Local Search and High Precision Gray Codes: Convergence Results and Neighborhoods

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Abstract

A proof is presented that shows how the neighborhood structure that is induced under a Gray Code representation repeats under shifting. Convergence proofs are also presented for steepest ascent using a local search bit climber and a Gray code representation: for unimodal 1-D functions and multimodal functions that are separable and unimodal in each dimension, the worst case number of steps needed to reach the global optimum is $\mathcal{O}(L)$ with a constant ≤ 2. We also show how changes in precision impact the Gray neighborhood. Finally, we also show how both the Gray and Binary neighborhoods are easily reachable from the Gray coded representation.

1 Introduction

A long-standing debate in the field of evolutionary algorithms involves the use of bit versus real-valued encodings for parameter optimization problems. The genetic algorithm community has largely emphasized bit representations. On the other hand, the *evolution strategies* (ES) community [10] [9] [10] [1] and, more recently, the *evolutionary programming* (EP) community [4] have emphasized the use of real-valued encodings. There are also application-oriented genetic algorithm researchers (e.g., [3]) who have argued for the use of real-valued representations.

Unfortunately, positions on both sides of the encoding debate are based almost entirely on empirical data. The trouble with purely empirical comparisons is that there are too many factors besides representation that can impact the interpretation of experimental results, such as the use of different genetic operators, or differences in experimental methodology.

This work provides a better theoretical foundation for understanding the neighborhoods induced by a commonly used bit representation: Standard Binary Reflected Gray Codes.

One disadvantage of bit representations is that they generally do not offer the same precision as real-valued encodings. Often, genetic algorithms use 10 bits per parameter, while ES/EP approaches use full machine precision. On the one hand, different levels of precision can impact how accurately the global optimum is sampled, and can even change the apparent location of the optimum. Higher precision results in greater accuracy. But higher precision enlarges the search space, and conventional wisdom suggests that a smaller search space is generally an easier search problem. Yet, this intuition may be wrong for parameter optimization problems where the number of variables is fixed but the precision is not. This work examines how the search space changes as precision is increased when using bit encodings. In particular, we focus on how neighborhood connectivity changes and how the number of local optima can change as encoding precision is increased.

While our research is aimed at a very practical representation issue, this paper explores several theoretical questions related to the use of Gray codes, and high precision Gray codes in particular. These results have the potential to dramatically impact the use of evolutionary algorithms and local search methods which utilize bit representations.

We also present proofs which demonstrate that strong symmetries exist in the Hamming distance-1 neighborhood structure for Gray code representations. Given an L-bit encoding, we then prove that the worst-case convergence time (in terms of number of evaluations) to a global optimum is $\mathcal{O}(L)$ for any unimodal 1-dimensional function encoded using a reflected Gray code and a specialized form of steepest ascent local search under a Hamming distance-1 neighborhood. Under standard steepest ascent, the worst-case number of evaluations needed to reach a global optimum is $\mathcal{O}(L^2)$ for any unimodal 1-dimensional function. In both cases, the number of actual steps required to reach a global optimum is at most $2L$. This $\mathcal{O}(L)$ convergence time also holds for multidimensional problems when each dimension is unimodal and the intersection of the optima for each dimension leads to the global optimum. This includes problems such as the sphere function. In addition, we note some limitations of both Gray and Binary neighborhoods; we then prove that the standard Binary neighborhood is easily accessible from Gray space using a special neighborhood (or mutation) operator.

2 Local Optima, Problem Complexity, and Representation

To compare representations, it is essential to have a measure of problem complexity. The complexity measure we propose is the number of local optima in the neighborhood search space. There is evidence that the number of local optima is a relatively useful measure of problem complexity, that it impacts problem complexity, and relates to other measures such as schema fitness and Walsh coefficients [8] for problems using bit representations.

Suppose we have N unique points in our search space, each with k neighbors, and a search operator that evaluates all k neighboring points before selecting its next move; similar results hold for most non-unique sets of values. A point is considered a local optimum from a steepest ascent perspective if its evaluation is better than all of its k-neighbors. We can sort these N points to create an ordinal ranking, $R = r_1, r_2, ..., r_N$, where r_1 is the global optimum of the search space and r_N is the worst point in the space. Using R, we

can compute the probability $P(i)$ that a point ranked in the i-th position in R is a local optimum under an arbitrary representation, given a neighborhood of size k:

$$P(i) = \frac{\binom{N-i}{k}}{\binom{N-1}{k}} \qquad [1 \leq i \leq (N-k)] \tag{1}$$

Proof:

For any point in the search space, there are $\binom{N-1}{k}$ possible sets of neighbors for that point. If the point is ranked in position r_1, then there are $\binom{N-1}{k}$ sets of neighbors that do not contain a point of higher evaluation than the point r_1. Therefore, the point ranked in position r_1 will always be a local optimum under all representations of the function. In the general case, a point in position r_i has only $\binom{N-i}{k}$ sets of neighbors that do not contain a point of higher evaluation than the point r_i. Therefore the probability that the point in position r_i remains a local optimum under an arbitrary representation is $\binom{N-i}{k} / \binom{N-1}{k}$. □

This proof also appears in an IMA workshop paper [7]. These probabilities enable us to count the expected number of local optima that should occur in any function of size N. The formula for computing the expected number of times a particular point will be a local optimum is simply $N! \times P(i)$. Therefore the expected number of optima over the set of all representations is:

$$\mathcal{E}(N,k) = \sum_{i=1}^{N-k} P(i) \times N! \tag{2}$$

Rana and Whitley [7] show that to find the expected number of local optima for a single representation instance, we divide $\mathcal{E}(N,k)$ by $N!$, which yields:

$$\mu(N,k) = \sum_{i=1}^{N-k} P(i) = \sum_{i=1}^{N-k} \frac{\binom{N-i}{k}}{\binom{N-1}{k}} = \frac{N}{k+1} \tag{3}$$

This result leads to the following general observation: in expectation, if we increase neighborhood size we decrease the number of local optima in the induced search space. Can we leverage this idea when constructing bit representations? In particular, can we construct bit representations that increase neighborhood size while also bounding or decreasing the number of local optima?

3 Gray and Binary Representations

Another much-debated issue in the evolutionary algorithms community is the relative merit of Gray code versus Standard Binary code bit representations. Generally, "Gray code" refers to Standard Binary Reflected Gray code [2]. In general, a Gray code is any bit encoding where adjacent integers are also Hamming distance-1 neighbors in the bit space. There are exponentially many Gray codes with respect to bit length L. Over all possible discrete functions that can be mapped onto bit strings, the space of all Gray codes and the space of all Binary representations are identical. Therefore, a "No Free Lunch" result must hold [13] [5]. If we apply all possible search algorithms to Gray coded representations of all possible functions and we apply all possible search algorithms to Binary representations of all possible functions, the behavior of the algorithms must be

identical for the two sets of representations since the set of all possible Gray coded and the set of all Binary coded functions are identical [11].

The empirical evidence suggests that Gray codes are usually superior to Binary encodings for practical optimization problems. It has long been known that Gray codes remove the Hamming Cliffs induced by the Standard Binary code, where adjacent integers are represented by complementary bit strings: e.g., 7 and 8 encoded as 0111 and 1000. Whitley et al. [12] note that every Gray code must preserve the connectivity of the original real-valued functions (subject to the selected discretization). Further, because of the increased neighborhood size, Gray codes induce additional connectivity which can potentially 'collapse' optima in the real-valued function. Therefore, for *every* parameter optimization problem, the number of optima in the Gray coded space must be less than or equal to the number of optima in the original real-valued function. Binary encodings offer no such guarantees. Binary encodings destroy half of the connectivity of the original real-valued function; thus, given a large basin of attraction with a globally competitive local optimum, most of the (non-locally optimal) points near the optimum of that basin become new local optima under a Binary encoding.

Recently, we proved that Binary encodings work better on average than Gray encodings on "worst case" problems [11]; a "worst case" function is such that when interpreted as a 1-D function, alternating points in the search space are local optima. "Better" means that the representation induces fewer local optima. (There is a definitional error in this proof; it does not impact "wrapping" functions, but does impact the definition of a worst case function for "non-wrapping" functions. See Appendix 1 for details and a correction.) A corollary to this result is that Gray codes on average induce fewer optima than Binary codes for all remaining functions. For small (enumerable) search spaces, it can also be proven that in general Gray codes are superior to Binary for the majority of functions with bounded complexity. A function with "lower complexity" in this case has fewer optima in real space. We use these theoretical results, as well as the empirical evidence to argue for the use of Gray codes.

But to be comparable to real-valued representations, bit representations must use higher precision. Higher precision can allow one to get "closer" to an optimum, and also creates higher connectivity around the optimum. But what happens when we use higher precision Gray codes?

We first establish some basic properties of Gray neighborhoods. We will assume that we are working with a 1-dimensional function, but results generally apply to the decoding of individual parameters.

4 Properties of the Reflected Gray Space

We begin by asking what happens when a function is "shifted." Since we are working with bit representations, we assume that a *decoder* function converts bits to integers, and finally to real space. Shifting occurs after the bits have been converted to integers, but before the integers are mapped to real values. If there are L bits then we may add any integer between 0 and $2^L - 1$ $(mod\, 2^L)$. The only effect of this operator is to shift which bit patterns are associated with which real values in the input domain. Also note the resulting representation is still a Gray code under any shift [6].

What happens when one shifts by 2^{L-1}? Under Binary, such a shift just flips the first bit, and the Hamming distance-1 neighborhood is unchanged. A reflected Gray code is a symmetric reflection. Shifting therefore also flips the leading bit of each string, but it also reverses the order of the mapping of the function values to strings in each half of the space. However, since the Gray code is a symmetric reflection, again the Hamming distance-1 neighborhood does not change. This will be proven more formally.

It follows that every shift from $i = 0$ to $2^{L-1} - 1$ is identical to the corresponding shift at $j = 2^{L-1} + i$. We next prove that shifting by 2^{L-2} will not change the neighborhood structure; in general, shifting by 2^{L-k} will change exactly $k - 2$ neighbors.

Theorem 1 *For any Gray encoding, shifting by 2^{L-k} where $2 \leq k \leq L$ will result in a change of exactly $k - 2$ neighbors for any point in the search space.*

Proof: Consider an arbitrary Gray code, and $k \geq 2$. Divide the 2^L points in the search space into 2^k continuous blocks of equal size, starting from the element labeled 0. Each block contains exactly 2^{L-k} elements corresponding to bit strings or integers (see Figure 1a). Consider an arbitrary block X and arbitrary element with label P within X. Exactly $L - k$ neighbors of P are contained in X. The periodicity of both Binary and Gray bit encodings ensures that the $L-k$ neighbors of P in X do not change when shifting by 2^{L-k}. Two of the remaining k neighbors are contained in the blocks preceding and following X, respectively. Since the adjacency between blocks does not change under shifting, the two neighbors in the adjacent blocks must stay the same.

The remaining $k-2$ neighbors are contained in blocks that are not adjacent to X. We prove that the rest of these $k-2$ neighbors change. Consider a block Y that contains a neighbor of P. For every Reflected Gray code there is a reflection point exactly halfway between any pair of neighbors. For all neighbors outside of block X which are not contained in the adjacent blocks, the reflection points must be separated by more than 2^{L-k} positions. Shifting X by 2^{L-k} will move it closer to the reflection point, while Y is moved exactly 2^{L-k} positions farther away from the reflection point (see Figure 1b). Point P in X must now have a new neighbor (also 2^{L-k} closer to the reflection point) in the block Z. If the reflection point between X and Z is at location R, then for the previous neighbor in Y to still be a neighbor of P in X it must have a reflection point at exactly $R + 2^{L-k}$. This is impossible since for all neighbors outside of block X which are not contained in the adjacent blocks, the reflection points must be separated by more than 2^{L-k} positions. A similar argument goes for the case when shifting by 2^{L-k} moves X farther away from the reflection point (while Y is moved closer). Thus, none of the previous $k - 2$ neighbors are neighbors after shifting by 2^{L-k}. □

Corollary of Theorem 1: In any reflected Gray code representation of a 1-dimensional function, or parameter of a multidimensional function, there are only 2^{L-2} unique shifts. When $k = 2$, $k - 2 = 0$ and 0 neighbors change. When $k = 1$, we can shift twice by 2^{L-2} and 0 neighbors change each time.

4.1 High Precision Gray Code and Longest Path Problems

We know that a Gray code preserves the connectivity of the real-valued space. If we think about search moving along the surface of the real-valued functions, then increased precision could cause a problem. The distance from any point in the search space and

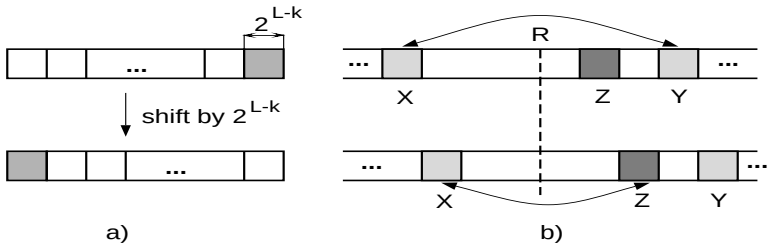


Figure 1 Shifting by 2^{L-k}. **a).** A representation of the Gray codes. **b).** For an arbitrary position in a block X, and an arbitrary neighbor of this position in the block Y, after shifting by 2^{L-k}, the neighbor moves from block Y to block Z.

the global optimum might grow exponentially as precision is increased. If we must step from one neighbor to the next, then as we increase the number of bits, L, used to encode the problem, the distance along this adjacent-neighbor path grows exponentially long as a function of L. On the other hand, we know that connectivity in a hypercube of dimension L is such that no two points are more than L moves away from one another. This lead us to ask what happens when we increase the precision for Gray coded unimodal functions? We prove that the number of steps leading to the optimum is $O(L)$.

4.2 Convergence Analysis for Unimodal and Sphere Functions

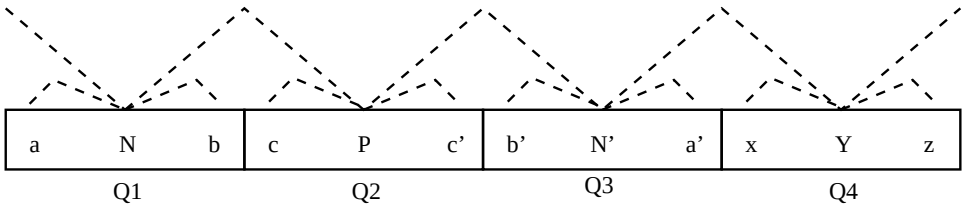
Consider any *unimodal real-valued* 1-dimensional function. Steepest ascent local search using the L-bit Hamming distance-1 neighborhood of any Reflected Gray-code representation of any unimodal real-valued function will converge to the global optimum after at most $2L$ steps or moves in the search space.

Lemma 1 *For any 1-dimensional unimodal real-valued function, steepest ascent local search using the L-bit Hamming distance-1 neighborhood of any Reflected Gray-code representation will converge to the global optimum after at most* $2L$ *steps.*

Proof: The proof assumes that all points in the search space have unique evaluations (to prevent search from being stuck on flat spots). We have already shown that for any Gray code representation shifting by 2^{L-2} does not change the structure of the search space. We can thus break the search space into four *quadrants*. This means we can assume the current point, `P` from which we are searching can be located in any quadrant, and the neighborhood structure is identical when `P` is shifted to the same position in any other quadrant of the search space.

Consider the following set of points: { `a, N, b, c, P, c', b', N' a', x, Y, z`}. The points {`N, P, N', Y`} are located in the four quadrants and for any reflected Gray code 2 adjacent points in the sequence `N, P, N', Y, N` are neighbors. Let points `a` and `b` be neighbors in the same quadrant as `N`, with `a` to the left and `b` to the right. The same holds for subsets {`c, P, c'`} {`b', N', a'`} and {`x, Y, z` } as shown in the following figure. The quadrants are labeled Q1, Q2, Q3 and Q4. Neighbors are connected by dashed lines.

Let `P` be the current position of the search. `P` has neighbors `c, c', N`, and `N'`. The neighbors `c` and `c'` are in the same quadrant as `P`, but `N` and `N'` must be in adjacent



quadrants of the space due to the reflected symmetry of Gray code. `Y` is in a position symmetric to `N` and reachable in 2 moves from `P`.

We now can decompose this problem into a series of cases. For any set of three points $\{w, x, y\}$, if we know that $w > x < y$ then we know that a minimum, and hence the global minimum, must lie between w and y. (Note we use the same symbol to represent a point and its evaluation.) In this way, each case either eliminates at least half of the search space from further consideration, or leads to at most 2 moves to a neighbor from which it is possible to eliminate at least half of the search space. The only moves that are considered are those that change from one quadrant to another. ("In quadrant" moves can be considered as part of the next move.)

POSITION	CASE	MOVE	QUADRANT TO ELIMINATE
P	c > P < c'	none	Q1, Q3, Q4
P	N > c < P	none	Q3, Q4
P	P > c'< N'	none	Q1, Q4
P	N'> N < c	goto N	
P	c'> N'< N	goto N'	
N	a > N < b	none	Q2, Q3, Q4
N	Y > a < N	none	Q2, Q3
N	N > b < c	none	Q3, Q4
N	N > Y < N'	goto Y	
Y	x > Y < z	none	Q1, Q2, Q3
Y	N'> x < Y	none	Q1, Q2
Y	Y > z < N	none	Q2, Q3

The cases for `N'` are a symmetric reflection of the cases for `N`. There are no other cases. Thus after 2 moves it is always possible to reduce the search space by at least half. Furthermore the remaining quadrants are always adjacent (which is true by inspection).

After discarding half of the search space, we can treat the space as having been reduced by 1 dimension in Hamming Space. This reduction in the dimensionality can be recursively applied until $L = 2$. For $L = 2$ the search space is reduced to four points (one of which is the optimum) and it takes at most two moves to go to the optimum. By summation, it follows that it takes at most $2L$ moves to go from any point in the space to the optimum. □

If the optimum can be reached after at most $2L$ moves, each move normally requires $L-1$ evaluations under steepest ascent. But if the function is unimodal we only need to evaluate four critical neighbors that are used in the preceding proof. Therefore

Theorem 2 *For any unimodal real-valued function, there exists a special form of steepest ascent local search using the L-bit Hamming distance-1 neighborhood of any Reflected Gray-code representation that will converge to the global optimum after at most $\mathcal{O}(L)$ evaluations.*

Proof: The result follows directly from the proof of Lemma 1. □

4.3 Multi-parameter Problems and Sphere Functions

The proofs only deal with 1 dimensional functions. However, every multi-parameter separable function can be viewed as a composition of real-valued subfunctions. If each real-valued sub-function is unimodal and encoded with at most l bits, a specialized form of steepest ascent Hamming distance-1 local search using any Reflected Gray-code representation will converge to the global optimum after at most $\mathcal{O}(l)$ steps in each dimension. If there are Q dimensions and exactly l bits per dimension, note that $Ql = L$, and the overall convergence is still bounded by $\mathcal{O}(L)$. It also follows that

Theorem 3 *Consider the sphere function, $c_0 + c_1 \sum_i^N (x_i - x_i^*)^2$, where $(x_i^*, ...x_n^*)$ denotes the minimum. For this sphere function, steepest ascent local search using the L-bit Hamming distance-1 neighborhood of any Reflected Gray-code representation will converge to the global optimum after at most $\mathcal{O}(L)$ steps.*

4.4 The Empirical Data

The proof obviously shows that regular steepest ascent, where all L neighbors are checked, will converge in $\mathcal{O}(L)$ steps and $\mathcal{O}(L^2)$ total evaluations. A set of experiments with different unimodal sphere functions encoded using a varying number of bits shows behavior exactly consistent with the proof. The number of *steps* of steepest ascent local search needed to reach the optimum is linear with respect to string length. This is shown in Figure 2. This figure also shows that the number of evaluations used by regular steepest ascent is order $\mathcal{O}(L^2)$ with respect to string length.

But what about next ascent? In the best case, next ascent will pick exactly the same neighbors as those selected under steepest ascent, and the number of steps needed to reach the optimum is $\mathcal{O}(L)$. However, in the worst case an adjacent point in real space is chosen at each move and thus the number of steps needed to reach the optimum is $\mathcal{O}(2^L)$. The linear-time best case and exponential-time worst case makes it a little less obvious what happens on average. The advantage of next ascent of course, is that there can be multiple improving moves found by the time that L neighborhoods have been evaluated. Informally, what are the odds that none of the improving moves which are found are long jumps in the search space? If, for example, one found a best possible move and a worst possible move after evaluating L neighborhoods, the convergence time is still closer to the $\mathcal{O}(L)$ steps and $\mathcal{O}(L^2)$ evaluations associated with blind steepest ascent. The empirical data seems to suggest that the average case is similar to the best case. The rightmost graph in Figure 2 shows that the empirical behavior of Random Bit Climbing appears to be bound by $L \log(L)$ on average. This is in fact better than the L^2 behavior that characterizes the number of *evaluations* required by steepest ascent. The variance is so small in both cases as to be impossible to be seen on the graphs shown here.

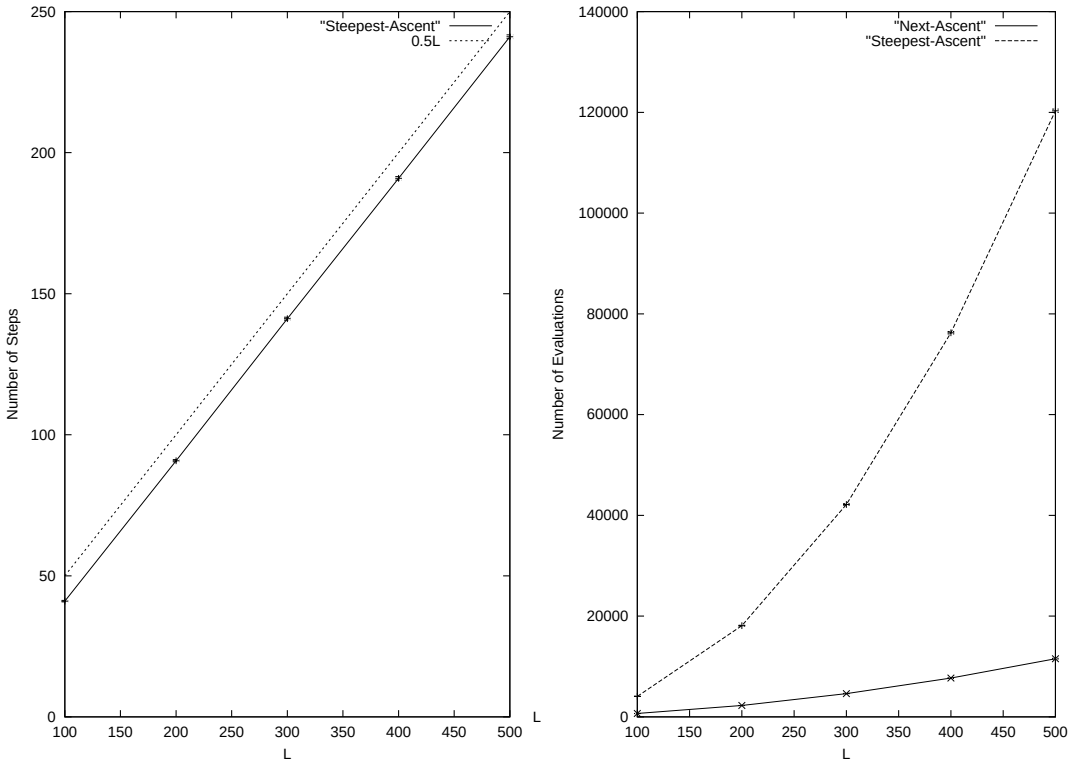


Figure 2 The leftmost graph shows the number of *steps* required by steepest-ascent local search to locate the global optimum for various sphere functions. The rightmost graph shows the number of *evaluations* required to locate the global optimum for sphere functions using both steepest-ascent and the next-ascent algorithm RBC. RBC requires far fewer evaluations. The results are averaged over 1000 initial starting locations. Each graph shows results for a single sphere function; the results for different sphere functions are indistinguishable.

We used Davis's Random Bit Climber (RBC) as our next ascent algorithm. RBC randomized the order in which the bits are checked. After every bit has been tested once, the order in which the bits are tested is again randomized. This randomization may be important in avoiding worst case behavior.

5 High Precision Gray Codes and Local Optima

Our results on the expected number of optima under a neighborhood search operator of size k confirm the intuitive notion that, *in expectation*, larger neighborhood sizes generally result in fewer optima. One way to increase the neighborhood size for bit-encoded parameter optimization problems is to increase the encoding precision of each parameter. This initially seems counter-intuitive, because it also increases the size of the search space. A 10 parameter optimization problem with a 10-bit encoding results in a search space of 2^{100} points, while a 20-bit encoding results in a search space of 2^{200} points. Generally, a smaller search space is assumed to be "easier" than a larger search space. But is this true?

Consider a parameter X with bounds X_{lb} and X_{ub}. From an L-bit representation, an integer y is produced by the standard Binary or Gray decoding process. This integer is then mapped onto an element $x \in X$ by : $x = X_{lb} + y\frac{X_{ub}-X_{lb}}{2^L-1}$. We refer to y as an integer point and x as the corresponding domain point.

We begin with an illustrative example. Let $X_{lb} = 0$ and $X_{ub} = 31$, and consider an L-bit Gray encoding of X, with $5 \leq L \leq 10$. Table 1 shows the L domain neighbors of the domain point *nearest* to 4.0; for reasons discussed below, 4.0 may not be exactly representable under an arbitrary L-bit encoding. Under a 5-bit Gray encoding, the integer neighbors of $y_5 = 4$ are 3, 5, 7, 11, and 27, as shown. And because of the domain bounds, these integers are also the domain neighbors of the point $x = 4.0$.

L	$n \sim 3$	n introduced by increases in precision					$n \sim 5$	$n \sim 7$	$n \sim 11$	$n \sim 27$
5	3.000						5.000	7.000	11.000	27.000
6	3.444					**4.429**	5.413	7.381	11.318	27.064
7	3.661				**4.149**	**4.638**	5.614	7.567	11.472	27.095
8	3.647			**3.890**	**4.133**	**4.619**	5.592	7.527	11.428	26.988
9	3.701		**3.943**	**4.065**	**4.186**	**4.671**	5.642	7.583	11.466	26.996
10	3.727	**3.969**	**4.030**	**4.091**	**4.212**	**4.697**	5.667	7.606	11.485	27.000

Table 1 Neighbors of the point nearest to $x = 4.0$ under a Gray encoding, $5 \leq L \leq 10$.

Table 1 shows that increasing the precision can influence the neighborhood structure under Gray encodings. The point of reference is x and its neighbors are n.

Two things are important about the pattern established in Table 1. First, as precision is increased, the set of neighbors when L = 5 continue to be represented by neighbors near to the original set of neighbors. Thus, all of the original neighbors are **approximately sampled** at higher precision. Second, note that when L = 5, the nearest neighbor of $x = 4.0$ are $n = 3.0$ and $n = 5.0$. All new neighbors of x fall between 3.0 and 5.0.

Observation 1 *Assume that a Gray code adequately samples a real valued function, such that every optimum and saddle in real space is represented in Hamming Space. Further*

assume that the small changes in this original discretization are not sufficient to change the number of local optima over the original set of neighborhood connections. Under these conditions, adding additional precision will not change the number of local optima in Hamming space.

This observation suggests that we might wish to consider the stability of the original set of neighborhoods as we increase precision. And it also suggests that higher precision does not necessarily change the number of optima, and thus, using higher precision does not hurt or help when "number of local optima" is used as a measure of complexity.

Note our observation makes strong assumptions. Table 1 shows that in fact there is considerable instability in the position of neighbors $3-11$, there is slight instability in the domain neighbor 27. A contributing cause, albeit minor, to the instability of the domain neighbors is due to the following

Theorem 4 *Let X_{lb} and X_{ub} denote the lower and upper bounds on the domain of a parameter X. Consider bit encodings (Gray or Binary) of X with precisions L and $L+1$. Define $z_L = X_{lb} + y_L \frac{X_{ub}-X_{lb}}{2^L-1}$ for some decoded integer y_L, $0 \leq y_L \leq 2^L - 1$; z_L is a point in the domain of X representable under an L-bit encoding. Then there exists no y_{L+1} (except for 0 and $2^{L+1}-1$) such that $z_L = z_{L+1}$ - i.e., identical points are not representable under bit encoding after changing the precision by one 1.*

Proof: Suppose that there exists y_{L+1} such that $z_L = z_{L+1}$ Using the definition for z_L we obtain:

$$\frac{y_L}{2^L-1} = \frac{y_{L+1}}{2^{L+1}-1} \quad \Leftrightarrow \quad (2^L-1)(y_{L+1}-y_L) = 2^L y_L$$

The equation above implies that (2^L-1) evenly divides $2^L y_L$, which is a contradiction if $y_{L+1} \neq 0$ and $y_{L+1} \neq 2^{L+1}-1$! Indeed, (2^L-1) does not evenly divide 2^L. The only 2 values of y_L which are evenly divided by (2^L-1) are 0 and (2^L-1). But if $y_L = 2^L-1$, then $z_L = z_{L+1} = X_{ub}$, and therefore $y_{L+1} = 2^{L+1}-1$ (value already accounted for by the theorem). Similarly, if $y_L = 0$ then $y_{L+1} = 0$. □

For example, consider a 10-bit encoding of a parameter X with $X_{lb} = 0$ and $X_{ub} = 16$ The decoded integer 512 maps to the domain value 8.993157. Increasing the precision to 11 bits, the nearest domain values are represented by the integers 1150 (8.988764) and 1151 (8.996580). While the difference is relatively minor (~ 0.004), altering the precision nonetheless changes the representable domain values. Further, this change is independent of the choice of Gray or Binary bit encodings. However note that *this proof does not preclude recycling of point at different precisions.* Table 1 shows that the same points can be resampled when the precision changes by more than 1 bit. Table 1 also shows that the change in distance from some *fixed* reference point *does not* change monotonically as precision is increased.

We can generate examples which prove that it is possible for minor changes in precision to either increase or decrease the number of optima which exists in Hamming Space due to small shifts in the locations of some "original" set of neighbors. Cases exists where two optima with similar evaluation exist at one level of precision in Gray space, and then collapse at higher precision. In addition, two optima in real space that were previously collapsed in Gray space at lower precision can again become separate optima in Gray space at higher precision. Nevertheless, the creation or collapse of an optimum under higher

precision appears to be a symmetric process–and we conjecture that in expectation, the creation and collapse of optima will be equal and that no change in the total number of optima would result.

Any remaining instability in the domain neighbors due to increases in precision must be explainable by changes in the neighborhood connectivity patterns. To characterize such changes, we divide the domain of a parameter X into 4 quadrants, denoted $Q1 - Q4$. Under both Gray and Binary encodings, a point in Q1 has a neighbor in Q2. Under a Gray code, the point in Q1 has a neighbor in Q4, and under Binary the same point has a neighbor in Q3. We can also "discard" Q3 and Q4 under both Binary and Gray encodings by discarding the first 1-bit. We can then cut the reduced space into 4 quadrants and the same connectivity pattern holds. (This connectivity pattern is also shown in Figures 3 and 4.)

First, we can show that increases in the precision fail to alter the location of neighbors from the quadrant viewpoint:

Theorem 5 *Consider the decoded integer y_L under an L-bit encoding, $L \geq 2$. Increasing the precision to $L+1$ yields $y_{L+1} = 2 \cdot y_L$. Let $Q^{y_L}_{neighbors}$ represent the set of quadrants in which neighbors of y_L reside. Then $Q^{y_L}_{neighbors} = Q^{y_{L+1}}_{neighbors}$.*

Proof: For the trivial case $y_L = y_{L+1} = 0$, the theorem is obviously true.

Consider $y_l \neq 0$, and z_L the domain point corresponding to y_L. Then, $z_L = X_{lb} + y_L \frac{X_{ub} - X_{lb}}{2^L - 1}$. If z_{L+1} is the domain point corresponding to y_{L+1}, then similarly: $z_{L+1} = X_{lb} + y_{L+1} \frac{X_{ub} - X_{lb}}{2^{L+1} - 1}$. We will prove that z_L and z_{L+1} reside in the same quadrant, this being equivalent to $Q^{y_L}_{neighbors} = Q^{y_{L+1}}_{neighbors}$.

In the real-valued domain, if z_L resides in the qth quadrant (where $q = 0..3$), then the following inequalities are satisfied:

$$X_{lb} + q\frac{X_{ub} - X_{lb}}{4} < z_L < X_{lb} + (q+1)\frac{X_{ub} - X_{lb}}{4} \tag{4}$$

First, we compute the difference between z_L and z_{L+1}:

$$z_L - z_{L+1} = X_{lb} + y_L \frac{X_{ub} - X_{lb}}{2^L - 1} - (X_{lb} + y_{L+1} \frac{X_{ub} - X_{lb}}{2^{L+1} - 1}) =$$

$$(X_{ub} - X_{lb})(\frac{y_L}{2^L - 1} - \frac{2y_L}{2^{L+1} - 1}) = y_L \frac{X_{ub} - X_{lb}}{(2^L - 1)(2^{L+1} - 1)} \tag{5}$$

Note that the difference is positive; therefore $z_{L+1} < z_L$.

Let z'_L be the domain point corresponding to $y_L - 1$. Then:

$$z_L - z'_L = \frac{X_{ub} - X_{lb}}{2^L - 1} \tag{6}$$

Since $\frac{y_L}{2^{L+1} - 1} < 1$, using (5) and (6), we can infer:

$$z'_L < z_{L+1} < z_L$$

If z_L is *not* the first point sampled in the qth quadrant by the L bit encoding, then z'_L must also be in the same quadrant with z_L. Therefore, from the above inequality it results that z_{L+1} must be in the same quadrant with z_L and z'_L.

Consider the case when z_L is the first point sampled in the qth quadrant by the L bit encoding. Since the $y_L = 0$ case was already considered, $q = 1..3$.

Suppose that z_{L+1} is *not* in the same quadrant with z_L. This means that the distance between z_{L+1} and z_L is larger than the distance from z_L to the starting point (in the real domain) of the qth quadrant:

$$z_L - z_{L+1} > z_L - (X_{lb} + q\frac{X_{ub} - X_{lb}}{4}) \quad \Leftrightarrow$$

$$y_L < \frac{(2^{L+1} - 1)q}{8} \quad \Leftrightarrow \quad y_L < \frac{q}{4}(2^L - \frac{1}{2}) \tag{7}$$

But, from (4):

$$y_L > \frac{q}{4}(2^L - 1) \tag{8}$$

Using (7) and (8), the difference between the two bounds discovered for y_L is:

$$\frac{q}{4}(2^L - \frac{1}{2}) - \frac{q}{4}(2^L - 1) = \frac{q}{8} \tag{9}$$

We distinguish 3 cases:

Case 1: $q = 1$

In this case $q(2^L - 1)$ is an odd number. Therefore, there exists an integer number p such that $q(2^L - 1) = 4p + 1$ or $q(2^L - 1) = 4p + 3$. Using (7), (8), and (9), we obtain:

$$p + \frac{1}{4} < y_L < p + \frac{1}{4} + \frac{1}{8} \tag{10}$$

or

$$p + \frac{3}{4} < y_L < p + \frac{3}{4} + \frac{1}{8} \tag{11}$$

(10), (11) can not be satisfied for any integer y_L.

Case 2: $q = 2$

In this case $\frac{q(2^L-1)}{2}$ is an odd number. Therefore, there exists an integer number p such that $\frac{q(2^L-1)}{2} = 2p + 1$. This implies:

$$p + \frac{1}{2} < y_L < p + \frac{1}{2} + \frac{2}{8} \tag{12}$$

Again, Case 2 (12) can not be satisfied for any integer y_L.

Case 3: $q = 3$

As for case 1, $q(2^L - 1)$ is an odd number. However, there exists no integer p such that $q(2^L - 1) = 4p + 3$. Indeed, suppose there exists an integer p such that $3(2^L - 1) = 4p + 3$.

This implies $2^{L-1} = (2/3)p + 1$, where the right hand side of the equality must be integer, and therefore is odd. But 2^{L-1} is an even number. The contradiction obtained confirms that for no integer p, $q(2^L - 1) = 4p + 3$. The only possibility left to express $q(2^L - 1)$ as an odd number is: $q(2^L - 1) = 4p + 1$ where p is integer. For y_L this implies:

$$p + \frac{1}{4} < y_L < p + \frac{1}{4} + \frac{3}{8} \tag{13}$$

It is clear that there exists no integer y_L satisfying (13).

The contradictions obtained for the three possible values of q resulted from the assumption that z_{L+1} is *not* in the same quadrant with z_L. Thus, we proved by contradiction that z_L and z_{L+1} reside in the same quadrant. □

Note that y_L and y_{L+1} are the decoded integers roughly corresponding to the same domain point (Theorem 4 prevents the exact correspondence to the same domain point). Theorem 5 establishes that increasing precision cannot change the quadrants sampled by the neighbors of a y_L, but it says nothing about how the relative densities of those neighbors change in the various quadrants, or how the neighbors can shift positions within quadrants.

To explore the question of neighbor density, we consider an L-bit encoding (Gray or Binary) and an integer y_{L-2} in a quadrant $Q_{y_{L-2}}$. There are $L-2$ neighbors of y_{L-2} in quadrant $Q_{y_{L-2}}$, and exactly one in two of the three remaining quadrants ($Q_{y\_adj\_left}$ and $Q_{y\_adj\_right}$).

Next, we increase the precision by one to $L+1$. Here, $L-2$ neighbors of y_{L-2} are compressed into $\frac{1}{8}$ of the domain, instead of $\frac{1}{4}$ under the L-bit encoding. The remaining 3 neighbors are allocated as follows: exactly one in two of the remaining three new quadrants ($Q_{y\_adj\_left}$ and $Q_{y\_adj\_right}$), and an additional neighbor in the quadrant $Q_{y_{L-2}}$. Because of this compression, we find an increased density of neighbors near x_{L-2} as the precision is increased. In summary:

Observation 2 *For a given integer y, increasing the encoding precision simply increases the density of neighbors near y. Loosely speaking, no new connectivity in introduced by the increased precision except new connectivity which is increasing closer to y.*

This observation is imprecise because the position of y also moves with the increased precision. This is clearly shown in Table 1. In addition to increased density, we see a 'migration' of domain neighbors within quadrants. Examining Table 1, we see that 3.0 under a 5-bit encoding migrates toward 3.7273 under a 10-bit encoding, and the migration is more than can be accounted for by Theorem 4. Consider a 4-bit Gray code and the integer 4, which has neighbors 3, 5, 7, and 11, and a corresponding domain point d_4. Next, increase the precision to 5 bits. Now the domain point nearest to 4.0, subject to Theorem 4, is produced by the integer 8, with neighbors 7, 9, 11, 15, and 23. Since we have roughly doubled the precision, these neighbors correspond roughly to 3.5, 4.5, 5.5, 7.5, and 11.5, respectively, for the integer 4.

6 Combining Gray and Binary Neighborhoods

The "Quadrant" decomposition used previously in this paper also provides a helpful way to visualize connectivity bias in the Gray and Binary neighborhoods. Figure 3 illustrates that

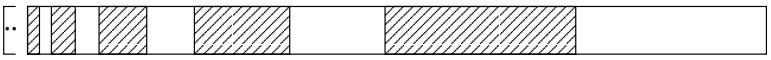


Figure 3 The search space is repeatedly broken into 4 quadrants. Assume the point of interest x is shifted to the first quadrant, discarding the third and fourth quadrants. The space is then reduced by 1 bit and the process is repeated. All Binary neighbors of some point of interest are in the dashed regions, Gray neighbors are in the undashed regions; the two regions are disjoint and complementary.

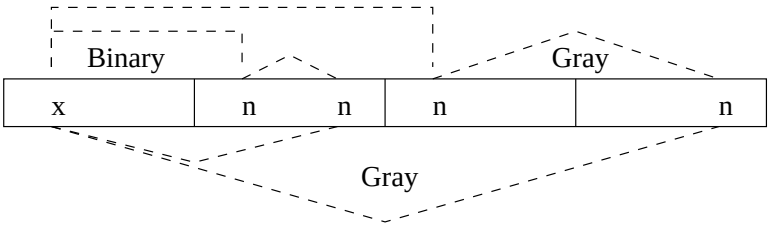


Figure 4 The search space is broken into 4 quadrants. The dashed "rectangular" connectors on the top of the figure locate binary neighbors of x. The dashed "triangular" of the bottom connects to Gray neighbors of x. Note there also the Gray "triangular" connectors on top; Binary neighbors are always two moves away in Gray space.

Binary and Gray neighbors reside in disjunct and complementary portions of the search space. We construct Figure 3 using our prior strategy of shifting any point of interest, x, to the first quadrant. Again, this can be done without changing the neighborhood structure of the space. x has exactly one Binary neighbor in the upper half of the space, in quadrant 3. Also, x has exactly one Gray neighbor in the upper half of the space, in quadrant 4. We recursively identify in the same way the location of the remaining Binary and Gray neighbors of x. First, we can discard quadrants 3 and 4 and consider the lower-dimensional problem. We then repeat the process of shifting the point of interest to the new lower-dimensional first quadrant. The lower dimensional neighborhood is unchanged.

Figure 3 shows how Gray and Binary codes connect x (via a Hamming distance-1 neighborhood) to complementary, disjoint portions of the search space. However, Figure 4 shows that the Hamming distance-1 neighbors under Binary are Hamming distance-2 neighbors in Gray space. Thus it is possible to construct a neighborhood of $2L - 1$ points that include both the Binary and Gray neighbors. The goal of constructing such a neighborhood is to reduce the complementary bias which exists in the Gray and Binary neighborhood structures.

We will show that flipping single bits accesses the Gray neighborhood and that flipping pairs of adjacent bits accesses the Binary neighborhood. Consider the following bit vector B as a binary string. Assume strings are numbered from right to left starting at zero: $B = B_{l-1}, ..., B_1, B_0$. In particular we are interested in the bit B_i. Now convert B to a Gray code using exclusive-or. This results in the following construction.

$$G_{l-1} = B_{l-1}, \;\; G_{l-2} = B_{l-2} \oplus B_{l-1}, \;\; \cdots, \; G_i = B_i \oplus B_{i+1},$$

$$G_{i-1} = B_{i-1} \oplus B_i, \;\; \cdots, \; G_0 = B_0 \oplus B_1$$

Now consider what happens when bit B_i is flipped, where $1 \leq i \leq l-1$. G changes at exactly two locations. Thus, we can access the Gray neighborhood by flipping individual bits and the Binary neighborhood by flipping adjacent pairs of bits. By combining Binary and Gray neighborhoods, we can never do worse than the original Gray space in terms of number of local optima which exist. To access these neighbors in a genetic algorithm, we would use a special mutation operator that flips adjacent pairs of bits.

7 Conclusions

We have presented four theoretical results which provide a better understanding of one of the most commonly used bit encodings: the family of Gray code representations. First, we showed that shifting the search space by $2^L - 2$ does not change the Gray code Hamming distance-1 neighborhood. Second, we showed that for any unimodal, 1-dimensional function encoded using a reflected L-bit Gray code, steepest-ascent local search under a Hamming distance-1 neighborhood requires only $\mathcal{O}(L)$ steps for convergence to the global optimum, in the worst case. We showed that this result also holds for multi-dimensional separable functions. Third, we demonstrated how increasing the precision of the encoding impacts on the structure of the search space. Finally, we show that there exists a complementary bias in the Gray and Binary neighborhood structures. To eliminate this bias, a new neighborhood can be constructed by combining Gray and Binary neighborhood structures.

References

[1] T. Bäck. *Evolutionary Algorithms in Theory and Practice.* Oxford University Press, 1996.

[2] James R. Bitner, Gideon Ehrlich, and Edward M. Reingold. Efficient Generation of the Binary Reflected Gray Code and Its Applications. *Communications of the ACM*, 19(9):517–521, 1976.

[3] Lawrence Davis. *Handbook of Genetic Algorithms.* Van Nostrand Reinhold, New York, 1991.

[4] D. B. Fogel. *Evolutionary Computation.* IEEE Press, 1995.

[5] N.J. Radcliffe and P.D. Surry. Fundamental limitations on search algorithms: Evolutionary computing in perspective. In J. van Leeuwen, editor, *Lecture Notes in Computer Science 1000.* Springer-Verlag, 1995.

[6] S. Rana and D. Whitley. Bit Representations with a Twist. In T. Bäck, editor, *Proc. of the 7th Int'l. Conf. on GAs*, pages 188–195. Morgan Kaufmann, 1997.

[7] S. Rana and D. Whitley. Search, representation and counting optima. In L. Davis, K. De Jong, M. Vose, and D. Whitley, editors, *Proc IMA Workshop on Evolutionary Algorithms.* Springer-Verlag, 1998.

[8] Soraya Rana. *Examining the role of Local Optima and Schema Processing in Genetic Search.* PhD thesis, Colorado State University, Department of Computer Science, Fort Collins, Colorado, 1999.

[9] Hans-Paul Schwefel. *Numerical Optimization of Computer Models.* Wiley, 1981.

[10] Hans-Paul Schwefel. *Evolution and Optimum Seeking.* Wiley, 1995.

[11] D. Whitley. A Free Lunch Proof for Gray versus Binary Encodings. In *GECCO-99*, pages 726–733. Morgan Kaufmann, 1999.

[12] Darrell Whitley, Keith Mathias, Soraya Rana, and John Dzubera. Evaluating Evolutionary Algorithms. *Artificial Intelligence Journal*, 85:1–32, August 1996.

[13] David H. Wolpert and William G. Macready. No free lunch theorems for search. Technical Report SFI-TR-95-02-010, Santa Fe Institute, July 1995.

Appendix 1

There is a definitional error in the proof that Binary encodings work better than Gray encodings on "worst case" problems [11].

First, "better" in this case means that over the set of "worst case" problems Binary induces fewer optima that a reflect Gray code. However, a No Free Lunch relationship holds between Gray codes and Binary codes. The total number of optima induced over all functions is the same. Thus, if binary induces fewer optima over the set of "worst case" problems then Gray code must induce fewer optima over the set of "non-worst case" problems

The problem lies in the definition of a "worst case" problems.

In the original proof, two definitions are used of function neighborhoods. For neighborhoods that wrap, adjacent points in real space are neighbors and the first point in the real valued space and the last point in the real valued space are also neighbors. For non-wrapping neighborhoods, adjacent points in real space are neighbors but the first point in the real valued space and the last point in the real valued space are *not* neighbors.

A worst case problem is defined as one where a) every other point in the real space is a local optimum and thus b) the total number of optima is N/2 when there are N points in the search space. For neighborhoods that wrap the two concepts that a) there are N/2 optima and b) every other point in the space is an optimum are identical. However for non-wrapping neighborhoods, these two concepts are not the same. For a non-wrapping neighborhood, there can be N/2 optima and yet there can be one set of optima that are separated by 2 intermediate points instead of one. This can happen when the first and last point in the space are both optima–which can't happen with a wrapping representation.

The proof relies on the fact that every other point in the space is an optimum. Thus, for non-wrapping neighborhoods, the definition of a worst case function must be restricted to the set of functions where every other point in the space is an optimum; with this restriction, the proof then stands. The proof is then unaffected for wrapping representations, since the "worst-case" definitions defines the same subset of functions.