

Squared Nearest-Neighbor Distances in the Unit Square

Let $p_1, \dots, p_n$ be labelled points in $U=[0,1]^2$; coincidences are allowed. Define $r_i = \min_{j \neq i} |p_i - p_j|$ and $S = \sum r_i^2$. Put $R = \max r_i$.

We use Pinelis's rectangle theorem: if a finite set of points lies in an $a \times b$ rectangle, then the sum of its squared nearest-neighbor distances is at most $2a^2 + 2b^2$. For labelled points with coincidences the same upper bound remains valid.

1. A very simple bound below 4

Theorem 1. For every $n \geq 5$,

$$S \leq 15/4 = 3.75 < 4.$$

1.1. Crude small-R disk estimate

For each i draw the closed disk D_i centered at p_i with radius $r_i/2$. The interiors of these disks are pairwise disjoint.

Every D_i lies in the $R/2$ -neighborhood of U , whose area is $1 + 2R + (\pi/4)R^2$. Hence

$$(\pi/4)S \leq 1 + 2R + (\pi/4)R^2, \text{ so } S \leq 4/\pi + 8R/\pi + R^2.$$

The right side is increasing. Therefore, if $R \leq 1/\sqrt{2}$,

$$S \leq 1/2 + 4(1 + \sqrt{2})/\pi = 3.573872177... < 15/4.$$

1.2. An easy adjacent-quarter lemma

Lemma 1. Let A be a nonempty collection of labelled points in one quarter-square, and let q lie in an adjacent quarter-square. If $\Sigma(A)$ denotes the sum of squared nearest-neighbor distances computed inside A , then

$$\Sigma(A) + \text{dist}(q, A)^2 \leq 7/4.$$

Proof. Scale lengths by 2. It is enough to prove the bound 7 in the 2×1 picture.

Move q horizontally to the right edge, so $q=(2,v)$. Translate A horizontally left until the left edge of its minimal bounding rectangle is $x=0$. Write this rectangle as $[0,x] \times [\gamma, \delta]$, with height $h \leq 1$.

Pinelis gives $\Sigma(A) \leq 2x^2 + 2h^2$. There is a point of A on the right side of the bounding rectangle. Its horizontal distance from q is $2-x$, and its vertical distance is at most 1. Hence

$$\text{dist}(q, A)^2 \leq (2-x)^2 + 1.$$

$$\text{Thus } \Sigma(A) + \text{dist}(q, A)^2 \leq 2x^2 + 2 + (2-x)^2 + 1 = 3x^2 - 4x + 7.$$

This quadratic is convex on $0 \leq x \leq 1$, so its maximum is at an endpoint. The endpoint values are 7 and 6. Therefore the scaled bound is 7, and scaling back gives $7/4$. QED.

1.3. Large-R estimate for Theorem 1

Assume $R > 1/\sqrt{2}$, choose q with $r_q = R$, and divide U into four quarter-squares. The quarter containing q is a singleton because a quarter-square has diameter $1/\sqrt{2}$. Any quarter containing at least two points contributes at most 1 internally by Pinelis.

If all three other quarters are nonsingletons, pair q with either adjacent quarter and use Lemma 1; the other two quarters contribute at most 1 each. Thus $S \leq 7/4 + 2 = 15/4$.

If exactly two other quarters are nonsingletons and the third is a singleton, pair the two singletons with the two nonsingleton quarters, giving $S \leq 2(7/4)=7/2$. If the third is empty, $S \leq 7/4+1=11/4$.

If exactly one other quarter is nonsingleton, Pinelis's Case 4/5 estimate gives $S \leq 3$. Combining these bounds with Section 1.1 proves Theorem 1.

2. A sharper disk-covering estimate

We now improve the small- R part by estimating more carefully how much the pairwise disjoint disks can cover outside U . Put $a=R/2$.

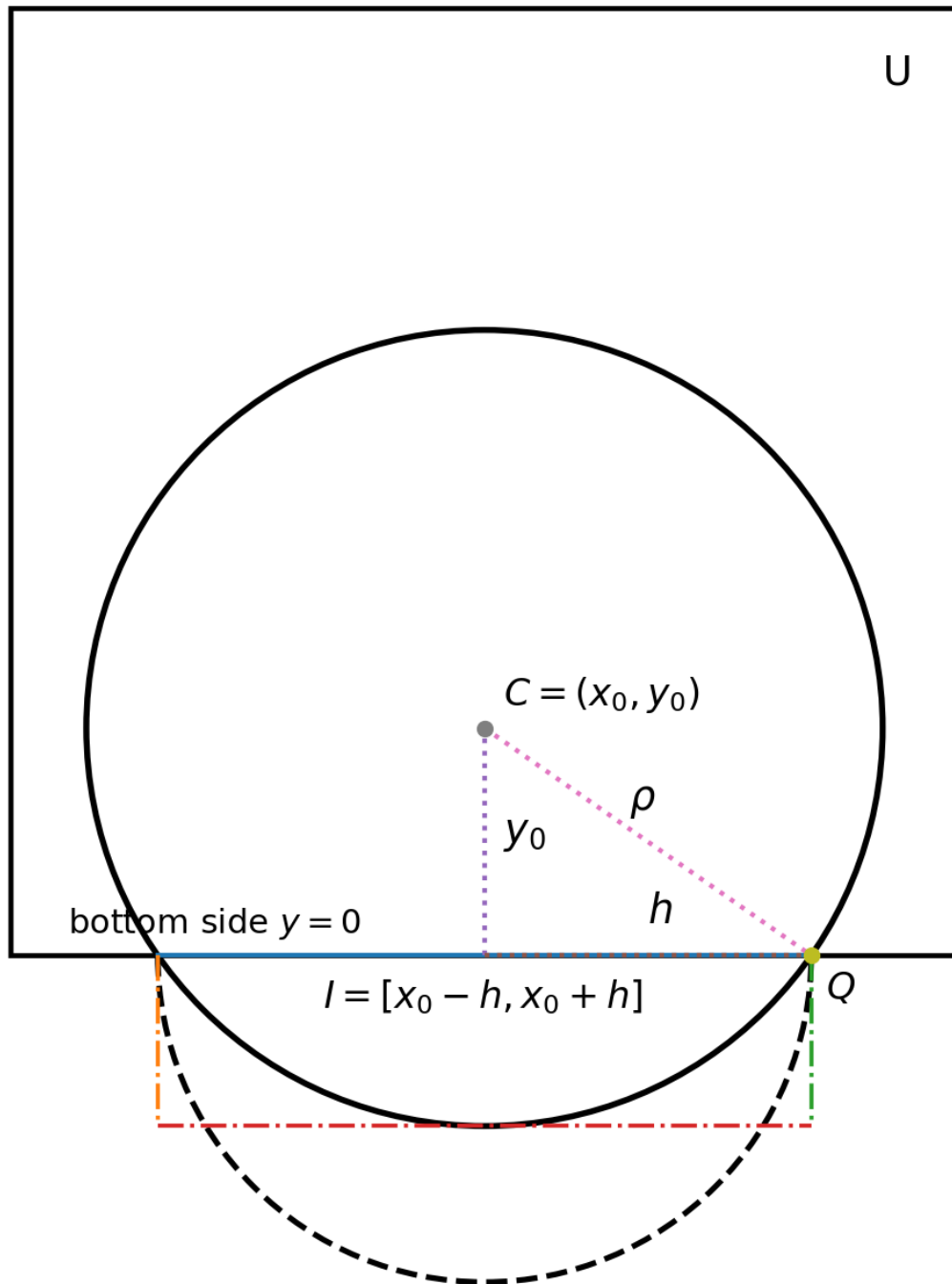
2.1. A cap below one side

Lemma 2. Let D be a disk of radius ρ centered at (x_0, y_0) , with $y_0 \geq 0$, and suppose D extends below $y=0$. Put $h = \sqrt{\rho^2 - y_0^2}$. Then the portion of D below $y=0$ has area at most

$$\min\{ (\pi/2)h^2, 2h(\rho - y_0) \}.$$

The cap is pointwise dominated by the lower semicircle of radius h centered at $(x_0, 0)$, and it also lies in a rectangle of width $2h$ and height $\rho - y_0$.

Figure 1: geometry in Lemma 1



dashed: lower semicircle of radius h

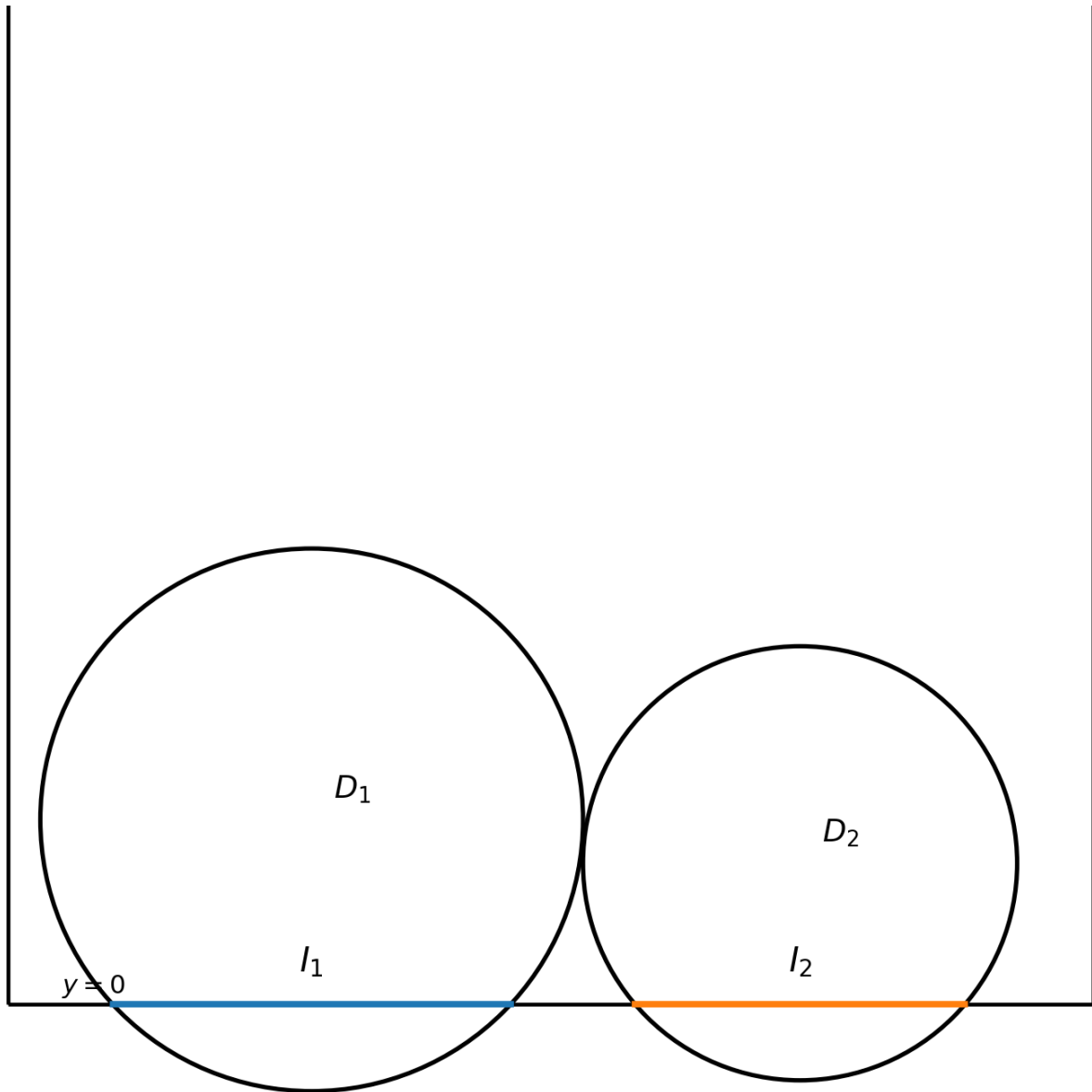
dash-dot: rectangle of height $\rho - y_0$

Definition. The chord interval is $I=[x_0-h, x_0+h]$.

Lemma 3. If two original disks are disjoint, then the interiors of their chord intervals are disjoint.

Indeed, an interior point common to both intervals would give a point $(x,0)$ lying strictly inside both disks.

Figure 2: disjoint discs give disjoint chord intervals



2.2. An endpoint estimate

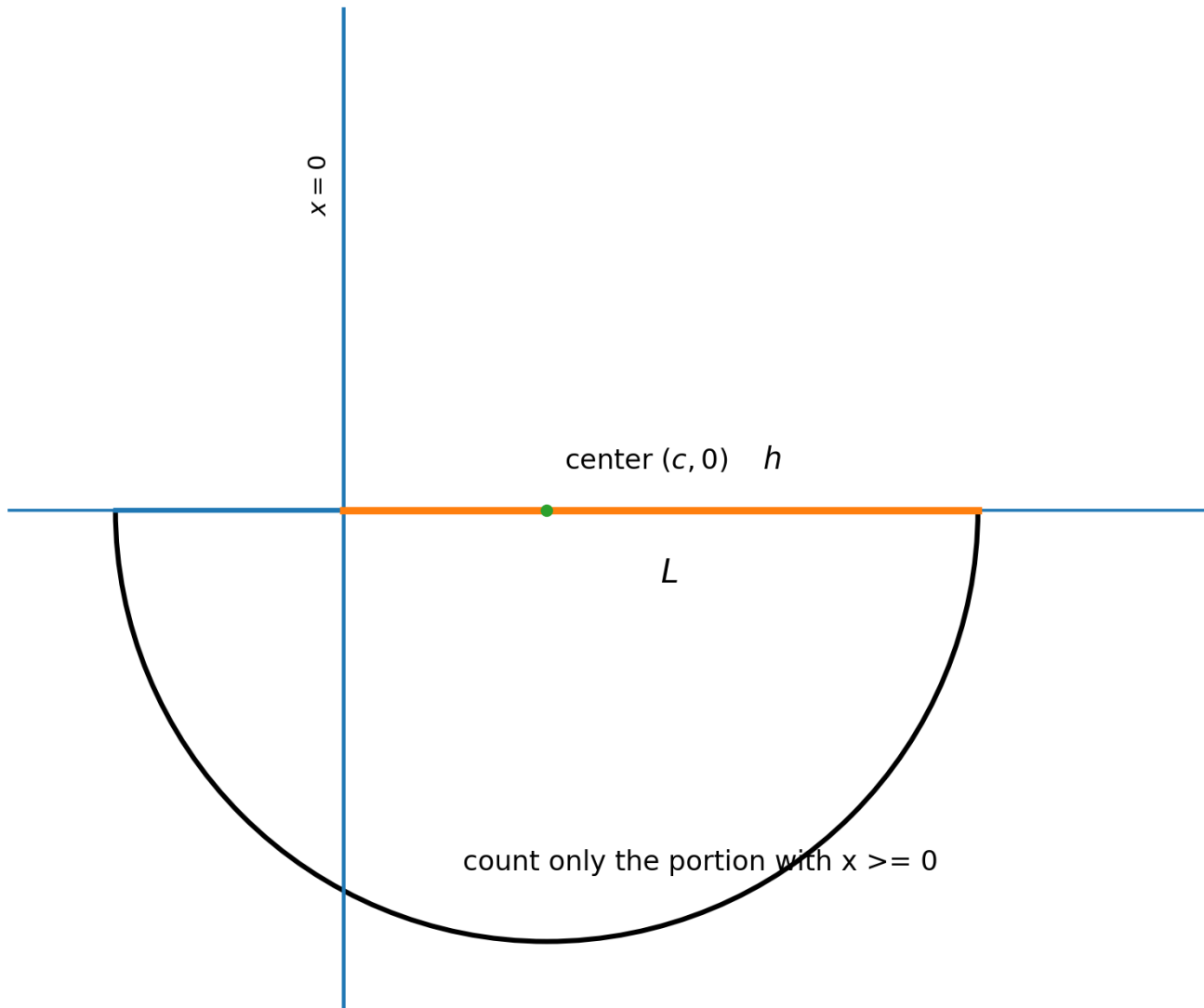
Define $t_0 = \sqrt{1 - \pi^2/16}$ and $e_0 = (1/2)\arcsin(t_0) - (\pi/8)t_0$.

Lemma 4. Let $0 = 0$ and let $L = c + h$. Then

$$A \leq (\pi a/4)L + a^2 e_0.$$

Put $t = c/h$ and $s = h/a$. Direct integration gives $A = h^2 [\pi/4 + (1/2)(t \sqrt{1-t^2} + \arcsin t)]$. For fixed t , the normalized excess over $(\pi a/4)L$ is a convex quadratic in s , so its maximum occurs at $s=0$ or $s=1$. At $s=1$ its derivative is $\sqrt{1-t^2} - \pi/4$, which is maximized at $t=t_0$.

Figure 3: the endpoint case in Lemma 3



2.3. One side strip

Lemma 5. In the bottom strip $B=\{(x,y):0\leq x\leq 1,y<0\}$, the total area covered by the original disks is at most

$$M(a)=\max\{\pi a/4 + 2a^2e_0, \pi a^2/2\}.$$

Apply Lemma 2 to the protruding caps. The chord intervals have disjoint interiors. For intervals inside $[0,1]$, bound the comparison semicircle by $(\pi a/4)$ times the chord length. For at most two endpoint-crossing intervals, use Lemma 4. If one interval contains all of $[0,1]$, the total is at most one full semicircle of radius a .

Figure 4A: original disjoint configuration

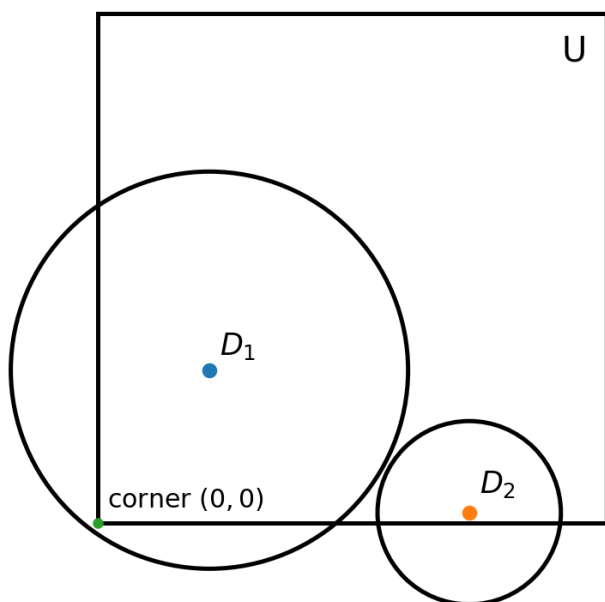
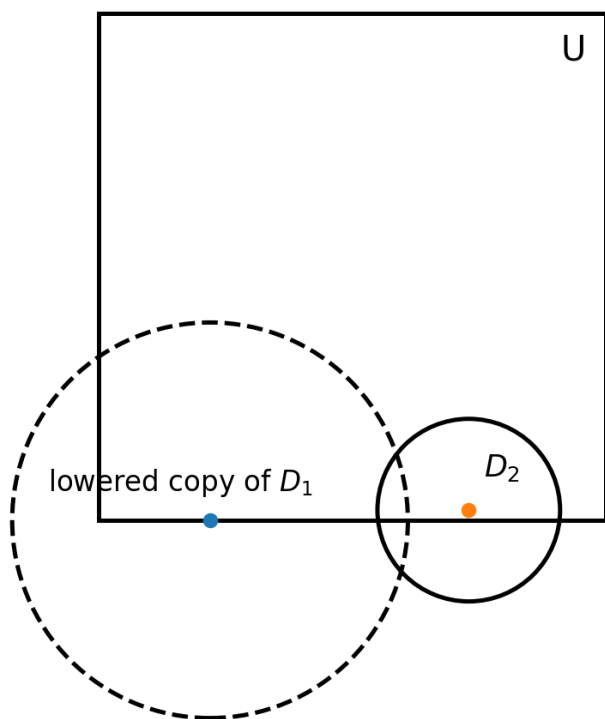


Figure 4B: lower only D_1 until its center lies on $y = 0$



2.4. The improved covering theorem

Put $C = \pi + 8e_0 = 3.86680427735\dots$

Theorem 2. Let $D_1, \dots, D_n$ be pairwise disjoint disks centered in U and of radii at most $R/2$. Then

$$\sum \text{area}(D_i) \leq 1 + \max\left\{ \left(\frac{\pi}{2}\right)R + \left(\frac{C}{4}\right)R^2, \left(\frac{3\pi}{4}\right)R^2 \right\}.$$

The part inside U has area at most 1. Each of the four corner quadrants contributes at most a quarter-disk of radius a , for a total of πa^2 . Each side strip contributes at most $M(a)$. Thus the total is at most $1 + \pi a^2 + 4M(a)$; substituting $a = R/2$ gives the theorem.

For the nearest-neighbor disks, $\sum \text{area}(D_i) = (\pi/4)S$, hence

$$S \leq 4/\pi + \max\left\{ 2R + \left(\frac{C}{\pi}\right)R^2, 3R^2 \right\}.$$

At $R = 1/\sqrt{2}$, this gives $S \leq 3.3028741218\dots$

3. The sharp adjacent-quarter lemma

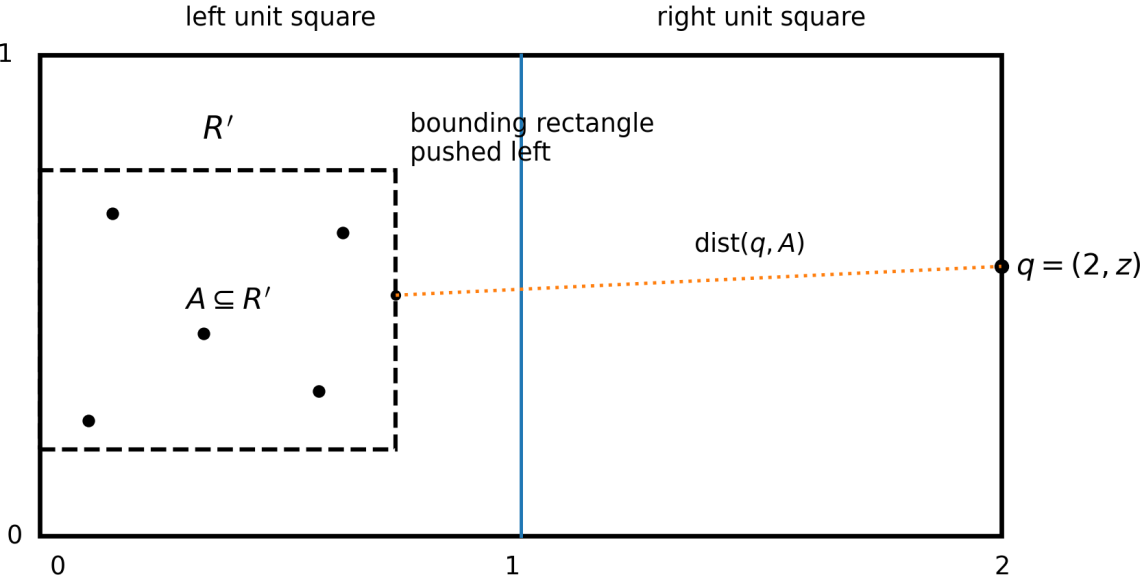
Lemma 6. Let A be a finite nonempty collection of labelled points in one quarter-square, and let q lie in an adjacent quarter-square. Then

$$\text{Sigma}(A) + \text{dist}(q, A)^2 \leq 25/16.$$

The constant $25/16$ is sharp.

Proof. Scale lengths by 2. Move q horizontally to the right edge, $q=(2,v)$. Translate A horizontally left until the left edge of its minimal bounding rectangle is $x=0$. Write that rectangle as $[0,x] \times [\gamma,\delta]$, with height $h \leq 1$.

Figure for Section 3.1: the 2×1 box, the bounding rectangle R' , and the point q



4. The Global Theorem

Theorem 3. Let $p_1, \dots, p_n$ be labelled points in the unit square, with $n \geq 5$. Let r_i be the distance from p_i to its nearest other point, and put $S = \sum r_i^2$. Then

$$S \leq 57/16 = 3.5625.$$

Proof. Put $R = \max r_i$. We divide the proof into two cases.

Case 1: $R \leq 1/\sqrt{2}$

For each i draw the disk D_i centered at p_i with radius $r_i/2$. These disks have pairwise disjoint interiors, and

$$\sum \text{area}(D_i) = (\pi/4)S.$$

Theorem 2 gives, for every $R \geq 0$,

$$\sum \text{area}(D_i) \leq 1 + \max\{(\pi/2)R + (C/4)R^2, (3\pi/4)R^2\},$$

where $C = \pi + 8e_0$. The resulting bound for S is increasing on $0 \leq R \leq 1/\sqrt{2}$, and at $R = 1/\sqrt{2}$ it is

$$S \leq 3.3028741218... < 57/16.$$

Therefore the theorem holds whenever $R \leq 1/\sqrt{2}$.

Case 2: $R > 1/\sqrt{2}$

Choose q with $r_q = R$, and divide the unit square into four quarter-squares of side $1/2$. A quarter-square has diameter $1/\sqrt{2}$, so no other labelled point can lie in the same quarter-square as q . Thus the quarter containing q is a singleton.

For any other quarter-square Q containing at least two points, let $\Sigma(Q)$ be the sum of the squared nearest-neighbor distances computed using only the points of Q . The nearest-neighbor distance of a point in the full configuration is no larger than its nearest-neighbor distance inside Q , so the contribution of Q to S is at most $\Sigma(Q)$. By Pinelis's rectangle theorem,

$$\Sigma(Q) \leq 2(1/2)^2 + 2(1/2)^2 = 1.$$

We also use Lemma 6. If A lies in a quarter-square adjacent to q 's quarter, then

$$\Sigma(A) + \text{dist}(q, A)^2 \leq 25/16.$$

Since $r_q \leq \text{dist}(q, A)$, we may use the weaker but more convenient form

$$\Sigma(A) + r_q^2 \leq 25/16.$$

There are three quarter-squares other than q 's singleton quarter. We classify the configuration by how many of these three quarters are nonsingletons.

The three occupancy cases in the large-R argument

All three are nonsingletons

singleton quarter	
q: 1	≥ 2
≥ 2	≥ 2

Exactly two are nonsingletons

singleton quarter	
q: 1	≥ 2
≥ 2	0 or 1

Exactly one is nonsingleton

singleton quarter	
q: 1	0 or 1
0 or 1	≥ 2

Large-R occupancy cases

All three are nonsingletons. Choose either nonsingleton quarter adjacent to q 's quarter and call its point set A . Lemma 6 gives $\text{Sigma}(A) + r_q^2 \leq 25/16$. Each of the remaining two nonsingleton quarters contributes at most 1. Hence

$$S \leq 25/16 + 1 + 1 = 57/16.$$

Exactly two are nonsingletons. If the third quarter is empty, at least one nonsingleton quarter is adjacent to q 's quarter. Pair it with q using Lemma 6; the other nonsingleton quarter contributes at most 1. Thus

$$S \leq 25/16 + 1 = 41/16.$$

If the third quarter is a singleton, there are two singleton quarters and two nonsingleton quarters. They can be paired so that each singleton is adjacent to one nonsingleton quarter. Applying Lemma 6 twice gives

$$S \leq 2(25/16) = 25/8.$$

Exactly one is nonsingleton. The other two quarters are singleton or empty. This is Pinelis's Case 4, with Case 5 allowing empty quarters. His stronger intermediate estimate gives $S \leq (3/2)(a^2 + b^2)$ for an $a \times b$ rectangle. For the unit square,

$$S \leq 3.$$

Thus in every large- R configuration, $S \leq 57/16$. Combining this with Case 1 proves Theorem 3. QED.

5. Conditional improvement from a 21/16 lemma

Suppose the following strengthening is true: whenever A contains at least three labelled points in a quarter-square and q lies in an adjacent quarter-square,

$$\text{Sigma}(A) + \text{dist}(q, A)^2 \leq 21/16.$$

Then for $n \geq 10$ one obtains a better bound. If an adjacent quarter contains at least three points, the conditional lemma together with the two remaining quarter bounds gives at most $21/16 + 1 + 1 = 53/16 = 3.3125$.

Otherwise the potentially worst occupancy is $1+2+2+m$. For $n \geq 10$ we have $m \geq 5$. Pair q with one 2-point adjacent quarter using Lemma 6, bound the other 2-point quarter by 1, and apply the proved $57/16$ theorem to the diagonal m -point quarter after scaling that quarter to a unit square. Its contribution is at most $(1/4)(57/16) = 57/64$.

$$\text{Therefore, conditionally, } S \leq 25/16 + 1 + 57/64 = 221/64 = 3.453125 \text{ for } n \geq 10.$$

For $n=8$, the remaining pattern $1+2+2+3$ gives $S \leq 25/16 + 1 + 13/16 = 27/8 = 3.375$. For $n=7$ and $n=9$, the patterns $1+2+2+2$ and $1+2+2+4$ are not eliminated merely by the conditional lemma.

Reference

I. Pinelis, "Exact upper bound on the sum of squared nearest-neighbor distances between points in a rectangle," *Mathematical Inequalities & Applications* 23 (2020), 663-670. DOI: 10.7153/mia-2020-23-54; arXiv:1904.11427.