# Integer Point Sets Minimizing Average Pairwise <br> $L_{1}$ Distance: What is the Optimal Shape of a Town? 

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#### Abstract

An $n$-town, $n \in \mathbb{N}$, is a group of $n$ buildings, each occupying a distinct position on a 2 -dimensional integer grid. If we measure the distance between two buildings along the axis-parallel street grid, then an $n$-town has optimal shape if the sum of all pairwise Manhattan distances is minimized. This problem has been studied for cities, i.e., the limiting case of very large $n$. For cities, it is known that the optimal shape can be described by a differential equation, for which no closed-form solution is known. We show that optimal $n$-towns can be computed in $O\left(n^{7.5}\right)$ time. This is also practically useful, as it allows us to compute optimal solutions up to $n=80$.


Key words: Manhattan distance, average pairwise distance, integer points, dynamic programming

## 1. Introduction

Selecting an optimal set of locations is a fundamental problem, not just in real estate, but also in many areas of computer science. Typically, the task is to choose $n$ sites from a given set of candidate locations; the objective is to pick a set that minimizes a cost function, e.g., the average distance between sites. As described below, there is a large variety of related results, motivated by different scenarios.

In general, problems of this type are hard, even to approximate, as the problem of finding a clique of given size is a special case. Some of the natural settings have a strong geometric flavor, so it is conceivable that more
positive results can be achieved by exploiting additional structures and properties. However, even seemingly easy special cases are still surprisingly difficult. Until now, there was no complexity result (positive or negative) for the scenario in which the candidate locations correspond to the full integer grid, with distances measured by the Manhattan metric (an n-town). Indeed, for the shape of area 1 with minimum average $L_{1}$ distance (the "optimal shape of a city", arising for the limit case of $n$ approaching infinity), no simple closedform solution is known, suggesting that finding sets of $n$ distinct grid points (the "optimal shapes of towns") may not be an easy task. This makes the problem mathematically challenging; in addition, the question of choosing $n$ grid positions with minimum average $L_{1}$ distance comes up naturally in grid computing, so the problem is of both practical and theoretical interest.

In this paper, we give the first positive result by describing an $O\left(n^{7.5}\right)$ algorithm for computing sets of $n$ distinct grid points with minimum average $L_{1}$ distance. Our method is based on dynamic programming, and (despite of its relatively large exponent) for the first time allows computing optimal towns up to $n=80$.

### 1.1. Related Work

Grid Computing. In grid computing, allocating a task requires selecting $n$ processors from a given grid, and the average communication overhead corresponds to the average Manhattan distance between processors; Mache and Lo $(1996,1997)$ and Leung et al. (2002) propose various metrics for measuring the quality of a processor allocation, including the average number of communication hops between processors. Leung et al. (2002) considered the problem of allocating processors on Cplant, a Sandia National Labs supercomputer; they applied and evaluated a scheme based on space-filling curves, and they concluded that the average pairwise Manhattan distance between processors is an effective metric to optimize.

The Continuous Version. Motivated by the problem of storing records in a 2-dimensional array, Karp et al. (1975) studied strategies that minimize average access time between successive queries; among other results, they described an optimal solution for the continuous version of our problem: What shape of area 1 minimizes the average Manhattan distance between two interior points? Independently, Bender et al. (2004) solved this problem in the setting of a city, inspiring the subtitle of this paper. The optimal

| $\begin{aligned} & n=2 \\ & c(S)=1 \\ & \hline \end{aligned}$ | $\begin{aligned} n & =3 \\ c(S) & =4 \end{aligned}$ | $\begin{aligned} &:: \\ & n=4 \\ & c(S)=8 \end{aligned}$ | $\begin{gathered} \because \quad:: \\ n=5 \\ c(S)=16 \end{gathered}$ | ::: $\begin{aligned} & n=6 \\ & c(S)=25 \\ & \hline \end{aligned}$ |
| :---: | :---: | :---: | :---: | :---: |
| : : $\begin{aligned} & n=7 \\ & c(S)=38 \\ & \hline \end{aligned}$ | $\begin{aligned} & n=8 \\ & c(S)=54 \\ & \hline \end{aligned}$ | ::: $\begin{aligned} n & =9 \\ c(S) & =72 \end{aligned}$ | $\begin{aligned} n & =10 \\ c(S) & =96 \end{aligned}$ | $\because:::::$ <br> -::: : :::: $\begin{aligned} n & =11 \\ c(S) & =124 \end{aligned}$ |
| $\begin{aligned} n & =12 \\ c(S) & =152 \end{aligned}$ | $\begin{aligned} n & =13 \\ c(S) & =188 \end{aligned}$ | $\begin{aligned} n & =14 \\ c(S) & =227 \end{aligned}$ | $\begin{aligned} n & =15 \\ c(S) & =272 \end{aligned}$ | $\begin{aligned} n & =16 \\ c(S) & =318 \end{aligned}$ |
| $\begin{aligned} n & =17 \\ c(S) & =374 \end{aligned}$ | $\begin{aligned} n & =18 \\ c(S) & =433 \end{aligned}$ | $\begin{aligned} n & =19 \\ c(S) & =496 \end{aligned}$ | $\begin{aligned} n & =20 \\ c(S) & =563 \end{aligned}$ | $\begin{aligned} n & =21 \\ c(S) & =632 \end{aligned}$ |

Figure 1: Optimal towns for $n=2, \ldots, 21$. All optimal solutions are shown, up to symmetries; $c(S)$ denotes the total distance between all pairs of points. The picture for $n=20$ also contains the symmetry axes from Lemma 3 .
solution is described by a differential equation, and no closed-form solution is known.

Selecting $k$ points out of $n$. Krumke et al. (1997) consider the discrete problem of selecting a subset of $k$ nodes from a network with $n$ nodes to minimize their average pairwise distance. They prove a 2 -approximation for metric distances and prove hardness of approximation for arbitrary distances. Bender et al. (2008) solve the geometric version of this problem, giving an efficient processor allocator for the Cplant setting described above, and a polynomialtime approximation scheme (PTAS) for minimizing the average Manhattan distance. For the reverse problem of maximizing the average Manhattan distance, see Fekete and Meijer (2003).

The $k$-median Problem. Given two sets $D$ and $F$, the $k$-median problem asks to choose a set of $k$ points from $D$ to minimize the average distance to the
points in $F$. For $k=1$ this is the classical Fermat-Weber problem. Fekete et al. $(2000,2005)$ considered the city-center problem: for a given city, find a point that minimizes the average Manhattan distance. They proved NPhardness for general $k$ and gave efficient algorithms for some special cases.

The Quadratic Assignment Problem. Our problem is a special case of the quadratic assignment problem (QAP): Given $n$ facilities, $n$ locations, a matrix containing the amount of flow between any pair of facilities, and a matrix containing the distances between any pair of locations. The task is to assign every facility to a location such that the cost function which is proportional to the flow between the facilities multiplied by the distances between the locations is minimized. For a survey see Loiola et al. (2007). The cost function in our problem and in the QAP are the same if we define the distances as the Manhattan distances between grid points and if we define all flows to be one. The QAP can not be approximated within any polynomial factor unless $P=N P$; see Sahni and Gonzalez (1976). Hassin et al. (2009) considered the metric version of this problem with the flow matrix being a $0 / 1$ incidence matrix of a graph. They state some inapproximability results as well as a constant-factor approximation for the case in which the graph has vertex degree two for all but one vertex.

The Maximum Dispersion Problem. The reverse version of the discrete problem, where the goal is to maximize the average distance between points, has also been studied: In the maximization version, called the maximum dispersion problem, the objective is to pick $k$ points from a set of size $n$ so that the pairwise distance is maximized. When the edge weights need not obey the triangle inequality, Kortsarz and Peleg (1993) give an $O\left(n^{0.3885}\right)$ approximation. Asahiro et al. (2000) improve this guarantee to a constant factor in the special case when $k=\Omega(n)$ and Arora et al. (1999) give a PTAS when $|E|=\Omega\left(n^{2}\right)$ and $k=\Omega(n)$.

When the edge weights obey the triangle inequality, Ravi et al. (1994) give a 4 -approximation that runs in $O\left(n^{2}\right)$ time and Hassin et al. (1997) give a 2-approximation that runs in $O\left(n^{2}+k^{2} \log k\right)$ time. For points in the plane and Euclidean distances, Ravi et al. (1994) give an approximation with performance bound arbitrarily close to $\pi / 2 \approx 1.57$. For Manhattan distances, Fekete and Meijer (2003) give an optimal algorithm for fixed $k$ and a PTAS for general $k$. Moreover, they provide a $(\sqrt{2}+\varepsilon)$-Approximation for Euclidean distances.

The Min-Sum k-Clustering Problem. Another related problem is called minsum $k$-clustering or minimum $k$-clustering sum. The goal is to separate a graph into $k$ clusters to minimize the sum of pairwise distances between nodes in the same cluster. For general graphs, Sahni and Gonzalez (1976) show that this problem is NP-hard to approximate within any constant factor for $k \geq 3$. In a metric space the problem is easier to approximate: Guttmann-Beck and Hassin (1998) give a 2-approximation, Indyk (1999) gives a PTAS for $k=2$, and Bartal et al. (2001) give an $O\left(1 / \epsilon \log ^{1+\epsilon} n\right)$-approximation for general $k$.

### 1.2. Our Results

We solve the $n$-town problem with an $O\left(n^{7.5}\right)$-time dynamic-programming algorithm. Our algorithm is based on some properties of an optimal town: an optimal $n$-town is convex in the sense that it contains all grid points within its convex hull (Lemma 2). It lies symmetric with respect to a horizontal and a vertical symmetry axis within a tolerance of $\pm 1$ that is due to parity issues (Lemma 3). Furthermore, it fits in an $O(\sqrt{n}) \times O(\sqrt{n})$ square (Lemma 5). We also present computational results and discuss the relation between the optimum continuous cities and their discretized counterparts ( $n$-towns, and $n$-block cities).

## 2. Properties of Optimal Towns

We want to find a set of $n$ distinct points from the integer grid $\mathbb{Z} \times \mathbb{Z}$ such that the sum of all pairwise Manhattan distances is minimized. A set $S \subset \mathbb{Z} \times \mathbb{Z}$ of cardinality $n$ is an $n$-town. An $n$-town $S$ is optimal if its cost

$$
\begin{equation*}
c(S):=\frac{1}{2} \cdot \sum_{s \in S} \sum_{t \in S}\|s-t\|_{1} \tag{1}
\end{equation*}
$$

is minimum. Figure 1 shows solutions for small $n$ and their cost, and Table 1 in Section 5 shows optimal cost values $c_{\text {town }}(n)$ for $n \leq 80$. We define the $x$-cost $c_{x}(S)$ as $\sum_{\{s, t\} \in S \times S}\left|s_{x}-t_{x}\right|$, where $s_{x}$ is the $x$-coordinate of $s ; y$-cost $c_{y}(S)$ is the sum of all $y$-distances, and $c(S)=c_{x}(S)+c_{y}(S)$. For two sets $S$ and $S^{\prime}$, we define $c\left(S, S^{\prime}\right)=\sum_{\left\{s, s^{\prime}\right\} \in S \times S^{\prime}}\left\|s-s^{\prime}\right\|_{1}$. If $S$ consists of a single point $t$, we write $c\left(t, S^{\prime}\right)$ instead of $c\left(\{t\}, S^{\prime}\right)$ for convenience. A town $S$ is convex if the set of grid points in the convex hull of $S$ equals $S$.

In proving various properties of optimal towns, we will often make a local modification by moving a point $t$ of a town to a different place $r$. The next lemma expresses the resulting cost change.

Lemma 1. Let $S$ be a town, $t \in S$ and $r \notin S$. Then,

$$
c((S \backslash t) \cup r)=c(S)-c(t, S)+c(r, S)-\|r-t\|_{1} .
$$

Proof. Let $p$ be a point in $S$. Then, its distance to $t$ is $\|t-p\|_{1}$ and the distance to $r$ is $\|r-p\|_{1}$. Hence, the change in the cost function is $\|r-p\|_{1}-\|t-p\|_{1}$. We need to subtract $\|r-t\|_{1}$ from the sum over all points in $S$ because $t$ is removed from $S$.

Lemma 2. An optimal n-town is convex.
The following proof holds in any dimension and with any norm for measuring the distance between points.

Proof. We prove that a non-convex $n$-town $S$ cannot be optimal. Take a grid point $x \notin S$ in the convex hull of $S$. Then there are points $x_{1}, x_{2}, \ldots, x_{k} \in$ $S$ such that $x=\lambda_{1} x_{1}+\lambda_{2} x_{2}+\cdots+\lambda_{k} x_{k}$ for some $\lambda_{1}, \lambda_{2}, \ldots, \lambda_{k} \geq 0$ with $\sum \lambda_{i}=1$. Because every norm is a convex function, and the sum of convex functions is again convex, the function $f_{S}(x)=c(x, S)=\sum_{s \in S}\|x-s\|_{1}$ is convex. Therefore,

$$
f_{S}(x) \leq \lambda_{1} f\left(x_{1}\right)+\lambda_{2} f\left(x_{2}\right)+\cdots+\lambda_{k} f\left(x_{k}\right)
$$

which implies $f_{S}(x) \leq f_{S}\left(x_{i}\right)$ for some $i$. Using Lemma 1 we get

$$
c\left(\left(S \backslash x_{i}\right) \cup x\right)=c(S)-f_{S}\left(x_{i}\right)+f_{S}(x)-\left\|x-x_{i}\right\|_{1}<c(S)
$$

This means that $S$ is not optimal.
Obviously, if we translate every point from an $n$-town by the same vector, the cost of the town does not change. We want to distinguish towns because of their shape and not because of their position inside the grid and, therefore, we will only consider optimal towns that are placed around the origin. Lemma 3 makes this more precise: an optimal $n$-town is roughly symmetric with respect to a vertical and a horizontal symmetry line, see Figure 2 for an illustration. Perfect symmetry is not possible since some rows or columns may have odd length and others even length.

We need some notation before: For an $n$-town $S$, the $i$-th column of $S$ is the set $C_{i}=\{(i, y) \in S: y \in \mathbb{Z}\}$ and the $i$-th row of $S$ is the set $R_{i}=\{(x, i) \in S: x \in \mathbb{Z}\}$.

Lemma 3 (Symmetry). In every optimal $n$-town $S$, the centers of all rows of odd length lie on a common vertical grid line $V_{o}$. The centers of all rows of even length lie on a common line $V_{e}$ that has distance $\frac{1}{2}$ from $V_{o}$. A corresponding statement holds for the centers of odd and even columns that lie on horizontal lines $H_{o}$ and $H_{e}$ of distance $\frac{1}{2}$. Moreover, without changing its cost, we can place $S$ such that $H_{o}$ and $V_{o}$ are mapped onto the $x$-axis and $y$-axis, respectively, and $H_{e}$ and $V_{e}$ lie in the negative halfplanes.

Proof. For a row $R_{j}$ and $r \in \mathbb{Z}$, let $R_{j}+(r, 0)$ be the row $R_{j}$ horizontally translated by $(r, 0)$. If two rows $R_{i}$ and $R_{j}$ are of the same parity, a straightforward calculation (using Lemma 1) shows that the cost $c\left(R_{i}, R_{j}+(r, 0)\right)$ is minimal if and only if the centers of $R_{i}$ and $R_{j}+(r, 0)$ have the same $x$ coordinate. If the parities differ, $c\left(R_{i}, R_{j}+(r, 0)\right)$ is minimized with centers having $x$-coordinates of distance $1 / 2$. The total cost is

$$
c(S)=c_{x}(S)+c_{y}(S)=\sum_{i, j} \sum_{s \in R_{i}, t \in R_{j}}\left|s_{x}-t_{x}\right|+c_{y}(S)
$$

If we translate every row $R_{i}$ of $S$ horizontally by some $\left(r_{i}, 0\right), c_{y}(S)$ does not change. The solutions that minimize $\sum_{s \in R_{i}, t \in R_{j}}\left|s_{x}+r_{i}-t_{x}+r_{j}\right|$ for all $i, j$ simultaneously are exactly those that align the centers of all rows of even length on a vertical line $V_{e}$ and the centers of all rows of odd length on a vertical line $V_{o}$ at offset $\frac{1}{2}$ from $V_{e}$. The existence of the lines $H_{o}$ and $H_{e}$ follows analogously.

We can translate $S$ such that $H_{o}$ and $V_{o}$ are mapped onto the $x$ - and the $y$-axis and rotate it by a multiple of $90^{\circ}$ degrees such that $H_{e}$ and $V_{e}$ lie in the negative halfplanes. These operations do not change $c(S)$.

From the convexity statement in Lemma 2 (together with Lemma 3) we know that $C_{0}$ is the largest column, and the column lengths decrease to both sides, and similarly for the rows. Our algorithm will only be based on this weaker property (orthogonal convexity); it will not make use of convexity per $s e$. We will, however, use convexity one more time to prove that the lengths of the columns are $O(\sqrt{n})$, in order to reduce the running time.

In the following we assume the symmetry property of the last lemma. For an $n$-town $S$, let the width of $S$ be $w(S)=\max _{i \in \mathbb{Z}}\left|R_{i}\right|$ and the height of $S$ be $h(S)=\max _{i \in \mathbb{Z}}\left|C_{i}\right|$. We will now show that the width and the height cannot differ by more than a factor of 2 . Together with convexity, this will imply that they are bounded by $O(\sqrt{n})$ (Lemma 5).

Lemma 4. For every optimal $n$-town $S$,

$$
w(S)>h(S) / 2-3 \text { and } h(S)>w(S) / 2-3
$$

Proof. Let $S$ be an $n$-town, $w=w(S)$, and $h=h(S)$, and assume $w \leq$ $h / 2-3$. Let $t=(0, l)$ be the topmost and $(k, 0)$ be the rightmost point of $S$, with $l=\left\lfloor\frac{h-1}{2}\right\rfloor$ and $k=\left\lfloor\frac{w-1}{2}\right\rfloor$. Let $r=(k+1,0)$. We show that $c((S \backslash t) \cup r)<c(S)$, and thus, $S$ is not optimal. By Lemma 1, the change in cost is $c(r, S)-c(t, S)-|k+l+1|$. We show that $c(r, S)-c(t, S) \leq$ 0 by calculating this difference column by column. This proves then that replacing $t$ with $r$ yields a gain of at least $|l+k+1| \geq 1$, and we are done. Let us calculate the difference $c\left(r, C_{j}\right)-c\left(t, C_{j}\right)$ for a column $C_{j}$ of height $\left|C_{j}\right|=s \leq h:$

$$
\begin{aligned}
c\left(r, C_{j}\right)-c\left(t, C_{j}\right) & =\sum_{i=-\left\lceil\frac{s-1}{2}\right\rceil}^{\left\lfloor\frac{s-1}{2}\right\rfloor}(|i|-(l-i))+s(k+1-j-|j|) \\
& =\sum_{i=0}^{\left\lfloor\frac{s-1}{2}\right\rfloor}(i-(l-i))+\sum_{i=1}^{\left\lceil\frac{s-1}{2}\right\rceil}(i-(l+i))+s(k+1-j-|j|) \\
& =2 \sum_{i=0}^{\left\lfloor\frac{s-1}{2}\right\rfloor} i-s l+s(k+1-j-|j|) \\
& \leq \frac{(s-1)(s+1)}{4}-s \frac{h-2}{2}+s(k+1) \leq \frac{s^{2}}{4}-s \frac{h-2}{2}+s \cdot \frac{w+1}{2} \\
& =\frac{s}{4}(s-2 h+2 w+6) \leq \frac{s}{2}(-h+2 w+6) \leq 0
\end{aligned}
$$

Lemma 5. For every optimal n-town we have

$$
\max \{w(S), h(S)\} \leq 2 \sqrt{n}+5
$$

Proof. Let $w=w(S)$ and $h=h(S)$. Assume without loss of generality that $h \geq w$. We know from Lemma 4 that $w>h / 2-3$. By Lemma 3, we choose a topmost, a rightmost, a bottommost, and a leftmost point of $S$ such that the convex hull of these four points is a quadrilateral with a vertical and horizontal diagonal, approximately diamond-shaped. Let $H$ be the set of all grid points contained in this quadrilateral. The area of the


Figure 2: The lines $V_{o}, V_{e}, H_{o}$, and $H_{e}$ from Lemma 3. The rectangle $R_{w}$ and the set of points above and below it with cardinality $U_{w}$ and $D_{w}$, respectively. The gray points are the corner points of $R_{w}$. In this example, the height $c_{w}$ of column $w$ is set to $c=4$.
quadrilateral equals $(w-1)(h-1) / 2$, and its boundary contains at least 4 grid points. Pick's theorem says that the area of a simple grid polygon equals the number of its interior grid points $H_{i}$ plus half of the number of the grid points $H_{0}$ on its boundary minus 1 . This implies $|H|=\left|H_{i}\right|+\left|H_{0}\right|=$ $\left(\left|H_{i}\right|+\left|H_{0}\right| / 2-1\right)+\left|H_{0}\right| / 2+1 \geq(w-1)(h-1) / 2+3$. Because of Lemma 2, all points in $H$ belong to $S$. Since $H$ consists of at most $n$ points, we have

$$
n \geq|H| \geq(w-1)(h-1) / 2+3>(h / 2-4)(h-1) / 2+3
$$

Solving the equation $h^{2}-9 h+20-4 n=0$ shows that

$$
h \leq 2 \sqrt{n+1 / 16}+9 / 2 \leq 2 \sqrt{n}+5 .
$$

## 3. Computing Optimal Solutions

We will now describe a dynamic-programming algorithm for computing optimal towns. A program for this algorithm is listed in Appendix A.

We denote by $c_{i}=\left|C_{i}\right|$ the number of selected points in column $i$ and by $c_{i}^{+}$and $c_{i}^{-}$the row index of the topmost and bottommost selected point in $C_{i}$, respectively. We have $c_{i}=c_{i}^{+}-c_{i}^{-}+1$; see Figure 2.

Lemma 6. Let $S$ be an optimal n-town (placed as described in Lemma 3) containing the points $\left(i, c_{i}^{+}\right)$and $\left(i, c_{i}^{-}\right)$, for $i \geq 0$. Then all points inside the rectangle $[-i, i] \times\left[c_{i}^{-}, c_{i}^{+}\right]$belong to $S$.

Similarly, if $S$ contains the points $\left(-i, c_{-i}^{+}\right)$and $\left(-i, c_{-i}^{-}\right)$, for $i \geq 1$, then it contains all points in the rectangle $[-i, i-1] \times\left[c_{-i}^{-}, c_{-i}^{+}\right]$.

Proof. If $\left(i, c_{i}^{+}\right)$and $\left(i, c_{i}^{-}\right)$are contained in $S$ then, by Lemma $3,\left(-i, c_{i}^{+}\right)$ and $\left(-i, c_{i}^{-}\right)$belong to $S$ as well. By Lemma 2 all points inside the convex hull of these four points are contained in $S$. The same arguments hold for the second rectangle.

Now we describe the dynamic program. It starts with the initial empty grid and chooses new columns alternating from the set of columns with nonnegative and with negative column index, i.e., in the order $0,-1,1,-2,2, \ldots$. Let $w \geq 0$ be the index of the currently chosen column and fix $c_{w}$ to a value $c$. We describe the dynamic program for columns with nonnegative index; columns with negative index are handled similarly. (In the program that is described in the appendix, we use a trick to avoid dealing with negative columns: they are mapped to columns with positive index by reflecting everything at the $y$-axis, with a proper adjustment to take into account that the placement of Lemma 3 is not invariant under this transformation.)

We know from Lemma 6 that in every optimal solution, every point inside the rectangle $R_{w}=[-w, w] \times\left[c_{w}^{-}, c_{w}^{+}\right]$is selected. We define

$$
\operatorname{cost}\left(w, c, \Delta_{w}^{\mathrm{UR}}, \Delta_{w}^{\mathrm{DR}}, \Delta_{w}^{\mathrm{UL}}, \Delta_{w}^{\mathrm{DL}}, U_{w}, D_{w}\right)
$$

as the minimum cost of a town with columns $-w, \ldots, w$ of height $c_{i} \geq c$ for $-w \leq i \leq w$ and $c_{w}=c$ where $U_{w}$ points lie above the rectangle $R_{w}$, having a total distance $\Delta_{w}^{\mathrm{UL}}$ and $\Delta_{w}^{\mathrm{UR}}$ to the upper-left and upper-right corner of $R_{w}$, respectively, and $D_{w}$ points lie below $R_{w}$, having a total distance $\Delta_{w}^{\mathrm{DL}}$ and $\Delta_{w}^{\mathrm{DR}}$ to the lower-left and lower-right corner of $R_{w}$. For a given $n$, we are looking for the $n$-town with minimum cost where $(2 w+1) c+U_{w}+D_{w}=n$. Next we show that $\operatorname{cost}\left(w, c, \Delta_{w}^{\mathrm{UR}}, \Delta_{w}^{\mathrm{DR}}, \Delta_{w}^{\mathrm{UL}}, \Delta_{w}^{\mathrm{DL}}, U_{w}, D_{w}\right)$ can be computed recursively.

Consider the current column $w$ with $c_{w}=c$. The cost from all points in this column to all points above $R_{w}$, in $R_{w}$, and below $R_{w}$ can be expressed

$$
\begin{aligned}
\sum_{k=c^{-}}^{c^{+}}\left(\Delta_{w}^{\mathrm{UR}}+\left(c^{+}-k\right) \cdot U_{w}\right)+\sum_{i=-w}^{w} \sum_{j=c^{-}}^{c^{+}} \sum_{k=c^{-}}^{c^{+}} & {[(w-i)+|k-j|] } \\
& +\sum_{k=c^{-}}^{c^{+}}\left(\Delta_{w}^{\mathrm{DR}}+\left(k-c^{-}\right) \cdot\left|D_{w}\right|\right)
\end{aligned}
$$

We can transform this into

$$
\begin{array}{r}
c \cdot\left(\Delta_{w}^{\mathrm{UR}}+\Delta_{w}^{\mathrm{DR}}+U_{w} \cdot c^{+}-D_{w} \cdot c^{-}\right)+c^{-} \cdot\left(D_{w}-U_{w}\right) \cdot((c+1) \bmod 2) \\
+\left(c^{2} w+\frac{c^{3}-c}{3}\right) \cdot(2 w+1)-\frac{c^{3}-c}{6} \tag{2}
\end{array}
$$

which, obviously, depends only on the parameters $w, c, \Delta_{w}^{\mathrm{UR}}, \Delta_{w}^{\mathrm{DR}}, U_{w}$, and $D_{w}$ (the two parameters $\Delta_{w}^{\mathrm{UL}}, \Delta_{w}^{\mathrm{DL}}$ are needed if we consider a column with negative index). We denote the expression (2) by $\operatorname{dist}\left(w, c, \Delta_{w}^{\mathrm{UR}}, \Delta_{w}^{\mathrm{DR}}, \Delta_{w}^{\mathrm{UL}}\right.$, $\left.\Delta_{w}^{\mathrm{DL}}, U_{w}, D_{w}\right)$ and state the recursion for the cost function:

$$
\begin{align*}
& \operatorname{cost}\left(w, c, \Delta_{w}^{\mathrm{UR}}, \ldots, \Delta_{w}^{\mathrm{DL}}, U_{w}, D_{w}\right) \\
& \quad=\min _{c_{-w} \geq c}\left\{\operatorname{cost}\left(-w, c_{-w}, \Delta_{-w}^{\mathrm{UR}}, \ldots, \Delta_{-w}^{\mathrm{DL}}, U_{-w}, D_{-w}\right)\right\} \\
& \tag{3}
\end{align*} \quad+\operatorname{dist}\left(w, c, \Delta_{w}^{\mathrm{UR}}, \ldots, \Delta_{w}^{\mathrm{DL}}, U_{w}, D_{w}\right) \text {. }
$$

By Lemma 6 it suffices to consider only previous solutions with $c_{-w} \geq c$. In the step before, we considered the rectangle $R_{-w}=[-w, w-1] \times\left[c_{-w}^{+}, c_{-w}^{-}\right]$. Hence, the parameters with index $-w$ can be computed from the parameters with index $w$ as follows:

$$
\begin{aligned}
U_{-w} & =U_{w}-2 w \cdot\left(c_{-w}^{+}-c^{+}\right), \\
D_{-w} & =D_{w}-2 w \cdot\left(c^{-}-c_{-w}^{-}\right), \\
\Delta_{-w}^{\mathrm{UR}} & =\Delta_{w}^{\mathrm{UR}}-\sum_{i=-w}^{w} \sum_{j=c^{+}+1}^{c_{-w}^{+}}\left[(w-i)+\left(j-c^{+}\right)\right] \\
& \quad-\left[U_{w}-U_{-w}\right] \cdot\left(c_{-w}^{+}-c^{+}+1\right),
\end{aligned}
$$

$$
\begin{gathered}
\Delta_{-w}^{\mathrm{DR}}=\Delta_{w}^{\mathrm{DR}}-\sum_{i=-w}^{w} \sum_{j=c^{-}-1}^{c_{-w}^{-}}\left[(w-i)+\left(c^{-}-j\right)\right] \\
-\left[D_{w}-D_{-w}\right] \cdot\left(c^{-}-c_{-w}^{-}+1\right) .
\end{gathered}
$$

The parameters $\Delta_{-w}^{\mathrm{UL}}$ and $\Delta_{-w}^{\mathrm{DL}}$ can be computed analogously and the cost function is initialized as follows:

$$
\operatorname{cost}(0, c, 0,0,0,0,0,0)= \begin{cases}\frac{c^{3}-c}{6}, & \text { if } 0 \leq c \leq 2 \sqrt{n}+5 \\ \infty, & \text { otherwise }\end{cases}
$$

The bound on $c$ has been shown in Lemma 5.
Theorem 7. An optimal n-town can be computed by dynamic programming in $O\left(n^{15 / 2}\right)$ time.

Proof. We have to fill an eight-dimensional array $\operatorname{cost}\left(w, c, \Delta^{\mathrm{UR}}, \Delta^{\mathrm{DR}}, \Delta^{\mathrm{UL}}\right.$, $\left.\Delta^{\mathrm{DL}}, U, D\right)$. Let $C_{\text {max }}$ denote the maximum number of occupied rows and columns in an optimum solution. By Lemma 5 , we know that $C_{\max }=O(\sqrt{n})$.

The indices $w$ and $c$ range over an interval of size $C_{\max }=O(\sqrt{n})$. Let us consider a solution for some fixed $w$ and $c$. The parameters $U$ and $D$ range between 0 and $n$. However, we can restrict the difference between $U$ and $D$ that we have to consider: If we reflect the rectangle $R=[-w, w] \times\left[c^{-}, c^{+}\right]$ about its horizontal symmetry axis, the $U$ points above $R$ and the $D$ points below $R$ will not match exactly, but in each column, they differ by at most one point, according to Lemma 3. It follows that $|U-D| \leq C_{\max }=O(\sqrt{n})$. (If the difference is larger, such a solution can never lead to an optimal $n$ town, and hence we need not explore those choices.) In total, we have to consider only $O(n \cdot \sqrt{n})=O\left(n^{3 / 2}\right)$ pairs $(U, D)$.

The same argument helps to reduce the number of quadruples ( $\Delta^{\mathrm{UL}}, \Delta^{\mathrm{UR}}$, $\left.\Delta^{\mathrm{DL}}, \Delta^{\mathrm{DR}}\right)$. Each $\Delta$-variable can range between 0 and $n \cdot 2 C_{\max }=O\left(n^{3 / 2}\right)$. However, when reflecting around the horizontal symmetry axis of $R$, each of the at most $D_{\max }$ differing points contributes at most $2 C_{\max }=O(\sqrt{n})$ to the difference between the distance sums $\Delta^{\mathrm{UL}}$ and $\Delta^{\mathrm{DL}}$. Thus we have $\left|\Delta^{\mathrm{UL}}-\Delta^{\mathrm{DL}}\right| \leq C_{\max } \cdot 2 C_{\text {max }}=O(n)$, and similarly, $\left|\Delta^{\mathrm{UR}}-\Delta^{\mathrm{DR}}\right|=O(n)$.

By a similar argument, reflecting about the vertical symmetry axis of $R$, we conclude that $\left|\Delta^{\mathrm{UL}}-\Delta^{\mathrm{UR}}\right|=O(n)$ and $\left|\Delta^{\mathrm{DL}}-\Delta^{\mathrm{DR}}\right|=O(n)$. In
summary, the total number of quadruples ( $\Delta^{\mathrm{UL}}, \Delta^{\mathrm{UR}}, \Delta^{\mathrm{DL}}, \Delta^{\mathrm{DR}}$ ) that the algorithm has to consider is $O\left(n^{3 / 2}\right) \cdot O(n) \cdot O(n) \cdot O(n)=O\left(n^{9 / 2}\right)$. In total, the algorithm processes $O(\sqrt{n}) \cdot O(\sqrt{n}) \cdot O\left(n^{3 / 2}\right) \cdot O\left(n^{9 / 2}\right)=O\left(n^{7}\right) 8$-tuples. For each 8 -tuple, the recursion (3) has to consider at most $C_{\max }=O(\sqrt{n})$ values $c_{-w}$, for a total running time of $O\left(n^{15 / 2}\right)$.

## 4. $n$-Towns, Cities, and $n$-Block Cities

For large values of $n, n$-towns converge towards the continuous weight distributions of cities. However, the arrangement of buildings in many cities are discretized in a different sense: An $n$-block city is the union of $n$ axisaligned unit squares ("city blocks"), see Figure 3 below. In the following, we discuss $n$-block cities, and we discuss the relation between $n$-towns and $n$-block cities.

For a planar region $R$, let $c^{\prime}(R)$ be the integral of Manhattan distances between all point pairs in $R$ :

$$
c^{\prime}(R):=\int_{p \in R} \int_{q \in R}\|p-q\| d p d q
$$

When $R$ has area 1 , this is the expected distance between two random points in $R$. Scaling a shape $R$ by a factor of $d$ increases the total cost by a factor of $d^{5}$, i.e., by a factor of $A^{2.5}$ for an area of $A$. This motivated Bender et al. (2004) to use the expression $D(R):=\frac{c^{\prime}(R)}{A(R)^{2.5}}$ as a scale-independent measure for the quality of the shape of a city. For example, a square $Q$ of any side length $a$ gets the same value

$$
D(Q)=\frac{1}{a^{5}}\left(a^{2} \cdot \int_{0}^{a} \int_{0}^{a}\left|x_{1}-x_{2}\right| d x_{2} d x_{1}+a^{2} \cdot \int_{0}^{a} \int_{0}^{a}\left|y_{1}-y_{2}\right| d y_{2} d y_{1}\right)=\frac{2}{3}
$$

A circle $C$ yields $D(C)=\frac{512}{45 \pi^{2.5}} \approx 0.6504$ and the optimal shape achieves a value of $\psi=0.650245952951 \ldots$

We will consider $n$-block cities $Q(S)$ consisting of unit squares ("blocks") centered at a set of $n$ grid points $S \subset \mathbb{Z} \times \mathbb{Z}$. We denote a unit square centered at point $s=\left(s_{x}, s_{y}\right)$ by $Q(s)=\left[s_{x}-\frac{1}{2}, s_{x}+\frac{1}{2}\right] \times\left[s_{y}-\frac{1}{2}, s_{y}+\frac{1}{2}\right]$, and then we have

$$
Q(S):=\bigcup_{s \in S} Q(s)
$$

The average distance $D(Q(S))$ of an $n$-block city can be decomposed into average distances between blocks:

$$
c^{\prime}(Q(S))=\int_{p \in Q(S)} \int_{q \in Q(S)}\|p-q\|_{1} d p d q=\sum_{s \in S} \sum_{t \in S} \int_{p \in Q(s)} \int_{q \in Q(t)}\|p-q\|_{1} d p d q
$$

Using the notation

$$
d^{\prime}(s):=\int_{p \in Q(s)} \int_{q \in Q(0)}\|p-q\|_{1} d p d q,
$$

we can express this as

$$
\begin{equation*}
c^{\prime}(Q(S))=\sum_{s \in S} \sum_{t \in S} d^{\prime}(s-t) . \tag{4}
\end{equation*}
$$

The average distance $d^{\prime}(s)$ between two square blocks at an offset $s$ can be expressed as follows: If the two blocks do not lie in the same row or column ( $s_{x} \neq 0$ and $s_{y} \neq 0$ ), the average distance is simply the distance $\|s\|_{1}$ between the centers, since positive and negative deviations from the block centers average out. When two blocks lie in the same column, then the $y$ distances average out to the $y$-distance between the centers, but the average $x$-distance is not the $x$-distance between the centers (which would be 0 ), but $\int_{-1 / 2}^{+1 / 2} \int_{-1 / 2}^{+1 / 2}\left|x_{1}-x_{2}\right| d x_{2} d x_{1}=\frac{1}{3}$. Similarly, for two blocks in the same row, we must add $\frac{1}{3}$ to the distance $\|s\|_{1}$ between the centers. Finally, for two identical blocks, we have already seen that the average distance is $\frac{2}{3}$. We can express this compactly as

$$
\begin{aligned}
d^{\prime}(s)=d^{\prime}\left(\left(s_{x}, s_{y}\right)\right) & =\left|s_{x}\right|+\frac{1}{3}\left[s_{x} \neq 0\right]+\left|s_{y}\right|+\frac{1}{3}\left[s_{y} \neq 0\right] \\
& =\|s\|_{1}+\frac{1}{3}\left[s_{x} \neq 0\right]+\frac{1}{3}\left[s_{y} \neq 0\right],
\end{aligned}
$$

where the notation $\left[s_{x} \neq 0\right]$ is 1 if the predicate $s_{x} \neq 0$ holds and 0 otherwise. With these conventions, the expression (4) for the cost $c^{\prime}(Q(S))$ of an $n$-block city $Q(S)$ looks very similar to (1) for the cost $c(S)$ of a town $S$, except for the correction terms $\frac{1}{3}$ in the summands and for the factor $\frac{1}{2}$. The factor $\frac{1}{2}$ accounts for the fact that in the sum $c(S)$ of a town, each pair of (distinct) points is counted once, whereas in the integral $c^{\prime}(R)$, each pair of points is considered twice, as two ordered pairs. To make these expressions better comparable, we introduce the factor $\frac{1}{2}$ and define

$$
c_{\mathrm{city}}(S):=\frac{1}{2} \cdot c^{\prime}(Q(S))=\frac{1}{2} \cdot \sum_{s \in S} \sum_{t \in S} d^{\prime}(s-t)
$$

The new "distance" $d^{\prime}$ is not a norm (for example, $d^{\prime}(0) \neq 0$ ), but the properties from Section 2 remain true for this new objective function. Thus, the dynamic programming formulation of Section 3 can be adapted to compute optimal $n$-block cities. As we shall now demonstrate, all lemmas of Section 2 hold verbatim for $n$-block cities, except that the formula for the change incurred by moving a single block to a different place (Lemma 1) must be adapted:

Lemma $\mathbf{1}^{\prime}$. Let $S \subset \mathbb{Z}^{2}$ be the set of centers of an $n$-block city, $t \in S$ and $r \notin S$. Then,

$$
c_{\mathrm{city}}((S \backslash t) \cup r)=c_{\mathrm{city}}(S)-c_{\mathrm{city}}(t, S)+c_{\mathrm{city}}(r, S)-d^{\prime}(r-t),
$$

where $c_{\text {city }}(p, S):=\sum_{q \in S} d^{\prime}(p-q)$.
The proof is the same as for Lemma 1. One can easily check that the distance $d^{\prime}$ from $t$ to itself and the distance from $r$ to itself are correctly accounted for.

Convexity of the optimum solution (Lemma 2) holds true for $n$-block cities. The proof goes through almost verbatim. The expression $d^{\prime}(p)$ is not a norm, but it is a convex function of $p$, and this is all that is needed. Approximate symmetry of the optimal solution (Lemma 3) remains true. The calculations (which have not been shown in detail anyway), are modified, but the conclusion is the same.

When comparing an $n$-town $S$ and a corresponding $n$-block city $Q(S)$, we have to add $1 / 6$ for each pair of blocks that are in the same column, and for each pair of blocks that are in the same row. Using the notation $r_{j}$ and $c_{i}$ of Section 3 for row and column lengths, and writing $c_{\text {town }}(S)$ instead of $c(S)$ for improved clarity, we get thus:

$$
\begin{equation*}
c_{\text {city }}(S)-c_{\text {town }}(S)=\Lambda(S):=\frac{1}{6}\left(\sum_{i} c_{i}^{2}+\sum_{j} r_{j}^{2}\right) \tag{5}
\end{equation*}
$$

This adjustment term accounts for the discretization effect. E.g., a 1-town has an average distance of 0 , as all the weight is concentrated in a single point, while a 1 -block city has an average distance of $2 / 3$, just like any other square, (and a $c_{\text {city }}$ value of $1 / 3$ ).

Using this expression, it is easy to show that the bound of 2 on the aspect ratio holds for $n$-block cities in the same form as in Lemma 4. The proof of Lemma 4 establishes that $c_{\text {town }}(S)$ decreases when a top-most point $t$ from
the longest column of height $h$ is added to the right of the longest row of length $w$. For an $n$-block city, the adjustment term $\Lambda(S)$ decreases by at least $h^{2}-(h-1)^{2}$ when $t$ is removed, and it increases by $(w+1)^{2}-w^{2}+1^{2}$ when $r$ is added. Under the assumption of the proof $(w \leq h / 2-3)$, the total change of $\Lambda$ is negative, and the modified solution is an improvement also when $S$ is regarded as an $n$-block city.

From Lemma 4 we conclude that the bound of $2 \sqrt{n}+5$ on the height and width of optimal $n$-block cities (Lemma 5) holds as well. (The argument of the proof of Lemma 5 is purely geometric: it is based on convexity and does not use the objective function.)

Thus, we conclude that the adjustment term (5) is asymptotically bounded by $\Lambda(S)=\Theta\left(n^{1.5}\right)$.

When considering the continuous weight distributions of $n$-block cities, we have to account twice for each pair of discrete block centers; hence, the appropriate measure for the quality of an $n$-town is $\Phi(S)=2 c(S) / n^{2.5}$. The measure for the corresponding $n$-block city is $\Psi(S)=2\left(c_{\text {town }}(S)+\Lambda(S)\right) / n^{2.5}$. Thus, the relative difference is $\Theta\left(\frac{1}{n}\right)$.

In Figure 3, we show the corresponding values for the small examples from Figure 1. Figure 5 shows results for some larger values $n$. One can observe how $\Phi(S)$ and $\Psi(S)$ converge from below and above towards the optimal city value $\psi$ of about 0.650245952 951. Note that convergence is not monotone, neither for $\Phi$ nor for $\Psi$.

## 5. Computational Results

Optimal $n$-towns and optimal $n$-block cities do not necessarily have the same shape. For $n \leq 21$, a comparison of Figures 1 and 3 shows that, while not all optimal $n$-towns are optimal $n$-block cities, every optimal $n$-block city is simultaneously an optimal $n$-town. However, this is not always true. In fact, for $n=72$, there are two shapes for optimal $n$-block cities, none of which is optimal for an $n$-town, see Figure 4 . This is the only instance of this phenomenon up to $n=80$, but we surmise it will be more and more frequent for larger $n$. We have more comments on this phenomenon at the end of this section.

We have calculated the optimal costs $c_{\text {town }}$ and $c_{\text {city }}$ up to $n=80$ points. The results are shown in Table 1. When there are several optimal solutions (except symmetries), this is indicated by a star, together with the multiplicity.

| $n$ | $c_{\text {town }} \quad E_{1}$ | $c_{\text {city }} \quad 3 E_{2}$ | $E_{3}$ | $n$ | $c_{\text {town }} \quad E_{1}$ | $c_{\text {city }} \quad 3 E_{2}$ | $E_{3}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0 | $0^{1 / 3} 30$ | 1 | 41 | 3446 | $3530{ }^{1 / 3} 3$ | 1 |
| 2 | 1 | 20 | 1 | 42 | 3662 | 3749 3 | 0 |
| 3 | $4^{*(2)} 0$ | $5^{2 / 3} \quad 1$ | 1 | 43 | 3886 2 | 3976 - 5 | 0 |
| 4 | 80 | $10^{2 / 3}-1$ | 1 | 44 | $4112-3$ | $4205^{1 / 3} 3-10$ | 0 |
| 5 | $16^{*(2)} 1$ | $19^{2 / 3} 3^{*(2)} 1$ | 1 | 45 | 4360*(2) 6 | $4456{ }^{2} / 3 \quad 17$ | 1 |
| 6 |  | $30-1$ | 1 | 46 | $4612{ }^{*(2)} 10$ | $4712 * * 2{ }^{* 2)} 31$ | 1 |
| 7 | 38 |  | 1 | 47 | $4868 *{ }^{(2)} 11$ | $4970{ }^{1 / 3} 3^{*(2)} 29$ | -2 |
| 8 | $54^{*(2)} 0$ | $61^{1 / 3}{ }^{*(2)} 0$ | 1 | 48 | 5128 | 523418 | -1 |
| 9 | $72-1$ | $81-3$ | 2 | 49 | 5398 4 | $5507{ }^{1 / 3} 311$ | -1 |
| 10 | $96 \quad 0$ | $106^{1 / 3} 30$ | 1 | 50 | 5675 | 5788 0 | 0 |
| 11 | $124 * *$ | $135{ }^{2} / 3^{*(2)} 3$ | 0 | 51 | $5960-4$ | $6076{ }^{1 / 3} 3-13$ | 0 |
| 12 | $152-1$ | $165^{1 / 3} 3-4$ | 1 | 52 | 6248 -14 | $6368-43$ | 1 |
| 13 | 1880 | $203-1$ | 1 | 53 | 6568 -1 | 6691 ²/3 3 -4 | 1 |
| 14 | 227 0 | $244-1$ | 1 | 54 | 6890 5 | $7017{ }^{1 / 3} 315$ | 2 |
| 15 | $272^{*(2)} 1$ | $290{ }^{2} / 3 \quad 3$ | 1 | 55 | $7222^{*(2)} 12$ | $7352^{1 / 3} 3$ 35 | 0 |
| 16 | 318 -1 | $338{ }^{2 / 3}-4$ | 1 | 56 | $7556{ }^{*(2)} 13$ | 7690 36 | 0 |
| 17 | $374 *$ *2) 1 | $396{ }^{1 / 3} 3$ | 0 | 57 | 789610 | $8033{ }^{2} / 3 \quad 28$ | 0 |
| 18 | $433 *$ *2) 2 | $4571 / 3$ | 0 | 58 | 8243 | $8384{ }^{2} / 314$ | 1 |
| 19 | $496{ }^{*(2)} 2$ | $522^{1 / 3}$ | 0 | 59 | 8604 4 | $8749^{1 / 3} 313$ | 1 |
| 20 | 563 0 | $5912 / 3$ 0 | 1 | 60 | 8968 -2 | $9117^{1 / 3} 3-6$ | 2 |
| 21 | $632-5$ | $663-15$ | 1 | 61 | 9354 3 | $9506{ }^{1 / 3} 3$ | 0 |
| 22 | 7160 | $749^{1 / 3} 3-1$ | 1 | 62 | 9749*(2) 9 | $9904{ }^{2} / 3^{*(2)} 24$ | -1 |
| 23 | $804^{*(2)} 2$ | $839^{1 / 3} 36$ | 1 | 63 | 10146 | $10305^{1 / 3} 3 \quad 17$ | -2 |
| 24 | 895 | 933 7 | 2 | 64 | 105568 | $10719^{1 / 3} 3 \quad 21$ | -1 |
| 25 | 992 2 | $1032^{1 / 3} 36$ | 1 | 65 | 10972 | $11139{ }^{2} / 3 \quad 15$ | 0 |
| 26 | 1091 -2 | $1134-5$ | 2 | 66 | 11400 5 | $115711^{2 / 3} \quad 14$ | 1 |
| 27 | 12042 | 1249 4 | 1 | 67 | $11836{ }^{*(2)} 3$ | $12011{ }^{2} / 3 \quad 7$ | 1 |
| 28 | 1318 | $1365{ }^{1 / 3} 3-1$ | 0 | 68 | $12280-2$ | $12460-4$ | 2 |
| 29 | 1442 | 1492 | 1 | 69 | $12728-12$ | $12912^{1 / 3} 3-34$ | 3 |
| 30 | 1570 | $1622^{2} / 3 \quad 4$ | 1 | 70 | 13209 | $13396{ }^{2} / 3 \quad 2$ | 1 |
| 31 | 1704 | 1759 ²/3 | 2 | 71 | $13700^{*(3)} 13$ | 13891 | -1 |
| 32 | $1840-6$ | 1898 $2 / 3-16$ | 3 | 72 | 1419317 | $14388 * *(2) 49$ | -1 |
| 33 | 1996 | 2057 | 2 | 73 | 1469015 | 14888 40 | -4 |
| 34 | 2153 | $2216{ }^{2} / 3 \quad 8$ | 1 | 74 | 1519511 | $15397^{1 / 3} 3 \quad 27$ | -4 |
| 35 | 2318 | 238412 | 0 | 75 | 15712 8 | $15918{ }^{1 / 3} 317$ | -4 |
| 36 | 2486 | $2554{ }^{2} / 36$ | -1 | 76 | $16232-3$ | $16442^{2} / 3-14$ | -4 |
| 37 | $2656-5$ | $2727^{2 / 3}-16$ | -1 | 77 | 16780 4 | 16995 7 | -3 |
| 38 | 2847 | $2921{ }^{2} / 3 \quad 3$ | 0 | 78 | $17335 \quad 7$ | $17554{ }^{2} / 3 \quad 18$ | -2 |
| 39 | 30402 | $3117{ }^{2} / 3 \quad 5$ | 0 | 79 | $17904 * *(2)$ | 18128 37 | -2 |
| 40 | 32413 | 33229 | 1 | 80 | 1847814 | $18706^{2} / 3 \quad 40$ | 0 |

Table 1: Optimal towns $c_{\text {town }}$ and $n$-block cities $c_{\text {city }} .{ }^{*}$ indicates multiple solutions.


Figure 3: Values of $\Phi$ and $\Psi$ for optimal $n$-block cities for $n=2, \ldots, 21$. All optimal solutions are shown, up to symmetries. These are simultaneously shapes of optimal $n$ towns, but for $n=3,11,15,17,18,19$, there are additional $n$-towns that are tied for the optimum (with the same value $\Psi$ ), cf. Figure 1.

It is clear that an optimal $n$-block city is never better than an optimal continuous city of area $n$ that has a value $\psi n^{5 / 2} / 2$. Empirically we found the approximation $c_{\text {city }} \approx \psi n^{5 / 2} / 2+0.115 \cdot n^{3 / 2}$ with $\psi=0.650245952951$. The order of magnitude of the "discretization penalty" $0.115 \cdot n^{3 / 2}=\Theta\left(n^{3 / 2}\right)$ is explained as follows: changing the continuous city of area $n$ into blocks affects $\Theta(\sqrt{n})$ squares along the boundary. For each adjustment in one of these squares, distances to $n$ other squares are affected.

Since $c_{\text {city }}$ is a multiple of $1 / 3$, we rounded our estimate to the nearest multiple of $1 / 3$ and used the approximation formula

$$
\bar{c}_{\text {city }}:=\left\lfloor 3 \psi n^{5 / 2} / 2+0.345 \cdot n^{3 / 2}\right\rceil / 3
$$

The notation $\lfloor\cdot\rceil$ denotes rounding to the nearest integer. Table 1 shows the error $E_{2}:=c_{\text {city }}-\bar{c}_{\text {city }}$ of this approximation. (Actually, the table shows $3 E_{2}$, which is an integer.)


Figure 4: The optimal $n$-town and the two optimal $n$-block cities for $n=72$.

For $n$-towns, on the other hand, we found the approximation $c_{\text {town }} \approx$ $\psi n^{5 / 2} / 2-0.205 \cdot n^{3 / 2}$. So this seems to approximate the optimal continuous city from below, but we do not have a proof of this fact.

The deviation $E_{1}$ between $c_{\text {town }}$ and its approximation formula

$$
\bar{c}_{\text {town }}:=\left\lfloor\psi n^{5 / 2} / 2-0.205 \cdot n^{3 / 2}\right\rceil
$$

is shown in Table 1.
Finally, we look at the difference between $c_{\text {city }}$ and $c_{\text {town }}$. For a given point set $S$, it is the quantity $\Lambda$ defined in (5). It is estimated as $0.32 \cdot n^{3 / 2}$. The table shows the error $E_{3}:=3 \cdot\left(c_{\text {city }}-c_{\text {town }}\right)-\left\lfloor 0.96 \cdot n^{3 / 2}\right\rceil$. Apart from the rounding, $E_{3}$ would equal $3\left(E_{2}-E_{1}\right)$.

One can see that the error $E_{3}$ is much smaller than one might expect from the random-looking fluctuations of $E_{1}$ and $E_{2}$. This can explained by the fact that the expression (5) for $\Lambda(S)$ is apparently not so sensitive to small deviations of the shape $S$.

Accordingly, Table 1 exhibits the tendency that the deviations of $c_{\text {town }}$ and $c_{\text {city }}$ "above" and "below average" occur for the same values of $n$ : $n$-towns and $n$-block cities with the same number $n$ suffer equally from the effects of discretization. A glance at the optimal solutions (Figures 1 and 3) shows that the costs are below average when the shapes are highly symmetric, for example $n=9,12,21$, but also $n=60$ (Figure 5). On the other hand, when there is no unique "very good" shape, one can expect a greater variation of different solutions that try to come close to the optimal continuous shape. Indeed, larger values of $E_{1}$ and $E_{2}$ in Table 1 tend to go hand in hand with a greater multiplicity of optimal solutions. The worst values of $E_{1}$ and $E_{2}$ occur for $n=72$; this is the first value of $n$ where optimal $n$-block cities and optimal $n$-towns differ (Figure 4). This is probably no coincidence: when

| - • | -•• | -••• |
| :---: | :---: | :---: |
|  | -••••• | -•••• |
| -•••• | - • | -••••••• |
|  |  |  |
| - . . . . - | - . • • • • | - •••••• |
| -••••••• | - | - |
|  |  |  |
| $n=58, c(S)=8243$ | $n=59, c(S)=8604$ | $n=60, c(S)=8968$ |
| $\Phi=0.6434$ | $\Phi=0.6436$ | $\Phi=0.6432$ |
| $\Psi=0.6546$ | $\Psi=0.6545$ | $\Psi=0.6539$ |

Figure 5: Optimal $n$-towns for $n=58,59,60$; these are simultaneously the shapes of the optimal $n$-block cities.
there is a greater variety of solutions that can compete for being best, the distinction of the objective function between $n$-block cities and $n$-towns is more likely to make a difference.

## 6. Outlook

We have shown that optimal $n$-towns can be computed in time $O\left(n^{7.5}\right)$. This is of both theoretical and practical interest, as it yields a method polynomial in $n$ that also allows extending the limits of the best known solutions; however, there are still some ways how the result could be improved.

Strictly speaking, the method is only pseudo-polynomial, as the input size is $O(\log n)$. It is not clear how the corresponding output could be described in polylogarithmic space; any compact encoding would lead to a good and compact approximation of the optimal (continuous) city curve, for which there is only a description by a differential equation with no known closedform solution. For this reason we are sceptical that a polynomial solution is possible.

We are more optimistic about lowering the number of parameters in our dynamic program, and thus the exponent, by exploiting convexity or stronger symmetry properties. This may also make it possible to compute optimal solutions for larger $n$. One possible avenue could arise if partial solutions would satisfy some monotonicity property; however, the unique optimal 9town is not contained in the unique optimal 12 -town. Thus, there is no way
for a town to organically grow and remain optimal at all times. Generally, an optimal $n$-town does not necessarily contain an optimal $(n-1)$-town. (The smallest example occurs for $n=35$, no optimal 35 -town contains an optimal 34-town.)

As discussed in the last section, there is still a variety of questions regarding the convergence of optimal solutions for growing $n$, approaching the continuous solution in the limit. As indicated, we have a pretty good idea how this continuous value is approximated from below and above by $n$-towns and $n$-block cities; however, we do not have a formal proof of the lower bound property of $n$-block cities.

It is easy to come up with good and fast approximation methods: In the continuous case, even a square is within $2.5 \%$ of the optimal shape; a circle reaches $0.02 \%$; consequently, simple greedy heuristics will do very well. Two possible choices are iteratively adding points to minimize the total cost, or (even faster) as close as possible to a chosen center.

As mentioned in the introduction, a closely related, but harder problem arises when $n$ locations are to be chosen from a given set of $k>n$ points, instead of the full integer grid. This was studied by Bender et al. (2008), who gave a PTAS, but were unable to decide the complexity. It is conceivable that a refined dynamic-programming approach may yield a polynomial solution; however, details can expected to be more involved, so we leave this for future work. The same holds for other metrics.

Finally, one can consider the problem in higher dimensions. A crucial property of our dynamic-programming solution is that the interface between the points in the columns that have already been constructed and the points to be added in the future can be characterized by a few parameters. A similar property does not hold in three dimensions, and therefore one cannot extend our dynamic-programming approach to higher dimensions. For the same reason, the Euclidean distance version cannot be solved by our method, since, unlike in the Manhattan case, the effect of the $U_{w}$ points on the upper side of the current rectangle on the distance to points that are inserted in the future cannot be summarized in the parameters $\Delta^{\mathrm{UR}}$ and $\Delta^{\mathrm{UL}}$. Moreover, in higher dimensions, there is no known solution for the continuous case; the corresponding calculus-of-variations problem will be harder to solve than in two dimensions.

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```
n_target = 40 # run up to this value of n
cost_array = {} # initialize data for "array"
from math import sqrt
width_limit = int(2*sqrt(n_target)+5)
for w in range(0,width_limit+2):
    for cc in range(width_limit,0,-1):
        cost_array [w,cc]={}
MAX = n_target**3 # "infinity", trivial upper bound on cost
opt = (n_target+1)*[MAX] # initialize array for optimal values
cost_array[0,width_limit][0,0,0,0,0,0]=0 # starting "town" with no columns
for w in range(0,width_limit+1):
    for cc in range(width_limit,0,-1):
        for (D_up_right, D_down_right, D_up_left, D_down_left,
            n_up, n_down), cost in cost_array[w,cc].items():
        D_up_left += n_up # add 1 horizontal unit to all left-distances
        D_down_left += n_down
        for c in range(cc,-1,-1): # decrease size c of new column one by one
            n = n_up+n_down + (w+1)*c # (w = previous value of w)
                if n <= n_target: # total number of occupied points so far
                    new_cost = cost + ( (D_up_left + D_down_left) * c +
                                    (n_up + n_down) * c*(c-1)/2 +
                                    (c+1)*c*(c-1)/6 * (2*W+1) +
                                    c*c * w*(w+1)/2 )
                    if c==0: # a completed town
                        opt[n] = min( new_cost, opt[n] )
                        else: # store cost of newly constructed partial town
                        ind = (D_up_left, D_down_left, D_up_right, D_down_right,
                            n_up, n_down) # exchange left and right when storing
                        cost_array[w+1, c] [ind] = min ( new_cost,
                        cost_array[w+1, c].get(ind, MAX) )
                # decrease c by 1:
                if (c%2)==1: # remove an element from the top of the leftmost column
                    n_up += w
                    D_up_left += n_up + w*(w+1)/2
                    D_up_right += n_up + w*(w-1)/2
                else: # remove from the bottom
                        n_down += w
                        D_down_left += n_down + w*(w+1)/2
                        D_down_right += n_down + w*(w-1)/2
for n in range(1,n_target+1): print n, opt[n]
```

Figure .6: Python program for computing optimal $n$-towns

## Appendix A. Program for Computing Optimal Towns

Figure .6 shows a short program in the programming language Python that implements our algorithm. The program calculates and prints the costs of optimal $n$-towns for all values of $n$ up to the specified limit $n=\mathrm{n}_{-}$target. Instead of an 8-dimensional array, the costs are stored as a dictionary in the variable cost_array [w, cc] [D_up_right, D_down_right, D_up_left, D_down_left, n_up, n_down]. This makes the program a lot simpler, since we do not have to worry about allocating arrays with explicit limits, and incurs little overhead, since internally, Python dictionaries are implemented as hash tables, providing constant expected access time.

Instead of adding rows alternately on the left and on the right, the program always adds a new row on the left side, but (implicitly) reflects the town about the $y$-axis when storing a cost value, achieving the same effect.

The main loop of the program does not use the recursion in the form (3), which calculates the optimum cost of a configuration from all partial solution that lead to it when a column is added. Instead, it makes a "forward" transfer, generating all successor configurations of a given configuration. This has the advantage that certain "impossible" parameter sets are automatically excluded. For example, in the running time analysis for Theorem 7, we argued that parameter pairs $U, D$ with $|U-D|>C_{\max }$ need not be considered. (The parameters $U$ and $D$ correspond to the variables n_up and $\left.n_{-} d o w n.\right)$ Since the program only adds columns which are (approximately) balanced about the $x$-axis, it will never generate solutions with such parameters.

The program can be adapted for computing optimal $n$-block cities. Then the additional cost $\Lambda$ from (5) between blocks in the same row or column must be taken into account. One simply has to extend the last line in the computation of new_cost:

```
c*c * w*(w+1)/2 )
```

to

```
c*c * w*(w+1)/2 ) * 6 + c*c + (cc-c)*w*w
```

The resulting cost is scaled by a factor of 6 , but the end result is then always even, so we could divide it by 2 (cf. Table 1: all values $c_{\text {city }}(n)$ are multiples of $1 / 3$ ).

For $n=40$, the program takes a few seconds, but for $n=80$ it takes hours. For larger $n$ the space becomes a more severe bottleneck than the running
time; thus it is important to release storage when it is no longer needed, for example by resetting cost_array $[\mathrm{w}, \mathrm{cc}]=\{ \}$ after each outer loop. There are several possibilities to speed up the program. The cost of some approximately circular solution can be taken as an initial upper bound. With this upper bound, one can then derive a stronger bound width_limit on the maximum height and width by ad-hoc methods. During the calculation, one can also prune cost values that are so large that they cannot possibly lead to a better solution. The given program computes only the optimum cost. We have extended it to also remember the optimal solutions. This program has 133 lines and was used to produce the data of Table 1.

