Three Points in the Unit Square

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ChatGPT was used extensively

1 Introduction

Notation 1.1 Let $p_1, \ldots, p_n$ be labelled points in the unit square, $[0,1] \times [0,1]$. Coincidences are allowed. Define

$$r_i = \min_{j \neq i} |p_i - p_j|,$$

Our goal is to find an upper bound on $\sum_{i=1}^3 r_i^2$. We seek a sharp bound, meaning that equality is attained by some set of points.

2 The Case of $n = 3$

Theorem 2.1 *There is a set of three points p_1, p_2, p_3 such that $\sum_{i=1}^3 r_i^2 = \frac{13}{4}$.*

Proof: Let
$p_1 = (0,0)$, $p_2 = (\frac{1}{2}, 1)$, $p_3 = (1,0)$.

$d(p_1,p_2)^2 = \frac{5}{4}$.
$d(p_1,p_3)^2 = 1$.
$d(p_2,p_3)^2 = \frac{5}{4}$.

$r_1^2 = 1$.
$r_2^2 = \frac{5}{4}$.
$r_3^2 = 1$.

$\sum_i r_i^2 = 1 + \frac{5}{4} + 1 = \frac{13}{4}$. ∎

We show that, for all p_1, p_2, p_3, $\sum_{i=1}^3 r_i^2 \leq \frac{13}{4}$.
We need the following well-known lemma.

Lemma 2.2

1. *A convex function of one variable on a closed interval has a maximum at an endpoint.*
2. *A convex function of two variables on a closed triangle in the plane has a maximum at one of the vertices of the triangle.*

We will use Lemma 2.2 without further comment.

Theorem 2.3 *Let p_1, p_2, p_3 be points in the unit square. Then $\sum_{i=1}^3 r_i^2 \leq \frac{13}{4}$.*

Proof: Let L be the leftmost point, R be the rightmost point, and M be the other point. Ties in the x-coordinate are allowed.

If L is not on the left boundary then moving it there will not decrease the distances from the other points and hence not decrease the sum. So we assume L is on the left boundary.

By the same reasoning we can assume R is on the right boundary.

We show that we can assume $L = (0, 0)$.

By reflecting the square across the horizontal midline if necessary, assume that L is no higher than R.

- If M is above (or on the same level as) L then we shift all three points down so that L is $(0, 0)$.
- If M is below L then do the following:

  a) Shift M to the bottom boundary. This does not decrease any nearest-neighbor distance.

  b) Shift R to the point $(1, 1)$. This does not decrease any nearest-neighbor distance.

  c) Reflect across $x + y = 1$. The old R becomes the new $L = (0, 0)$. The old M becomes the new R on the right edge. The old L becomes the new M on the top edge.

Case 1: L and R are on the same horizontal line, so $L = (0, 0)$ and $R = (1, 0)$. If M is not on the top boundary then moving it there will not decrease the sum. So we assume M is on the top boundary. Let $M = (x, 1)$.

$L = (0, 0)$, $R = (1, 0)$, and $M = (x, 1)$.
$r_L^2 = 1$
$r_R^2 = 1$.
$r_M^2 = \min\{x^2 + 1, (1 - x)^2 + 1\}$.
The sum is

$$3 + \min\{x^2, (1 - x)^2\}.$$

It is easy to see that this quantity is maximized when $x = \frac{1}{2}$. Hence the maximum is

$$3 + \min\left\{\frac{1}{4}, \frac{1}{4}\right\} = \frac{13}{4}.$$

Case 2: M is lower than, or on the same level as, R. Hence $R = (1, y_R)$, $M = (x, y)$ and $y \leq y_R$. If R is not $(1, 1)$ then moving it there will not decrease the sum. So we assume $R = (1, 1)$.

$L = (0, 0)$, $R = (1, 1)$ and $M = (x, y)$.

$r_L^2 = x^2 + y^2$
$r_R^2 = (1 - x)^2 + (1 - y)^2$
$r_M^2 = \min\{x^2 + y^2, (1 - x)^2 + (1 - y)^2\}$
There are two cases.

- $x + y \leq 1$. Then $x^2 + y^2 \leq (1-x)^2 + (1-y)^2$. The sum is

$$3x^2 + 3y^2 - 2x - 2y + 2$$

We maximize the expression over the triangle with vertices $(0,0)$, $(0,1)$, and $(1,0)$. Since it is convex, its maximum is achieved at one of those vertices. By plugging in the numbers we see that the max is $3 < \frac{13}{4}$.

- $x + y \geq 1$. Set $u = 1 - x$ and $v = 1 - y$. Then $u + v \leq 1$, and the sum becomes $3u^2 + 3v^2 - 2u - 2v + 2$. This is now the $x + y \leq 1$ case, hence the maximum will be $3 \leq \frac{13}{4}$.

Case 3: M is higher than R. Moving M to the top boundary will not decrease either of its distances to L and R. Hence $L = (0,0)$, $R = (1,y)$, $M = (x,1)$. By reflecting across $y = x$ and relabeling the point on the right edge as R if necessary, we may assume $x \leq y$.
$r_L^2 = \min\{y^2 + 1, x^2 + 1\} = x^2 + 1$
$r_R^2 = \min\{y^2 + 1, (x-1)^2 + (y-1)^2\}$
$r_M^2 = \min\{x^2 + 1, (x-1)^2 + (y-1)^2\}$

Case 3.1 $(x-1)^2 + (y-1)^2 \leq x^2 + 1$.
Since $x \leq y$ we also have
$(x-1)^2 + (y-1)^2 \leq x^2 + 1 \leq y^2 + 1$.
Hence the sum is

$$x^2 + 1 + (x-1)^2 + (y-1)^2 + (x-1)^2 + (y-1)^2 = (3x^2 - 4x) + (2y^2 - 4y) + 5.$$

The premise of this case determines which term realizes the minimum in both r_R^2 an r_M^2. Hence we will not have to deal with a function with a min in it.

A Lower Bound on y
From the premise of this case we have:
$(x-1)^2 + (y-1)^2 \leq x^2 + 1$
$y^2 - 2y + 1 \leq 2x$ (We will use this later to get a bound on x.)
Since $x \leq y$ we have
$y^2 - 2y + 1 \leq 2y$ (We will use this now to get an Interval For y.)
$y^2 - 4y + 1 \leq 0$. Hence

$$y \in [2 - \sqrt{3}, 2 + \sqrt{3}].$$

However, the problem restricts $y \in [0,1]$. Hence

$$y \in [2 - \sqrt{3}, 1].$$

An Interval For x
Now we get back to x. Recall that $y^2 - 2y + 1 \leq 2x$. Hence

$$x \in \left[\frac{(y-1)^2}{2}, y\right].$$

Goal: Maximize

$$(3x^2 - 4x) + (2y^2 - 4y) + 5 \text{ with constraints } y \in [2-\sqrt{3}, 1] \text{ and } x \in \left[\frac{(y-1)^2}{2}, y\right].$$

We deal with x first. The maximum of $3x^2 - 4x$ is achieved at one of the endpoints. There are two cases.

Case 3.1.1 The maximum of $3x^2 - 4x$ occurs when $x = \frac{(y-1)^2}{2}$

$$(3x^2 - 4x) = 3\left(\frac{(y-1)^2}{2}\right)^2 - 4\left(\frac{(y-1)^2}{2}\right) = \frac{3(y-1)^4 - 8(y-1)^2}{4}$$

Hence our goal is to maximize

$$\frac{3(y-1)^4 - 8(y-1)^2}{4} + 2y^2 - 4y + 5 = \frac{3}{4}(y-1)^4 + 3$$

Since the second derivative of $\frac{3}{4}(y-1)^4 + 3$ is $9(y-1)^2$, which is ≥ 0, $\frac{3}{4}(y-1)^4 + 3$ is convex. Hence it achieves its maximum at one of the endpoints.

$y = 2 - \sqrt{3}$:

$$\frac{3}{4}(y-1)^4 + 3 = \frac{3}{4}(1-\sqrt{3})^4 + 3 = 24 - 12\sqrt{3} \leq 3.216 < \frac{13}{4}.$$

$y = 1$:

$$\frac{3}{4}(y-1)^4 + 3 = \frac{3}{4}(1-1)^4 + 3 = 3 < \frac{13}{4}.$$

Case 3.1.2 The maximum occurs when $x = y$.

$$(3x^2 - 4x) + (2y^2 - 4y) + 5 = (3y^2 - 4y) + (2y^2 - 4y) + 5 = 5y^2 - 8y + 5.$$

Since the second derivative of $5y^2 - 8y + 5$ is 10 which is ≥ 0, $5y^2 - 8y + 5$ is convex. Hence it achieves its maximum at one of the endpoints.

$y = 2 - \sqrt{3}$: $5y^2 - 8y + 5 = 24 - 12\sqrt{3} < 3.216 < \frac{13}{4}$.

$y = 1$: $5y^2 - 8y + 5 = 2 < \frac{13}{4}$.

Case 3.2 $x^2 + 1 \leq (x-1)^2 + (y-1)^2$.

The premise tells us which term is the minimum in r_M^2 but not r_M^2.

The sum is

$$x^2 + 1 + \min\{y^2 + 1, (x-1)^2 + (y-1)^2\} + y^2 + 1.$$

We simplify and use this sum later.

An Upper Bound on x

The premise yields:

$x^2 + 1 \leq x^2 - 2x + 1 + y^2 - 2y + 1$

$x \leq \frac{(y-1)^2}{2}$

Since we also know $x \leq y$ we have $x \leq \min\left\{\frac{(y-1)^2}{2}, y\right\}$

The Bounds on y Affect the Bounds on x

We need to determine for which values of y, $y \leq \frac{(y-1)^2}{2}$.

$y \leq \frac{(y-1)^2}{2}$

$0 \leq y^2 - 4y + 1.$

The roots of this equation are $2 \pm \sqrt{3}$.

So we have, if $y \in [0, 1]$ then

- $0 \leq y \leq 2 - \sqrt{3}$ iff $\min\left\{\frac{(y-1)^2}{2}, y\right\} = y$. In this case $x \leq y \leq 2 - \sqrt{3}$, so $x \leq 2 - \sqrt{3}$. Takeaway: If y is small then x is small.
- $2 - \sqrt{3} \leq y \leq 1$ iff $\min\left\{\frac{(y-1)^2}{2}, y\right\} = \frac{(y-1)^2}{2}$. In this case, $x \leq \frac{(y-1)^2}{2}$. Since $\frac{(y-1)^2}{2}$ is maximized at $2 - \sqrt{3}$ we get $x \leq \frac{(2-\sqrt{3}-1)^2}{2} = 2 - \sqrt{3}$. Takeaway: If y is large then x is small. This will not be good enough since y is still large. We will use this when we have more constraints.

We will *not* make these our two cases. Instead, we will take cases based on resolving $\min\{x^2 + 1, (x-1)^2 + (y-1)^2\}$ and within those cases have cases based on the two bullet points above. For the sake of sanity we won't number those sub-sub-cases. We will instead use bullet points.

$r_L^2 = \min\{y^2 + 1, x^2 + 1\} = x^2 + 1$

$r_R^2 = \min\{y^2 + 1, (x-1)^2 + (y-1)^2\}$

$r_M^2 = \min\{x^2 + 1, (x-1)^2 + (y-1)^2\} = x^2 + 1$ (This is by the premise of Case 3.2.)

Goal Maximize

$$2x^2 + 2 + \min\{y^2 + 1, (x-1)^2 + (y-1)^2\} \text{ with constraints } 0 \leq x \leq \frac{(y-1)^2}{2} \text{ and } 0 \leq y \leq 1.$$

Case 3.2.1: $y^2 + 1 \leq (x-1)^2 + (y-1)^2$.

Goal Maximize

$$2x^2 + y^2 + 3 \text{ with constraints } 0 \leq x \leq \frac{(y-1)^2}{2} \text{ and } 0 \leq y \leq 1.$$

An Upper Bound on x

$y^2 + 1 \leq (x-1)^2 + (y-1)^2$.

$y^2 + 1 \leq (x-1)^2 + y^2 - 2y + 1$
$0 \leq (x-1)^2 - 2y$
$\sqrt{2y} \leq |1-x|$. Since $x \leq 1$, $|1-x| = 1-x$.

$$x \leq 1 - \sqrt{2y}$$

Two Bulleted Cases

- $0 \leq y \leq 2 - \sqrt{3}$. Since $x \leq 2 - \sqrt{3}$.

$$2x^2 + y^2 + 3 \leq 3(2-\sqrt{3})^2 + 3 = 24 - 12\sqrt{3} \leq 3.216 < \frac{13}{4}.$$

- $2 - \sqrt{3} \leq y \leq \frac{1}{2}$. Since $x \leq 1 - \sqrt{2y}$. $2x^2 + y^2 + 3 \leq y^2 + 4y - 4\sqrt{2y} + 5$.

  Let $f(y) = y^2 + 4y - 4\sqrt{2y} + 5$. A simple calculation shows that, for all y, $f''(y) \geq 0$ in the interval $[2-\sqrt{3}, \frac{1}{2}]$. Hence f is convex in that interval. By Lemma 2.2 f achieves its maximum at one of the endpoints.

  $y = 2 - \sqrt{3}$:

  $(2-\sqrt{3})^2 + 4(2-\sqrt{3}) - 4\sqrt{2(2-\sqrt{3})} + 5 = 20 - 8\sqrt{3} - 4\sqrt{4-2\sqrt{3}}$

  One can show that $\sqrt{4-2\sqrt{3}} = \sqrt{3} - 1$ by squaring both sides. So we get:

  $= 20 - 8\sqrt{3} - 4\sqrt{4-2\sqrt{3}}$

  $= 24 - 12\sqrt{3} \leq 3.216 < \frac{13}{4}$.

  $y = \frac{1}{2}$:

  $(\frac{1}{2})^2 + 4(\frac{1}{2}) - 4\sqrt{2(\frac{1}{2})} + 5 = \frac{1}{4} + 2 - 4 + 5 = \frac{13}{4}$.

Case 3.2.2: $(x-1)^2 + (y-1)^2 \leq y^2 + 1$.

The sum is

$$x^2 + 1 + (x-1)^2 + (y-1)^2 + x^2 + 1 = 3x^2 + y^2 - 2x - 2y + 4.$$

Lower Bounds on y

Since we are in Case 3.2 we have $x \leq \frac{(y-1)^2}{2}$. We will use this later.
Since $(x-1)^2 + (y-1)^2 \leq y^2 + 1$ we get
$(x-1)^2 + y^2 - 2y + 1 \leq y^2 + 1$
$(x-1)^2 - 2y \leq 0$
$(x-1)^2 \leq 2y$.
$2y \geq (x-1)^2$
Since $(x-1)^2$ is a decreasing function on the interval $[0,1]$ and $x \leq y$ we have
$2y \geq (x-1)^2 \geq (y-1)^2$
$y^2 - 4y + 1 \leq 0$
The roots of $y^2 - 4y + 1$ are $2 \pm \sqrt{3}$. Since $y \in [0,1]$ we have

$$y \geq 2 - \sqrt{3}.$$

Upper Bound on y

The remaining bound is $y \leq 1$.

Upper Bound on x

We have $x \leq \frac{(y-1)^2}{2}$. The right hand side is a decreasing function of y. Since $y \geq 2 - \sqrt{3}$

$$x \leq \frac{(1-\sqrt{3})^2}{2} = 2 - \sqrt{3}.$$

Lower Bound on x

Recall from above $(x-1)^2 \leq 2y$.

We use this inequality to obtain a new lower bound on x.

$x^2 - 2x + 1 \leq 2y$

$x^2 - 2x + (1 - 2y) \leq 0$.

Viewing this as a quadratic in x:

$$x \geq 1 - \sqrt{2y}.$$

Summary

We want to maximize

$3x^2 + y^2 - 2x - 2y + 4$ with constraints $y \in [2 - \sqrt{3}, 1]$ and $x \in [\max\{0, 1 - \sqrt{2y}\}, 2 - \sqrt{3}]$.

We will need two cases: $y < \frac{1}{2}$, and $y \geq \frac{1}{2}$.

The following observation will cut down on the cases.

Let $F(x, y) = 3x^2 + y^2 - 2x - 2y + 4$

$\frac{\partial F}{\partial x} = 6x - 2$.

$\frac{\partial^2 F}{\partial x^2} = 6 > 0$.

We record the following as the *Left Endpoint Fact*:

- For fixed y, $\frac{\partial^2 F}{\partial x^2} = 6 > 0$, so F is convex as a function of x. Therefore its maximum on a closed x-interval is achieved at an endpoint.
- The first partial derivative with respect to x is 0 at $x = 1/3$. Hence, for fixed y, the function $F(x, y)$ decreases as x runs from 0 to 1/3. The interval for x has right endpoint $2 - \sqrt{3} < \frac{1}{3}$. Hence, in all cases where we want to choose x to maximize the function, we will pick the left endpoint (it might be bigger than 0).

Case 3.2.2.1: $y \leq \frac{1}{2}$. Then the problem is to maximize

$$3x^2 + y^2 - 2x - 2y + 4 \text{ with constraints } y \in [2 - \sqrt{3}, \frac{1}{2}] \text{ and } x \in [1 - \sqrt{2y}, 2 - \sqrt{3}].$$

Fix y. By *Left Endpoint Fact* the maximum is achieved when x is at the left endpoint which is $1-\sqrt{2y}$.

$3x^2+y^2-2x-2y+4 = 3(1-\sqrt{2y})^2+y^2-2(1-\sqrt{2y})-2y+4 = y^2+4y-4(2y)^{1/2}+5$

Let $f(y) = y^2+4y-4(2y)^{1/2}+5$. Then $f''(y) = 2+\frac{4}{(2y)^{3/2}}$ which is always ≥ 0. Hence f is convex, so it achieves its maximum at one of the endpoints.

$y = 2-\sqrt{3}$: $(2-\sqrt{3})^2+4(2-\sqrt{3})-4\sqrt{2(2-\sqrt{3})}+5$

Since $\sqrt{2(2-\sqrt{3})} = \sqrt{3}-1$, we obtain

$$(2-\sqrt{3})^2+4(2-\sqrt{3})-4(\sqrt{3}-1)+5 = 24-12\sqrt{3} < 3.216 < \frac{13}{4}.$$

$y = \frac{1}{2}$: $(\frac{1}{2})^2+4(\frac{1}{2})-4(1)^{1/2}+5 = \frac{1}{4}+2-4+5 = \frac{13}{4}$.

Case 3.2.2.2: $y \geq \frac{1}{2}$. We now use the constraints on x:

$x \in [\max\{0, 1-\sqrt{2y}\}, 2-\sqrt{3}]$

Since $y \geq \frac{1}{2}$ the left endpoint for x is 0. So we want to maximize

$$3x^2+y^2-2x-2y+4 \text{ with constraints } y \in [\frac{1}{2}, 1] \text{ and } x \in [0, 2-\sqrt{3}].$$

Fix y. By *Left Endpoint Fact* the maximum is achieved when x is at the left endpoint which is 0.

When $x = 0$, the expression is $g(y) = y^2-2y+4$. Since $g''(y) = 2 > 0$, g is convex and hence achieves its maximum at one of the endpoints.

$x = 0$ and $y = \frac{1}{2}$: $3x^2+y^2-2x-2y+4 = \frac{1}{4}-1+4 = \frac{13}{4}$.

$x = 0$ and $y = 1$: $3x^2+y^2-2x-2y+4 = 1-2+4 = 3 < \frac{13}{4}$.

∎