some structure matrix A) the linear program (81) possesses non-integral solutions as well. In general, there will be no direct relationship between the Superb N-triangles and the local maxima corresponding to these non-integral solutions. Consequently, one may conclude that Perfect N-triangles are globally maximal, but there may be other globally maximal N-triangles as well.

A much cleaner situation which does not presume uniqueness is the following alternative to Conjecture 2. This alternative is stronger than Alternative 1, but still weaker than Conjecture 2.

Alternative 2 *For every structure matrix A, all basic solutions to the linear program (81) are integral.*[6]

Assume for the moment that Alternative 2 is true and denote the set of basic solutions by $\{q_i\}$. Then each q_i is also a solution to the integer linear program (80); hence, each q_i is Superb. If any other Superb N-triangles (with the same structure) exist, they must have the same irregularity as the q_i's; therefore, one can again conclude that all Superb N-triangles are locally maximal. Furthermore, the set $\{q_i\}$ consists of precisely those Superb N-triangles which have the vertex property. The set of all rational solutions to the linear program (81) is simply the rational convex hull of the basic solutions $\{q_i\}$. By using Definition 3.1 and Theorem 7.13, it is not difficult to show that p is locally maximal if and only if

$$p \approx \sum_i k_i q_i, \tag{84}$$

where k_i is any set of non-negative integers which are not all zero. This is a rather nice generalization of the analogous proposition in Theorem 7.14. Moreover, provided that no two *Perfect* N-triangles share the same structure, Alternative 2 (like Conjecture 2) implies Conjecture 1. If this is not the case, one simply forms integral combinations of

[6] A basic solution is a solution which is a vertex of the underlying polyhedron [7].

those Perfect N-triangles which do share the same structure (by using equation (84)) in order to generate the complete set of globally maximal N-triangles.

We conclude this section with a brief discussion of four additional conjectures which are logically interrelated with Conjecture 2 and its alternatives. These conjectures are consistent with one another, with Conjecture 2, and with all available empirical evidence.

First, note that Conjecture 2 implies that there exists a *unique* Superb N-triangle corresponding to each structure. We state this assertion independently as the following conjecture.

Conjecture 4 *For each structure matrix A, there is a unique Superb N-triangle.*

The only difference between Conjecture 2 and Alternative 2 is with regard to this uniqueness. In fact, Alternative 2 together with Conjecture 4 is equivalent to Conjecture 2.

According to Conjecture 2, the unique Superb N-triangle corresponding to each structure is a vertex of the structure polyhedron. On the other hand, it has been proved that Superb N-triangles have unit index (Corollary 7.6) and posses the index reduction property (Theorem 7.7). We conjecture that these properties taken together completely characterize Superb N-triangles.

Conjecture 5 *Suppose $p \in P_N$. Then p is Superb if and only if p has the vertex property, p has the index reduction property, and* $\mathrm{In}\, p = 1$.

By Definition 7.7, if p has the vertex property and $\mathrm{In}\, p = 1$ then p is actually a vertex of the underlying structure polyhedron. However, even assuming Conjecture 2, the fact that p is an integral vertex of the underlying structure polyhedron is not sufficient in itself to make p Superb; i.e., in some cases integral vertices exist which are not locally maximal (see Section 9).

A simply stated assertion which would guarantee that Alternative 2 holds is given by the following conjecture.

Conjecture 6 *Every structure polyhedron $\wp$ is an integral polyhedron.*

Since structure polyhedra are pointed, a structure polyhedron $\wp$ is integral if and only if each vertex of $\wp$ is integral. As remarked above, in some cases integral vertices exist which are not locally maximal. For this reason, Alternative 2 is *not* equivalent to Conjecture 6 — the latter assertion is stronger. Taken together, Conjecture 6 and Conjecture 4 imply Conjecture 2.

Conjecture 6 is more than just wishful thinking based on empirical evidence; polyhedra which arise from combinatorial problems frequently turn out to be integral [7]. For structure polyhedra, the vector on the right-hand side of the system of inequalities is always the same — its components are all equal to one. Thus, whether or not a structure polyhedron is integral depends only on the properties of the structure matrix.

A particularly simple class of matrices which yield integral polyhedra (assuming the vector on the right-hand side of the system of inequalities is integral) is the class of *totally unimodular* matrices [7]. A matrix is totally unimodular if and only if every possible square submatrix has determinant 0 or ± 1. Since structure matrices consist only of the elements 0 and ± 1 they are prime candidates for total unimodularity. Unfortunately, this is not the case in general (see Section 9). However, there is somewhat weaker condition on structure matrices which also guarantees integral structure polyhedra.

Let A be a structure matrix and $\wp$ the associated structure polyhedron. Suppose that every maximal square submatrix of A (i.e., every square submatrix of order $N+1$) has determinant 0 or ± 1. Since each vertex of $\wp$ is determined by $N+1$ linearly independent equations from the system $Ap = 1$ [7], this guarantees that all vertices of $\wp$ are integral.[7] A square matrix is said to be *unimodular* if its elements are integral and its determinant is ± 1. According to the usual definition of unimodularity applicable to more general matrices [7], a structure matrix A will have the above property precisely when the transpose of A is unimodular. We conjecture that this is, in fact, the case.

Conjecture 7 *For every structure matrix A, the transpose of A is unimodular.*

This purpose of replacing Conjecture 6 by this stronger statement is that presumedly Conjecture 7 can be proved more directly since the theory of unimodular matrices is well developed. However, as discussed in Section 7.4, a complete characterization of the class of structure matrices is needed first.

8 Convexity and the Irregularity Function

We now interpret some of the results of Sections 7 in the context of the continuous irregularity function $F_N(x)$. In one sense this is trivial, since equation (46) (together with the N-triangle bijection T) gives the complete story as far as translating between the continuous and N-triangle domains. What is interesting is the naturalness with which standard convexity statements in the continuous domain translate into statements about N-triangles. This is the fundamental reason that the present work should stimulate further progress on the widely applicable Golomb Ruler Problem.

Before demonstrating how convexity translates from one domain to the other, we make two additional remarks regarding $\approx$-equivalence. Firstly, Theorem 3.1 implies that $p \approx T(x)$ if and only if $x = T^{-1}(p)$. We will normally write the former relation. Secondly, by summing both sides of equation (32), it follows that if $p = T(x)$ then $\operatorname{Tr} p = C_x$. If $p \approx T(x)$ then the latter equality does not hold; nevertheless, equation (36) implies

$$p_j = \operatorname{Tr} p\,(x_{j+1} - x_j). \tag{85}$$

We begin our discussion of convexity in the usual way. Let $x, y \in X_N$ and define the *open segment* spanned by x and y according to

$$(x, y) \equiv \{z \mid z = \lambda x + (1-\lambda)y; \quad \lambda \in (0,1) \cap \mathbb{Q}\} \tag{86}$$

This is identical to the standard definition of convex analysis [8] except that our underlying space is rational. It is easy to see that $(x, y) \subset X_N$; i.e., X_N is convex. In equation (58), we defined the open segment spanned by p and q, where $p, q \in P_N$. We justify this redundant use of terminology by the following theorem.

Theorem 8.1 *Let $x, y \in X_N$ and $p, q \in P_N$, and suppose that $p \approx T(x)$ and $q \approx T(y)$. Then*

$$(p, q) \approx T\Big((x, y)\Big). \tag{87}$$

<u>Proof</u>

Let $r \in (p, q)$ so that $r = mp + nq$ for some $m, n \in \mathbb{N}$. Define

$$\lambda = \frac{m \operatorname{Tr} p}{m \operatorname{Tr} p + n \operatorname{Tr} q} \tag{88}$$

[7] Consider Cramer's rule.

and put $z = \lambda x + (1-\lambda)y$ so that $z \in (x,y)$. Then, for $0 \le j \le N+1$,

$$\begin{aligned} z_j &= \lambda x_j + (1-\lambda)y_j \\ &= \frac{m \operatorname{Tr} p\, x_j + n \operatorname{Tr} q\, y_j}{m \operatorname{Tr} p + n \operatorname{Tr} q} \\ &= \frac{m \sum_{k=0}^{j-1} p_k + n \sum_{k=0}^{j-1} q_k}{m \operatorname{Tr} p + n \operatorname{Tr} q} \\ &= \frac{1}{\operatorname{Tr} r} \sum_{k=0}^{j-1} r_k. \end{aligned} \tag{89}$$

Therefore $r \approx T(z) \in T\Big((x,y)\Big)$.

Now let $z \in (x,y)$ so that $z = \lambda x + (1-\lambda)y$ where $\lambda = s/t$ for some $s,t \in \mathbb{N}$ satisfying $0 < s < t$. Define

$$\begin{aligned} m &= s \operatorname{Tr} q, \\ n &= (t-s) \operatorname{Tr} p \end{aligned} \tag{90}$$

and put $r = mp + nq$ so that $r \in (p,q)$ and

$$\begin{aligned} \operatorname{Tr} r &= m \operatorname{Tr} p + n \operatorname{Tr} q \\ &= t \operatorname{Tr} p \operatorname{Tr} q. \end{aligned} \tag{91}$$

Then, for $0 \le j \le N+1$,

$$\begin{aligned} z_j &= \lambda x_j + (1-\lambda)y_j \\ &= \frac{s x_j + (t-s) y_j}{t} \\ &= \frac{s \operatorname{Tr} q \sum_{k=0}^{j-1} p_k + (t-s) \operatorname{Tr} p \sum_{k=0}^{j-1} q_k}{t \operatorname{Tr} p \operatorname{Tr} q} \\ &= \frac{m \sum_{k=0}^{j-1} p_k + n \sum_{k=0}^{j-1} q_k}{t \operatorname{Tr} p \operatorname{Tr} q} \\ &= \frac{1}{\operatorname{Tr} r} \sum_{k=0}^{j-1} r_k. \end{aligned} \tag{92}$$

Therefore $T(z) \approx r \in (p,q)$.

□

This theorem allows us to identify convex subsets of X_N with convex subsets of P_N (in the sense of the discussion following equation (58)) via the N-triangle bijection.

It should not be taken for granted that the concept of an open segment in X_N translates so naturally into the language of N-triangles. Suppose, for instance, that $x, y \in X_N$ and $y = \alpha x$ for some (positive rational) constant α. Then $p = T(x)$ and $q = T(y)$ are not as simply related. Neither are p and q as simply related if $y = x + \epsilon$ for some (integral) vector ϵ. Thus, the N-triangle bijection T is particularly nice in that it respects statements concerning convexity. Another important example of this phenomenon is given by the following theorem.

Theorem 8.2 *Let $x, y \in X_N$ and $p, q \in P_N$, and suppose that $p \approx T(x)$ and $q \approx T(y)$. Let $z \in (x, y)$ and $r \in (p, q)$, and (according to Theorem 8.1) suppose that $r \approx T(z)$. Then*

$$F_N(z) \geq \lambda F_N(x) + (1-\lambda) F_N(y) \Longleftrightarrow \operatorname{In} r \geq m \operatorname{In} p + n \operatorname{In} q. \tag{93}$$

Proof

We know $r = mp + nq$ for some $m, n \in \mathbb{N}$ and $z = \lambda x + (1-\lambda)y$ for some $\lambda \in (0,1) \cap \mathbb{Q}$. Because $T^{-1}(r)$ is uniquely defined, m, n, and λ must be related by equation (88). Therefore, as a consequence of equations (46) and (88), the inequality on the left-hand side of the implication is equivalent to

$$\frac{\operatorname{In} r}{\operatorname{Tr} r} \geq \frac{m \operatorname{Tr} p}{\operatorname{Tr} r} \cdot \frac{\operatorname{In} p}{\operatorname{Tr} p} + \frac{n \operatorname{Tr} q}{\operatorname{Tr} r} \cdot \frac{\operatorname{In} q}{\operatorname{Tr} q}. \tag{94}$$

By cancelling appropriate factors, this is also equivalent to the inequality on the right-hand side of the implication.

□

Remarkably, the inequality on the right-hand side of the implication involves only the index, not the trace.

We can now reinterpret Theorems 7.1–7.3 with the help of the previous two results. Theorem 7.1 says that each connected component of X'_N (the inverse image under T of a structure equivalence class) is convex. Theorem 7.2 says that $F_N(x)$ restricted to any connected component of X'_N is concave. Theorem 7.3 says that two vectors x and y ($x, y \in X'_N$) belong to the same connected component of X'_N if and only if $F_N(z) > 0$ on the entire open segment spanned by x and y. In the reverse direction, it is interesting to note how these intuitive statements about $F_N(x)$ translate into non-intuitive but simple and useful facts about N-triangles.

From the discussion at the beginning of Section 7.1, we know that the closure of each connected component of X'_N is an N-dimensional polyhedron. Each facet of one of these polyhedra is the intersection of the polyhedron itself with an $(N-1)$-dimensional hyperplane of the form $f_{i,j,k,l}(x) = 0$. Thus, each of these polyhedra is determined by a set of inequalities, each of which is of the form

$$x_i - x_j - x_k + x_l \geq 0 \tag{95}$$

for some admissible i, j, k, l. It follows that each of these polyhedra can be described as $\{x \mid Bx \geq 0\}$, where B is some matrix whose elements can only be 0, ± 1, or ± 2. It is important to note that, in this representation, x must include the component $x_{N+1} = 1$, so that the column order of B is $N+1$. Consequently, the system of inequalities is not really homogeneous, and therefore does not describe a *polyhedral cone* [7] in X_N. Of course, these polyhedra must be intimately related to the structure polyhedra introduced in Section 7.1. We make this relationship explicit as follows.

The first step is to establish the relationship between the structure matrix A and the matrix B, which turns out to be trivial. Each row of B represents the difference between two entries in the triangle of Figure 5; whereas, each row of A represents the difference between two entries in the triangle of Figure 6. Since these two triangles differ only by a normalization factor of $\operatorname{Tr} p$, we have

$$\frac{1}{\operatorname{Tr} p} \sum_{j=0}^{N} A_{i,j} p_j = \sum_{j=1}^{N+1} B_{i,j} x_j. \tag{96}$$

Then, by using equation (85), it is easy to show that

$$B_{i,j} = \begin{cases} A_{i,j-1} - A_{i,j}, & 1 \le j \le N \\ A_{i,N}, & j = N+1 \end{cases} \tag{97}$$

and

$$A_{i,j} = \sum_{k=j+1}^{N+1} B_{i,k}, \qquad 0 \le j \le N; \tag{98}$$

i.e., the matrices A and B are related by elementary column operations.

Suppose A and B are related in the above manner and let $\wp$ be the structure polyhedron defined by A. Then the interior of the polyhedron $\{x \mid Bx \ge 0\}$ is the inverse image (with respect to T) of the integral vectors in $\wp$; in other words,

$$T(\{x \mid Bx > 0\}) \approx \{p \mid Ap \ge 1;\ p \text{ integral}\}. \tag{99}$$

This, however, is not the most useful interpretation of the structure polyhedron $\wp$. Its primary importance comes from its relationship to the hypograph of $F_N(x)$ restricted to $\{x \mid Bx \ge 0\}$. We denote this object by χ; i.e.,

$$\chi = \{(x, z) \mid Bx \ge 0; \quad 0 \le z \le F_N(x)\}. \tag{100}$$

As previously remarked, $F_N(x)$ restricted to $\{x \mid Bx \ge 0\}$ is polyhedral; i.e., χ itself is an $(N+1)$-dimensional polyhedron. In order to see this, note that if $Bx \ge 0$ then

$$F_N(x) = \min_i \left\{ \sum_{j=1}^{N+1} B_{i,j} x_j \right\}. \tag{101}$$

This is just the continuous analogue of equation (77). It follows that χ can also be written in the (manifestly polyhedral) form

$$\chi = \{(x, z) \mid Bx \ge z \ge 0\}. \tag{102}$$

In Section 7.5, we established a relationship between the vertices of $\wp$ (or N-triangles with the vertex property) and local maximality. The following theorem, which establishes a relationship between χ and $\wp$, both explains and generalizes this earlier result.

Theorem 8.3 *Let $\wp$ be a structure polyhedron and χ the corresponding polyhedral component of the hypograph of $F_N(x)$. Then (x, z) is a vertex of χ satisfying $z > 0$ if and only if $p = T(x)$ has the vertex of property.*

Proof

Let (x, z) be a vertex of χ satisfying $z > 0$ and let $p = T(x)$. Then there is a submatrix $\tilde{B}$ consisting of $N+1$ linearly independent rows of B such that $\tilde{B}x = z$. Being a vertex, (x, z) must certainly lie on the boundary of χ; therefore, as $z > 0$, one must conclude that $z = F_N(x)$. By using equations (46) and (96), it follows that there is a submatrix $\tilde{A}$ consisting of $N+1$ linearly independent rows of A such that $\tilde{A}p = \text{In}\, p$. This means precisely that p has the vertex property; i.e., $\rho = p/\text{In}\, p$ is a vertex of the structure polyhedron $\wp$. The converse argument is analogous.

□

Thus, the structure polyhedra formulation suppresses those points where $F_N(x)$ vanishes while simultaneously capturing all of the interesting behavior of $F_N(x)$ as vertices. This is precisely why the N-triangle method is so powerful in analyzing $F_N(x)$.

We conclude this section with the following theorem, which partially answers the uniqueness question for local maxima.

Theorem 8.4 *The polyhedron $\{x \mid Bx \geq 0\}$ is an N-dimensional simplex if and only if the corresponding polyhedron χ is an $(N+1)$-dimensional simplex.*

Proof

Suppose $\{x \mid Bx \geq 0\}$ is an N-dimensional simplex. Then, possibly after removing some redundant inequalities, we may assume that the matrix B has $N+1$ rows [7]. Thus, after removing the corresponding redundant inequalities, the matrix A also has $N+1$ rows. From Theorem 7.11, we know that $\wp$ is pointed; hence, it must have at least one vertex. On the other hand, as there are only $N+1$ inequalities which define $\wp$, it cannot have more than one vertex. Thus $\wp$ has exactly one vertex. Then, as a consequence of Theorem 8.3, χ must be an $(N+1)$-dimensional simplex. The converse implication is trivial.

$\square$

The proof is interesting in that is uses the structure polyhedron $\wp$ as an intermediary between the other two polyhedra. If either of the propositions are true then $F_N(x)$ attains a unique local maximum on $\{x \mid Bx \geq 0\}$.

9 Two Examples

We will now consider two examples. In addition to illustrating many of the concepts thus far presented, we will develop (but not attempt to formalize) a procedure for parameterizing the set of all N-triangles with a given structure. For both examples, we take as a starting point the structure triangle introduced by Definition 7.5.

9.1 Example I

Consider the $N = 3$ structure triangle shown in Figure 10. This structure triangle specifies

$$\begin{array}{cccc}
1 & & & \\
 & 4 & & \\
3 & & 8 & \\
 & 7 & & 10 \\
5 & & 9 & \\
 & 6 & & \\
2 & & &
\end{array}$$

Figure 10: Structure Triangle for Example I

one of the 61 (modulo conjugacy) admissible orderings for the 10 distinct elements of a Good 3-triangle; hence it defines an equivalence class of P_3'. As usual, denote the associated structure matrix and structure polyhedron by A and $\wp$, respectively. By following the previously explained procedure for constructing A, the matrix equation $Ap \geq 1$ (which defines $\wp$) can be written out explicitly as

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \\ 0 & 1 & 0 & -1 \\ -1 & -1 & 1 & 0 \end{bmatrix} \begin{bmatrix} p_0 \\ p_1 \\ p_2 \\ p_3 \end{bmatrix} \geq \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}. \tag{103}$$

In other words, not counting the 1 (which determines the first row of A), there are only three consecutive independent pairs: 1–2, 2–3, and 4–5. This is the minimal number of rows for a $N = 3$ structure matrix, as A must contain sufficient information for ordering the four components of the generator. The matrix B (related to A by equation (96)) is given by

$$B = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 0 & -1 & 1 \\ -1 & 1 & 1 & -1 \\ 0 & -2 & 1 & 0 \end{bmatrix}. \tag{104}$$

The fact that B has only four rows implies that the polyhedron $\{x \mid Bx \geq 0\} \subset X_N$ is a simplex. The structure polyhedron itself cannot be a simplex as it is unbounded. In order to see exactly what $\wp$ looks like, we proceed as follows.

Suppose $p \in \wp \cap P_N$. The first inequality in (103) says that p_0 must be positive. Thus, for any $\alpha \in \mathbb{N}$, we can put $p_0 = \alpha$. The second inequality in (103) says that $p_3 - p_0$ must be positive. Thus, for any $\beta \in \mathbb{N}$, we can put $p_3 = \alpha + \beta$. Continuing in this manner, for any $\gamma, \delta \in \mathbb{N}$, we can put $p_1 = \alpha + \beta + \gamma$ and $p_2 = 2\alpha + \beta + \gamma + \delta$. So we have

$$\begin{bmatrix} p_0 \\ p_1 \\ p_2 \\ p_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 2 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{bmatrix}. \tag{105}$$

This parameterizes the structure equivalence class in terms of a single vector with arbitrary positive integral components.[8] Moreover, we have

$$\begin{aligned} \operatorname{Tr} p &= 5\alpha + 3\beta + 2\gamma + \delta; \\ \operatorname{In} p &= \min\{\alpha, \beta, \gamma, \delta\}. \end{aligned} \tag{106}$$

Thus, it is trivial to prove the existence of a unique Superb N-triangle — just put $\alpha = \beta = \gamma = \delta = 1$. This yields the first $N = 3$ Perfect N-triangle listed in Appendix A. As it happens, this N-triangle can be mechanically obtained from the structure triangle of Figure 10 by increasing the numbers 6 through 10 by 1.

If we drop the integrality constraint on the parameter-vector, the structure polyhedron itself is parameterized by the same equation (each component must still be greater than or equal to one). Therefore, with reference to Theorems 7.12 and 7.13, the unique Superb N-triangle must also be a unique locally maximal N-triangle.[9] Furthermore, the unique Superb N-triangle is clearly a vertex of $\wp$, as all four inequalities in (103) are saturated. In fact, as there are only four inequalities from which to choose, it is the only vertex of $\wp$; hence, $\wp$ is integral. Of course, this situation is in accordance with (and provides an excellent illustration of) Theorem 8.3.

[8]According to reference [7], the concept of an *integral Hilbert basis* can be used to give a parametric representation of the integral vectors in any rational polyhedron.

[9]This is also easy to prove directly by using equation (106) and Definition 7.3.

In light of the above considerations, the structure polyhedron $\wp$ can be visualized as an unbounded, four-sided, cone-like polyhedron, situated in the space $(\mathbb{R}^+)^4$, whose apex (which is the unique Superb N-triangle) is the closest point in $\wp$ to the origin. The N-dimensional generalization of this picture is actually a rather accurate description for *any* structure polyhedron, except that there may be more than $N+1$ sides and/or there may be more than one vertex. Both of these situations are illustrated in Example II.

This example (and the next one) supports the point of view that, once restricted to a particular structure polyhedron, finding Superb N-triangles and proving their correspondence with local maxima are relatively easy — the real challenge is determining how the connected components of X'_N are put together. The following observation, which at least on the surface is truly remarkable, takes this point of view to its extreme.

Consider the column vectors of the matrix in equation (105). It can be readily verified that these vectors are the generators of the (necessarily not Good) N-triangles corresponding to the four vertices of the simplex $\{x \mid Bx \geq 0\}$. Recall that this polyhedra is only 3-dimensional; hence, each vertex must saturate three of the inequalities and merely satisfy the fourth. This is remarkable because the unique Superb N-triangle is given by the sum of the four N-triangles corresponding to these vertices. We state this property formally as the following conjecture.

Conjecture 8 *Restricted to each polyhedron $\{x \mid Bx \geq 0\}$, $F_N(x)$ attains a unique local maximum — whose corresponding (Superb) N-triangle is given by the sum of the N-triangles corresponding to the vertices of $\{x \mid Bx \geq 0\}$.*

In addition to this example, it can be verified case by case that this conjecture is universally true for $N = 1$ and $N = 2$. If it is true in general, then knowledge of the vertices defining the connected components of X'_N gives immediate knowledge of the local maxima. However, Conjecture 8 may be true only if $\{x \mid Bx \geq 0\}$ is a simplex, or if it is weakened in some other way.

Finally, we remark that, for this example, it is easy to verify that the structure matrix A is *totally unimodular*. With reference to the discussion following Conjecture 6, this provides a direct proof that this particular structure polyhedron is integral.

9.2 Example II

Now consider the $N = 3$ structure triangle shown in Figure 11. We proceed as in Exam-

$$\begin{array}{cccc}
2 & & & \\
 & 4 & & \\
1 & & 7 & \\
 & 5 & & 10 \\
3 & & 9 & \\
 & 8 & & \\
6 & & &
\end{array}$$

Figure 11: Structure Triangle for Example II

ple I, but only comment on those aspects which are different from the previous analysis.

The matrix equation $Ap \geq 1$ written out explicitly is

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 1 & 1 & -1 & 0 \\ 0 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix} \begin{bmatrix} p_0 \\ p_1 \\ p_2 \\ p_3 \end{bmatrix} \geq \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}. \tag{107}$$

In this case, there are five consecutive independent pairs of N-triangle elements (not counting the 1).

Suppose $p \in \wp \cap P_N$. Proceeding as in Example I, the first three inequalities in (107) give $p_1 = \alpha$, $p_0 = \alpha + \beta$, and $p_2 = \alpha + \beta + \gamma$. The fourth inequality then tells us that

$$(2\alpha + \beta) - (\alpha + \beta + \gamma) = \alpha - \gamma \geq 1. \tag{108}$$

We satisfy this inequality by defining $\alpha = \alpha' + \gamma$, where $\alpha' \in \mathbb{N}$. Substituting into the first three inequalities gives $p_1 = \alpha' + \gamma$, $p_0 = \alpha' + \beta + \gamma$, and $p_2 = \alpha' + \beta + 2\gamma$. The fifth inequality then gives $p_3 = 2\alpha' + \beta + 3\gamma + \delta$. Finally, the sixth inequality tells us that

$$(3\alpha' + 2\beta + 4\gamma) - (2\alpha' + \beta + 3\gamma + \delta) = \alpha' + \beta + \gamma - \delta \geq 1. \tag{109}$$

Thus, by dropping the prime on α, we have

$$\begin{bmatrix} p_0 \\ p_1 \\ p_2 \\ p_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 2 & 0 \\ 2 & 1 & 3 & 1 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{bmatrix}. \tag{110}$$

This parameterizes the structure equivalence class in terms of a single vector with positive integral components; however, these components must satisfy the additional constraint $\alpha + \beta + \gamma - \delta \geq 1$. In this case, we have

$$\begin{aligned} \mathrm{Tr}\, p &= 5\alpha + 3\beta + 7\gamma + 1\delta; \\ \mathrm{In}\, p &= \min\{\alpha, \beta, \gamma, \delta, \alpha + \beta + \gamma - \delta\}. \end{aligned} \tag{111}$$

The inequality $p_1 \geq 1$ is not represented in the formula for the index. This is because it is *redundant* [8]; i.e., it is implied by the other inequalities.

Again, it is trivial to prove the existence of a unique Superb N-triangle by putting $\alpha = \beta = \gamma = \delta = 1$. The resulting N-triangle will be denoted by p, and is shown in Figure 12. As in Example I, there are several ways to see that p must also be a unique locally maximal N-triangle. First, we note that p is again a vertex of $\wp$, as four inequalities in (107) are saturated. In this case, however, there is a second N-triangle which is also a vertex of $\wp$, but is not Superb. This peculiar N-triangle is obtained by putting $\alpha = \beta = \gamma = 1$ and $\delta = 2$ so that $\alpha + \beta + \gamma - \delta = 1$ is the fourth saturated inequality. The resulting N-triangle will be denoted by q, and is also shown in Figure 12. It is not difficult to argue that p and q are the only vertices of the structure polyhedron $\wp$; hence, $\wp$ is integral. The conclusion that p is the unique locally maximal N-triangle with the given structure then follows from the analysis of Section 7.5.

For this example, whether or not the column vectors of the matrix in equation (110) correspond to vertices of the polyhedron $\{x \mid Bx \geq 0\}$ has not been checked. However, from Theorems 8.3 and 8.4 and the fact that the structure polyhedron $\wp$ has two vertices,

$$p = \left\{ \begin{array}{cccc} 3 & & & \\ & 5 & & \\ 2 & & 9 & \\ & 6 & & 16 \\ 4 & & 13 & \\ & 11 & & \\ 7 & & & \end{array} \right. \qquad q = \left\{ \begin{array}{cccc} 3 & & & \\ & 5 & & \\ 2 & & 9 & \\ & 6 & & 17 \\ 4 & & 14 & \\ & 12 & & \\ 8 & & & \end{array} \right.$$

Figure 12: N-Triangles with the Vertex Property for Example II

we know that $\{x \mid Bx \geq 0\}$ is *not* a simplex. Thus, it must have at least five vertices, and therefore, the column vectors of the matrix in equation (110) cannot give the whole story. Nevertheless, Conjecture 8 may still be true.

Incidentally, for this example, the structure matrix A is *not* totally unimodular, as it contains 2×2 submatrices with determinant ± 2.

10 The Recurrence Property

We now return temporarily to the continuous domain in order to point out an interesting property of the irregularity function $F_N(x)$. As a consequence of this digression, we will be able to identify a sizable family of structures whose Superb N-triangles cannot possibly be Perfect. In order to illustrate this property, we refer to the slice of $F_3(x)$ shown in Figure 13. This figure is interesting in that it contains an exact scaled reproduction of the graph of $F_2(x)$ (shown in Figure 2) in the lower left-hand corner. We will call this phenomenon the *recurrence property* of $F_N(x)$. In order to understand this property, we proceed as follows.

For each $x \in X_N \setminus \{0\}$, define $x' \in X_{N-1}$ by

$$x' \equiv (x_1/x_N, \cdots, x_{N-1}/x_N). \tag{112}$$

We then ask for which values of $x \in X_N \setminus \{0\}$ the following recurrence relation holds:

$$F_N(x) = x_N \, F_{N-1}(x'). \tag{113}$$

This question can be most easily answered after translation into the language of N-triangles. With reference to Figure 6, let p' denote the $(N-1)$-triangle obtained by deleting the bottom diagonal of the N-triangle p so that $p'_{i,j} = p_{i,j}$ for $0 \leq i \leq j \leq N-1$. From the definition of T, it follows easily that[10]

$$p = T(x) \Longrightarrow p' \approx T(x'). \tag{114}$$

By using equation (46), the recurrence relation translates directly into

$$\frac{\operatorname{In} p}{\operatorname{Tr} p} = \frac{\operatorname{Tr} p'}{\operatorname{Tr} p} \cdot \frac{\operatorname{In} p'}{\operatorname{Tr} p'}. \tag{115}$$

This equation (and hence the recurrence) holds precisely when $\operatorname{In} p = \operatorname{In} p'$. It is automatically true that $\operatorname{In} p \leq \operatorname{In} p'$; thus, this condition is equivalent to saying that the minimum

[10] In the first equation $T : X_N \to P_N$; whereas in the second, $T : X_{N-1} \to P_{N-1}$; thus technically, the notation should distinguish between the two mappings.

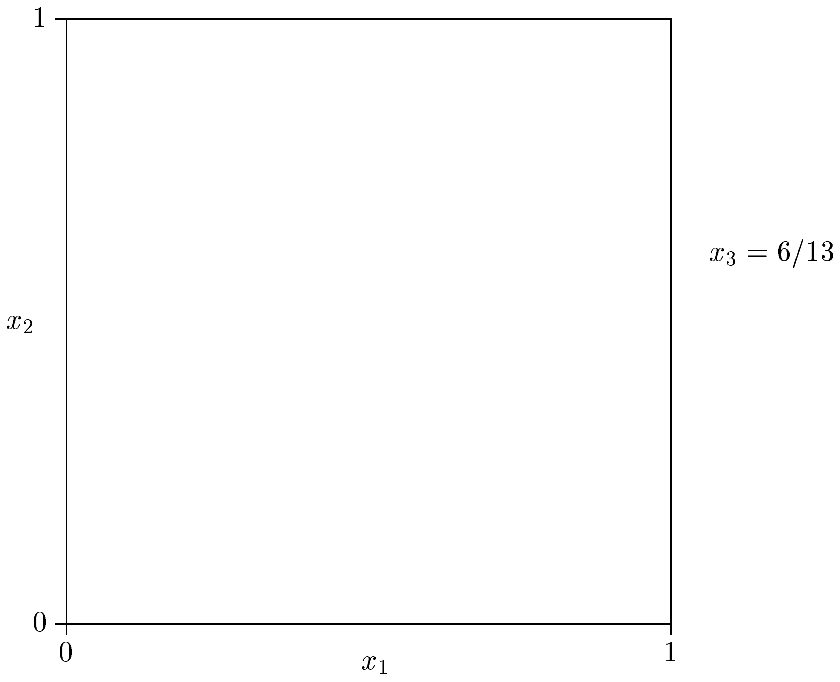

Figure 13: The Recurrence Property

difference (which determines the index of p) is attained between two elements which lie in p'. We will not attempt to characterize the entire subset of X_N where this condition holds, but only a portion thereof. In particular, it is easy to see that

$$p_N \geq \operatorname{Tr} p' + \operatorname{In} p' \Longrightarrow \operatorname{In} p = \operatorname{In} p'. \tag{116}$$

The translation of the left-hand side of this implication back into the continuous domain is

$$x_N \leq \frac{1}{2 + F_{N-1}(x')}. \tag{117}$$

The term $F_{N-1}(x')$ in the denominator may be replaced by anything larger in order to obtain a simple sufficient condition for the recurrence relation to hold. The strongest such condition that depends only on x_N is given by the following theorem.

Theorem 10.1 *For all $x \in X_N \setminus \{0\}$ satisfying $x_N \leq [2 + \max F_{N-1}(x)]^{-1}$, the recurrence relation (113) holds.*

According to this theorem, the value $x_3 = 6/13$ used in Figure 13 is the largest possible value which guarantees that the recurrence property holds. The breakdown of this property for $6/13 < x_3 \leq 1/2$ is illustrated in Figure 14. The reason for this breakdown is that $F_3(x)$ is determined by the component function $|1 - 2x_3|$ near $x_3 = 1/2$. In the figure, this component function manifests itself as a black surface of constant height. As x_3 approaches unity, another exact scaled image of $F_2(x)$ appears in the upper right-hand corner of the graph, as can be seen in Figure 3. This new recurrence can be easily understood in terms of the symmetry properties of $F_N(x)$; however, it is of no interest in the present development, as the image falls outside of the ordered-x simplex. Finally, we remark

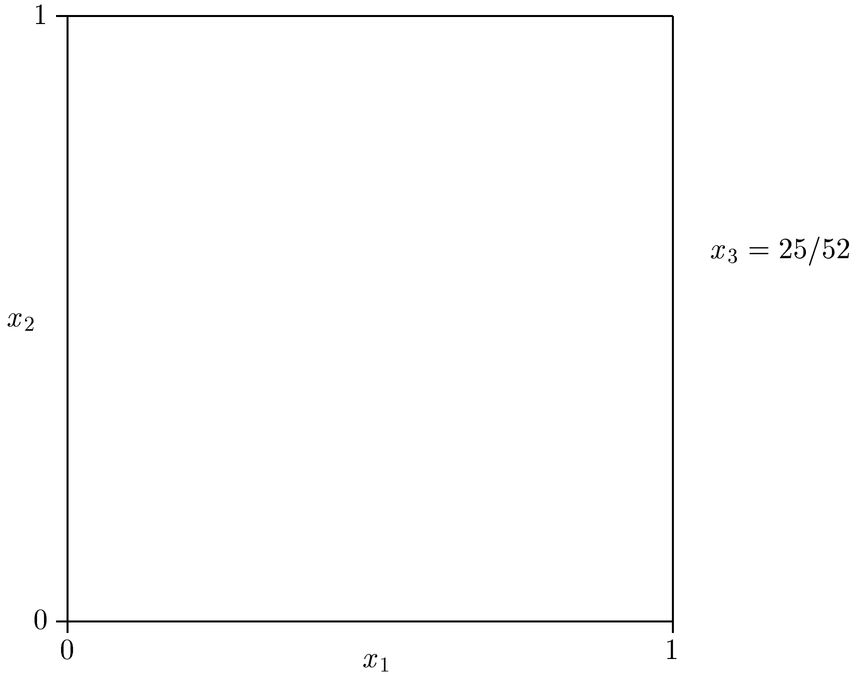

Figure 14: Breakdown of the Recurrence Property

that Theorem 10.1 can be applied recursively. For example, if $x_3 \le 6/13$ and $x_2/x_3 \le 3/7$ then $F_3(x) = x_2 F_1(x)$. If, in addition, $x_1/x_2 \le 1/3$ then $F_3(x) = x_1$, at which point the recurrence property has become trivial.

The constraining value of x_N in Theorem 10.1 approaches $1/2$ monotonically from below as N tends to infinity. Thus, in the region $x_N < 1/2$, it is reasonable to suppose that $F_N(x)$ possesses local maxima corresponding to the local maxima of $F_{N-1}(x')$ via the recurrence relation (113). We will argue informally (by means of an example) that these are the only local maxima in the region $x_N < 1/2$ and that they cannot possibly be global maxima. The formal motivation behind this informal argument is Theorem 10.2, which is written in the language of N-triangles. Instead of treating local maximality, however, the theorem treats the closely related vertex property.

Let $x \in X_N$ and $p = T(x)$. First we note how the condition $x_N < 1/2$ is translated into a condition on p. As before, let p' denote the $(N-1)$-triangle obtained by deleting the bottom diagonal of the N-triangle p. By using the fact that $p_N = \operatorname{Tr} p\,(1 - x_N)$, it is easy to show that

$$x_N < 1/2 \iff 2p_N - \operatorname{Tr} p > 0 \iff p_N - \operatorname{Tr} p' > 0. \tag{118}$$

In other words, $x_N < 1/2$ if and only if the generator component p_N is greater than the sum of all the other generator components. We can now give a recursive characterization of the vertex property for those N-triangles which satisfy this condition.

Theorem 10.2 *Let $p \in P_N$ and suppose that the inequalities in (118) hold. Then p has the vertex property if and only if p' has the vertex property and*

$$p_N - \operatorname{Tr} p' = \operatorname{In} p'. \tag{119}$$

Proof

The inequality $p_N - \mathrm{Tr}\, p' > 0$ implies that the structure matrices of p and p' are related by

$$A = \begin{bmatrix} & & & 0 \\ & A' & & \vdots \\ & & & 0 \\ -1 & \cdots & -1 & 1 \end{bmatrix} \tag{120}$$

Assume p has the vertex property. Then there is a submatrix $\tilde{A}$ consisting of $N+1$ linearly independent rows of A such that $\tilde{A}p = \mathrm{In}\, p$. One of these rows must be the bottom row of A since otherwise $\tilde{A}$ would be singular; therefore, $p_N - \mathrm{Tr}\, p' = \mathrm{In}\, p$. The other N rows must be contained in A'; i.e., there is a submatrix $\tilde{A}'$ consisting of N linearly independent rows of A' such that $\tilde{A}'p' = \mathrm{In}\, p$. Trivially, $\mathrm{In}\, p \leq \mathrm{In}\, p'$. On the other hand, with the help of equation (77), we can conclude the reverse inequality; therefore, $\mathrm{In}\, p = \mathrm{In}\, p'$. It follows that p' has the vertex property and $p_N - \mathrm{Tr}\, p' = \mathrm{In}\, p'$.

Now assume p' has the vertex property and $p_N - \mathrm{Tr}\, p' = \mathrm{In}\, p'$. Then there is a submatrix $\tilde{A}'$ consisting of N linearly independent rows of A' such that $\tilde{A}'p' = \mathrm{In}\, p'$. Together with $p_N - \mathrm{Tr}\, p' = \mathrm{In}\, p'$ (corresponding to the bottom row of A), these form a submatrix $\tilde{A}$ consisting of $N+1$ linearly independent rows of A such that $\tilde{A}p = \mathrm{In}\, p'$. In this case, it is immediate that $\mathrm{In}\, p = \mathrm{In}\, p'$. It follows that p has the vertex property.

□

Equation (119) implies that $\mathrm{In}\, p = \mathrm{In}\, p'$ and $\mathrm{Tr}\, p = 2\mathrm{Tr}\, p' + \mathrm{In}\, p'$. We remark that it easy to produce an N-triangle with the same index and trace (and thus the same irregularity) which does *not* have the vertex property. Indeed, consider the N-triangle generated by

$$q_k = \begin{cases} \mathrm{In}\, p', & k = 0 \\ 2p'_{k-1}, & 1 \leq k \leq N \end{cases}. \tag{121}$$

Theorem 10.2 and the preceding remark are significant for the following reason. Suppose Conjecture 2 is true. Then the phrase "has the vertex property" can be replaced by either "is Superb" or "is locally maximal" in both the theorem and the remark. This implies that, among other things, the Superb N-triangles corresponding to the family of structures described by equation (118) cannot possibly be Perfect. Thus, for each successive value of N, the part of $F_N(x)$ which is easily understood in terms of $F_{N-1}(x)$ is irrelevant in solving Problem 1.

As an example, let p' be the Perfect 2-triangle given in Appendix A. We know from previous considerations that this Perfect 2-triangle has the vertex property and is globally maximal. According to Theorem 10.2, we can form a 3-triangle p with the vertex property by appending $p_3 = 7$. This 3-triangle is shown in Figure 15. By carrying out an analysis similar to that of Section 9, it is easy to show that p is both Superb and locally maximal. However, by using equation (121), we can construct an N-triangle q (also shown in Figure 15) which lacks the vertex property and thus cannot be Superb. It follows that the Superb N-triangle with the same structure as q has a smaller trace than p; hence, p is *not* Perfect.[11]

[11] Of course, from Appendix A, we know p is not Perfect.

$$p = \left\{ \begin{array}{cccc} 1 & & & \\ & 4 & & \\ 3 & & 6 & \\ & 5 & & 13 \\ 2 & & 12 & \\ & 9 & & \\ 7 & & & \end{array} \right. \qquad q = \left\{ \begin{array}{cccc} 1 & & & \\ & 3 & & \\ 2 & & 9 & \\ & 8 & & 13 \\ 6 & & 12 & \\ & 10 & & \\ 4 & & & \end{array} \right.$$

Figure 15: Example ($N = 3$) of Theorem 10.2

Finally, we remark that, as a consequence of the conjugate symmetry, analagous results must hold for the region $x_1 > 1/2$. If any of the other elementary differences exceed $1/2$; i.e., $x_{j+1} - x_j > 1/2$ for some j satisfying $1 \leq j \leq N-1$, then again we would expect that the irregularity is not particularly large. In this situation, one can show that no vertices (and hence, certainly no local maxima) can exist.

11 Upper Bounds on D_N and the VG-Algorithm

11.1 An Exponential Bound

Because D_N is, by definition, the minimal trace attained among all Good N-triangles, the trace of any particular Good N-triangle which can be exhibited is an upper bound on D_N. As will be detailed in Section 11.3, for a fixed value of N, there is a simple algorithm for producing a large supply of Good N-triangles. However, this algorithm does not readily yield an explicit formula for the dependence of the trace on N, and consequently, an analytical bound on D_N. Thus, there are really two issues at hand: (1) finding an analytical bound on D_N which is valid for all N and (2) for a fixed value of N, exhibiting an N-triangle whose trace is as near minimal as possible. Section 11.3 addresses the second problem.

In order to solve the first problem, one must find an algorithm which yields Good N-triangles for every N, and for which an explicit formula for the trace can be produced. Perhaps the simplest such algorithm is to proceed sequentially assigning to each generator the integer one greater than the sum of all of the previous ones. This procedure, as illustrated by Figure 16, yields the following simple theorem and corollary:

Theorem 11.1 *The N-triangle with generator*

$$p_k = 2^k, \qquad 0 \leq k \leq N \tag{122}$$

is Good.

Corollary 11.2

$$D_N \leq 2^{N+1} - 1. \tag{123}$$

As might be expected, one can do much better than this exponential bound.

$$
\begin{array}{cccccc}
1 & & & & & \\
 & 3 & & & & \\
2 & & 7 & & & \\
 & 6 & & 15 & & \\
4 & & 14 & & 31 & \\
 & 12 & & 30 & & \ddots \\
8 & & 28 & & & \\
 & 24 & & \ddots & & \\
16 & & & & & \\
 & \ddots & & & &
\end{array}
$$

Figure 16: N-triangle Expansion for Theorem 11.1

$$
\begin{array}{lllll}
a & & & & \\
 & 2a+1 & & & \\
a+1 & & 3a+3 & & \\
 & 2a+3 & & & \\
a+2 & & & & \\
\vdots & \vdots & \vdots & \cdots & (N+1)(a+N/2) \\
a+N-2 & & & & \\
 & 2a+2N-3 & & & \\
a+N-1 & & 3a+3N-3 & & \\
 & 2a+2N-1 & & & \\
a+N & & & &
\end{array}
$$

Figure 17: N-triangle Expansion for Theorem 11.3

11.2 Cubic Bounds

We here prove an analytical bound on D_N which is cubic in N. The idea is to use a generator consisting of linearly-ordered consecutive integers with the smallest integer chosen so as to guarantee that the N-triangle is Good. This procedure yields the following theorem:

Theorem 11.3 *The N-triangle with generator*

$$p_k = a + k, \qquad 0 \leq k \leq N \tag{124}$$

is Good provided that $a > N^2/4$.

<u>Proof</u>

The N-triangle expansion of the generator (124) is shown in Figure 17. Define m_j and M_j to be respectively the smallest and largest elements in the j^{th} column ($0 \leq j \leq N$) of this N-triangle. Then the N-triangle will be Good provided that a can be chosen to

26										
	53									
27		81								
	55		110							
28		84		140						
	57		114		171					
29		87		145		203				
	59		118		177		236			
30		90		150		210		270		
	61		122		183		244		305	
31		93		155		217		279		341
	63		126		189		252		315	
32		96		160		224		288		
	65		130		195		260			
33		99		165		231				
	67		134		201					
34		102		170						
	69		138							
35		105								
	71									
36										

Figure 18: Example ($N = 10$) of Theorem 11.3

guarantee that $m_j - M_{j-1}$ is strictly positive for $1 \leq j \leq N$. From Figure 17, it is easy to see that $m_j = p_{0,j}$ and $M_j = p_{N-j,N}$. A simple calculation then gives

$$m_j = (j+1)(a + j/2) \tag{125}$$

and

$$M_j = (j+1)(a + N - j/2), \tag{126}$$

so that

$$m_j - M_{j-1} = a - j(N-j). \tag{127}$$

By elementary calculus, the right-hand side cannot be any smaller than when $j = N/2$, so

$$m_j - M_{j-1} \geq a - N^2/4. \tag{128}$$

Thus choosing $a > N^2/4$ guarantees that the N-triangle is Good.

□

Figure 18 illustrates an application of this theorem for $N = 10$ with the smallest possible choice of a. Note that this results in an N-triangle with $N+1$ independent occurrences of the index — N times within the generator and once between 170 and 171.

A direct consequence of Theorem 11.3 is that

Corollary 11.4

$$D_N \leq (N+1)\left\{ \left\lceil \frac{N^2}{4} \right\rceil + \frac{N}{2} \right\}; \tag{129}$$

$$
\begin{array}{lllll}
a & & & & \\
 & 2a+2 & & & \\
a+2 & & 3a+6 & & \\
 & 2a+6 & & & \\
a+4 & & & & \\
 & & & & \\
\vdots & \vdots & \vdots & \cdots & (N+1)(a+N/2) \\
 & & & & \\
a+5 & & & & \\
 & 2a+8 & & & \\
a+3 & & 3a+9 & & \\
 & 2a+4 & & & \\
a+1 & & & &
\end{array}
$$

Figure 19: N-triangle Expansion for Theorem 11.5

therefore, D_N is bounded above by a cubic polynomial in N. The following theorem demonstrates that the coefficient of N^3 in this bound can be improved somewhat. Again, a generator composed of consecutive integers is used, but now these integers are mixed up "as much as possible" rather than linearly ordered. The priced paid for this improved bound is a slightly more complicated proof.

Theorem 11.5 *The N-triangle with generator*

$$
p_k = \begin{cases} a + 2k, & 0 \le k \le N/2 \\ a + 2(N-k) + 1, & N/2 < k \le N \end{cases} \tag{130}
$$

is Good provided that $a > (2N-1)^2/24$.

Proof

The N-triangle expansion of the generator (130) is shown in Figure 19. The same strategy will be adopted which was used to prove the previous theorem. Define m_j and M_j as before. Again, as can be seen from Figure 19, $m_j = p_{0,j}$ and a simple calculation gives

$$
m_j = \begin{cases} (j+1)(a+j), & 0 \le j \le N/2 \\ (j+1)a + (N+1)N/2 - (N-j)^2, & N/2 < j \le N \end{cases} . \tag{131}
$$

The largest element of each column of the N-triangle expansion of Figure 19 occurs roughly in the middle of that column. Explicit formulas for the indices of this element (which attains M_j) are tedious and unnecessary, as it is evident that M_j is just the sum of the $j+1$ largest elements in the generator; and thus, it is again given by (126).

First assume that $1 \le j \le N/2$; i.e., m_j is given by the first part of (131). In this case

$$
m_j - M_{j-1} = a - \frac{1}{2}[(2N-1)j - 3j^2]. \tag{132}
$$

By elementary calculus, the right-hand side cannot be any smaller than when $j = (2N - 1)/6$, so

$$
m_j - M_{j-1} \ge a - (2N-1)^2/24. \tag{133}
$$

16										
	34									
18		54								
	38		76							
20		60		100						
	42		84		126					
22		66		110		151				
	46		92		135		174			
24		72		117		158		195		
	50		97		140		179		214	
26		75		120		161		198		231
	51		98		141		180		215	
25		74		119		160		197		
	48		95		138		177			
23		69		114		155				
	44		88		131					
21		63		105						
	40		80							
19		57								
	36									
17										

Figure 20: Example ($N = 10$) of Theorem 11.5

Thus choosing $a > (2N-1)^2/24$ guarantees that $m_j - M_{j-1}$ is strictly positive for $1 \leq j \leq N/2$. It remains to be shown that the same condition will also guarantee that $m_j - M_{j-1}$ is strictly positive for $N/2 < j \leq N$; i.e., when m_j is given by the second part of (131). In this case

$$m_j - M_{j-1} = a - \frac{1}{2}[j^2 - (2N-1)j + N(N-1)]. \tag{134}$$

□

Figure 20 illustrates an application of this theorem for $N = 10$ with the smallest possible choice of a. Note that this again results in an N-triangle with $N+1$ independent occurrences of the index — N times within the generator and once between 75 and 76. The upper bound corresponding to Theorem 11.5 is given by

Corollary 11.6

$$D_N \leq (N+1)\left\{ \left\lceil \frac{(2N-1)^2}{24} \right\rceil + \frac{N}{2} \right\}. \tag{135}$$

This is the best analytical bound on D_N which is currently known by this author.

11.3 The VG-Algorithm and the Quadratic Bound Conjecture

As previously mentioned, finding Perfect N-triangles (or Golomb rulers) is not the objective of the present work. For completeness, however, we do present a simple algorithm for constructing Good N-triangles whose trace is not too large. A special case of this algorithm has been previously studied in connection with the Golomb Ruler Problem. The original idea was conceived by S. W. Golomb under the name of the "midsegment algorithm", and later refined by D. S. Robertson. For an overview and numerous examples, see reference [3].

The basic idea is to fill in the components of the generator in some pre-chosen order and in such a way that, at each step, all the N-triangle elements that can be calculated are distinct. We formalize this idea by defining the *VG-algorithm*[12] for generating a Good N-triangle.

Definition 11.1 *Let $\{j_m\}_{m=0}^N$ be a permutation of $\{0, 1, \cdots, N\}$ and define $p \in P'_N$ as follows. Let $p_{j_0} = 1$. For $1 \le m \le N$, proceed sequentially choosing each p_{j_m} to be the smallest integer strictly greater than $p_{j_{m-1}}$ which guarantees that all of the N-triangle elements which have only p_{j_0} through p_{j_m} as summands are distinct. We then say that p is generated by the* <u>*VG-algorithm*</u> *using the permutation $\{j_m\}_{m=0}^N$.*

Golomb's "midsegment algorithm" is recovered by using the permutation

$$\{j_m\}_{m=0}^N = \{0, N, 1, N-1, 2, N-2, \cdots\}. \tag{136}$$

As first noted by Golomb, the N-triangle generated by the VG-algorithm using this permutation is particularly Good. In fact, it is Perfect for $N \le 5$. For $N = 6$, the VG-algorithm using the above permutation yields a 6-triangle with $\operatorname{Tr} p = 36$ as compared to the Perfect trace $D_6 = 34$.

As an explicit example, the 10-triangle generated by the VG-algorithm using the permutation given by equation (136) is shown in Figure 21. Note that, using this particular permutation, the N-triangle generated by the VG-algorithm can be obtained from the analogous $(N-1)$-triangle by adding a new component to the "middle" of the generator. Thus, Figure 21 also tells us the components of the generators of the analogous N-triangles for $N \le 9$.

The VG-algorithm is important because it gives a rich supply of Good N-triangles with relatively little effort. In applications where optimality is not necessarily needed, these N-triangles may serve the required purpose. This is the situation for the problem of constructing radar signals with sharply peaked ambiguity functions [1].

The VG-algorithm is also important for the following reason. It is easy to see that if p is an N-triangle generated by the VG-Algorithm (using any permutation) then p has the vertex property, p has the index reduction property, and $\operatorname{In} p = 1$. Thus, if Conjecture 5 is true then these N-triangles are all Superb; and if, in addition, Conjecture 2 is true then they are also locally maximal. This is most probably the case. However, the VG-algorithm can find only $(N+1)!/2$ (one for each permutation modulo conjugacy) out of a total of S_N Superb N-triangles.[13] Nevertheless, supported by all known Perfect N-triangles, we make the following conjecture.

Conjecture 9 *Every Perfect N-triangles can be generated by the VG-algorithm using a suitable permutation.*

If this conjecture is true, one can simply apply the VG-algorithm to each of the $(N+1)!/2$ permutations; those resulting N-triangles with minimal trace will be the Perfect N-triangles. Moreover, one may be able to eliminate certain classes of permutations a priori by using arguments similar to those of Section 10.

[12] Very Good

[13] Here, we are assuming Conjecture 4 is true.

1										
	4									
3		10								
	9		21							
6		20		40						
	17		39		64					
11		36		63		87				
	30		60		86		101			
19		54		83		100		109		
	43		77		97		108		114	
24		66		91		105		113		116
	47		80		99		110		115	
23		61		88		104		112		
	37		69		93		106			
14		45		74		95				
	22		50		76					
8		27		52						
	13		29							
5		15								
	7									
2										

Figure 21: Example ($N = 10$) of the VG-Algorithm

Finally, in Table 2, we give a summary of the various upper bounds which have been discussed, in comparison with the actual values of D_N. We know (from Corollaries 5.9 and 11.4) that D_N is bounded below by a quadratic in N and bounded above by a cubic in N. However, as D_N seems to be diverging from the cubic bounds (and based on other analytical and empirical evidence), we conjecture that D_N is, in fact, bounded above by a quadratic in N. Of course, for this to be true, it is sufficient (but not necessary) for the trace of the N-triangle generated by the VG-algorithm using the permutation given by equation (136) (the sixth column in Table 2) to be bounded above by a quadratic in N. If it is true, this latter assertion may be easier to prove. Without loss of generality, we state the quadratic bound conjecture as

Conjecture 10 *There exists some $\alpha \in \mathbb{R}$ such that $D_N \leq \alpha C_N$ for all $N \in \mathbb{N}$.*

For the purpose of comparison, we tabulate this pseudo-bound for $\alpha = 1.5$ in the last column of Table 2; we do not claim that this value of α works for all $N \in \mathbb{N}$.

12 Conclusion and Open Problems

To conclude, we first summarize the key results concerning the relationship between maximizing irregularity (Problem 1) and the Golomb Ruler Problem (Problem 2). We then collect into one place the many interesting unresolved issues which have arisen, and supplement them with a few miscellaneous problems and conjectures.

A summary of the main results contained herein can conveniently be organized around the following four assertions, which we will call the *X–P equivalence theorems*:

N	C_N	D_N	Cor. 11.4	Cor. 11.6	VG-Alg.	$\lfloor 1.5C_N \rfloor$
0	1	1	1	1	1	1
1	3	3	3	3	3	4
2	6	6	9	6	6	9
3	10	11	18	14	11	15
4	15	17	35	25	17	22
5	21	25	57	39	25	31
6	28	34	91	63	36	42
7	36	44	132	92	50	54
8	45	55	189	126	69	67
9	55	72	255	175	92	82
10	66	85	341	231	116	99
11	78	106	438	294	141	117
12	91	127	559	377	172	136

Table 2: Comparison of Upper Bounds on D_N

1. $T(X_N) \approx P_N$ (Theorem 3.1)
2. $T(X'_N) \approx P'_N$ (Theorem 3.2)
3. $T(X''_N) \approx P''_N$ (Conjecture 2)
4. $T(X'''_N) \approx P'''_N$ (Conjecture 1).

The first step in the analysis was to map the study of the continuous irregularity function $F_N(x)$ onto the study of discrete N-triangles (or "rulers" in the terminology of the Golomb Ruler Problem). The first X–P equivalence theorem says that X_N, the natural domain of $F_N(x)$, can be mapped bijectively onto ($\approx$-equivalence classes of) P_N, the space of N-triangles. Together with equation (46), which provides an explicit formula for calculating $F_N(x)$ directly from $p = T(x)$, this theorem allows one to translate any statement about $F_N(x)$ into an equivalent statement about N-triangles (and vice versa).

The second X–P equivalence theorem is a trivial consequence of the first. It says that an N-triangle $p = T(x)$ is Good (i.e., all its elements are distinct) if and only if $F_N(x) > 0$. Although trivial to prove, this theorem is important for two reasons. Firstly, many statements about $F_N(x)$ are more naturally formulated on $X'_N \equiv \{x \in X_N \mid F_N(x) > 0\}$ than X_N; and similarly, many statements about N-triangles are more naturally formulated on $P'_N \equiv \{p \in P_N \mid p \text{ is Good}\}$ than P_N. Secondly, it serves as a simple prelude for the more substantial X–P equivalence theorems which follow.

The fourth X–P equivalence theorem is an abstract statement of the assertion that maximizing irregularity and finding Golomb rulers are equivalent problems. It says that an N-triangle $p = T(x)$ is Perfect (i.e., it is a Golomb ruler) if and only if $F_N(x)$ attains a global maximum at the point x. This is precisely what we want to prove; however, we have been completely successful only for $N \leq 4$. For the general case, we have focused instead on the stronger assertion given by the third X–P equivalence theorem.

The third X–P equivalence theorem is a localized version of the fourth. In order to achieve this localization, we defined *structure* equivalence classes of P_N which correspond (via the N-triangle bijection T) to open polyhedral regions of X_N on which $F_N(x)$ is strictly positive and concave. The third X–P equivalence theorem says that an N-triangle $p = T(x)$ is Superb (i.e., it is a Golomb ruler *relative to a particular structure equivalence* *class*) if and only if $F_N(x)$ attains a *local* maximum at the point x. Therefore, the third X–P equivalence theorem is much stronger than what we originally set out to prove; it implies the fourth X–P equivalence theorem.

Nevertheless, for the following reasons, the third X–P equivalence theorem has been the focal point of the present work. First, all empirical evidence indicates that it is true, thus suggesting that the issue in question is more closely related to local maximality than global maximality. Secondly, as has been demonstrated, the methods of convex analysis and linear programming can be applied to the localized version, thus allowing us to obtain a deeper understanding of it content as compared to the global version. This deeper understanding is manifested by the similarity between Theorems 7.12 and 7.13, which, in turn, gives us the additional proposition in Theorem 7.14 as compared to Theorem 5.6. This additional proposition — which relates the third X–P equivalence theorem to the theory of integral polyhedra — leads directly to a deeper understanding of the continuous irregularity function $F_N(x)$, as reflected by Theorem 8.3. Finally, though we do not actually succeed in proving the third X–P equivalence theorem, we are able to tie it logically to more traditional mathematical assertions, like Conjectures 6 and 7.

We conclude with a list of open problems. First, we have Conjectures 1–10 which are given throughout the paper. The proofs of these conjectures are likely to range from easy (Conjecture 3) to difficult (Conjecture 8). It is important to keep in mind that many of these are logically interdependent, especially those in Section 7.5. Although all have been tested to some extent, they do carry differing degrees of conviction. For example, it is strongly believed that Conjectures 4 and 6 are true, which, in turn, implies that Conjecture 2 (and hence Conjecture 1) is true. On the other hand, Conjectures 8–10 are more speculative.

In addition to these formal conjectures, we have mentioned the following three problems.

1. For fixed N, determine the largest value of M that can be attained in Theorem 7.10. In other words, what is the maximum number of consecutive independent pairs of elements that any Good N-triangle can have?

2. For fixed N, find a complete characterization of the class of structure matrices.

3. Determine S_N for $N \geq 4$ and/or its asymptotic behavior.

The first problem is relatively easy; whereas, the second is likely to be difficult. The third problem is purely combinatorial; the next few values of S_N should be easily accessible by computer. Another interesting problem is to determine the distribution of those points in X_N whose corresponding N-triangles have unit index. Preliminary investigations for $N = 2$ have been quite intriguing.

Thirdly, we have the following miscellaneous conjecture.

Conjecture 11 *Suppose* $p \in P_N$ *and* $\operatorname{In} p \geq 2$*. Then, for some* $q, r \in P_N$*,* p *can be decomposed as* $p = q + r$*, where* $\operatorname{In} q = \operatorname{In} p - 1$ *and* $\operatorname{In} r = 1$*.*

This is an example of an "algebraic" assertion about N-triangles, in the sense that it has nothing do with maximizing irregularity or Golomb Rulers, at least on the surface. Many interesting conjectures of this type can be formulated. This one is particularly interesting in that it actually implies Conjecture 1 without implying Conjecture 2. It is easy to prove for $N = 1$ and no counter examples have yet been found for $N \geq 2$.

Finally, of course, we have the problem of actually finding Perfect N-Triangles (Golomb rulers) for $N \geq 12$. This problem is discussed in more detail in the references [3, 4]. We also have the closely related problem of determining D_N and/or the number of distinct Perfect N-triangles (as a function of N) either exactly or asymptotically. The present work may stimulate further progress in this direction, at least for the asymptotic results.

A Perfect N-Triangles for $N \leq 9$

$\underline{N=1}$

1	
	3
2	

$\underline{N=2}$

1		
	4	
3		6
	5	
2		

$\underline{N=3}$

1			
	4		
3		9	
	8		11
5		10	
	7		
2			

2			
	7		
5		8	
	6		11
1		9	
	4		
3			

$\underline{N=4}$

1				
	4			
3		10		
	9		15	
6		14		17
	11		16	
5		13		
	7			
2				

1				
	4			
3		10		
	9		12	
6		11		17
	8		16	
2		13		
	7			
5				

1				
	8			
7		11		
	10		13	
3		12		17
	5		16	
2		9		
	6			
4				

1				
	8			
7		12		
	11		14	
4		13		17
	6		16	
2		9		
	5			
3				

$\underline{N = 5}$

1					
	4				
3		10			
	9		18		
6		17		23	
	14		22		25
8		19		24	
	13		21		
5		15			
	7				
2					

1					
	11				
10		16			
	15		19		
5		18		23	
	8		22		25
3		12		24	
	7		14		
4		9			
	6				
2					

1					
	7				
6		11			
	10		20		
4		19		23	
	13		22		25
9		16		24	
	12		18		
3		14			
	5				
2					

2					
	3				
1		10			
	8		16		
7		14		21	
	13		19		25
6		18		23	
	11		22		
5		15			
	9				
4					

2					
	7				
5		13			
	11		21		
6		19		22	
	14		20		25
8		15		23	
	9		18		
1		12			
	4				
3					

$\underline{N=6}$

1						
	4					
3		9				
	8		15			
5		14		22		
	11		21		32	
6		18		31		34
	13		28		33	
7		23		30		
	17		25			
10		19				
	12					
2						

$\underline{N=7}$

1							
	5						
4		12					
	11		25				
7		24		27			
	20		26		35		
13		22		34		41	
	15		30		40		44
2		23		36		43	
	10		29		39		
8		16		32			
	14		19				
6		17					
	9						
3							

$\underline{N=8}$

1								
	6							
5		10						
	9		23					
4		22		26				
	17		25		34			
13		20		33		41		
	16		28		40		53	
3		24		35		52		55
	11		31		47		54	
8		18		43		49		
	15		30		45			
7		27		32				
	19		29					
12		21						
	14							
2								

<u>$N = 9$</u>

1									
	4								
3		13							
	12		28						
9		27		33					
	24		32		47				
15		29		46		54			
	20		43		53		64		
5		34		50		63		70	
	19		41		60		69		72
14		26		51		66		71	
	21		36		57		68		
7		31		42		59			
	17		37		44				
10		23		39					
	16		25						
6		18							
	8								
2									

1									
	9								
8		19							
	18		24						
10		23		31					
	15		30		52				
5		22		51		56			
	12		43		55		58		
7		33		47		57		69	
	28		37		49		68		72
21		32		39		60		71	
	25		34		50		63		
4		27		45		53			
	6		38		48				
2		17		41					
	13		20						
11		16							
	14								
3									

B Proof of Conjecture 1 for $N \leq 4$

We first develop a few general results, after which, the cases $N = 1$ and $N = 2$ will follow immediately.[14] The case $N = 3$ will then be proved completely and the case $N = 4$ will be outlined. The detailed treatment of the case $N = 4$ is quite involved; the generalization to $N = 5$ is not immediately apparent.

We take as a starting point the form of Conjecture 1 given by the second proposition in Theorem 5.6. We abbreviate this as

$$p = kq, \quad q \in P_N''' \Longleftrightarrow p \in T(X_N'''), \tag{B.1}$$

where throughout this section, we assume k is some positive integer. We wish to develop another equivalent form of this proposition which will be easier to prove.

First, from Corollary 5.2 and Theorem 5.5, we know that if $q \in P_N'''$ and $p = kq$ then p has irregularity D_N^{-1}. It follows that (B.1) is equivalent to

$$p \neq kq, \quad q \in P_N''' \Longrightarrow \frac{\operatorname{In} p}{\operatorname{Tr} p} < \frac{1}{D_N}. \tag{B.2}$$

Secondly, we remark that the inequality on the right-hand side of (B.2) is equivalent to

$$\operatorname{Tr} p \leq k' D_N \Longrightarrow \operatorname{In} p < k'. \tag{B.3}$$

Moreover, without loss of generality, the left-hand side of (B.3) may be replaced by

$$(k' - 1) D_N < \operatorname{Tr} p \leq k' D_N. \tag{B.4}$$

This defines k' uniquely for any given $p \in P_N$. If p satisfies this inequality and $p = kq$ with $q \in P_N'''$ then the only possibility is that $k = k'$. It follows that (B.2) is equivalent to

$$\left. \begin{aligned} (k-1) D_N < \operatorname{Tr} p \leq k D_N \\ p \neq kq, \quad q \in P_N''' \end{aligned} \right\} \Longrightarrow \operatorname{In} p < k. \tag{B.5}$$

This is the form in which we will prove Conjecture 1. If $\operatorname{Tr} p \leq D_N$ and p is not Perfect then (by the definition of D_N) $\operatorname{In} p = 0$. Therefore, we may assume $k \geq 2$. We now commence with the proof proper by using the method of *reductio ad absurdum.*

Let $p \in P_N$ and suppose

$$\begin{aligned} &(k-1) D_N < \operatorname{Tr} p \leq k D_N, \quad k \geq 2; \\ &p \neq kq, \quad q \in P_N'''; \\ &\operatorname{In} p \geq k. \end{aligned} \tag{B.6}$$

Define q and r to be the quotient and remainder (respectively) resulting from the division of p by k; i.e., for $0 \leq j \leq N$, put $q_j = \lfloor p_j / k \rfloor$ and $r_j = p_j - k q_j$ so that

$$p_j = k q_j + r_j, \quad 0 \leq r_j \leq k - 1. \tag{B.7}$$

From the assumptions (B.6), it follows that neither q nor r can be identically zero; therefore, $q \in P_N$ and $r \in P_N$. We then have

$$\operatorname{Tr} p = k \operatorname{Tr} q + \operatorname{Tr} r \leq k D_N. \tag{B.8}$$

[14] That Conjecture 1 holds for these trivial cases should come as no surprise — the existence of a unique global maximum corresponding to the unique Perfect N-triangle (on the conjugate-free ordered-x simplex) is apparent in Figures 1 and 2.

This, in turn, implies

$$\operatorname{Tr} q < D_N \tag{B.9}$$

so that q is *not* Good. Nevertheless, q cannot be too bad in the following sense.

Let $\{j_m\}_{m=0}^N$ be a permutation of $\{0, 1, \cdots, N\}$ such that

$$p_{j_0} < p_{j_1} < \cdots < p_{j_N}. \tag{B.10}$$

Then, for $1 \leq m \leq N$,[15]

$$k \leq \operatorname{In} p \leq p_{j_m} - p_{j_{m-1}} = k(q_{j_m} - q_{j_{m-1}}) + (r_{j_m} - r_{j_{m-1}}). \tag{B.11}$$

So

$$q_{j_m} - q_{j_{m-1}} \geq 1 - \frac{r_{j_m} - r_{j_{m-1}}}{k} \geq 1 - \frac{k-1}{k} > 0. \tag{B.12}$$

In other words, the components of the generator of q are distinct positive integers with the same relative ordering as the components of the generator of p.

At this point, we can obtain an absurdity (and thus conclude the proof) for the cases $N = 1$ and $N = 2$. Recall that for these two cases, $D_N = C_N$; hence, (B.9) becomes $\operatorname{Tr} q < C_N$. On the other hand, if the components of the generator of q are distinct positive integers then $\operatorname{Tr} q \geq C_N$. Thus the existence of q is absurd.

The reason that Conjecture 1 can be proved for $N = 3$ and $N = 4$ is that the number of possibilities for q is relatively small, and each leads to an absurdity. Our basic strategy for uncovering this absurdity is as follows. Since q is not Good, we can find *independent* (see Definition 6.1) elements $q_{i,j}$ and $q_{i',j'}$ satisfying $q_{i,j} = q_{i',j'}$, in which case

$$|p_{i,j} - p_{i',j'}| = |r_{i,j} - r_{i',j'}|. \tag{B.13}$$

We will then show $|r_{i,j} - r_{i',j'}| \leq k - 1$, which contradicts the assumption that $\operatorname{In} p \geq k$.

Consider $N = 3$. As the components of the generator of q must be distinct positive integers satisfying $\operatorname{Tr} q < D_3 = 11$, the only possibility is a permutation of $\{1, 2, 3, 4\}$. Therefore $q_{j_m} - q_{j_{m-1}} = 1$ and (B.11) implies $r_{j_m} - r_{j_{m-1}} \geq 0$, or more explicitly

$$0 \leq r_{j_0} \leq r_{j_1} \leq r_{j_2} \leq r_{j_3} \leq k - 1. \tag{B.14}$$

We now consider three exhaustive (but non-mutually exclusive) cases.

Case Ia: p_{j_0} and p_{j_1} are adjacent

For some $p_{i,j}$ (with $j = i$) and some $p_{i',j'}$ (with $j' = i' + 1$) we have $p_{i,j} = p_{j_2}$ and $p_{i',j'} = p_{j_0} + p_{j_1}$. Since $q_{j_2} - q_{j_0} - q_{j_1} = 0$ and (B.14) gives $0 \leq r_{j_2} - r_{j_1} \leq k - 1$ and $0 \leq r_{j_0} \leq k - 1$, it follows that

$$|p_{i,j} - p_{i',j'}| = |(r_{j_2} - r_{j_1}) - r_{j_0}| \leq k - 1. \tag{B.15}$$

This contradicts the assumption that $\operatorname{In} p \geq k$.

Case Ib: p_{j_0} and p_{j_2} are adjacent

For some $p_{i,j}$ (with $j = i$) and some $p_{i',j'}$ (with $j' = i' + 1$) we have $p_{i,j} = p_{j_3}$ and $p_{i',j'} = p_{j_0} + p_{j_2}$. Since $q_{j_3} - q_{j_0} - q_{j_2} = 0$ and (B.14) gives $0 \leq r_{j_3} - r_{j_2} \leq k - 1$ and $0 \leq r_{j_0} \leq k - 1$, it follows that

$$|p_{i,j} - p_{i',j'}| = |(r_{j_3} - r_{j_2}) - r_{j_0}| \leq k - 1. \tag{B.16}$$

This contradicts the assumption that $\operatorname{In} p \geq k$.

[15] For completeness, this and all similar arguments should also be applied to the special case obtained by making the replacement $p_{j_m} - p_{j_{m-1}} \to p_{j_0}$.

Case Ic: p_{j_0} and p_{j_3} are adjacent *and* p_{j_1} and p_{j_2} are adjacent

For some $p_{i,j}$ (with $j = i+1$) and some $p_{i',j'}$ (with $j' = i'+1$) we have $p_{i,j} = p_{j_1} + p_{j_2}$ and $p_{i',j'} = p_{j_0} + p_{j_3}$. Since $q_{j_1} + q_{j_2} - q_{j_0} - q_{j_3} = 0$ and (B.14) gives $0 \le r_{j_1} - r_{j_0} \le k-1$ and $0 \le r_{j_3} - r_{j_2} \le k-1$, it follows that

$$|p_{i,j} - p_{i',j'}| = |(r_{j_1} - r_{j_0}) - (r_{j_3} - r_{j_2})| \le k-1. \tag{B.17}$$

This contradicts the assumption that $\operatorname{In} p \ge k$.

This concludes the proof for $N = 3$.

Now consider $N = 4$. In this case, the components of the generator of q must be distinct positive integers satisfying $\operatorname{Tr} q < D_4 = 17$; therefore, q is either a permutation of $\{1,2,3,4,5\}$ or a permutation of $\{1,2,3,4,6\}$. For the first possibility, the proof can be carried out in essentially the same way as before. The crucial point is that (B.11) again implies

$$0 \le r_{j_0} \le r_{j_1} \le r_{j_2} \le r_{j_3} \le r_{j_4} \le k-1. \tag{B.18}$$

One possible breakdown into an exhaustive set of cases is as follows.

Case Ia: p_{j_0} and p_{j_1} are adjacent

Case Ib: p_{j_0} and p_{j_2} are adjacent

Case Ic: p_{j_0} and p_{j_3} are adjacent

Case Id: p_{j_1} and p_{j_2} are adjacent

Case Ie: p_{j_0} and p_{j_4} are adjacent *and* p_{j_1} and p_{j_3} are adjacent

Each of these cases can be treated exactly as was done for $N = 3$.

The second possibility is that q is a permutation of $\{1,2,3,4,6\}$. In this case, we have $q_{j_4} - q_{j_3} = 2$, which means that (B.11) allows us to conclude (B.14) but not (B.18). In other words, the only thing we know about r_{j_4} is that $0 \le r_{j_4} \le k-1$. Again, we propose an exhaustive set of cases.

Case IIa: p_{j_0} and p_{j_1} are adjacent

Case IIb: p_{j_0} and p_{j_2} are adjacent

Case IIc: p_{j_0} and p_{j_3} are adjacent *and* p_{j_1} and p_{j_2} are adjacent

Case IId: p_{j_1} and p_{j_3} are adjacent

Case IIe: p_{j_0} and p_{j_5} are adjacent *and* p_{j_2} and p_{j_3} are adjacent

Case IIf: $q = (1,4,3,6,2)$ (modulo conjugacy)

Cases IIa–IIc can be treated exactly as was done for $N = 3$ because, with reference to the discussion preceding equation (B.13), $|p_{i,j} - p_{i',j'}|$ does not depend on r_{j_4}. Cases IId–IIf require a different argument, and we procede as follows.

From (B.8), we know $\operatorname{Tr} r \le k(D_N - \operatorname{Tr} q) = k$. Therefore, again with reference to the discussion preceding equation (B.13), we know

$$k \le \operatorname{In} p \le |p_{i,j} - p_{i',j'}| = |r_{i,j} - r_{i',j'}| \le \operatorname{Tr} r \le k. \tag{B.19}$$

Thus we conclude

$$|r_{i,j} - r_{i',j'}| = k. \tag{B.20}$$

Note that the application of the triangle inequality relies critically on the independence of $r_{i,j}$ and $r_{i',j'}$.

We now apply (B.20) to obtain an absurdity for Case IId. There are two subcases corresponding to the two choices of sign arising from the absolute value.

Case IId: p_{j_1} and p_{j_3} are adjacent

For some $p_{i,j}$ (with $j = i$) and some $p_{i',j'}$ (with $j' = i' + 1$) we have $p_{i,j} = p_{j_4}$ and $p_{i',j'} = p_{j_1} + p_{j_3}$. Since $q_{j_4} - q_{j_1} - q_{j_3} = 0$ and by using (B.20), we have

$$|p_{i,j} - p_{i',j'}| = |r_{j_4} - r_{j_1} - r_{j_3}| = k. \tag{B.21}$$

If the argument of the absolute value is postive then

$$\begin{aligned} r_{j_4} = r_{j_1} + r_{j_3} + k &\implies \\ \operatorname{Tr} r = r_{j_0} + 2r_{j_1} + r_{j_2} + 2r_{j_3} + k \leq k &\implies \\ r_{j_0} = r_{j_1} = r_{j_2} = r_{j_3} = 0 &\implies \\ r_{j_4} = k. & \end{aligned} \tag{B.22}$$

The last equality contradicts the assumption that $r_{j_4} \leq k-1$. Similarly, if the argument of the absolute value is negative then

$$\begin{aligned} r_{j_1} + r_{j_3} = r_{j_4} + k &\implies \\ \operatorname{Tr} r = r_{j_0} + r_{j_2} + 2r_{j_4} + k \leq k &\implies \\ r_{j_0} = r_{j_1} = r_{j_2} = r_{j_4} = 0 &\implies \\ r_{j_3} = k. & \end{aligned} \tag{B.23}$$

The last equality contradicts the assumption that $r_{j_3} \leq k-1$; we have used (B.14) to obtain $r_{j_1} = 0$.

For Cases IIe and IIf, the above method can be applied to the subcases corresponding to one choice of sign arising from the absolute value. For the subcases corresponding to the other choice of sign, the method fails; one can only conclude that $r_{j_0} = r_{j_1} = r_{j_4} = 0$ and $r_{j_2} + r_{j_3} = k$, which is not manifestly contradictory. However, there are only four possible permutations (modulo conjugacy) which are covered exclusively by these two cases. For each one, we obtain a contradiction as follows.

Case IIe.1: $q = (2, 6, 1, 4, 3)$

$$p_{3,4} = (4k + r_{j_3}) + (3k + r_{j_2}) = 8k = p_{0,1}. \tag{B.24}$$

Case IIe.2: $q = (1, 6, 2, 3, 4)$

$$p_{3,4} = (3k + r_{j_2}) + (4k + r_{j_3}) = 8k = p_{1,2}. \tag{B.25}$$

Case IIe.3: $q = (1, 6, 4, 3, 2)$

$$\begin{aligned} p_{2,4} &= (4k + r_{j_3}) + (3k + r_{j_2}) + 2k = 10k, \\ p_{1,2} &= 6k + (4k + r_{j_3}) = 10k + r_{j_3}; \end{aligned} \tag{B.26}$$

$$\implies$$

$$p_{1,2} - p_{2,4} = r_{j_3} \leq k - 1. \tag{B.27}$$

Case IIf: $q = (1, 4, 3, 6, 2)$

$$p_{1,2} = (4k + r_{j_3}) + (3k + r_{j_2}) = 8k = p_{3,4}. \tag{B.28}$$

This concludes (the outline of) the proof for $N = 4$.

The proof is not elegant; no one argument will work for all of the various cases. Also, for both $N = 3$ and $N = 4$, we have used either $\mathrm{Tr}\, q = C_N$ or $\mathrm{Tr}\, q = D_N - 1$ in each of the arguments. Since for $N = 5$, there will be cases where neither of these hold, the generalization of the proof is not immediately apparent. Presumedly, this lack of elegance is due to the fact that we are trying to prove a property based on the globally maximal nature of an N-triangle, when in actuality, it is the locally maximal nature which gives rise to the property.

Acknowledgements

Above all, the author would like to thank Alex Grossmann for introducing him to the concept of irregularity, for supplying the graphics software, and for patiently discussing most of the preliminary results. Thanks are also due to N. J. Sloane for identifying the sequence $\{1, 3, 6, 11, 17, \cdots\}$, and to S. W. Golomb for supplying some of the references. Finally, the author would like to thank everyone at the Centre de Physique Théorique, in particular Maryse Cohen-Solal, for making his stay in Marseille productive and enjoyable.

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