Colorings for Efficient Derivative Computation on Grids with Periodic Boundaries *

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Abstract

Computing the first derivatives of a discretized nonlinear partial differential equation (PDE) can be made more efficient given colorings of the lattice points of the plane, cylinder, or torus that assign different colors to all vertices within some specified stencil. Goldfarb and Toint showed how to efficiently color the lattice points of the plane, but their results do not extend to the cases of cylinders or toruses, as arise in the case of discretizing PDEs with periodic boundary conditions on a Cartesian grid. We give colorings for the $(4l-3)$-point star and the $l \times l$ square stencils (for all l) in the plane, on the cylinder, and on the torus. We also give colorings for the $(6l-5)$-point star in $\mathbb{Z}^3$ and for the $l \times l \times l$ cube in $\mathbb{Z}^3$ with periodic boundary conditions in 0 and 1 dimensions. We show that all colorings are optimal or near-optimal.

Keywords: Jacobian, Hessian, automatic differentiation, finite differences, graph coloring

1 Introduction and Motivation

Many numerical methods require the evaluation of the Jacobian. The *Jacobian* is an $M \times N$ matrix J of partial derivatives of a vector-valued function $F : \mathbb{R}^N \mapsto \mathbb{R}^M$.

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The Jacobian entry in row i and column j is nonzero only if the ith component $F(x)$ depends on x_j.

The Jacobian is frequently computed by using automatic differentiation [4] or approximated by using finite differences. These techniques are often necessary because the function F is available only in the form of a computer program. Both approaches compute a set of directional derivatives of F. When we choose the direction to be the unit vector e_j in the jth coordinate direction, we compute the jth column of J. By taking the directions to be the standard basis of $\mathbb{R}^N$, we can compute J using N directional derivatives of F.

In many cases, however, the Jacobian matrix is sparse. When the sparsity pattern is known, the ith and jth columns of J can be computed simultaneously whenever they are structurally orthogonal. A pair of columns i and j of a matrix are *structurally orthogonal* if in each row of the matrix at most one of the columns contains a nonzero entry.

If columns i and j are structurally orthogonal, we compute them simultaneously by taking the derivative of F in the direction $e_i + e_j$. Then for each row k, at most one of J_{ki} and J_{kj} is nonzero. This nonzero entry is equal to the kth component of the derivative vector.

This idea can be extended to larger sets of pairwise structurally orthogonal columns. If columns $i_1, i_2, \ldots, i_p$ are structurally orthogonal, we can compute them simultaneously by taking the derivative of F in the direction $e_{i_1} + e_{i_2} + \cdots + e_{i_p}$. Again, for each row k, at most one column has a nonzero entry in the kth row. This nonzero entry is equal to the kth component of the derivative vector.

We are now interested in partitioning the columns of J into structurally orthogonal sets. All the columns in a set can be computed simultaneously. To minimize the cost of computing J, we must minimize the number of sets in the partition.

It turns out to be more useful (and to offer better intuition) if we view the problem as points on a torus, rather than columns of a matrix [6]. Rather than partitioning the columns into structurally orthogonal sets, we speak of coloring the points on the torus so that no two points receive the same color unless their corresponding columns in the Jacobian are structurally orthogonal. If we take the points of the torus as a vertex set and add an edge between two points whenever their corresponding columns are not structurally orthogonal, we have a standard graph coloring problem. Motivated by viewing the problem as points on a torus, we also refer to the points by the more natural (i, j) to denote the point in the ith row and jth column.

Unfortunately, finding an optimal coloring of a general graph is NP-complete. Therefore, research has focused on approximation algorithms for graphs with random adjacency patterns [2, 1, 5] and optimal (or near-optimal) algorithms for structured graphs [3].

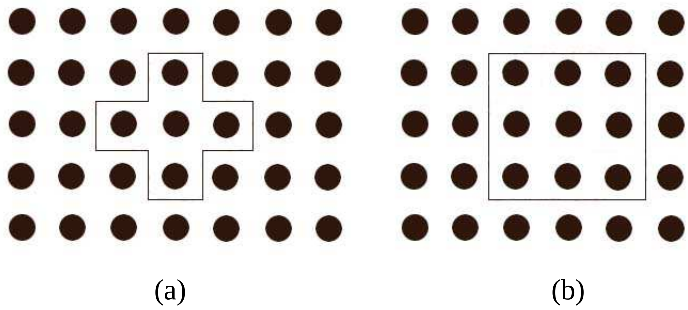

Figure 1: (a) The 5-point star stencil on the 5×7 torus. It is important to distinguish between the torus and the Jacobian. The Jacobian will be 35×35, since each point on the torus corresponds to a column in the Jacobian. (b) The 3×3 square stencil on the 5×6 torus. The Jacobian for this torus will be 30×30.

We now examine the problem more in detail. We want to find the derivative of a function that maps the surface of a torus to itself, $F : T \mapsto T$. Since we don't have an analytical form of the function, we approximate it at selected points. We select mn points in the shape of an $m \times n$ lattice on the surface of the torus. In the Jacobian, each row and column corresponds to a sample point on the torus. (This means that the Jacobian matrix, J, actually has dimensions $mn \times mn$.) We refer to the point corresponding to column (and row) i as point i. The derivative at a point can be approximated by using the value of the function at that point and at nearby points.

We use the term *stencil* to specify those points near point i which our approximation of the derivative at i will depend on. Because we use the same stencil for every point on the torus, the sparsity pattern of the Jacobian is very structured. In particular, J_{ij} is nonzero only if point i lies within the stencil of point j. Thus, two columns are structurally orthogonal only if their corresponding points never lie in the same stencil. Thus, the number of structurally orthogonal sets in the column partition must be at least equal to the number of points in the stencil.

Goldfarb and Toint [3] give optimal colorings (a coloring is optimal if it is uses a minimum number of colors) for a variety of sparsity patterns arising from the stencil-based discretization of partial differential equations on Cartesian grids. Goldfarb and Toint demonstrate that in many cases the size of the coloring need not be any larger than the size of the stencil. However, all of the cases they consider are in the plane. This significantly simplifies matters, because it avoids difficulties with boundary conditions.

In this paper, we examine the problem for $(4l-3)$-point star and square stencils on both the torus and the cylinder. We use the term $m \times n$ torus (cylinder) to mean the discrete torus (cylinder) with height m and width n. For the cylinder, the height is the dimension that does not wrap around.

In three dimensions, we look at $(6l-5)$-point star and cube stencils. We consider two cases. First, we color the points of $\mathbb{Z}^3$, the three-dimensional latice without wrap-around in any dimension. Second, we color the points of $\mathbb{Z}^2 \times \mathbb{Z}_m$, a three-dimensional lattice with wrap-around in a single dimension of size m.

In Section 2, we present a preliminary result that is helpful in constructing the colorings in Section 3. In Section 3, we present colorings for $(4l-3)$-point and $(6l-5)$-point star stencils and for square and cube stencils. In Section 4, we present lower bounds and show that in all cases they are tight or nearly tight for $l \times l$ square stencils and $(4l-3)$-star stencils. We offer some concluding remarks in Section 5.

2 Preliminaries

To build all the colorings in this paper, we partition into smaller rectangles the region to be colored. We color each rectangle so that when the rectangles are reassembled into the initial region, the resulting coloring is valid. In general, the rectangles have two different heights and two different widths: $h_1 \times w_1$, $h_2 \times w_1$, $h_1 \times w_2$, and $h_2 \times w_2$. In addition to each coloring being valid for the specified stencil, these colorings also have the property that if two rectangles with the same height are placed side by side or if two rectangles with the same width are placed one atop the other, the coloring of this new larger rectangle is valid for the same stencil. To color a torus with dimensions $h \times w$, we will write h as a nonnegative integer linear combination of h_1 and h_2 and write w as a nonnegative integer linear combination of w_1 and w_2. (Throughout this paper, the term *linear combination* will mean linear combination with nonnegative integer coefficients.) We write $a|b$ to denote that a divides b.

We want to know when an integer n can be written as a linear combination of two smaller integers p and q. Let $r(p,q)$ be the smallest positive integer such that if $n \geq r(p,q)$, then n can be written as a linear combination of p and q. The following result is known as *Sylvester's theorem*. For a proof, see [7].

Lemma 1 (Sylvester's Theorem [7])**.** *If p and q are relatively prime positive integers, then $r(p,q) = (p-1)(q-1)$.*

We say that a coloring (of a torus or the plane) is *valid* for a given stencil if, under that coloring, all points within each copy of that stencil receive distinct

$$\begin{bmatrix} 4 & 5 & 6 & 7 & 8 & 0 & 1 & 2 & 3 \\ 7 & 8 & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 0 \\ 4 & 5 & 6 & 7 & 8 & 0 & 1 & 2 & 3 \\ 7 & 8 & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 0 \\ 4 & 5 & 6 & 7 & 8 & 0 & 1 & 2 & 3 \\ 7 & 8 & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 0 \end{bmatrix}$$

Figure 2: A coloring of the 9×9 torus for the 3×3 square stencil.

colors. We say that a valid coloring (for stencil S) of an $h \times w_1$ torus and a valid coloring (for S) of an $h \times w_2$ torus are *vertically compatible* if, when placed side by side, the two form a valid coloring (for stencil S) of the $h \times (w_1 + w_2)$ torus. Analogously, we define *horizontally compatible* colorings of $h_1 \times w$ and $h_2 \times w$ tori. When the meaning is clear, we will refer to both vertically compatible and horizontally compatible simply as *compatible*. We also extend these definitions to three dimensions in the obvious way.

3 Colorings for Square Stencils

The simplest coloring for the 3×3 square stencil, on an $m \times n$ torus with $3|m$ and $3|n$, is given by $C(i, j) = (3i + j) \bmod 9$, as shown in Figure 2.

This coloring was given by Goldfarb and Toint [3] and can easily be extended to the $l \times l$ square stencil by letting $C(i, j) = (li + j) \bmod l^2$. If we are coloring rectangles rather than tori, this coloring suffices for all m and n. For the torus, however, we require $l|m$ and $l|n$. So now we need to look for valid colorings for the $l \times l$ square stencil in instances when $l \nmid m$ or $l \nmid n$.

The colorings we use are similar to the coloring in Figure 2. We define a general family of colorings:

$$C(i, j, l, m, n) = ((li \bmod m + j) \bmod n).$$

Each time we use coloring C, the parameters l, m, and n remain fixed, while the parameters i and j vary to indicate which entry is being colored. As we move to the right in a row, each entry is larger than the previous entry by 1. Similarly, as we move downward in a column, each entry is larger than the previous entry by l. As a result, the period of the coloring in the rows is n, and the period in the columns is

$\gcd(l,m)$. For Theorem 2 through Lemma 5, we consider the case when the height and width of the torus are given by $m = l^2 + b$ and $n = l^2 + c$, where b and c are at most l.

Theorem 2. *If $l^2 \le m \le n \le l^2 + l$, then $C(i, j, l, m, n)$ is a valid coloring of the $m \times n$ torus for the $l \times l$ square stencil.*

Proof. Since the tiling is periodic in both directions, it suffices to show that the coloring is valid for the plane. If this coloring is invalid, then there exist two entries (i_1, j_1) and (i_2, j_2) that lie within the same $l \times l$ square and receive the same color, that is, $|i_1 - i_2| < l$, $|j_1 - j_2| < l$, and $(li_1 \bmod m + j_1) \equiv (li_2 \bmod m + j_2) \bmod n$. Without loss of generality, assume that $(li_1 \bmod m) \ge (li_2 \bmod m)$. Let

$$\begin{aligned} T &= (li_1 \bmod m) - (li_2 \bmod m) + j_1 - j_2, \\ U &= li_1 - li_2 + j_1 - j_2. \end{aligned}$$

Since $n|T$ and $-n < T < 2n$, we see that $T \in \{0, n\}$. Clearly $m|(T-U)$, and by assumption, $T \ge U$. Since $|li_1 - li_2| \le l|i_1 - i_2| < l^2 \le m$, we see that $T - U \in \{0, m\}$. Thus $U \in \{T, T-m\}$, and hence $U \in \{0, -m, n, n-m\}$. Since $|i_1 - i_2| < l$ and $|j_1 - j_2| < l$, we see that $|U| \le |li_1 - li_2| + |j_1 - j_2| = l|i_1 - i_2| + |j_1 - j_2| < l^2 \le m \le n$; so $U \notin \{-m, n\}$. Since $U = 0$ implies that $(i_1, j_1) = (i_2, j_2)$, we must have $U = n - m$ and $n \ne m$. Thus (i_1, j_1) is one of $(i_2 + 1, j_2), (i_2, j_2 + n - m)$, or $(i_2 + 1, j_2 + n - m - l)$. Both of the first two cases can be easily seen to assign distinct colors to (i_1, j_1) and (i_2, j_2). We now show that the third case also assigns distinct colors to (i_1, j_1) and (i_2, j_2).

The key is to determine the difference $(li_1 \bmod m) - (li_2 \bmod m)$. We consider two possibilities: either there exists an integer g such that $li_2 < gm \le l(i_2 + 1) = li_1$, or there does not exist such a g. Let $N = li_2 \bmod m$. If there exists such an integer g, then $li_1 \bmod m = N + l - m$. In this case, $(li_1 \bmod m + j_1) \bmod n = (N + l - m + j_2 + n - m - l) \bmod n = (li_2 \bmod m + j_2) \bmod n = N + j_2 \bmod n$. After simplifying, this gives $n - 2m \equiv 0 \bmod n$, which is impossible, since $l^2 \le m \le n \le l^2 + l$ and $n \ne m$. Thus, there does not exist such an integer g. Since no such g exists, $(li_1 \bmod m) = (li_2 \bmod m) + l$. By substituting this equality into the congruence $(li_1 \bmod m + j_1) \bmod n \equiv (li_2 \bmod m + j_2) \bmod n$, we reach the implication $m = n$, which is a contradiction. Hence, the tiling of the plane is valid, and so is the tiling of the torus. □

Corollary 3. *If $l|m$ and $l|n$, then the coloring $C(i, j, l, l^2, l^2)$ is a valid l^2-coloring of the plane and the $m \times n$ torus for the $l \times l$ square stencil.*

Proof. Apply Theorem 2, with $m = l^2$ and $n = l^2$. Immediately, we see that the coloring is valid for an $l \times l$ torus and the $l \times l$ square stencil. If a coloring is valid for a torus for a given stencil, then that coloring remains valid for that stencil if two copies of the torus are placed side by side or one atop the other. By placing copies of the $l \times l$ torus next to and atop one another, we can construct an $m \times n$ torus. Thus, the given coloring is valid for the $m \times n$ torus and the $l \times l$ square stencil. $\square$

In the next two lemmas, we show that the colorings given for the smaller rectangles can indeed be assembled to give larger colorings that are valid.

Lemma 4. *If $l^2 \leq m \leq n_1 \leq n_2 \leq l^2 + l$, then colorings $C(i, j, l, m, n_1)$ and $C(i, j, l, m, n_2)$ are vertically compatible for the $l \times l$ square stencil.*

Proof. Let t_1 be an $m \times n_1$ rectangle colored by $C(i, j, l, m, n_1)$, and let t_2 be an $m \times n_2$ rectangle colored by $C(i, j, l, m, n_2)$. The entries in a row of t_1 are (beginning from the first column) $x \bmod n_1$, $(x+1) \bmod n_1$, $(x+2) \bmod n_1, \ldots$, where $x < m$. The entries in the same row of t_2 are $x \bmod n_2$, $(x+1) \bmod n_2$, $(x+2) \bmod n_2, \ldots$. As a result, the colors from a row of t_1 appear in the same order within that row of t_2. The difference is that since $n_2 \geq n_1$, there may be additional colors in t_2. So in each row of t_2, no color is closer to the edge of t_1 than it would be if t_2 were replaced with a second copy of t_1. Let v_1 be an entry in t_1 and v_2 be an entry in t_2. If v_1 and v_2 receive the same color and lie in the same row, then they are at least as far apart as any two nearest entries in t_1 that receive the same color and lie in the same row. Thus, the colorings are compatible. $\square$

Lemma 5. *If $l^2 \leq m_1 \leq m_2 \leq n \leq l^2 + l$, then colorings $C(i, j, l, m_1, n)$ and $C(i, j, l, m_2, n)$ are horizontally compatible for the $l \times l$ square stencil.*

Proof. Since $li < m_1 \leq m_2$ for all $0 \leq i < l$, the first l rows of the two colorings are identical. Thus, the colorings are compatible for the $l \times l$ square stencil. $\square$

Finally, we put together all of the pieces we have proved. We now show that

1. any sufficiently large torus can be partitioned into smaller rectangles,
2. those rectangles can be colored using few colors, and
3. the smaller colorings can be assembled to give a valid coloring for the torus.

Theorem 6. *For all $m \geq (l-1)l^2$ and $n \geq l^2(l^2+1)$, there is an (l^2+2)-coloring of the $m \times n$ torus that is valid for the $l \times l$ square stencil.*

Proof. By using Sylvester's theorem, we find $a_1, a_2, b_1, b_2 \in \mathbb{N}$ such that $m = a_1 l + a_2(l^2+1)$ and $n = b_1(l^2+1) + b_2(l^2+2)$. Using these linear combinations, we partition the $m \times n$ torus into rectangles with heights $h \in \{l, l^2+1\}$ and with widths $w \in \{l^2+1, l^2+2\}$. From Theorem 2, we get colorings of tori with these four sizes. We then apply the appropriate coloring to each rectangle in the partition of the $m \times n$ torus. The resulting coloring uses at most l^2+2 colors and is valid for the $m \times n$ torus as guaranteed by Lemmas 4 and 5. □

This technique used to prove Theorem 6 yields an even better bound for coloring the cylinder. A coloring of a torus with any height can be used to color a cylinder, since we need not worry about boundary conditions in the height dimension. If we use the coloring for a torus with height l, then we need to use only $l \times l$ and $l \times (l^2+1)$ rectangles in our partition of the torus. This partition results in a coloring with l^2+1 colors.

Theorem 7. *There is an (l^2+1)-coloring of the $m \times n$ cylinder for the $l \times l$ square stencil when $n \geq (l-1)l^2$.*

4 Colorings for Star Stencils

Now we give colorings for the torus that are valid for the $(4l-3)$-point star stencils. To prove that our colorings are valid for the star stencil, we need only show that the colorings are valid for the $l \times l$ square stencil, the $(2l-1) \times 1$ rectangle stencil, and the $1 \times (2l-1)$ rectangle stencil, since any pair of points that lies in a $(4l-3)$-point star also lies in one of these three stencils.

If $m \geq l^2(l^2+1)$ and $n \geq (l^2+1)(l^2+2)$, then by Lemma 1 we can partition the torus into rectangles with heights $h \in \{l^2+1, l^2+2\}$ and widths $w \in \{l^2+2, l^2+3\}$. We use the colorings for each of the rectangles that are valid for the $l \times l$ stencil that are given in Theorem 2. When the colorings for these rectangles are combined, we get a coloring for the torus. Call this coloring $\hat{C}$ and call the partition into rectangles P.

Lemma 8. *The coloring $\hat{C}$ is valid for the $l \times l$ square stencil.*

Proof. This follows immediately from Theorem 2 and Lemmas 4 and 5. □

Lemma 9. *The coloring $\hat{C}$ is valid for the $(2l-1) \times 1$ rectangle stencil.*

Proof. If $\hat{C}$ were invalid for the $(2l-1) \times 1$ stencil, then there would exist two points (i_1, j) and (i_2, j) in the same $(2l-1) \times 1$ stencil that receive the same color. We show that situation is impossible.

$$
\begin{bmatrix}
4 & 5 & 6 & 7 & 8 & 9 & A & 0 & 1 & 2 & 3 \\
7 & 8 & 9 & A & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\
A & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & A & 0 & 1 \\
5 & 6 & 7 & 8 & 9 & A & 0 & 1 & 2 & 3 & 4 \\
8 & 9 & A & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\
0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & A \\
3 & 4 & 5 & 6 & 7 & 8 & 9 & A & 0 & 1 & 2 \\
6 & 7 & 8 & 9 & A & 0 & 1 & 2 & 3 & 4 & 5 \\
9 & A & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & A & 0
\end{bmatrix}
\quad
\begin{bmatrix}
4 & 5 & 6 & 7 & 8 & 9 & A & B & 0 & 1 & 2 & 3 \\
7 & 8 & 9 & A & B & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\
A & B & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & A & B & 0 & 1 \\
5 & 6 & 7 & 8 & 9 & A & B & 0 & 1 & 2 & 3 & 4 \\
8 & 9 & A & B & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\
0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & A & B \\
3 & 4 & 5 & 6 & 7 & 8 & 9 & A & B & 0 & 1 & 2 \\
6 & 7 & 8 & 9 & A & B & 0 & 1 & 2 & 3 & 4 & 5 \\
9 & A & B & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & A & B & 0
\end{bmatrix}
$$

$$
\begin{bmatrix}
4 & 5 & 6 & 7 & 8 & 9 & A & 0 & 1 & 2 & 3 \\
7 & 8 & 9 & A & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\
A & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
3 & 4 & 5 & 6 & 7 & 8 & 9 & A & 0 & 1 & 2 \\
6 & 7 & 8 & 9 & A & 0 & 1 & 2 & 3 & 4 & 5 \\
9 & A & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & A & 0 & 1 \\
5 & 6 & 7 & 8 & 9 & A & 0 & 1 & 2 & 3 & 4 \\
8 & 9 & A & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & A & 0
\end{bmatrix}
\quad
\begin{bmatrix}
4 & 5 & 6 & 7 & 8 & 9 & A & B & 0 & 1 & 2 & 3 \\
7 & 8 & 9 & A & B & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\
A & B & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
3 & 4 & 5 & 6 & 7 & 8 & 9 & A & B & 0 & 1 & 2 \\
6 & 7 & 8 & 9 & A & B & 0 & 1 & 2 & 3 & 4 & 5 \\
9 & A & B & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & A & B & 0 & 1 \\
5 & 6 & 7 & 8 & 9 & A & B & 0 & 1 & 2 & 3 & 4 \\
8 & 9 & A & B & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & A & B & 0
\end{bmatrix}
$$

Figure 3: The colorings of four rectangles used to construct a coloring of the torus for the $(4l-3)$-point star stencil. The colorings shown are from Theorem 11, when $l = 3$.

We can assume that (i_1, j) and (i_2, j) lie in different rectangles in P, since it is easy to see that different entries within the same column of a rectangle receive different colors. We consider the entries of column j modulo l. As we move down a column, we encounter in succession all the entries that lie in the same equivalence class modulo l. Additionally, we encounter the entries in the same equivalence class in increasing order. That is, as we move down a column of height $h \geq l^2+1$, we encounter l blocks of entries, where each block consists of entries that lie in the same equivalence class. Each block of entries is of length l or $l+1$. The only exception is that beginning at the top of a column, we may be partway through a block. The preceding portion of this block will appear at the bottom of the column, so that the block, when viewed as a torus, appears whole and in order.

The important insight is that for a fixed column, each rectangle in the partition P has the same first l entries in that column. As we move down the column, we must cross a boundary between two rectangles. Both the rectangle above the boundary and the one below it have the same first l rows. Hence, as we cross the boundary from one rectangle to another, all the blocks are whole and in order. The column of each rectangle contains $l \geq 2$ of these blocks (if $l = 1$, the lemma is trivial). If two entries receive the same color, they must be in different blocks, and there must be at least one additional block between them. Hence, the second entry must appear at least $2l$ positions after the first. □

Lemma 10. *The coloring $\hat{C}$ is valid for the $1 \times (2l-1)$ rectangle stencil.*

Proof. If $\hat{C}$ were invalid for the $1 \times (2l-1)$ rectangle stencil, then there would exist (i, j_1) and (i, j_2) that lie in the same $1 \times (2l-1)$ rectangle. Either both points are colored by using the same coloring (i.e., in the partition they lie within rectangles of the same size), or they are colored by using two different colorings. First, we assume they are colored by using the same coloring. However, we know that within a row, each coloring is cyclic with period $w \geq l^2+2$. In addition, we know that each color appears only once every w entries. Thus, if (i, j_1) and (i, j_2) receive the same color, then they must be at a distance of at least $w \geq l^2+2 > 2l-1$.

Now consider the case where (i, j_1) and (i, j_2) are colored by using different colorings; suppose that (i, j_1) is colored by $C_1 = C(i, j, l, w, l^2+2)$, and (i, j_2) is colored by $C_2 = C(i, j, l, w, l^2+3)$. Let d_1 be the color used on (i, j_1). If both points were colored with the same coloring, the next occurence of color d_1 to the right of (i, j_1) would be at (i, j_1+w). However, the first appearance of a color in each row of coloring C_2 is no closer to the boundary between colorings C_1 and C_2 than if we were to continue using C_1 (see Lemma 4). As a result, no color can appear at two positions that are in the same row and are distance less than $w \geq l^2+2 > 2l-1$ apart. □

Theorem 11. *If $m \geq l^2(l^2+1)$ and $n \geq (l^2+1)(l^2+2)$, then there is an (l^2+3)-coloring of the $m \times n$ torus that is valid for the $(4l-3)$-point star stencil.*

Proof. This follows immediately from Lemmas 8, 9, and 10. $\square$

5 Three-Dimensional Stencils

In this section, we consider the three-dimensional version of our problem. In the three-dimensional case, the lattices we study are $\mathbb{Z}^3$ and $\mathbb{Z}^2 \times \mathbb{Z}_m$. We are motivated to look at colorings of these lattices for the $l \times l \times l$ cube. We also consider colorings of $\mathbb{Z}^3$ for the $(6l-5)$-point star. Apart from the 7-point star considered by Goldfarb and Toint [3], we are unaware of any treatment of these cases in the literature.

The intution for Theorem 12 is as follows. We assume that two points receive the same color under the specified coloring. We proceed to show that they cannot lie inside the same $(6l-5)$-point star stencil. Because we are giving a single coloring for all of $\mathbb{Z}^3$ (and not considering boundary conditions for discrete tori), there are no issues of compatibility between different colorings.

Theorem 12. *Let $M = l^2+l+1$, and define the coloring $C(i,j,k,l) = (i + l^2 j + (l^2+1)k) \bmod M$. Coloring $C(i,j,k,l)$ is a valid coloring of $\mathbb{Z}^3$ for the $(6l-5)$-point star and uses M colors.*

Proof. If the coloring is invalid, then there are two points $p_1 = (i_1, j_1, k_1)$ and $p_2 = (i_2, j_2, k_2)$ that receive the same color and lie within the same copy of a $(6l-5)$-point star stencil. Each point of a star differs in only one coordinate from the center of the star, so if p_1 and p_2 lie in the same star, then p_1 and p_2 agree in at least one coordinate.

First, consider the case where p_1 and p_2 agree in two coordinates. We simplify the expression $(i_1 + l^2 j_1 + (l^2+1)k_1) \equiv (i_2 + l^2 j_2 + (l^2+1)k_2) \bmod M$ by substituting in two of the three equalities: $i_1 = i_2$, $j_1 = j_2$, and $k_1 = k_2$. Depending on which two of the three equalities we assume to be true, we get one of three possibilities: $i_1 \equiv i_2 \bmod M$, $l^2 j_1 \equiv l^2 j_2 \bmod M$, or $(l^2+1)k_1 \equiv (l^2+1)k_2 \bmod M$. Since $1, l^2$, and (l^2+1) are all relatively prime to M, we see that $M|(i_1 - i_2)$, $M|(j_1 - j_2)$, or $M|(k_1 - k_2)$. However, we know that $|i_1 - i_2| < 2l-1$, $|j_1 - j_2| < 2l-1$, and $|k_1 - k_2| < 2l-1$; since $M > 2l-1$, we conclude that $p_1 = p_2$, which is a contradiction. Thus, if p_1 and p_2 lie inside the same star and receive the same color, then they agree in exactly one coordinate.

Now consider the case where p_1 and p_2 agree in exactly one coordinate. We must have $|i_1 - i_2| < l$, $|j_1 - j_2| < l$, $|k_1 - k_2| < l$, and one of the following.

$$(i_1 + l^2 j_1) \equiv (i_2 + l^2 j_2) \bmod M$$

$$\begin{aligned}(i_1+(l^2+1)k_1) &\equiv (i_2+(l^2+1)k_2) \bmod M\\ (l^2 j_1+(l^2+1)k_1) &\equiv (l^2 j_2+(l^2+1)k_2) \bmod M\end{aligned}$$

We rewrite these as follows.

$$\begin{aligned}(i_1-(l+1)j_1) &\equiv (i_2-(l+1)j_2) \bmod M\\ (i_1-lk_1) &\equiv (i_2-lk_2) \bmod M\\ (-lj_1+k_1) &\equiv (-lj_2+k_2) \bmod M\end{aligned}$$

The third equation follows by multiplying through by $(l+1)$. Those equations then imply (respectively) that one of the following is true.

$$\begin{aligned}M &\mid (i_1-i_2-(l+1)(j_1-j_2))\\ M &\mid (i_1-i_2-l(k_1-k_2))\\ M &\mid (k_1-k_2-l(j_1-j_2))\end{aligned}$$

In each case (making use of $|i_1-i_2|<l$, $|j_1-j_2|<l$, and $|k_1-k_2|<l$), we see that the quantity that M is supposed to divide has absolute value less than M. This implies that each quantity must be 0 and hence that $(i_1, j_1, k_1) = (i_2, j_2, k_2)$. This is a contradiction. Hence, the coloring is valid. □

Now we turn our attention to the $l\times l\times l$ cube stencil. Because we want to color $\mathbb{Z}^2\times\mathbb{Z}_m$, we need to give a coloring for all of the $l^3\times l^3\times(l^3+b)$ three-dimensional cylinders ($0\le b\le l$), rather than just the $l^3\times l^3\times l^3$ three-dimensional torus. The proof takes the same form as before. We assume that there are two points that lie within a cube and receive the same color; eventually we reach a contradiction. Define the coloring

$$C(i,j,k,l,b) = ((l^2 i+lj) \bmod l^3+k) \bmod (l^3+b).$$

Theorem 13. *If $0\le b\le l$, then $C(i,j,k,l,b)$ is a valid coloring of the $l^3\times l^3\times(l^3+b)$ three-dimensional cylinder for the $l\times l\times l$ cube. $C(i,j,k,l,b)$ uses l^3+b colors.*

Proof. If the coloring is invalid, then there are two points $p_1=(i_1,j_1,k_1)$ and $p_2=(i_2,j_2,k_2)$ that receive the same color and lie inside the same $l\times l\times l$ cube. As a result, p_1 and p_2 satisfy constraints (3.1) and (3.2) below:

$$|i_1-i_2|<l,\quad |j_1-j_2|<l,\quad |k_1-k_2|<l \tag{1}$$
$$(((l^2 i_1+lj_1) \bmod l^3)+k_1) \equiv ((l^2 i_2+lj_2) \bmod l^3+k_2)(\bmod (l^3+b)). \tag{2}$$

Without loss of generality, assume $(l^2 i_1 + l j_1) \bmod l^3 \geq (l^2 i_2 + l j_2) \bmod l^3$. Let $T = ((l^2 i_1 + l j_1) \bmod l^3 - (l^2 i_2 + l j_2) \bmod l^3 + (k_1 - k_2))$. Then T is divisible by $l^3 + b$ and $-(l^3+b) < T < 2(l^3+b)$. In particular, $T \in \{0, l^3+b\}$. Let $U = l^2(i_1 - i_2) + l(j_1 - j_2) + (k_1 - k_2)$. Then $U \in \{0, -l^3, l^3+b, b\}$. Making use of (3.1), we see that $|U| < l^3$. If $U = 0$, we immediately get $(i_1, j_1, k_1) = (i_2, j_2, k_2)$. This leaves only the case $U = b$. To have a solution other than $(i_1, j_1, k_1) = (i_2, j_2, k_2)$, we need $0 < b$. Again using (3.1) and the fact that $b \leq l$, we see that the only possible solutions are the following.

$$
\begin{array}{lll}
l^2 i_1 + l j_1 = l^2 i_2 + l j_2 & k_1 = k_2 + b & (i) \\
l^2 i_1 + l j_1 = l^2 i_2 + l j_2 + l & k_1 = k_2 + (b - l) & (ii)
\end{array}
$$

We need to show that none of these pairs of points actually receive the same colors. It is easy to see that no pair of points satisfying (i) receives the same color.

Consider pairs of points satisfying (ii). The key is to determine the difference $(l^2 i_1 + l j_1) \bmod l^3 - (l^2 i_2 + l j_2) \bmod l^3$. Let $N = (l^2 i_2 + l j_2) \bmod l^3$. There are two possibilities. Either there exists a positive integer d such that $l^2 i_2 + l j_2 < d l^3 \leq l^2 i_2 + l j_2 + l$, or there does not exist such an d. If there does not exist such an d, then $(l^2 i_1 + l j_1) \bmod l^3 = N + l$. This leads to $(N + k_2) \bmod (l^3 + b) = (N + l + k_2 + b - l) \bmod (l^3 + b)$. This implies that $b \equiv 0 \bmod (l^3 + b)$. However, since $0 < b \leq l$, this is a contradiction. Hence, there must exist such an integer d.

Consider (ii) when there exists a positive integer d such that $l^2 i_2 + l j_2 < d l^3 \leq l^2 i_1 + l j_1$. Then $(l^2 i_1 + l j_1) \bmod l^3 = N + l - l^3$. This leads to $(N + k_2) \equiv (N + l - l^3 + k_2 + b - l) \bmod (l^3 + b)$. Simplifying, we get $l^3 \equiv b \bmod (l^3 + b)$. However, $0 < b \leq l$, so we reach a contradiction. Hence, there are no pairs of points receiving the same color and also satisfying constraint (ii). Thus, there is no pair of points $(i_1, j_1, k_1), (i_2, j_2, k_2)$ receiving the same color and also lying inside the same $l \times l \times l$ cube. As a result, the coloring is valid. □

Corollary 14. *There exists a l^3-coloring of $\mathbb{Z}^3$ that is valid for the $l \times l \times l$ cube.*

Proof. $C(i, j, k, l, 0)$ is valid for a $l \times l \times l$ cube and uses l^3 colors. It is easy to see that this coloring also works for the points of $\mathbb{Z}^3$. □

Lemma 15. *Define the colorings $C_1 = C(i, j, k, l, b_1)$ and $C_2 = C(i, j, k, l, b_2)$. If $0 \leq b_1 \leq b_2$ then C_1 and C_2 are compatible.*

Proof. Analogous to rows and columns, we define towers to be the set of lattice points for which i, j are fixed and k varies. Under C_1, as k increases in a tower, we get the repeating sequence $0, 1, 2, \ldots, l^3 + b_1 - 2, l^3 + b_1 - 1$. Under C_2, as k increases in a tower, we get the repeating sequence $0, 1, 2, \ldots, l^3 + b_2 - 2, l^3 + b_2 - 1$. The key insight is that in a tower, under C_2, no color is closer to the boundary between C_1 and C_2 than if we were to continue using C_1. Suppose we have one point (i_1, j_1, k_1), colored by C_1, and another point (i_2, j_2, k_2), colored by C_2, which make the colorings incompatible. Instead of changing from C_1 to C_2 at the boundary between them, we could continue using C_1 for all the points and find a point (i_3, j_3, k_3), which makes C_1 incompatible with itself. Since C_1 is not incompatible with itself, C_1 and C_2 must be compatible. $\square$

Theorem 16. *Suppose l and m are positive integers that satisfy $m \geq l^3$. Define q to be the least nonnegative integer for which m can be written as a linear combination of $l^3, l^3+1, \ldots, l^3+q-1, l^3+q$. There is an (l^3+q)-coloring of $\mathbb{Z}^2 \times \mathbb{Z}_m$, that is valid for the $l \times l \times l$ cube.*

Proof. Following the ideas of Theorem 6, we partition $\mathbb{Z}^2 \times \mathbb{Z}_m$ into copies of $\mathbb{Z}^2 \times \mathbb{Z}_{b_i}$, where b_i can differ in different copies but $l^3 \leq b_i \leq l^3+q$ for all copies. We color each copy of $\mathbb{Z}^2 \times \mathbb{Z}_{b_i}$ using the coloring given by Theorem 13. By Lemma 15, these colorings are compatible, so the total coloring is valid. $\square$

Corollary 17. *Let l and m be positive integers such that $m \geq l^3(l^3-1)$. There is an (l^3+1)-coloring of $\mathbb{Z}^2 \times \mathbb{Z}_m$, that is valid for the $l \times l \times l$ stencil.*

Proof. This follows from Theorem 16 and Lemma 1 (setting $q = 1$). $\square$

6 Lower Bounds

We give lower bounds that prove that our colorings for the square and cube stencils are either optimal or within one color of being optimal.

Theorem 18. *Any valid coloring of the $m \times n$ torus for the $l \times l$ square stencil requires l^2+1 colors unless $l|m$ and $l|n$.*

Proof. Consider an $m \times l$ subcylinder (the dimension of size m is the one that wraps around). If our coloring uses at most l^2 colors, then by the pigeon-hole principle there is some color class of size at least $\lceil \frac{m \times l}{l^2} \rceil = \lceil \frac{m}{l} \rceil$. However, a color class can have size at most $\lfloor \frac{m \times l}{l^2} \rfloor = \lfloor \frac{m}{l} \rfloor$ (since two entries in the same color class must be at least l rows apart). If $l|m$, these quantities are equal. Otherwise, we need at least l^2+1 colors. An analagous argument shows that we need $l|n$. $\square$

Slight variations of this proof lead to the following theorems.

Theorem 19. *Any valid coloring of the $m \times n$ cylinder for the $l \times l$ square stencil requires l^2+1 colors unless $l|n$.*

$$\begin{bmatrix} 1 & 2 & 3 & 4 & 5 & \\ 6 & 7 & 8 & 9 & 10 & + \\ 11 & 12 & 13 & 14 & 15 & + \\ 16 & 17 & 18 & 19 & 20 & + \\ 21 & 22 & 23 & 24 & 25 & + \\ & * & * & * & * & \end{bmatrix}$$

Figure 4: The proof of Theorem 21 for $l = 5$.

Theorem 20. *Any valid coloring of $\mathbb{Z}^2 \times \mathbb{Z}_m$ for the $l \times l \times l$ cube requires $l^3 + 1$ colors unless $l|m$.*

Now we give a bound on the number of colors needed for star stencils.

Theorem 21. *If $m > l$ and $n > l$, then we need at least $l^2 + 1$ colors to color an $m \times n$ rectangle such that no two points with the same color lie in a $(4l-3)$-point star.*

Proof. It is easy to see that no vertices in a $l \times l$ square can receive the same color. We begin by coloring these all differently. For ease of reference, we will refer to the vertices as entries of a $m \times n$ matrix, where a_{ij} denotes the vertex in the ith row and jth column.

The only colors available to color entries of column $l+1$ are those used in column 1. To color entries $a_{1,l+1}, a_{2,l+1}, \ldots, a_{l,l+1}$, we must use each color in the set $\{1+kl : 0 \le k < l\}$ exactly once. Since $(1,1) = 1$, we see that $(1, l+1) \neq 1$. So there exists i with $2 \le i \le l$ and $(i, l+1) = 1$ (one of the entries denoted by + in the diagram). The only colors available to color row $l+1$ are those used in row 1. To color $(l+1,2), (l+1,3), \ldots, (l+1,l)$ (those entries denoted by * in the diagram), we must use every color in the set $\{2,3,\ldots,l\}$ exactly once. However, this leaves no color for $(l+1,1)$. Color 1 cannot be used because $(1,1) = 1$ and all other colors are already assigned to some (i,j) with $2 \le i \le l+1$ and $1 \le j \le l$. Thus, we need an additional color for $(l+1,1)$, so at least $(l+1)^2 + 1$ colors are required. $\square$

Theorem 22. *The coloring given for the $(6l-5)$-point star is asymptotically the best possible.*

Proof. Every (axis-aligned) cross-section of the coloring for the $(6l-5)$-point star must be a valid coloring for the $(4l-3)$-point star. Thus, we have a lower bound of l^2+1 colors. We use $l(l+1)+1$ colors. The ratio of upper and lower bound is $(1+\frac{1}{l-1})$, which approaches 1 as l gets large. $\square$

7 Conclusion

We have given colorings for the $(4l-3)$-point star and the $l \times l$ square stencils (for all l) in the plane, on the cylinder, and on the torus. On the torus, we have proved that the colorings for the $(4l-3)$-point star are within at most 2 colors of optimality. On the cylinder, they are within at most 1 color of optimality. In the plane all star colorings are optimal. On the torus and the cylinder, our colorings for the square stencils are within at most 1 color of optimality. The colorings for square stencils in the plane are optimal.

We have given colorings for the $l \times l \times l$ cube stencils for $\mathbb{Z}^3$ and $\mathbb{Z}^2 \times \mathbb{Z}_m$. Both are optimal. We have also given colorings of $\mathbb{Z}^3$ for the $(6l-5)$-point star, which are asymptotically the best possible.

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