Faster DBSCAN and HDBSCAN in Low-Dimensional Euclidean Spaces

Paper: Mark de Berg, Ade Gunawan, Marcel Roeloffzen

Slides: Thomas van Dijk

Noon seminar: 15th Feb 2018

Julius-Maximilians-UNIVERSITÄT WÜRZBURG

Lehrstuhl für INFORMATIK I Effiziente Algorithmen und wissensbasierte Systeme

Institut für Informatik

Clustering

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Fundamental problem in data mining, but not uniquely defined.

What are you clustering? What are you trying to do with the data?

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Distance: Euclidean? Metric?

How many clusters? What can clusters look like?

Clustering

1956

MATHÉMATIQUE

Sur la division des corps matériels en parties

par

H. STEINHAUS

Présenté le 19 Octobre 1956

Un corps Q est, par définition, une répartition de matière dans l'espace, donnée par une fonction $f(P)$; on appelle cette fonction la *densité* du corps en question; elle est définie pour tous les points P de l'espace; elle est non-négative et mesurable. On suppose que *l'ensemble caracté-*

Clustering

1967

SOME METHODS FOR CLASSIFICATION AND ANALYSIS OF MULTIVARIATE OBSERVATIONS

J. MacQUEEN
University of California, Los Angeles

1. Introduction

The main purpose of this paper is to describe a process for partitioning an N-dimensional population into k sets on the basis of a sample. The process, which is called 'k-means,' appears to give partitions which are reasonably efficient in the sense of within-class variance. That is, if p is the probability mass function for the population, $S = \{S_1, S_2, \cdots, S_k\}$ is a partition of E_N, and u_i,

Clustering

DBSCAN

1996

A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases with Noise

Martin Ester, Hans-Peter Kriegel, Jörg Sander, Xiaowei Xu

Institute for Computer Science, University of Munich
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$\geqslant 8 \times 10^3$ citations

KDD "test of time award" 2014

Open source implementations available in many languages

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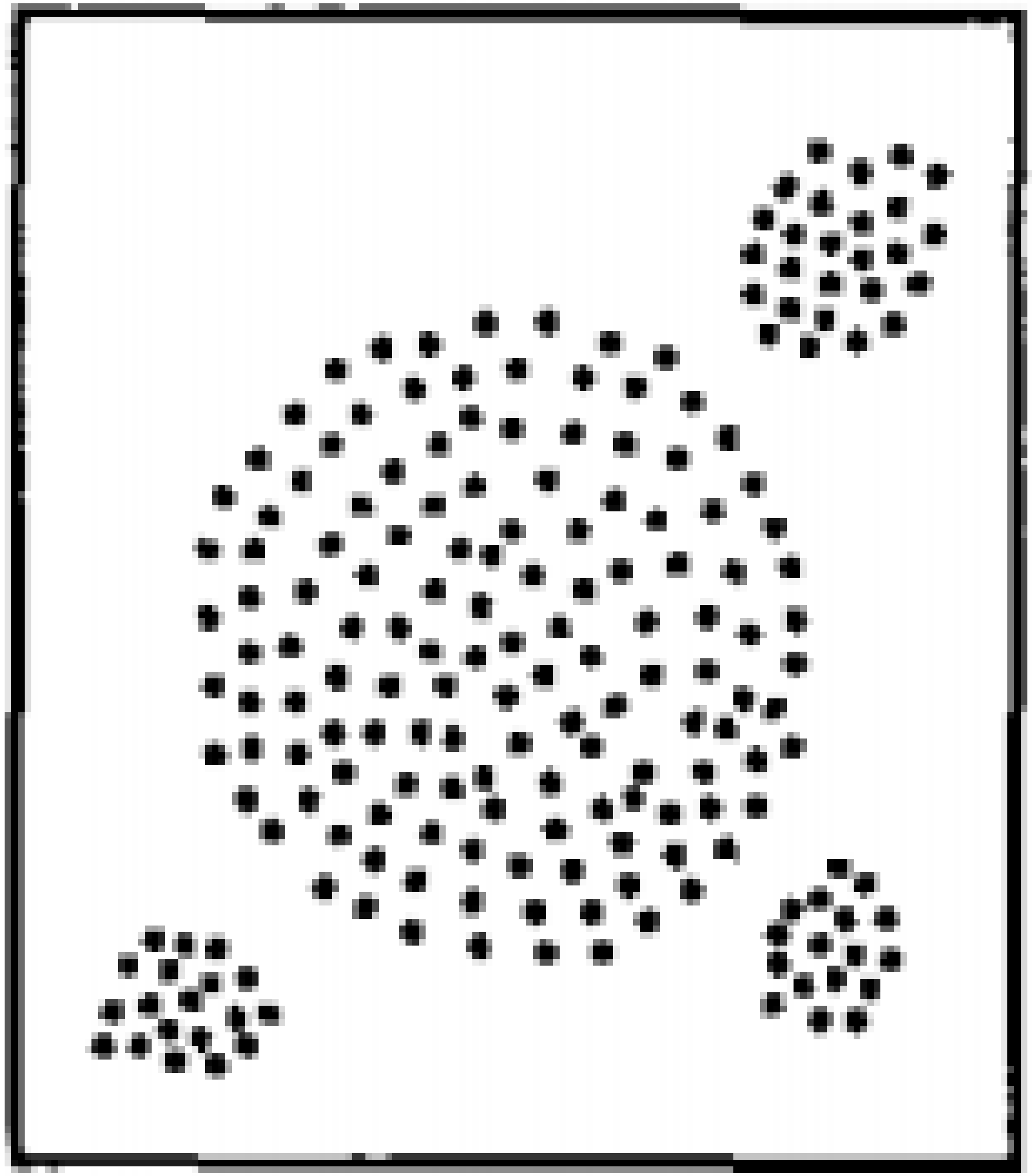
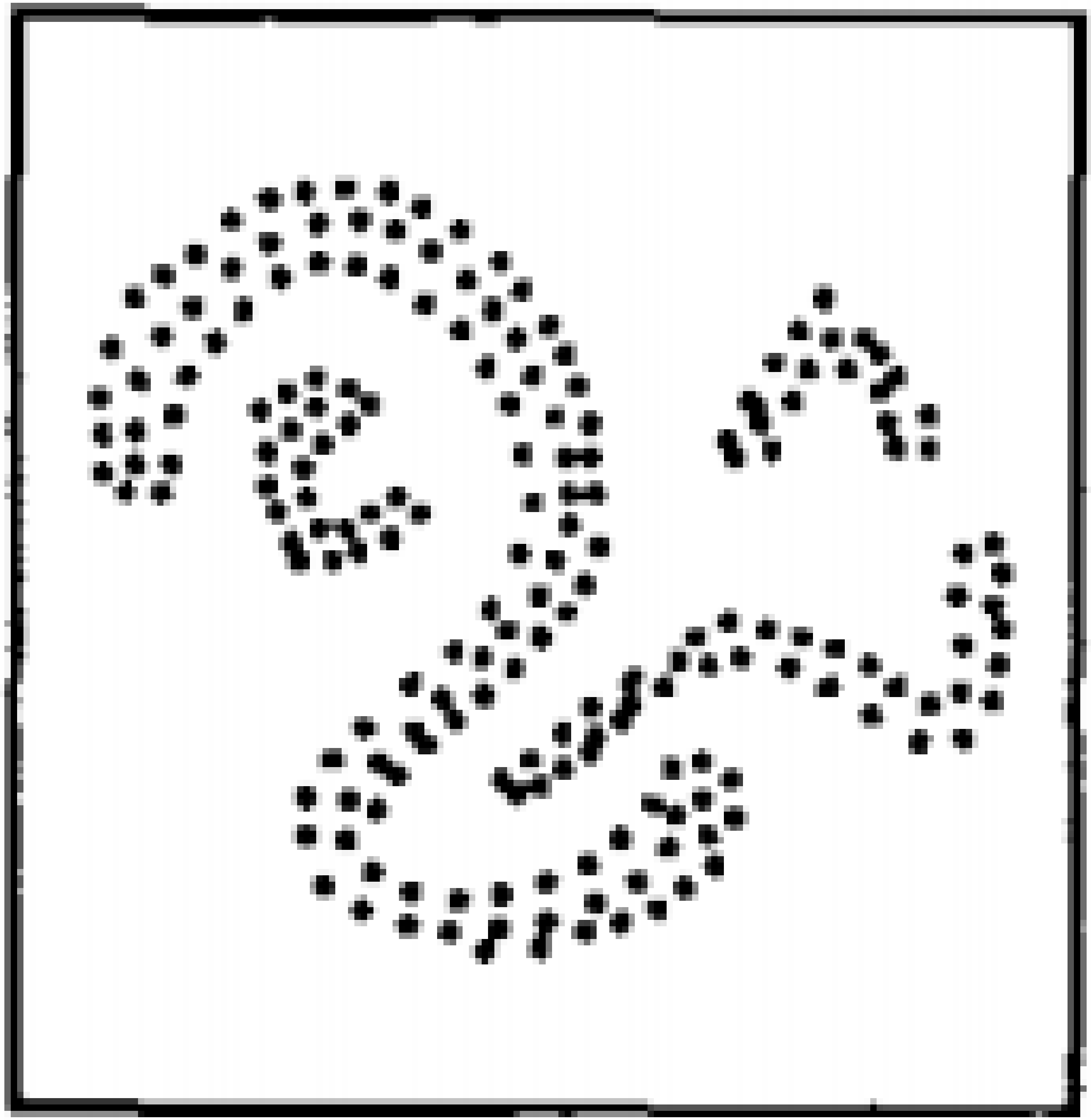
ing an appropriate value for it. It discovers clusters of arbitrary shape. Finally, DBSCAN is efficient even for large spatial databases. The rest of the paper is organized as follows.

Clustering



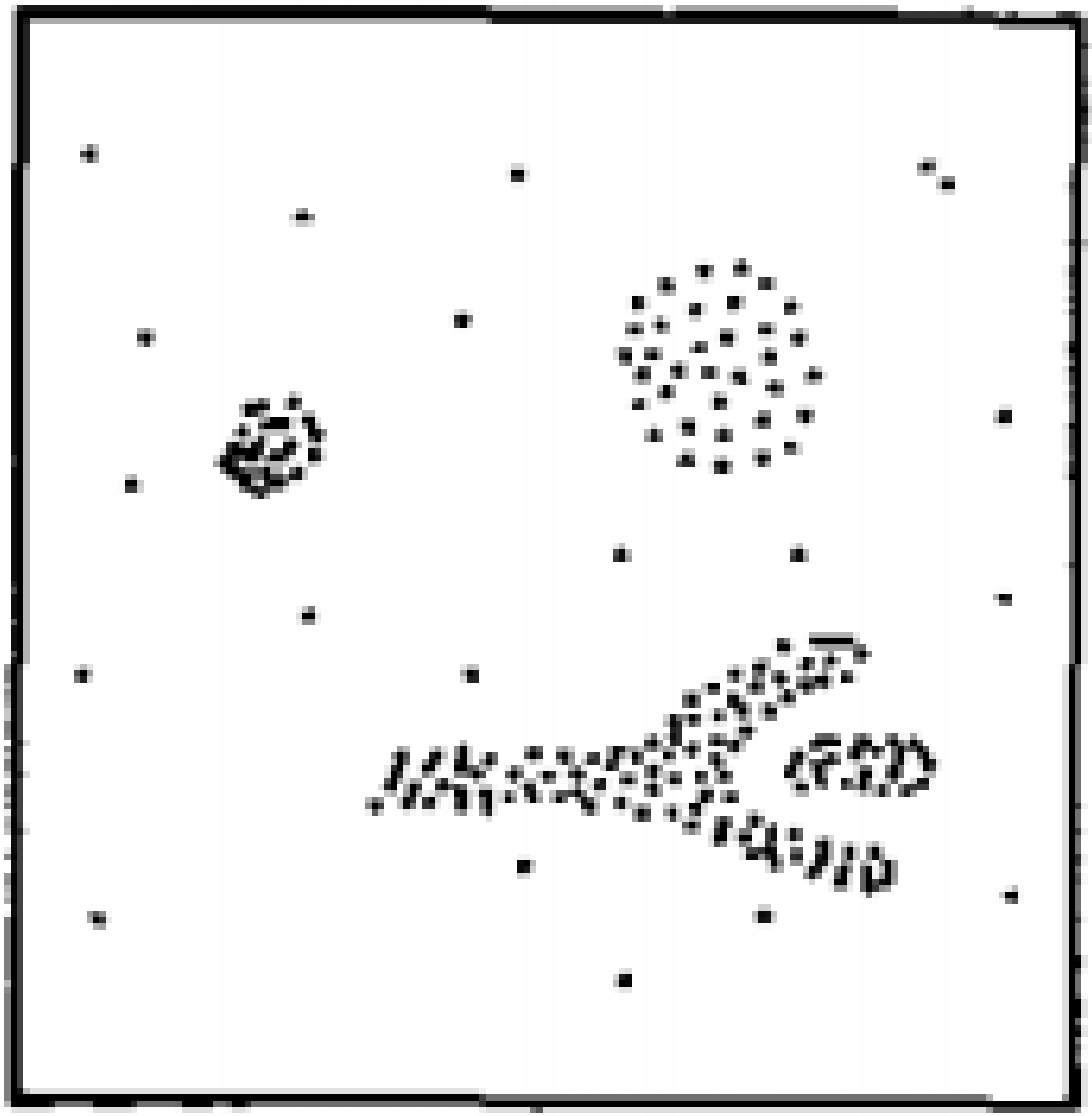
database 1

Clustering



database 2

Clustering



database 3

DBSCAN: Objectives

1. “Minimal requirements of domain knowledge to determine the input parameters, because appropriate values are often not known in advance when dealing with large databases.”

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2. “Discovery of clusters with arbitrary shape, because the shape of clusters in spatial databases may be spherical, drawn-out, linear, elongated etc.”

3. “Good efficiency on large databases, i.e. on databases of significantly more than just a few thousand objects.”

DBSCAN

Given: data points X, distance function $d(\cdot, \cdot)$, thresholds ε and k.

DBSCAN

"Eps" "MinPts"

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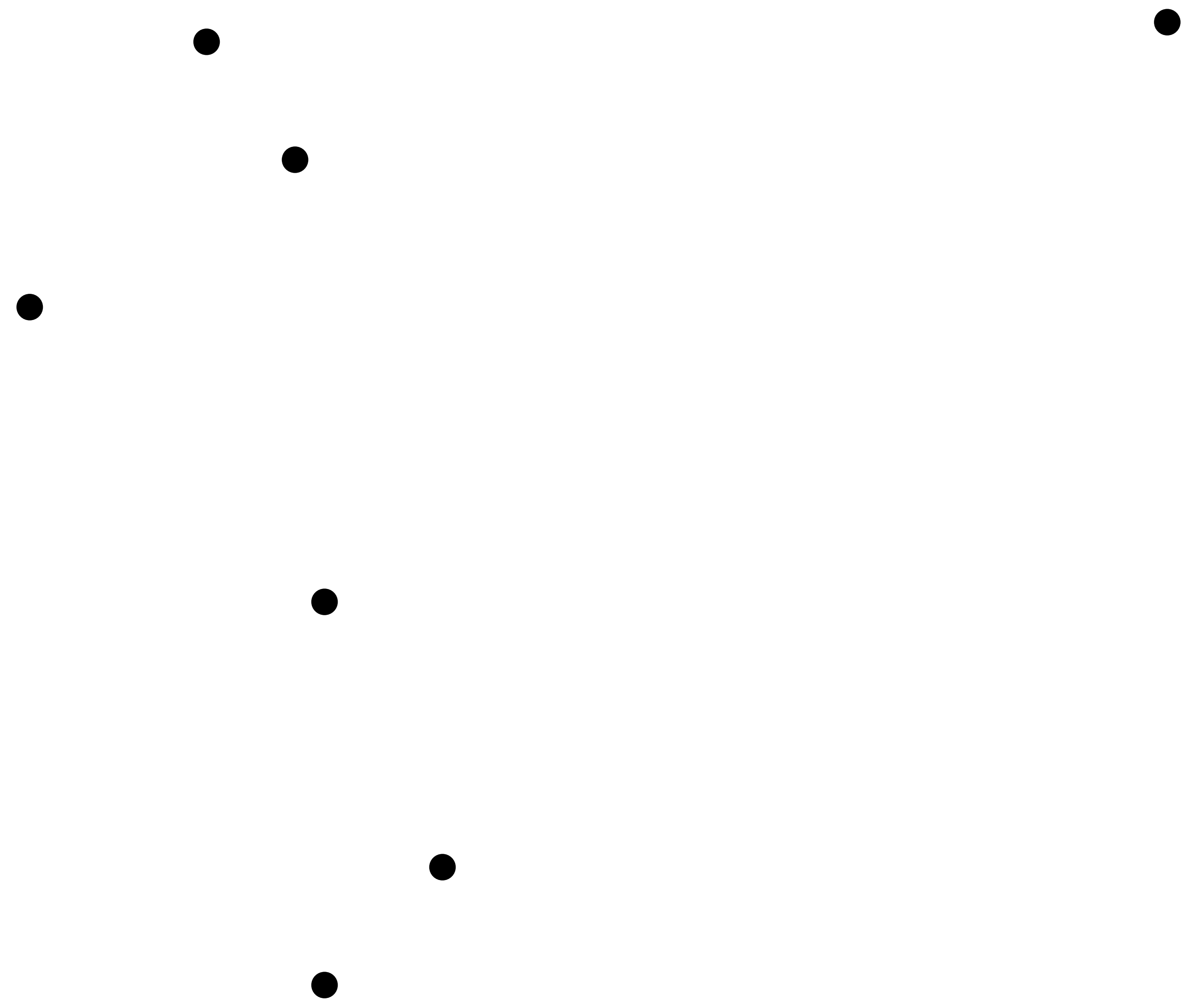
Def. A point $p \in X$ is **density connected** to a point q if there exists a (core) point r such that both p and q are density-reachable from r.

DBSCAN example

Legend

$k = 3$

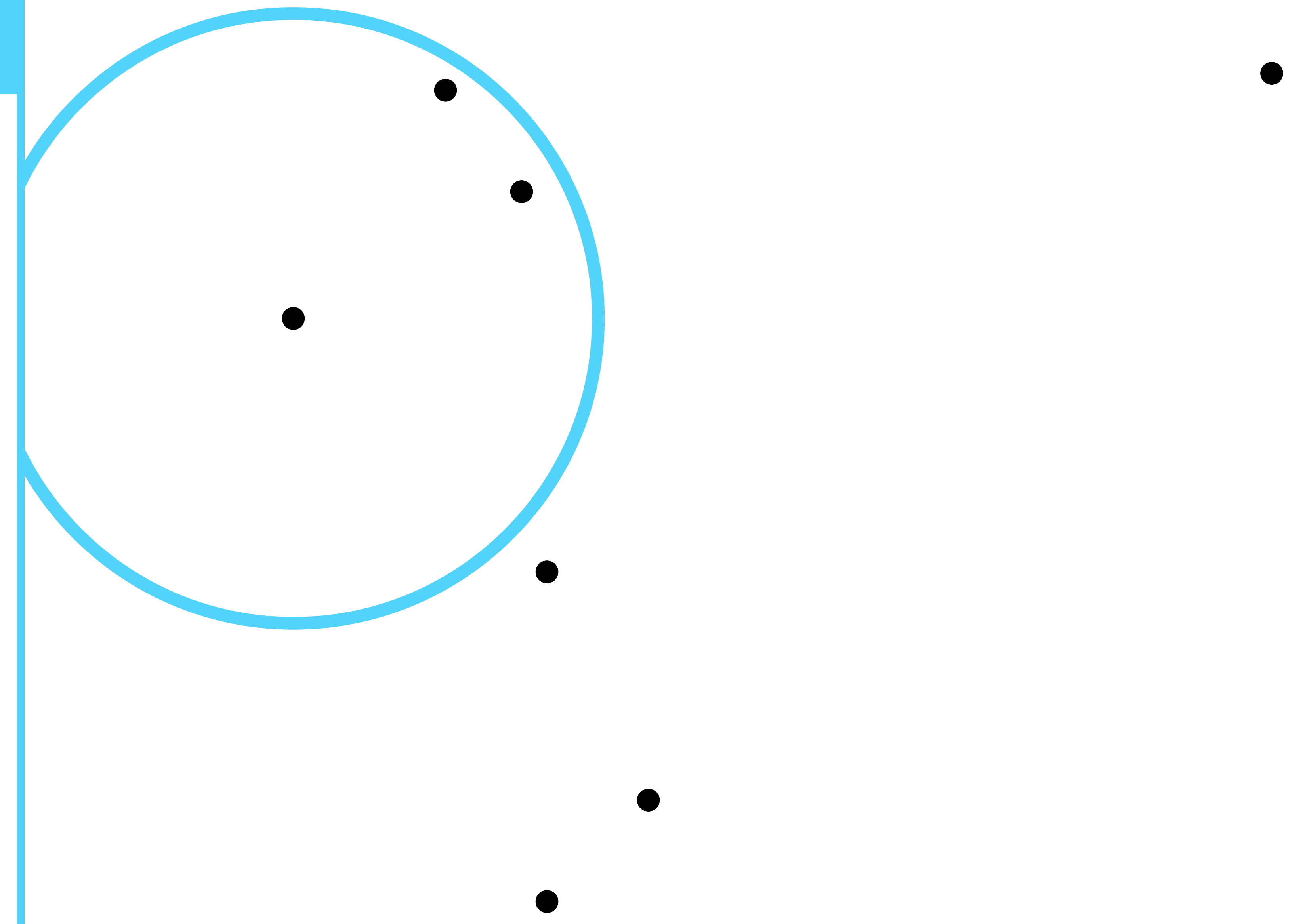


DBSCAN example

Legend

$k = 3$

Distance ε



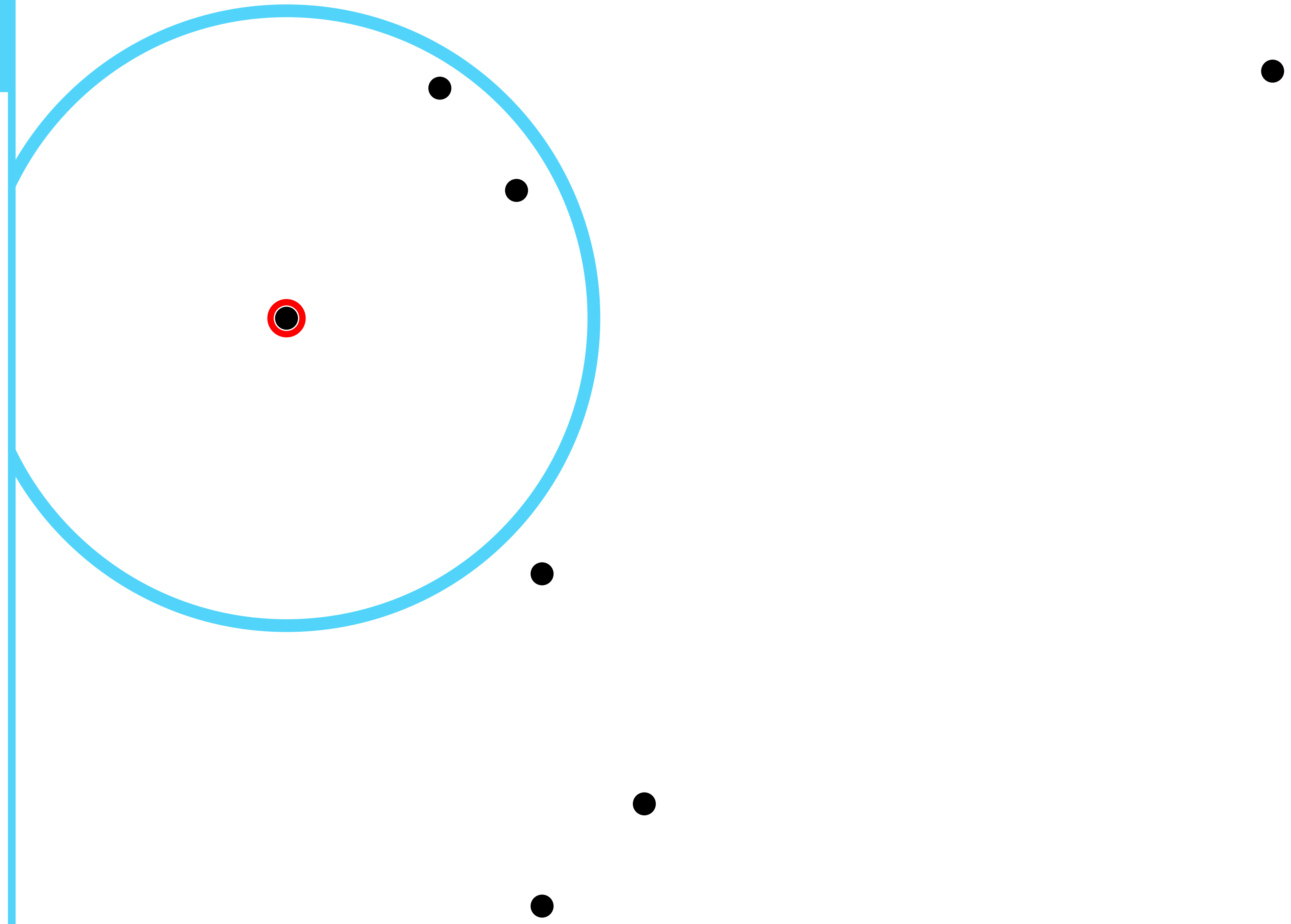
DBSCAN example

Legend

$k = 3$

Distance ε

Core points



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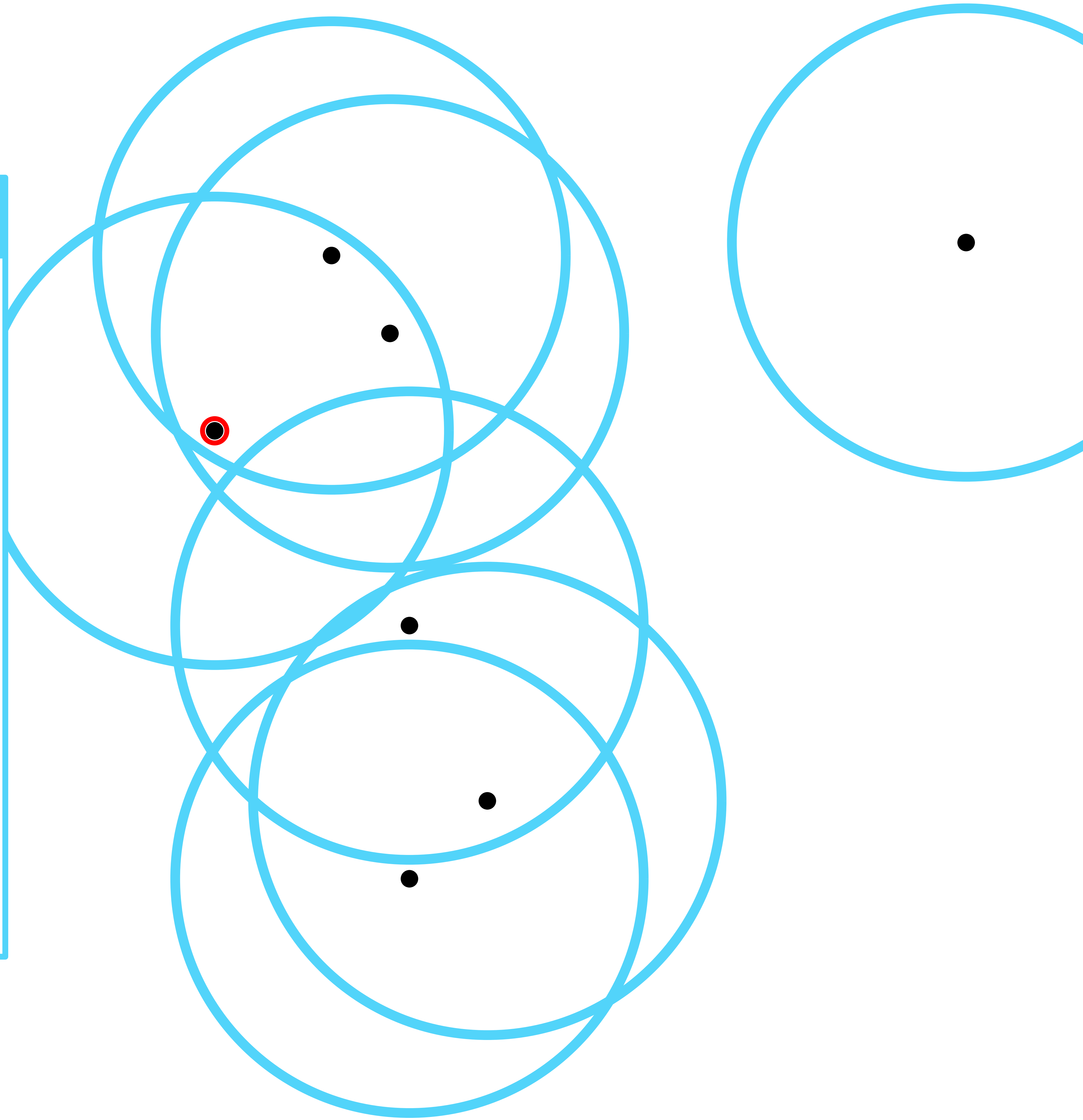

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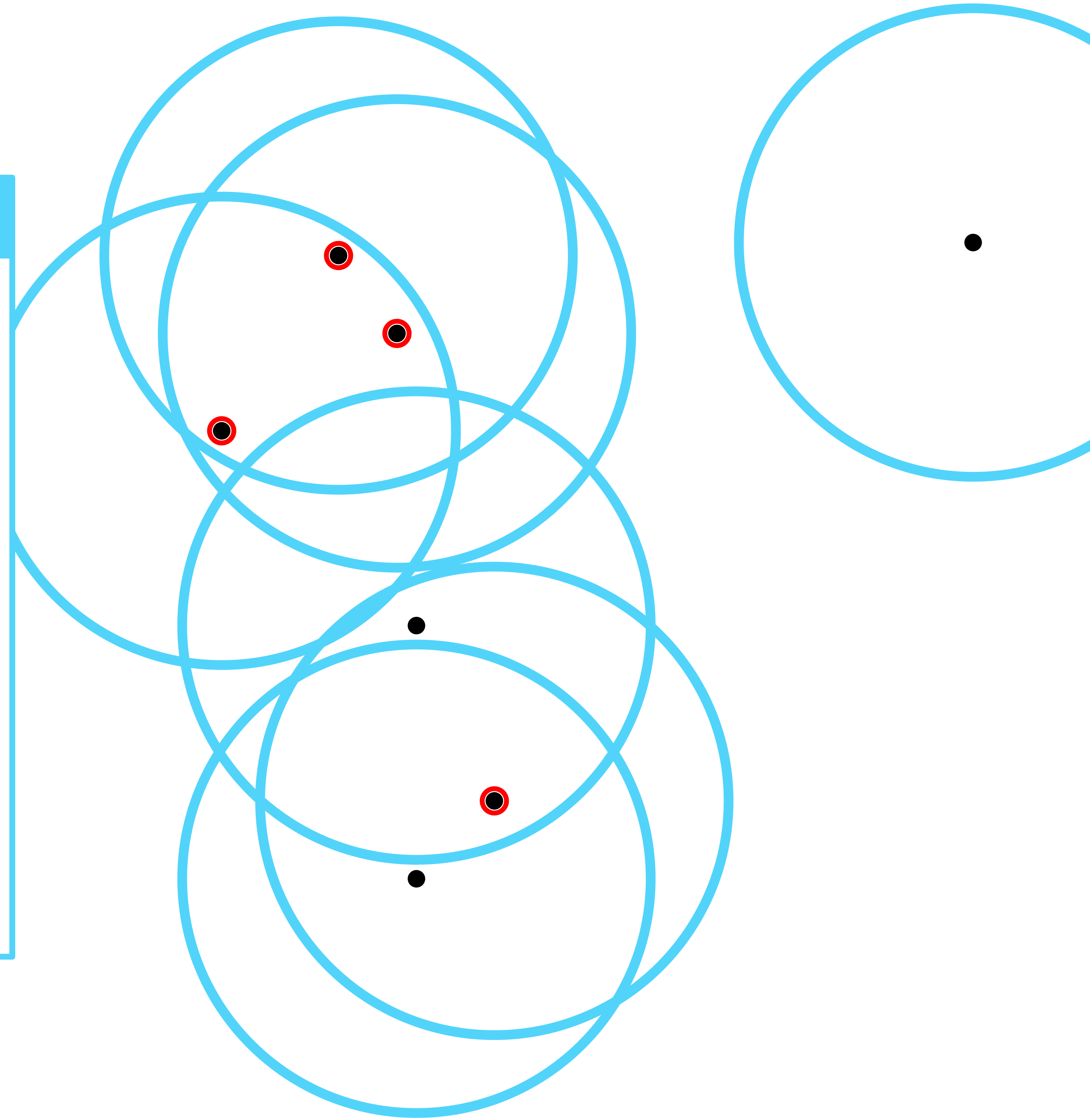

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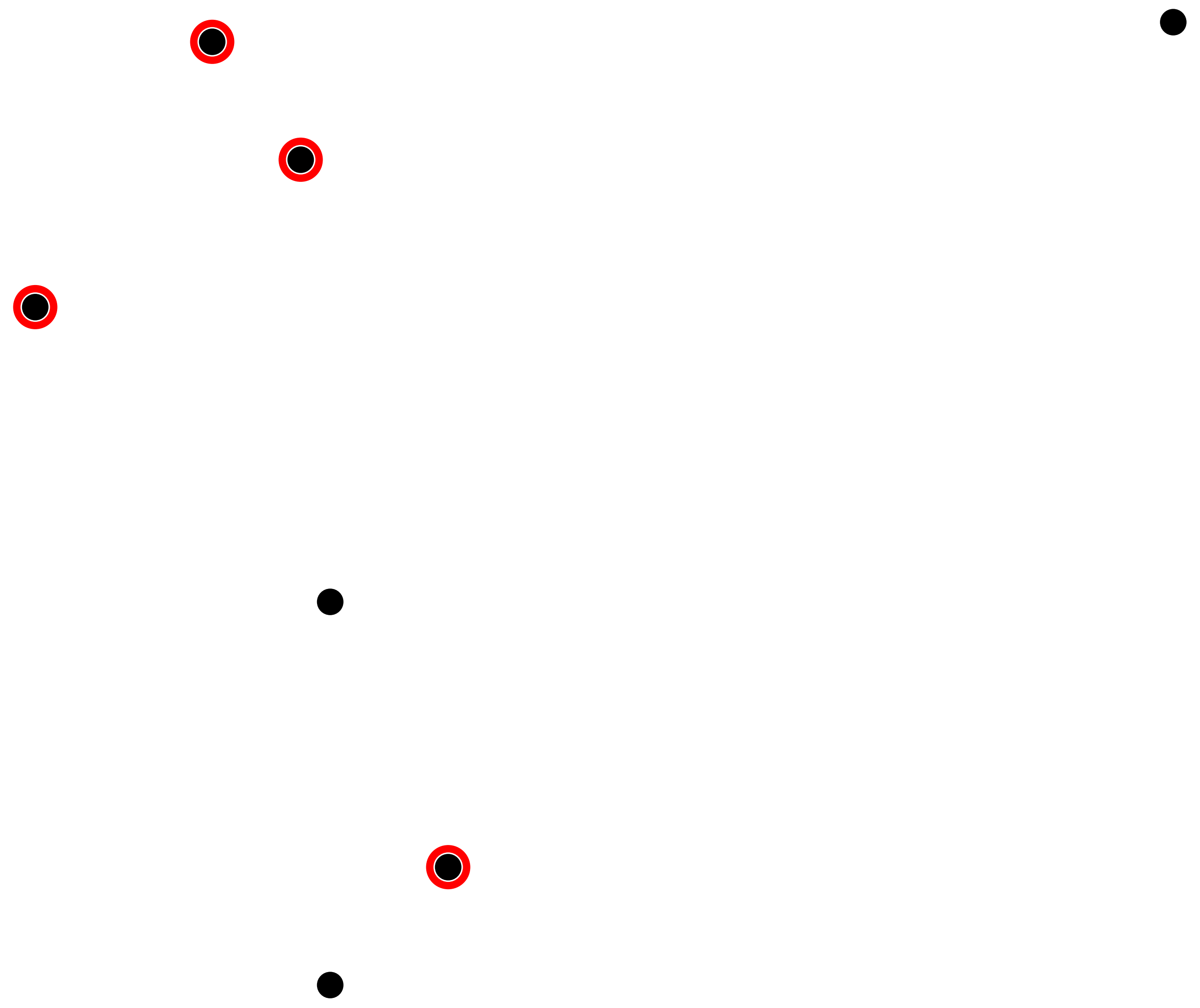

DBSCAN example

Legend

$k = 3$

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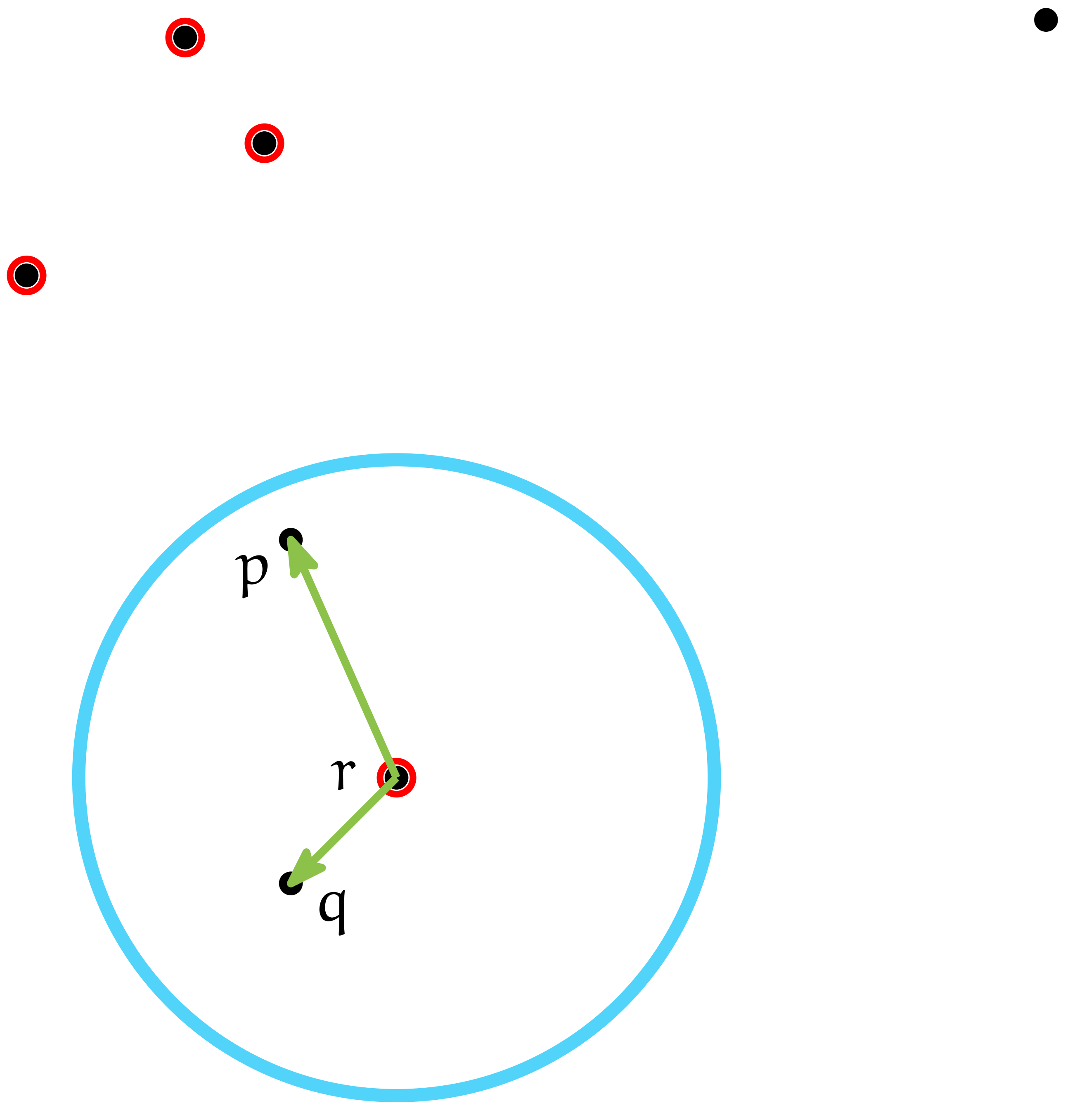
Core points

Density connected



DBSCAN example

Legend

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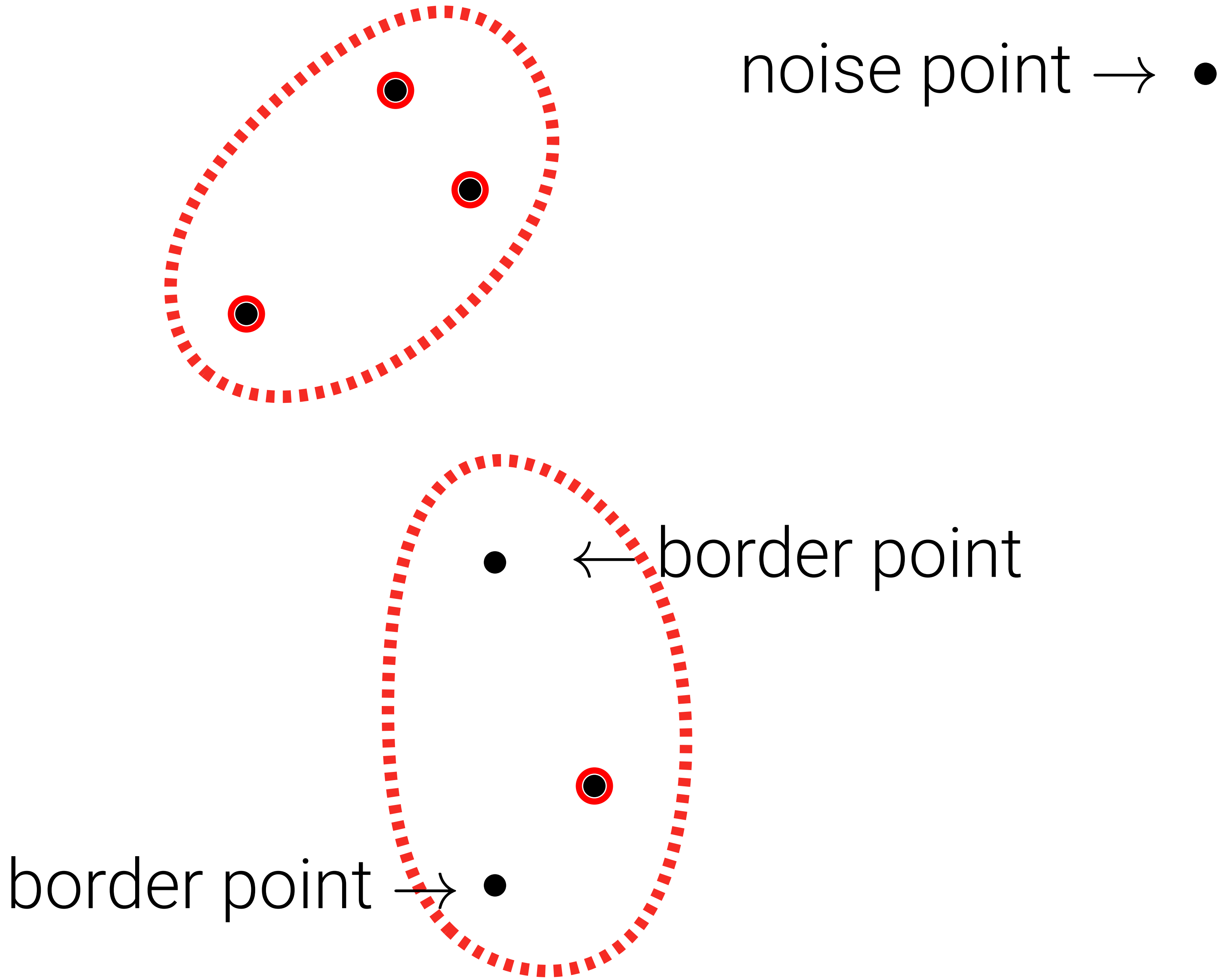
Core points

Density connected

DBSCAN clustering



DBSCAN example

Legend

$k = 3$

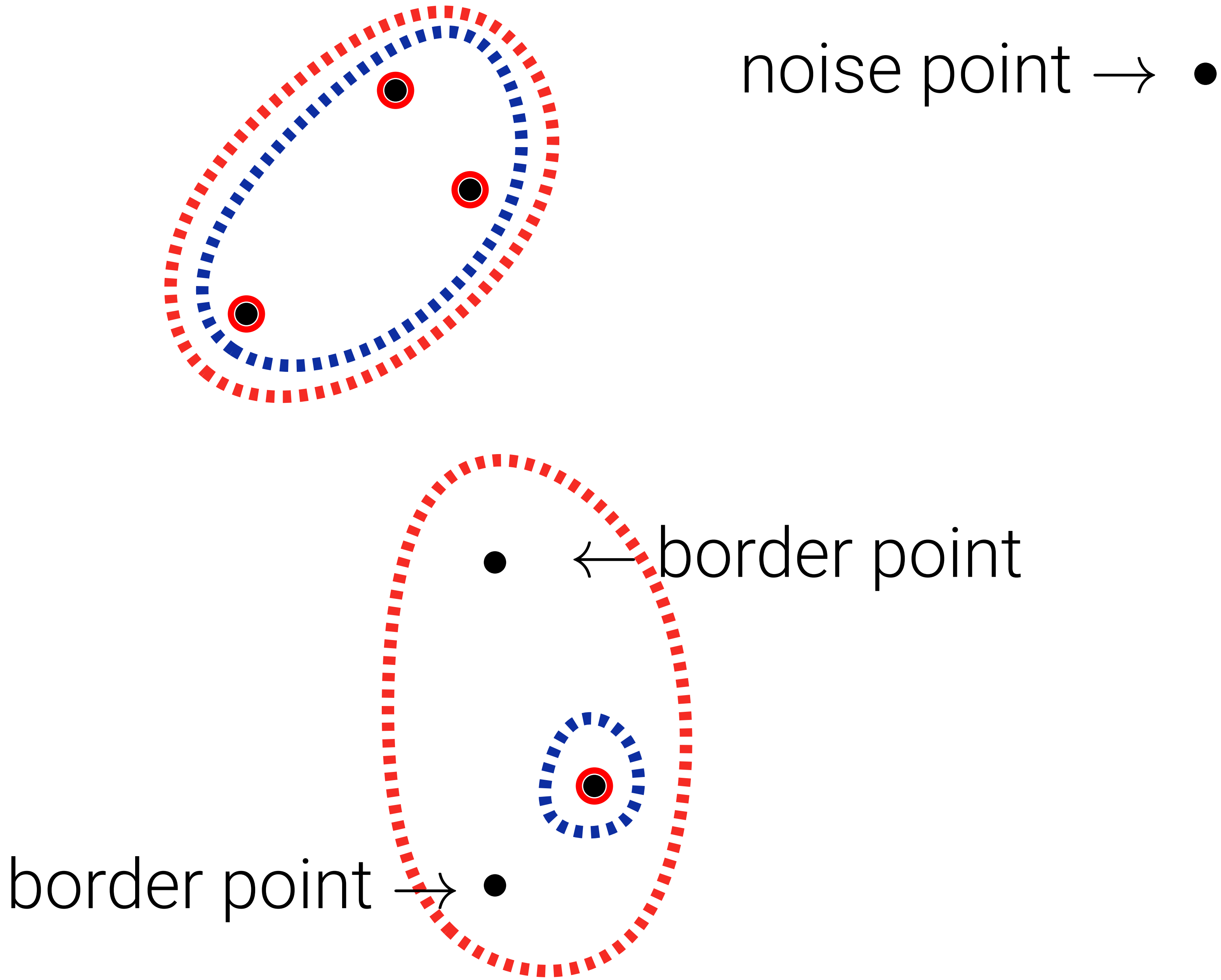
Distance ε

Core points

Density connected

DBSCAN clustering

DBSCAN* clustering



DBSCAN example

Legend

$k = 3$

Distance ε

Core points

Density connected

DBSCAN clustering

DBSCAN* clustering

border

Runtime

Naive algorithm runs in $\mathcal{O}(n^2)$ time.

DBSCAN example

Legend

$k = 3$

Distance ε

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DBSCAN clustering

DBSCAN* clustering

Runtime

Naive algorithm runs in $\mathcal{O}(n^2)$ time.

“Since the Eps-Neighborhoods are expected to be small compared to the size of the whole data space, the average run time complexity of a single region query is $\mathcal{O}(\log n)$. (...) Thus, the average run time complexity of DBSCAN is $\mathcal{O}(n * \log n)$.”

Results

Everywhere: ε free, k fixed constant, Euclidean distances

	2D	dD
DBSCAN	$\mathcal{O}(n \log n)$	$\mathcal{O}(n^{2-\frac{2}{\lceil d/2 \rceil + 1}+\gamma})$ $\gamma > 0$
HDBSCAN	$\mathcal{O}(n \log n)$ expected	$\times$

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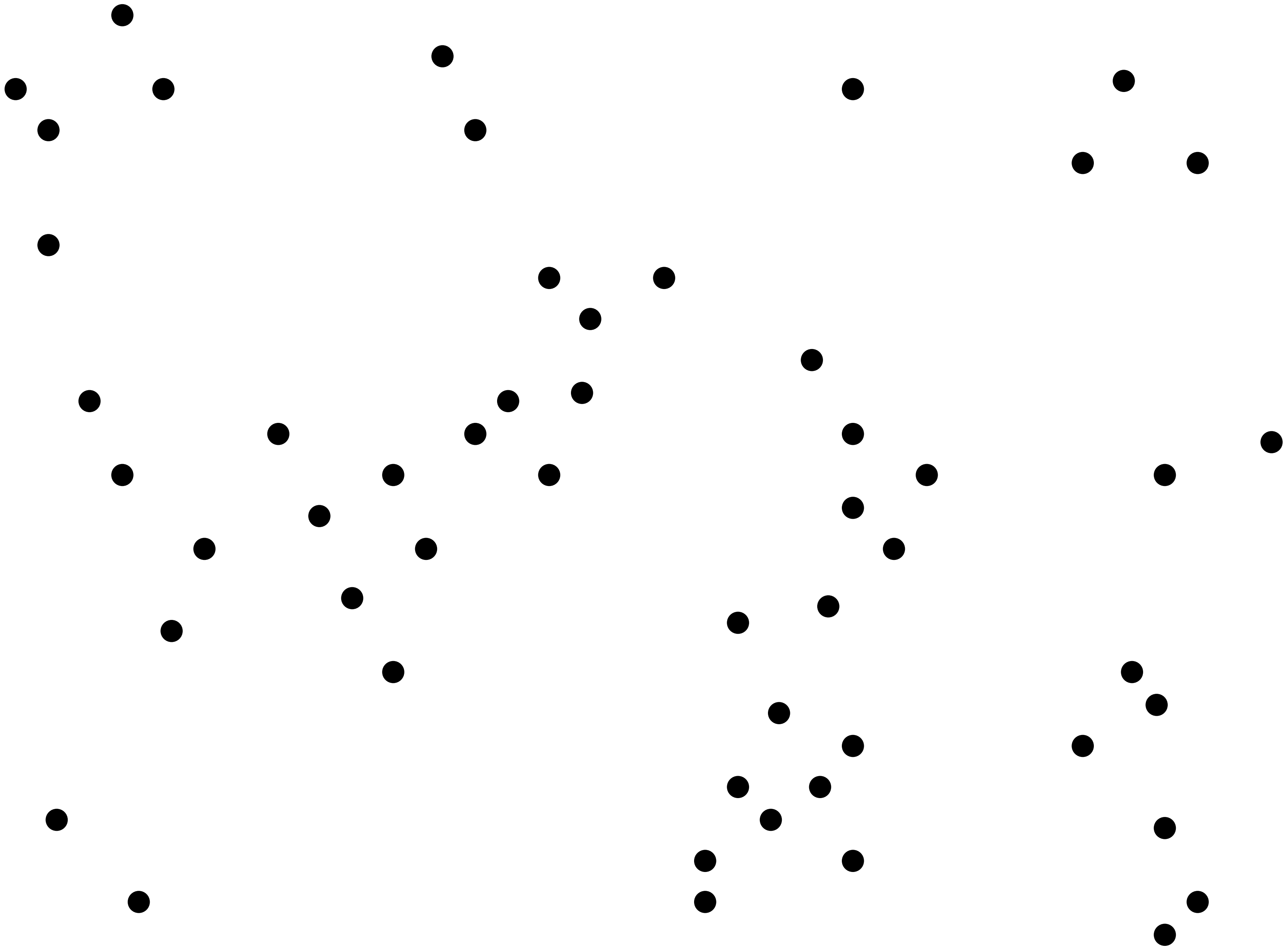
Box graph $\mathcal{G}_{\text{box}}$



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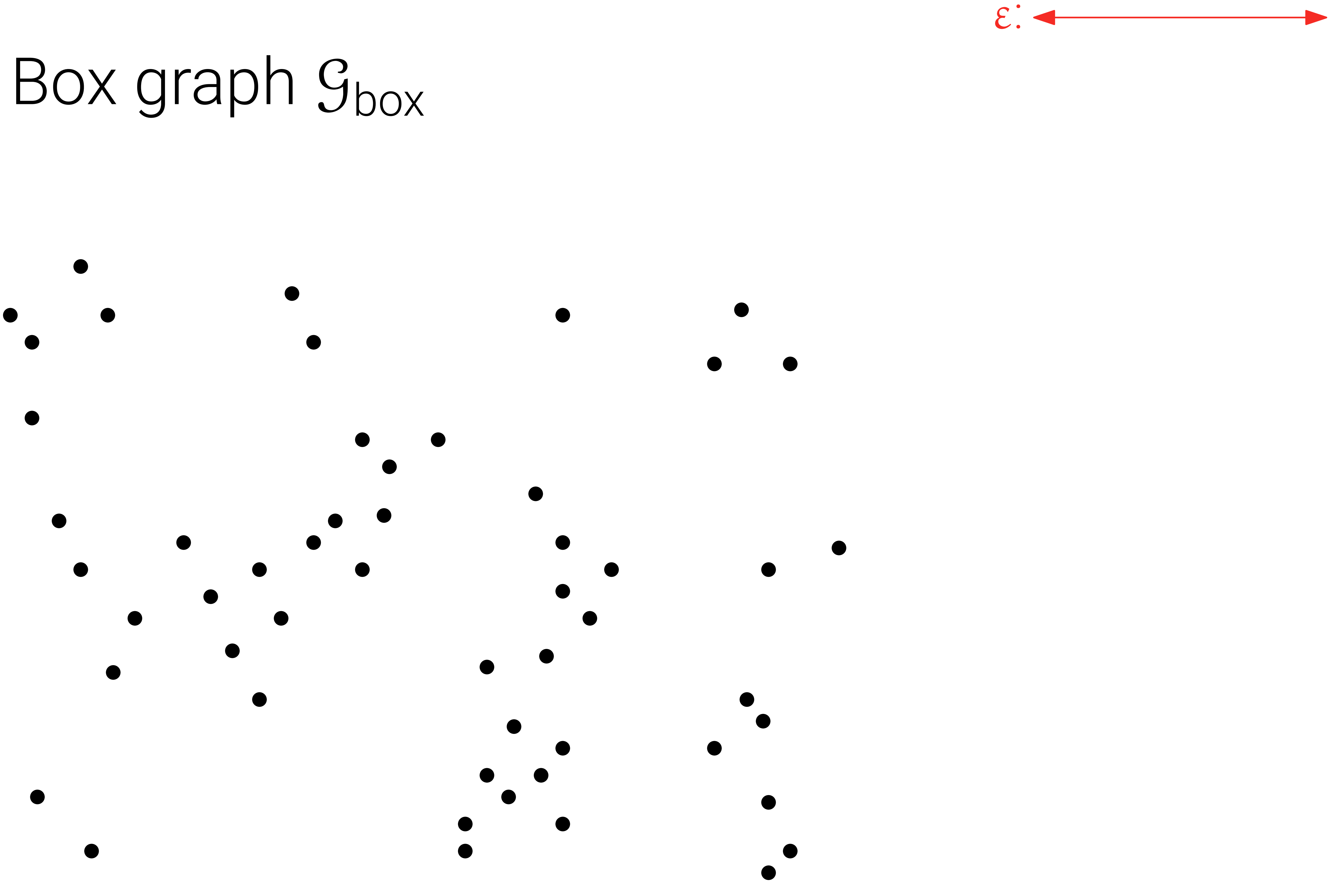

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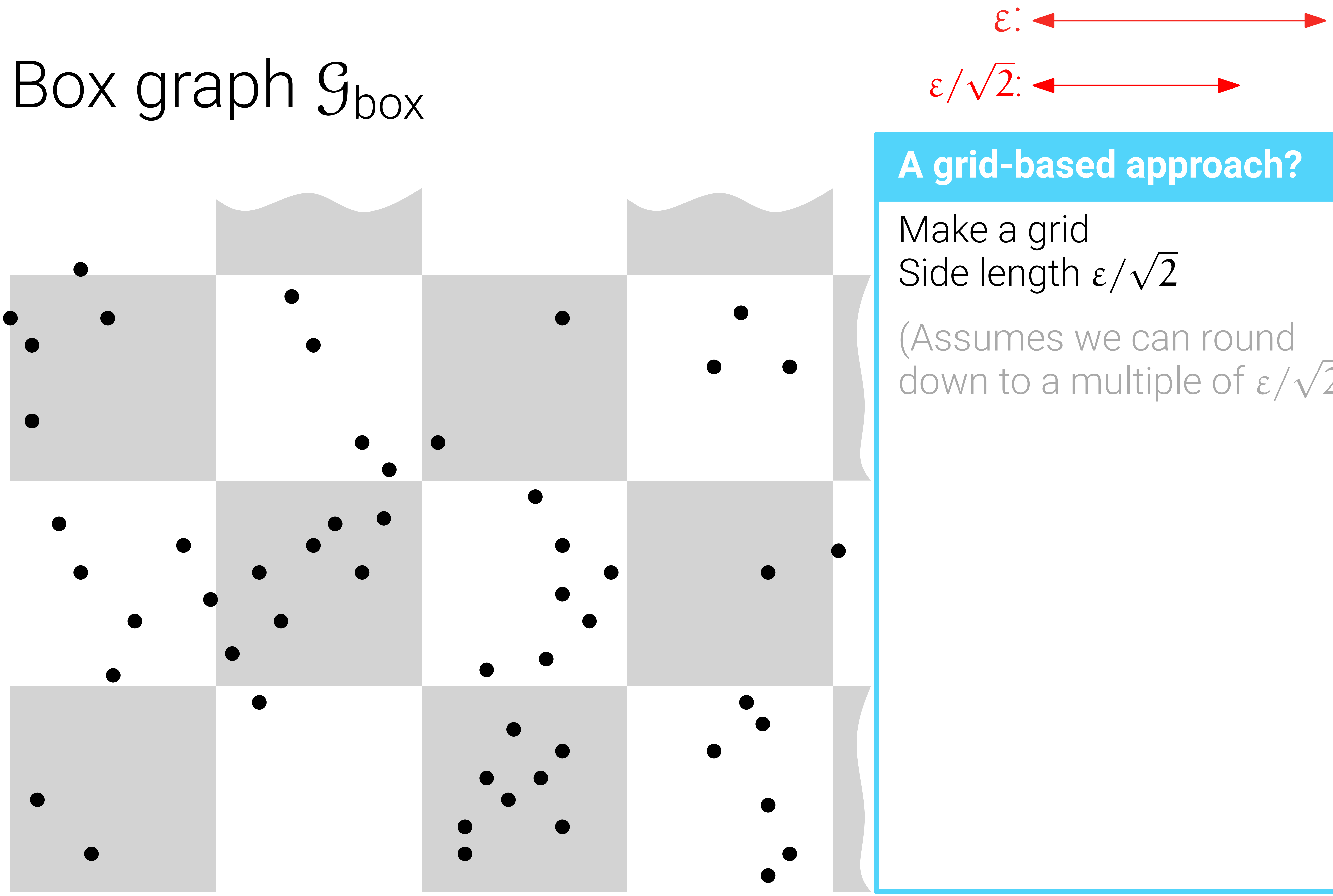

A grid-based approach?

Make a grid
Side length $\varepsilon/\sqrt{2}$

(Assumes we can round down to a multiple of $\varepsilon/\sqrt{2}$)

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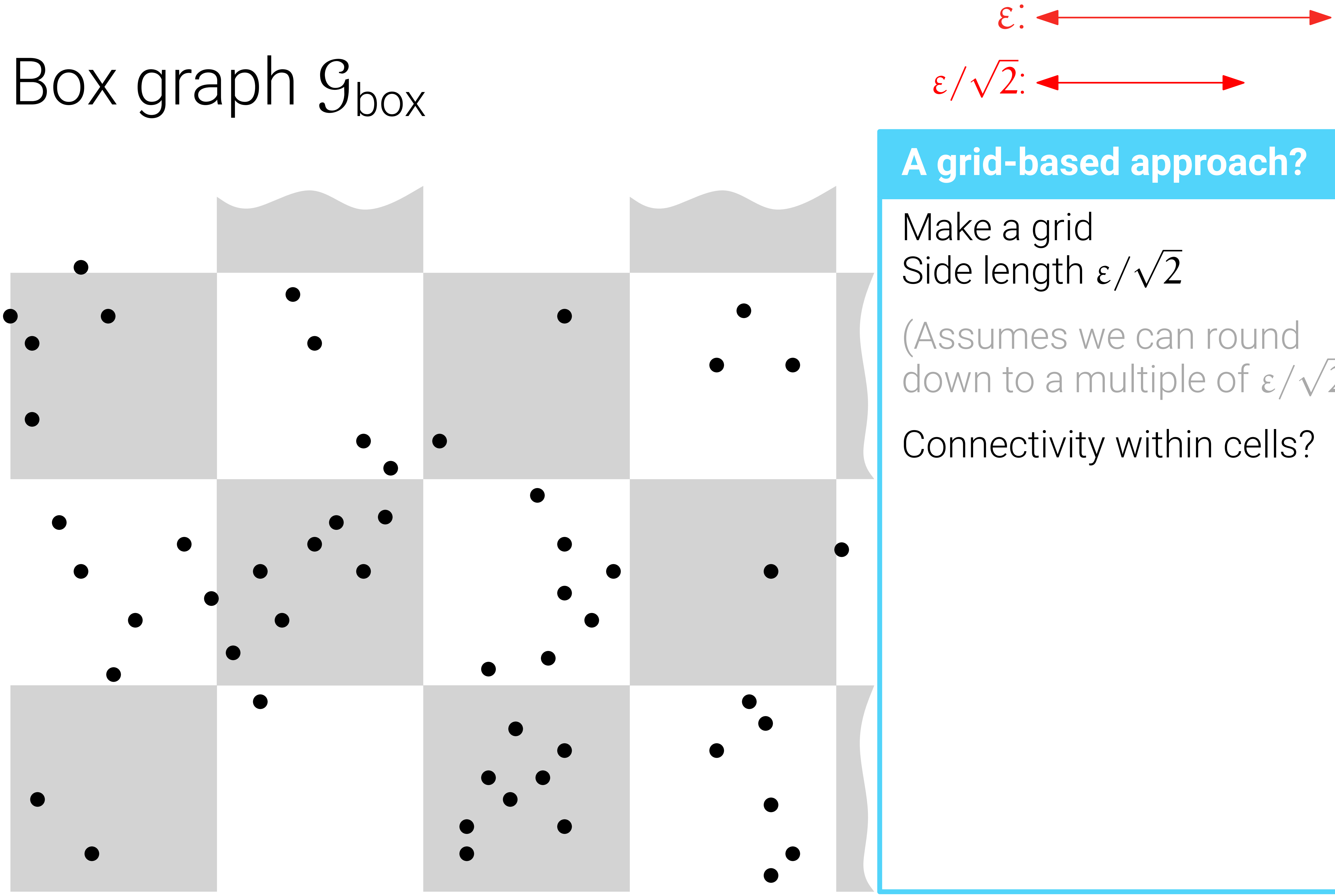

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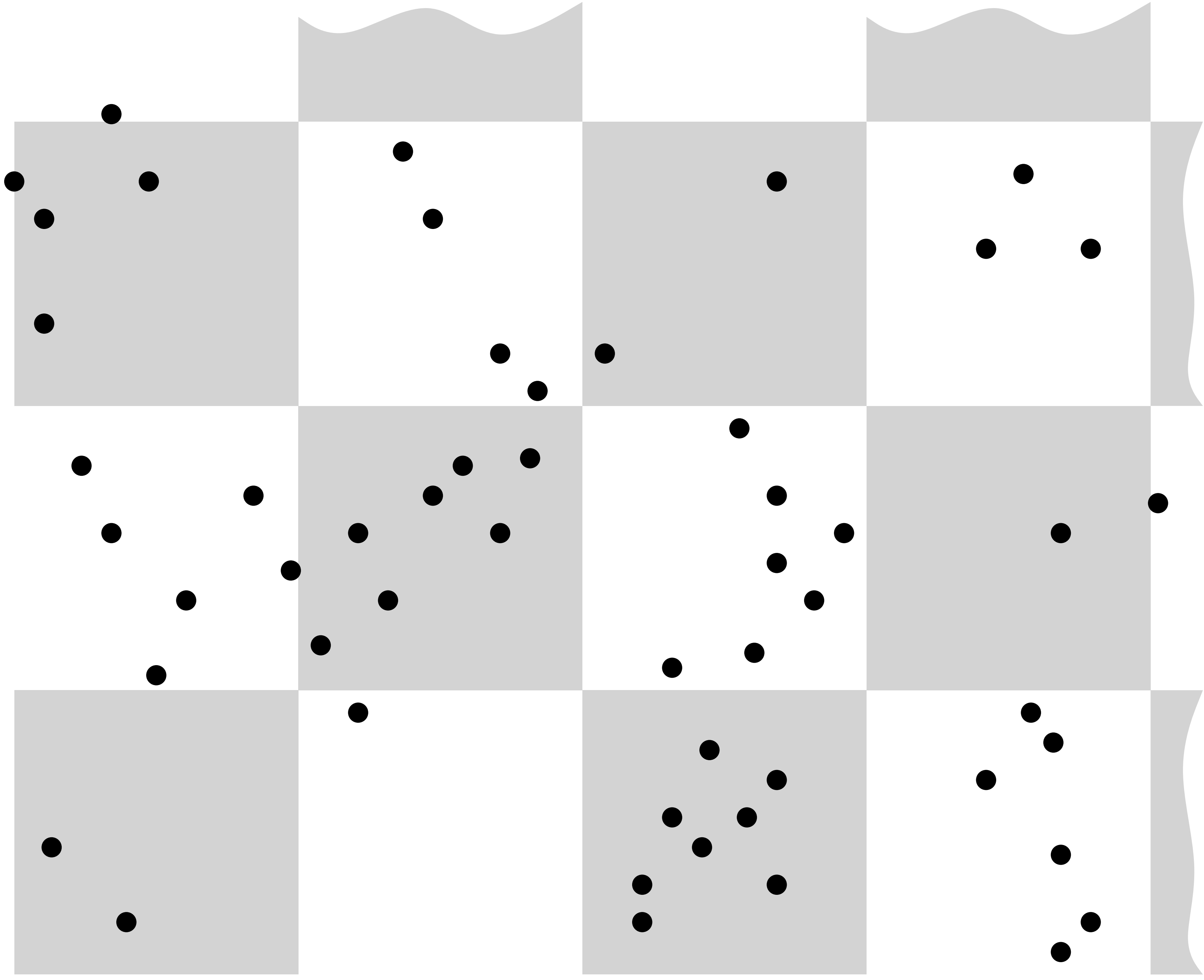

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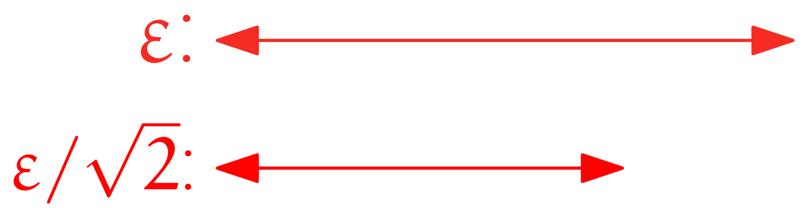

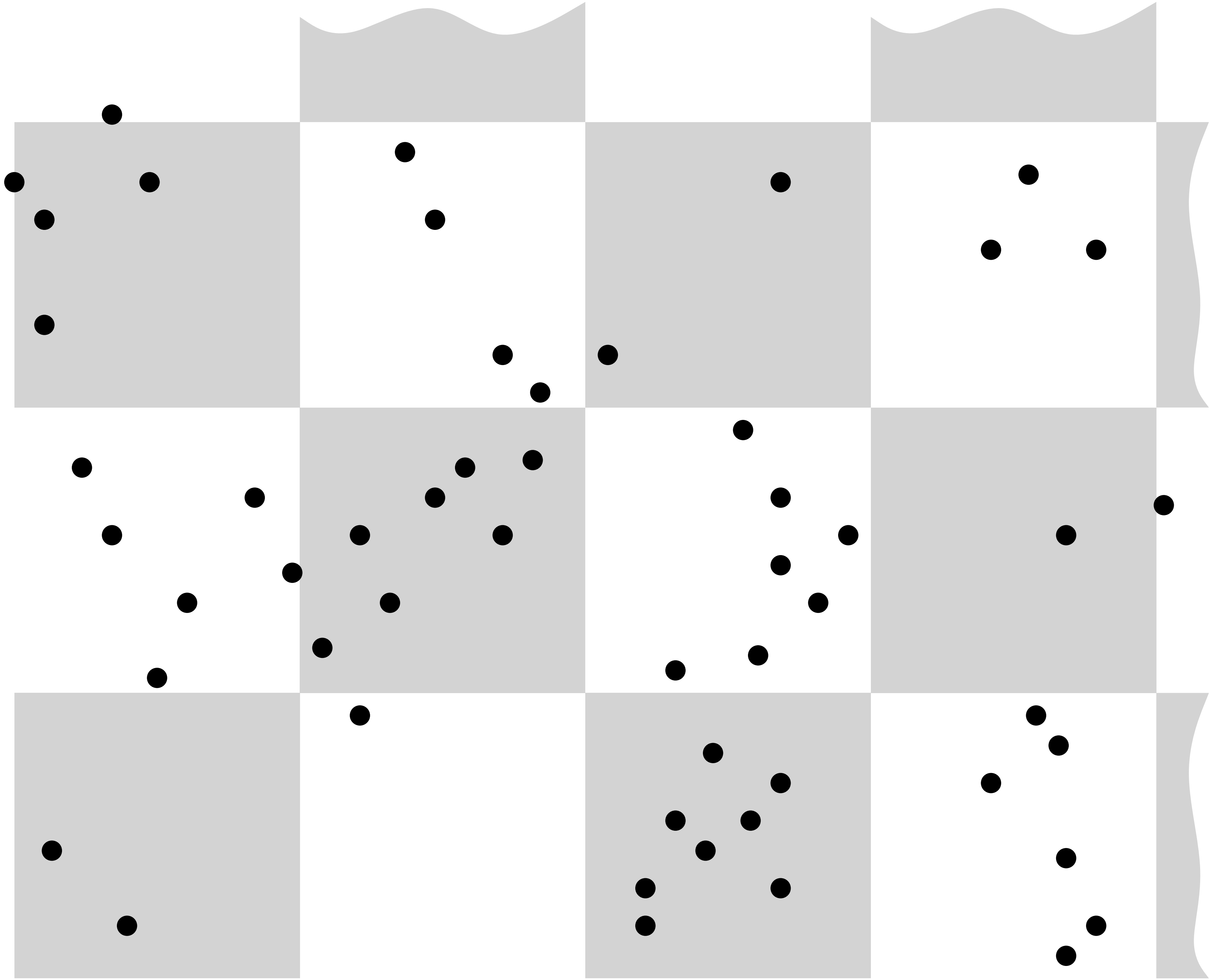

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Not clear how to get a runtime bound in n without assumption on the distribution.

Be more flexible...

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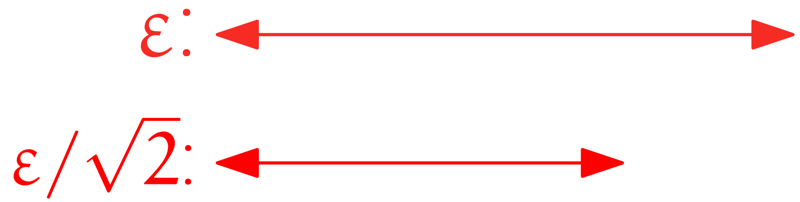

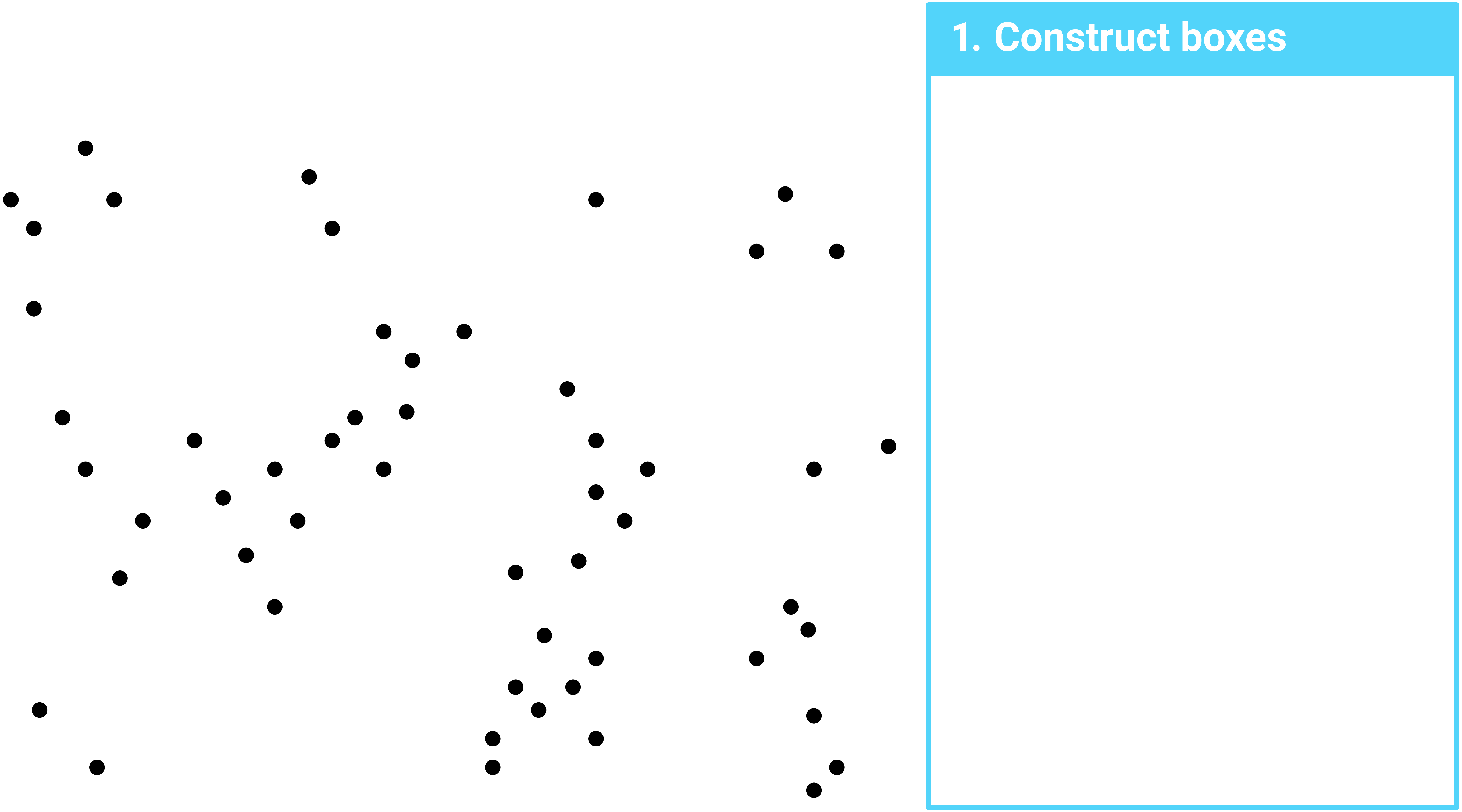

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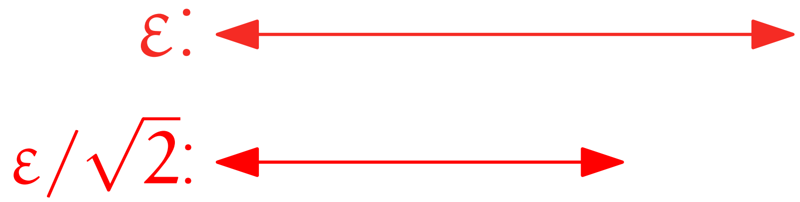
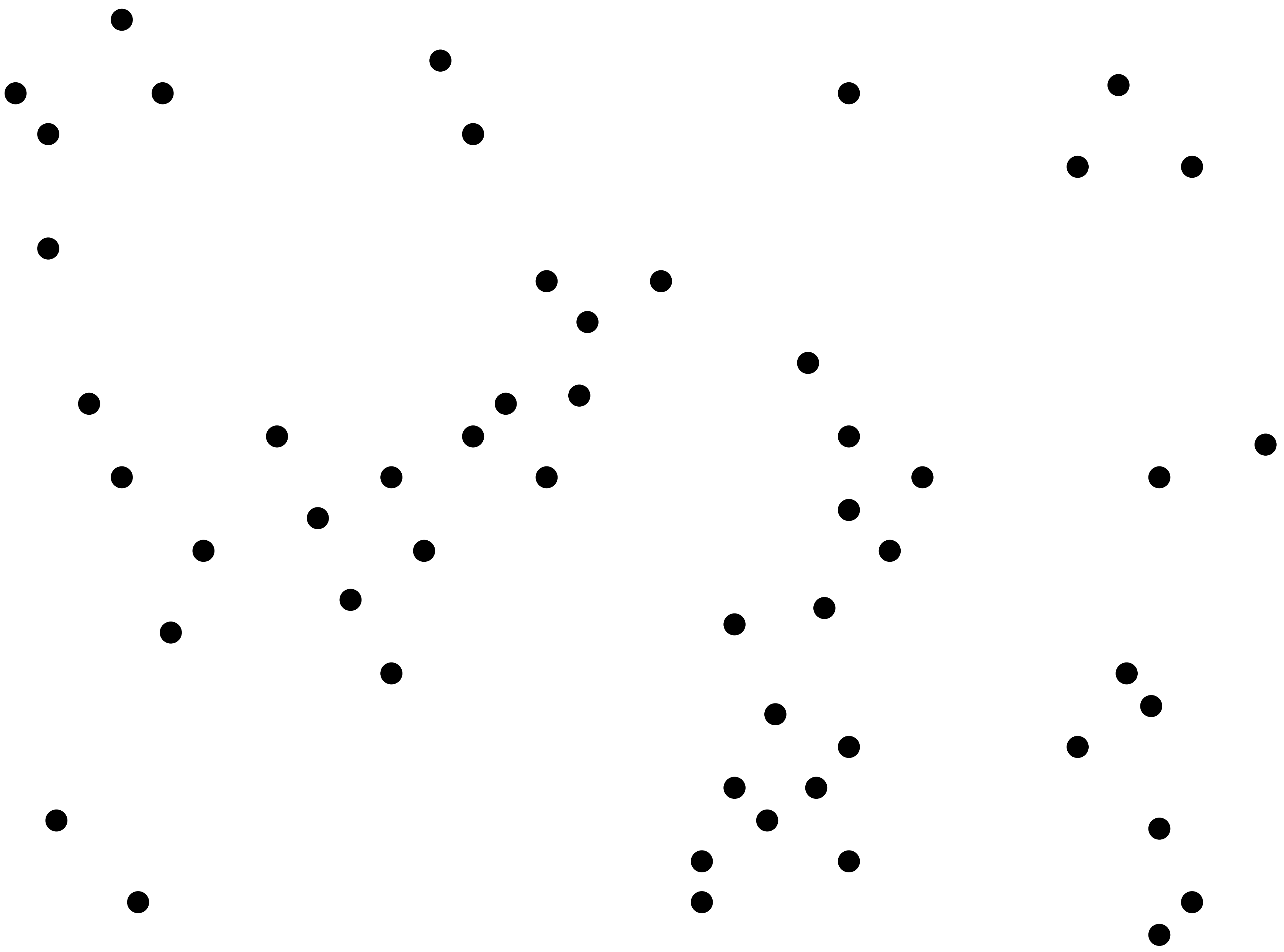
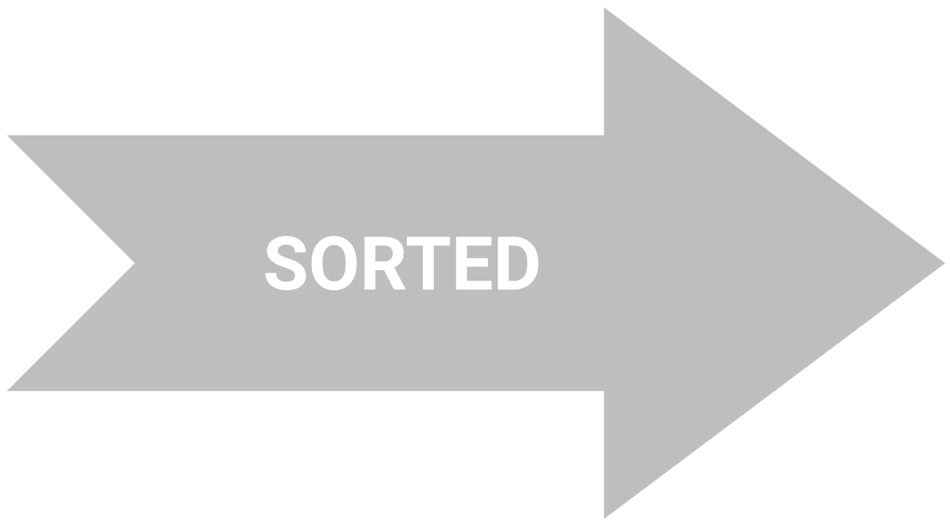




1. Construct boxes

Add points as long as strip width $\leqslant \varepsilon/\sqrt{2}$.



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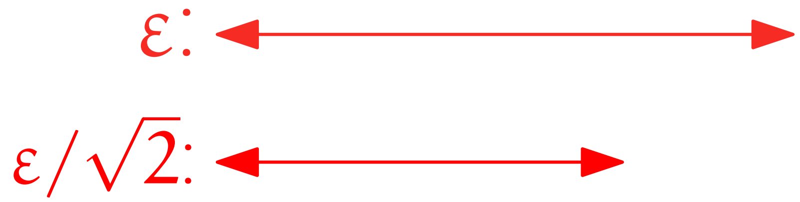

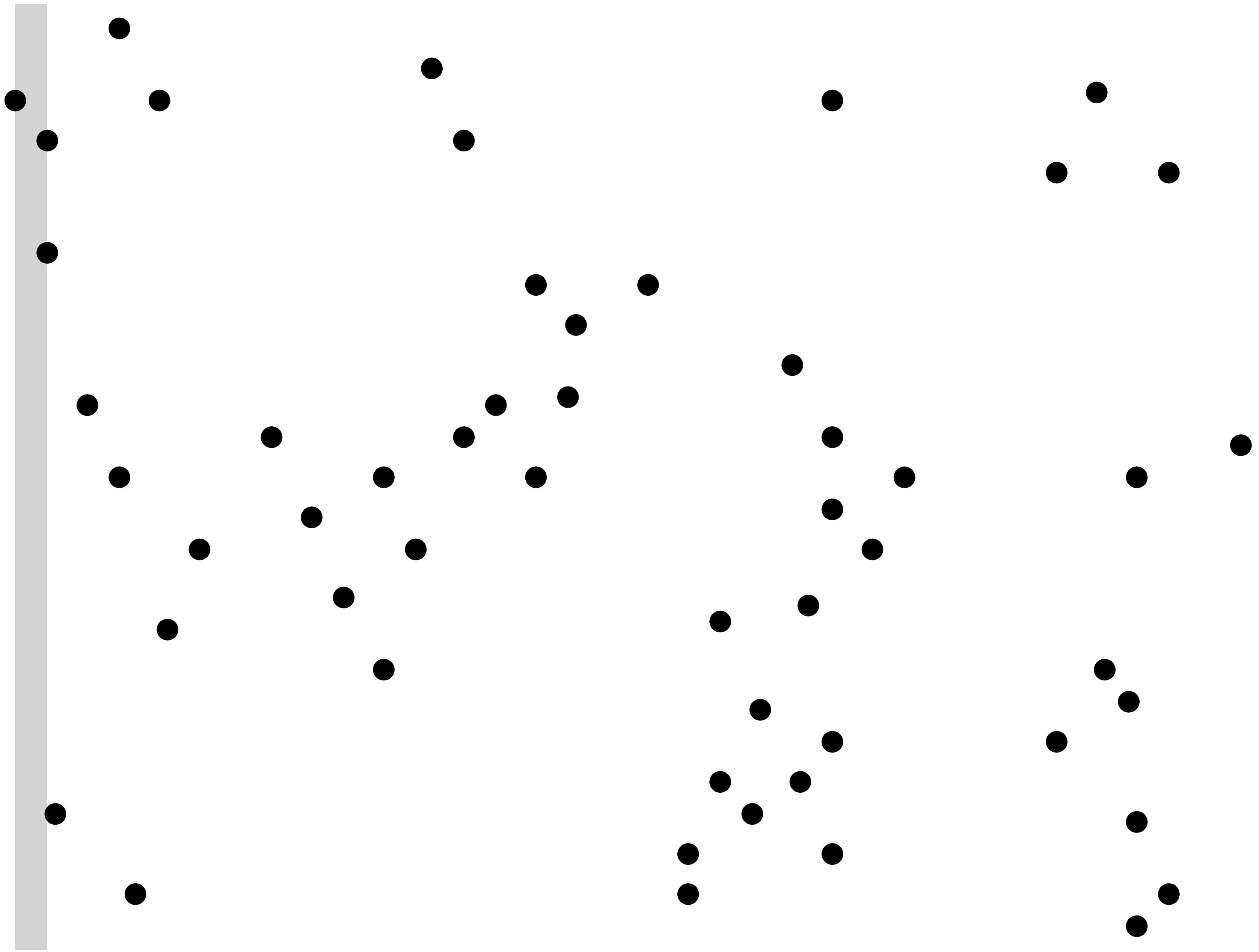

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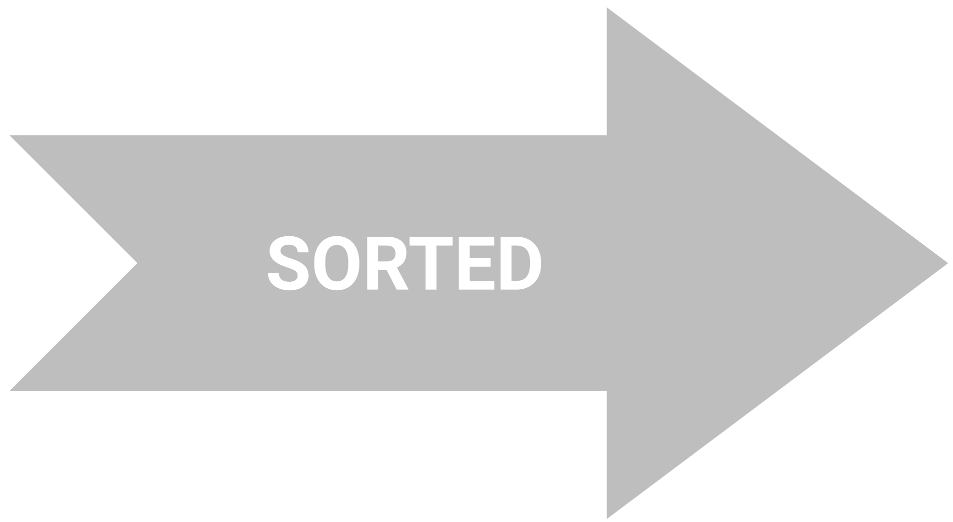

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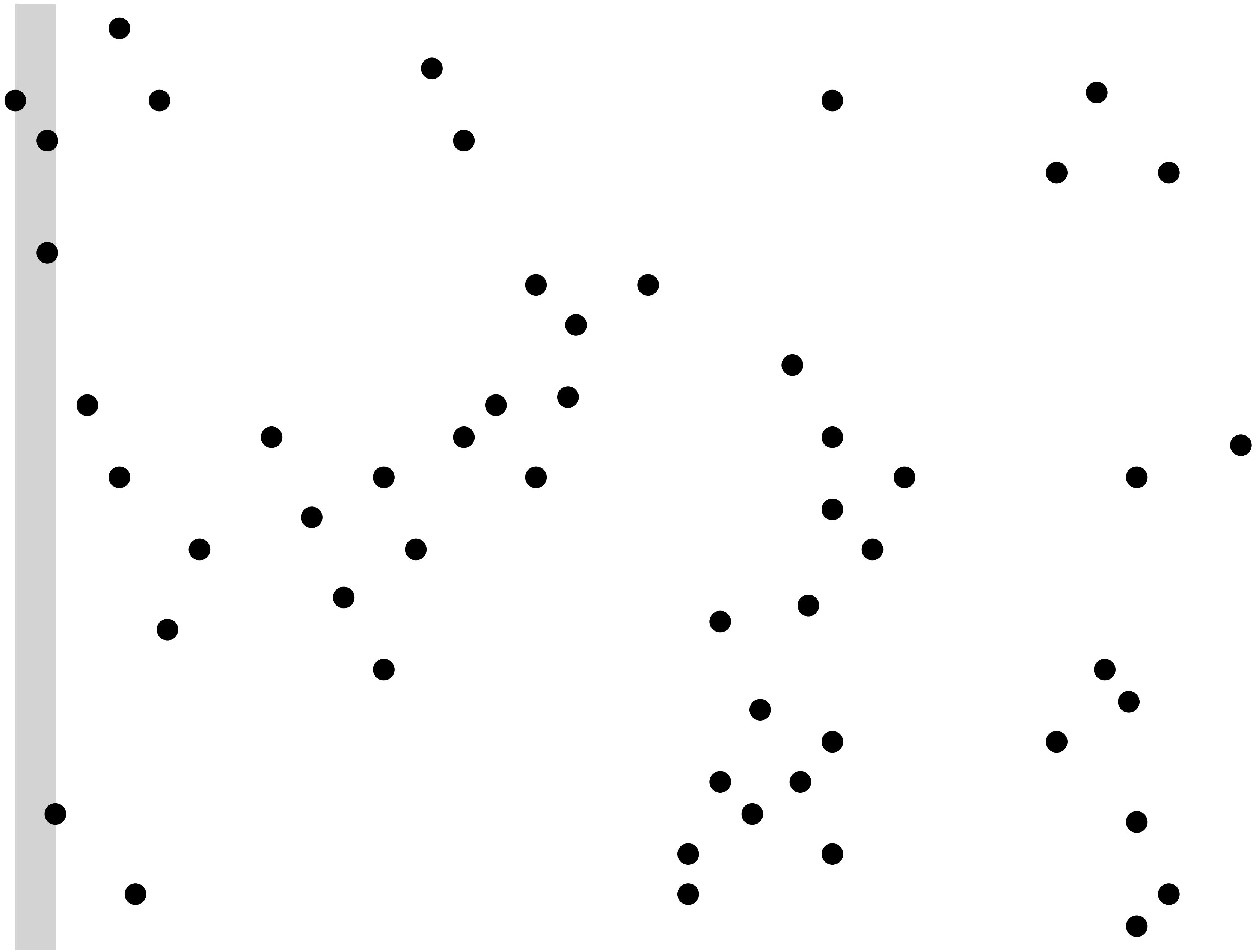

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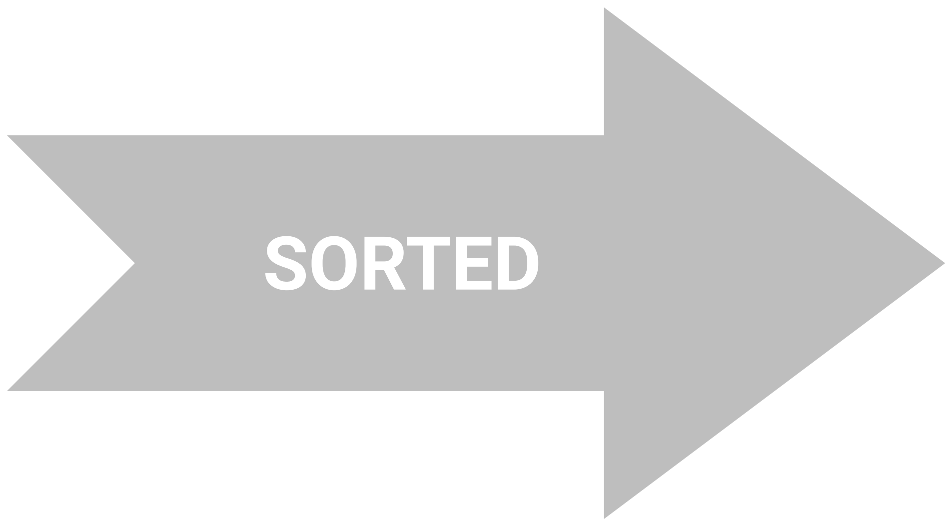

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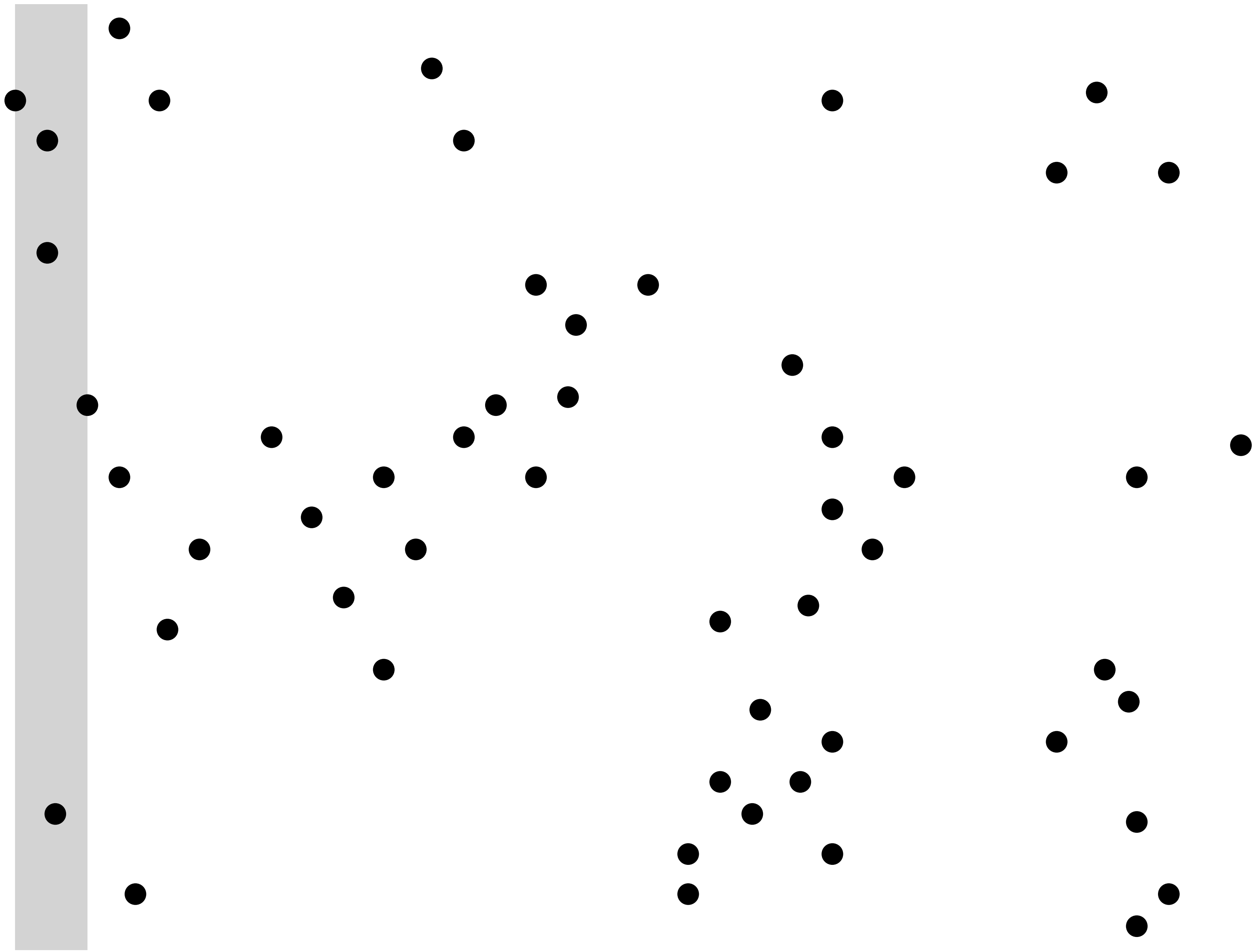

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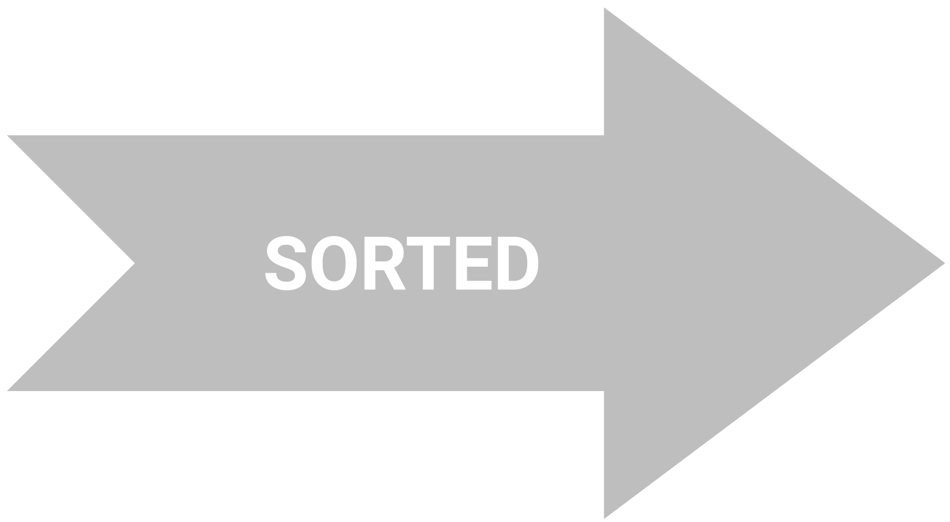

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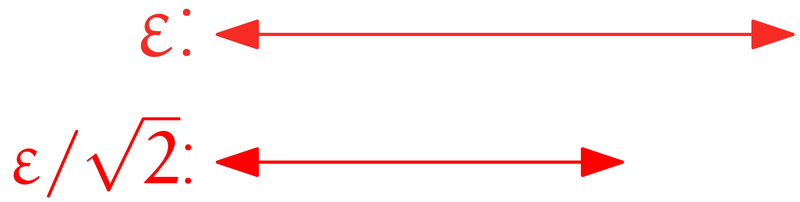

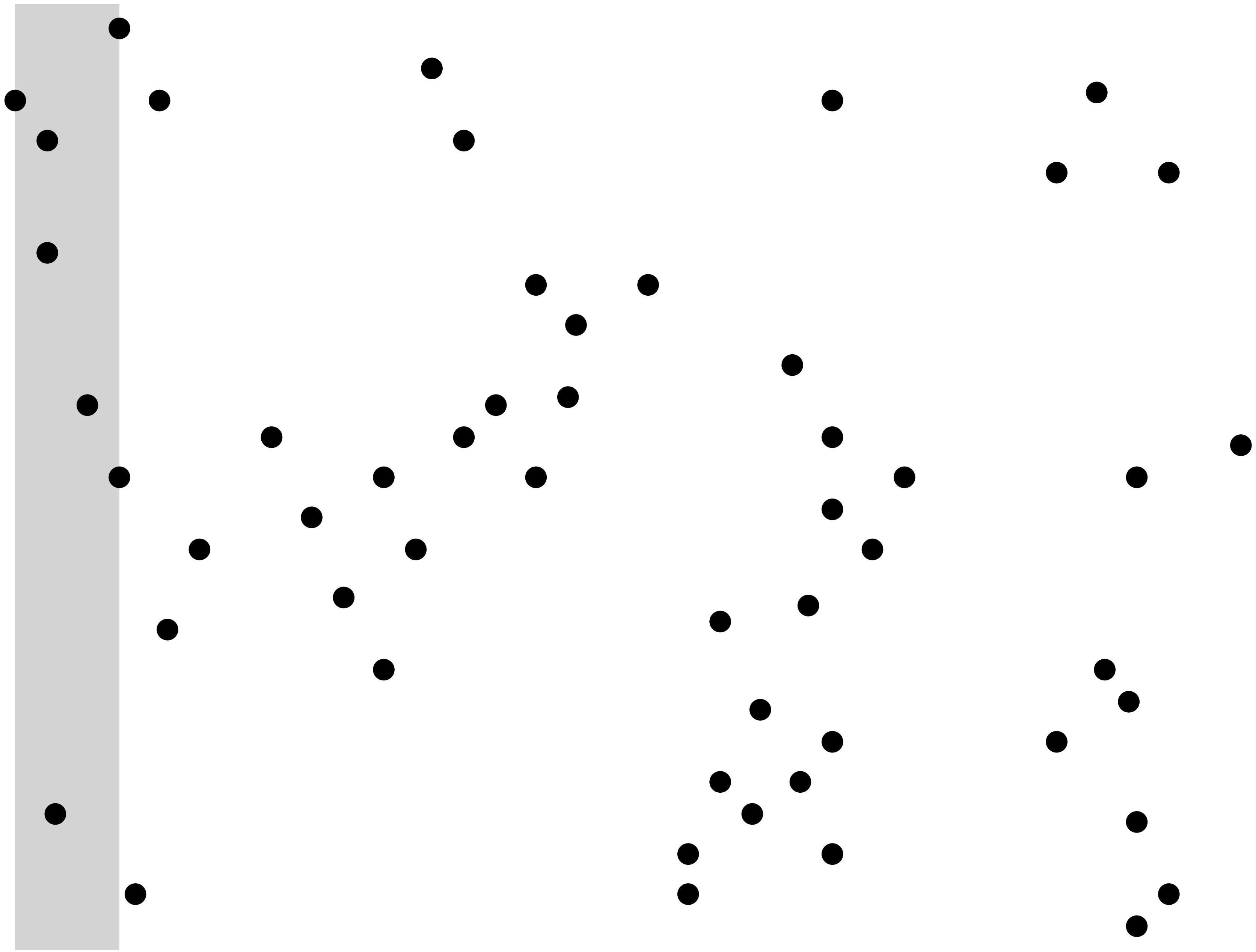

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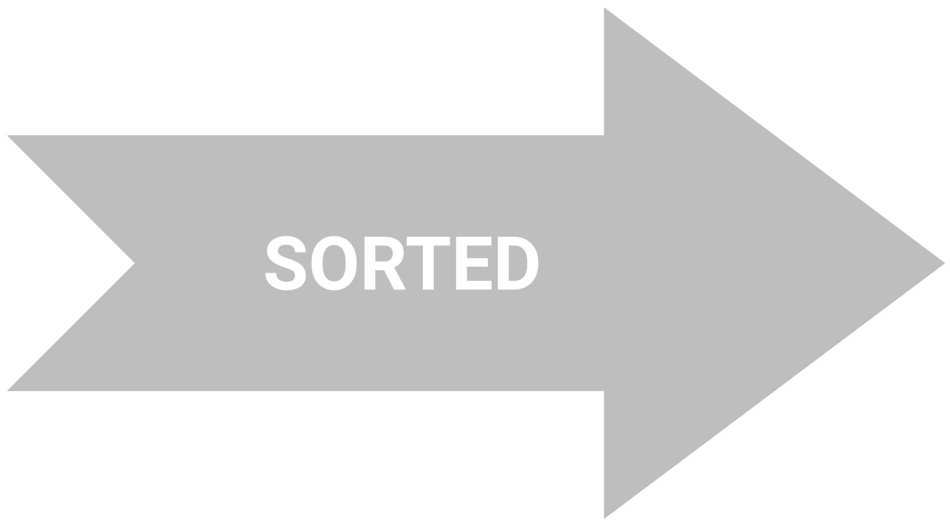

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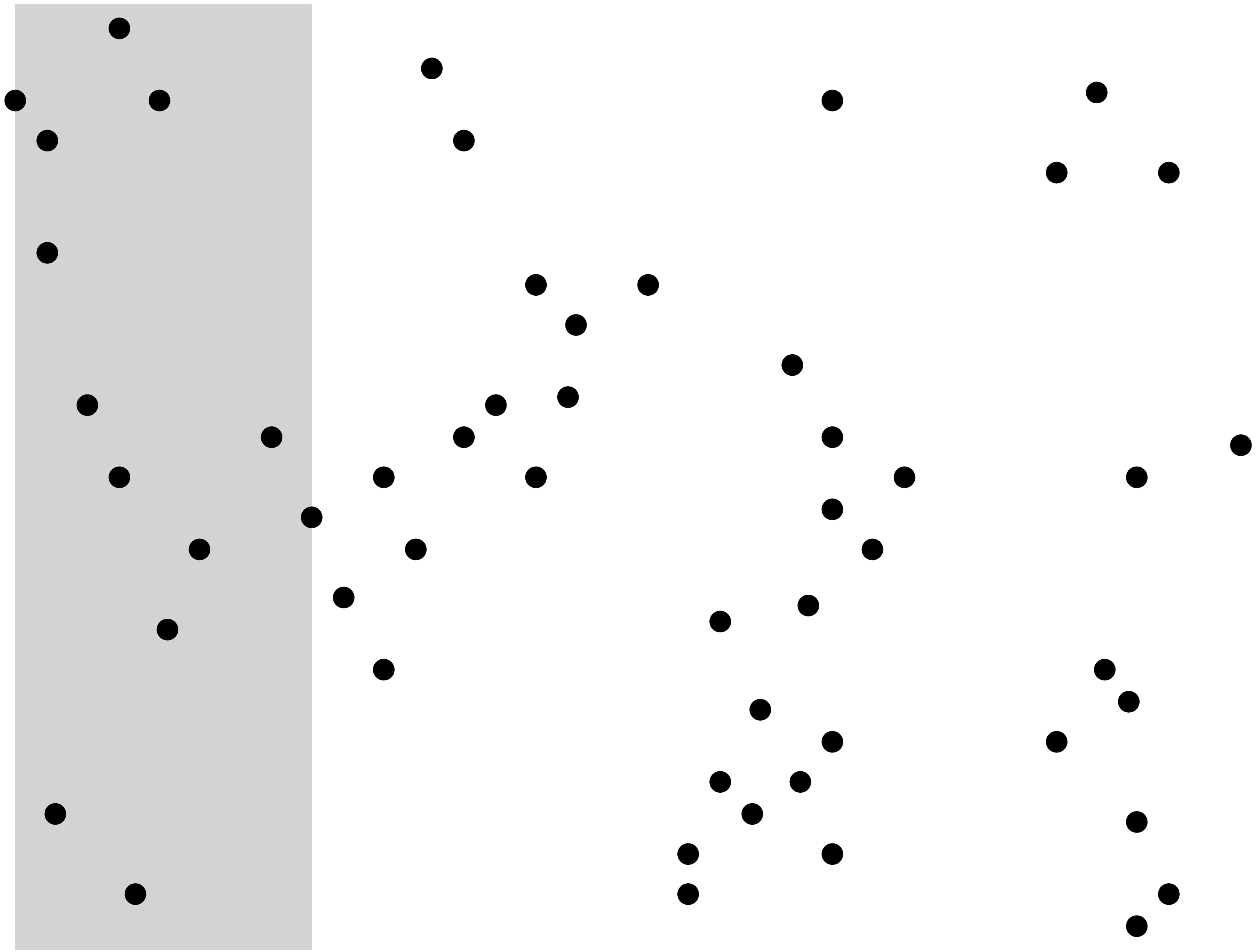

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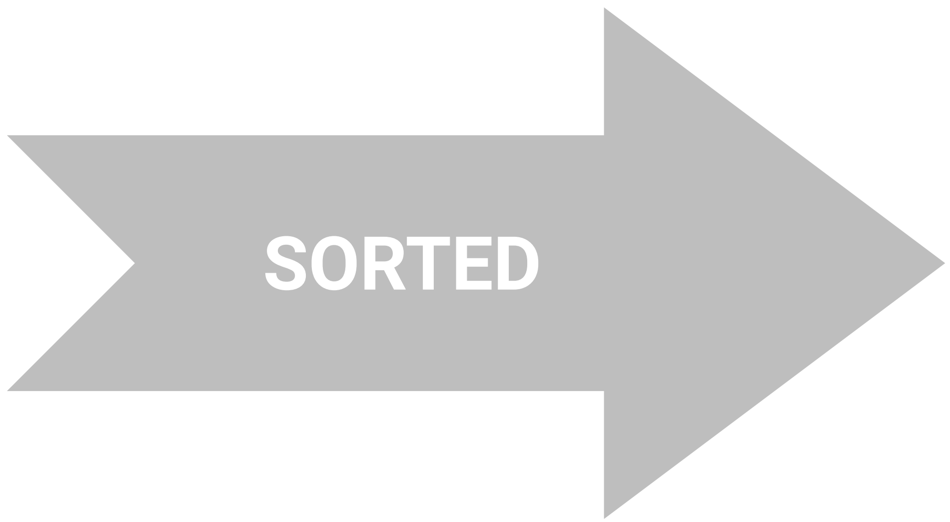

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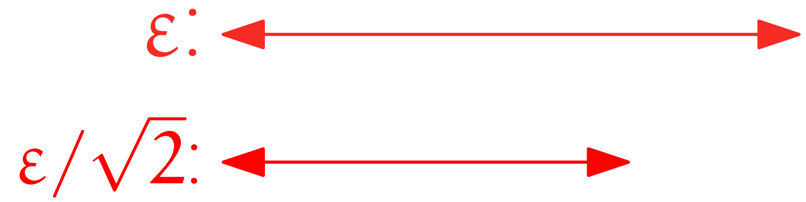

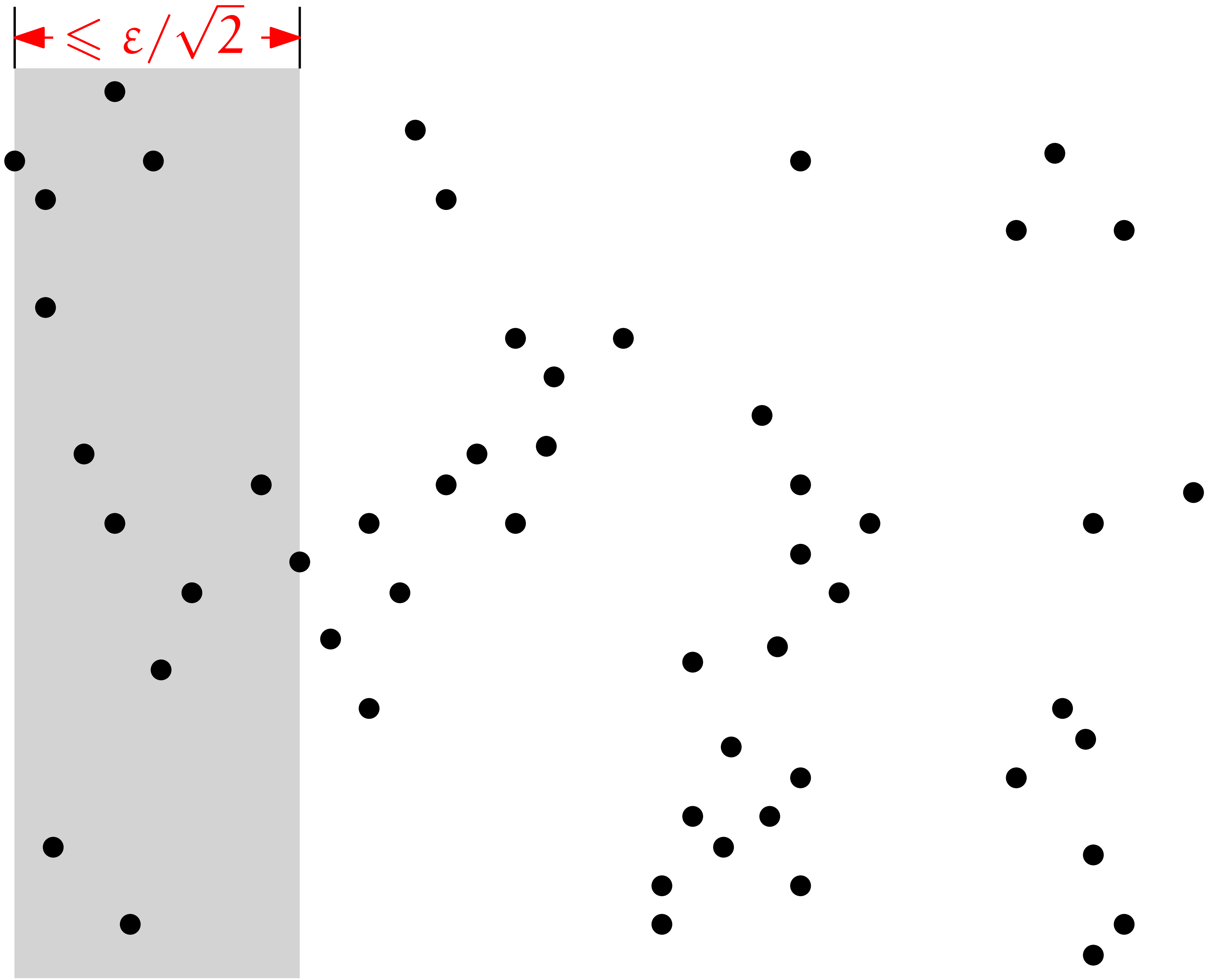

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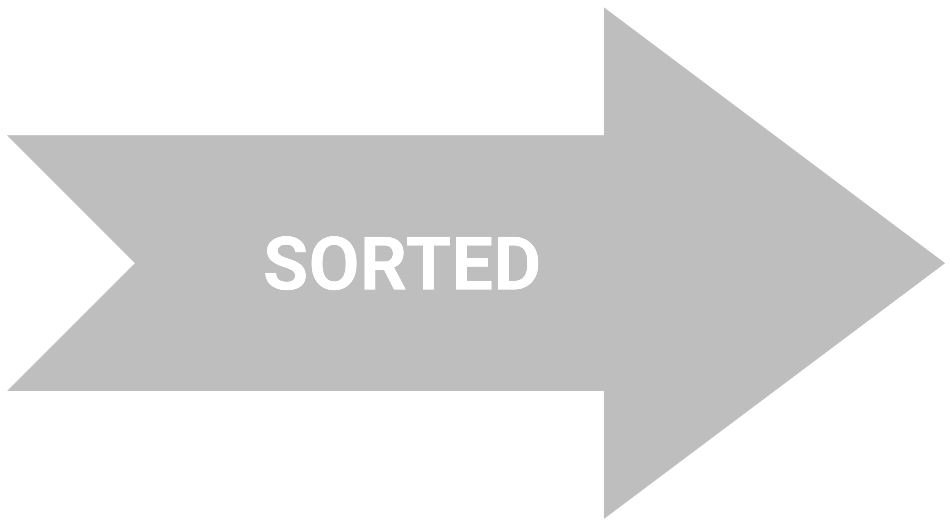

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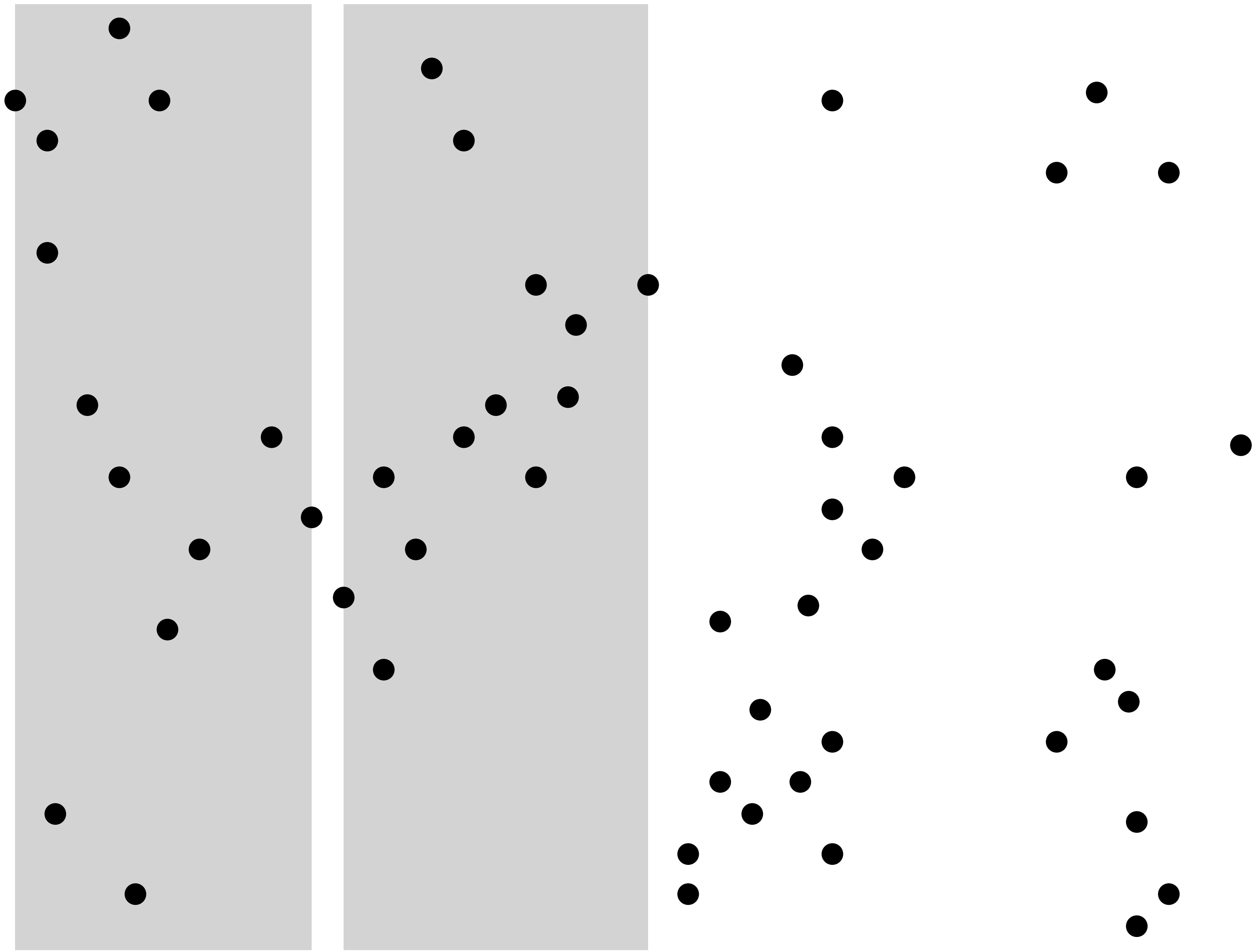

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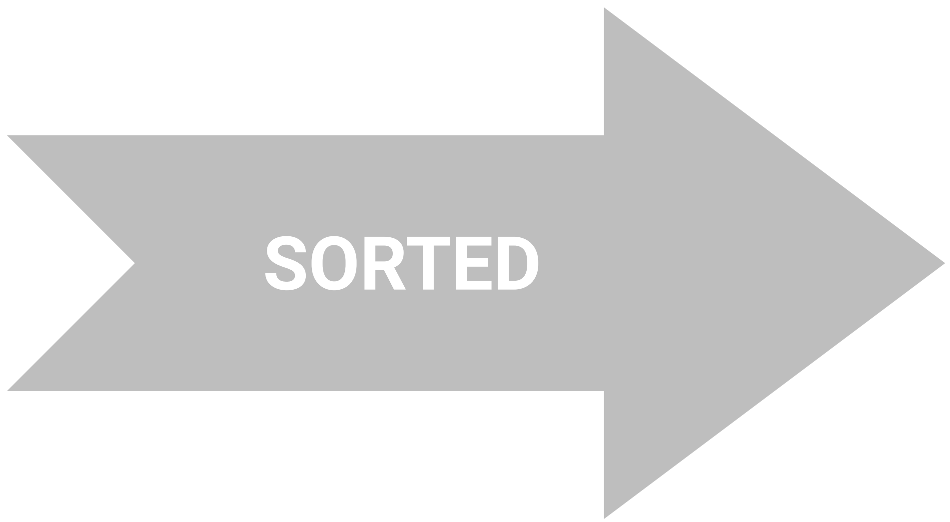

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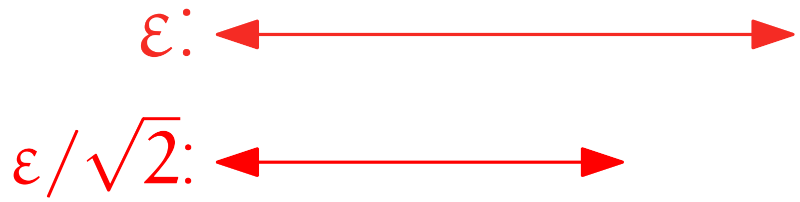
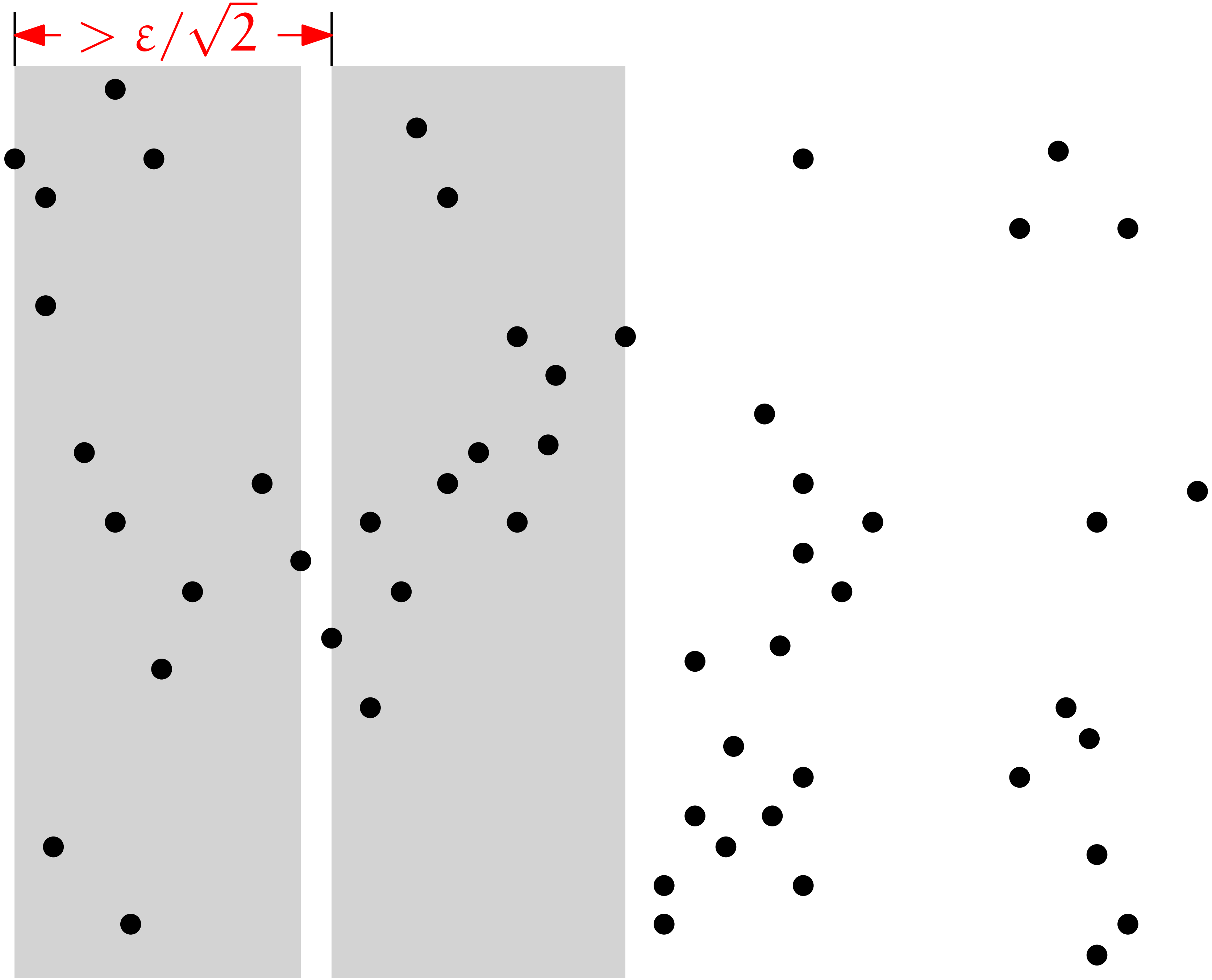
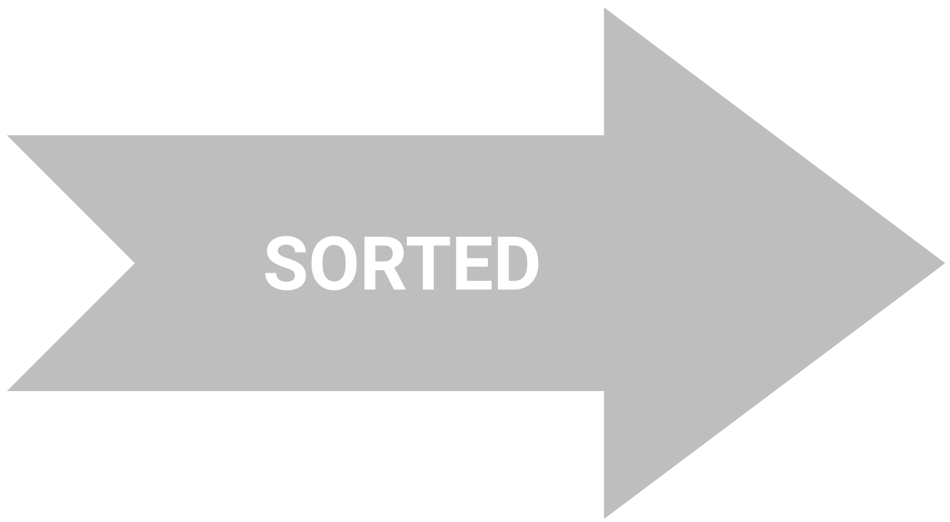




1. Construct boxes

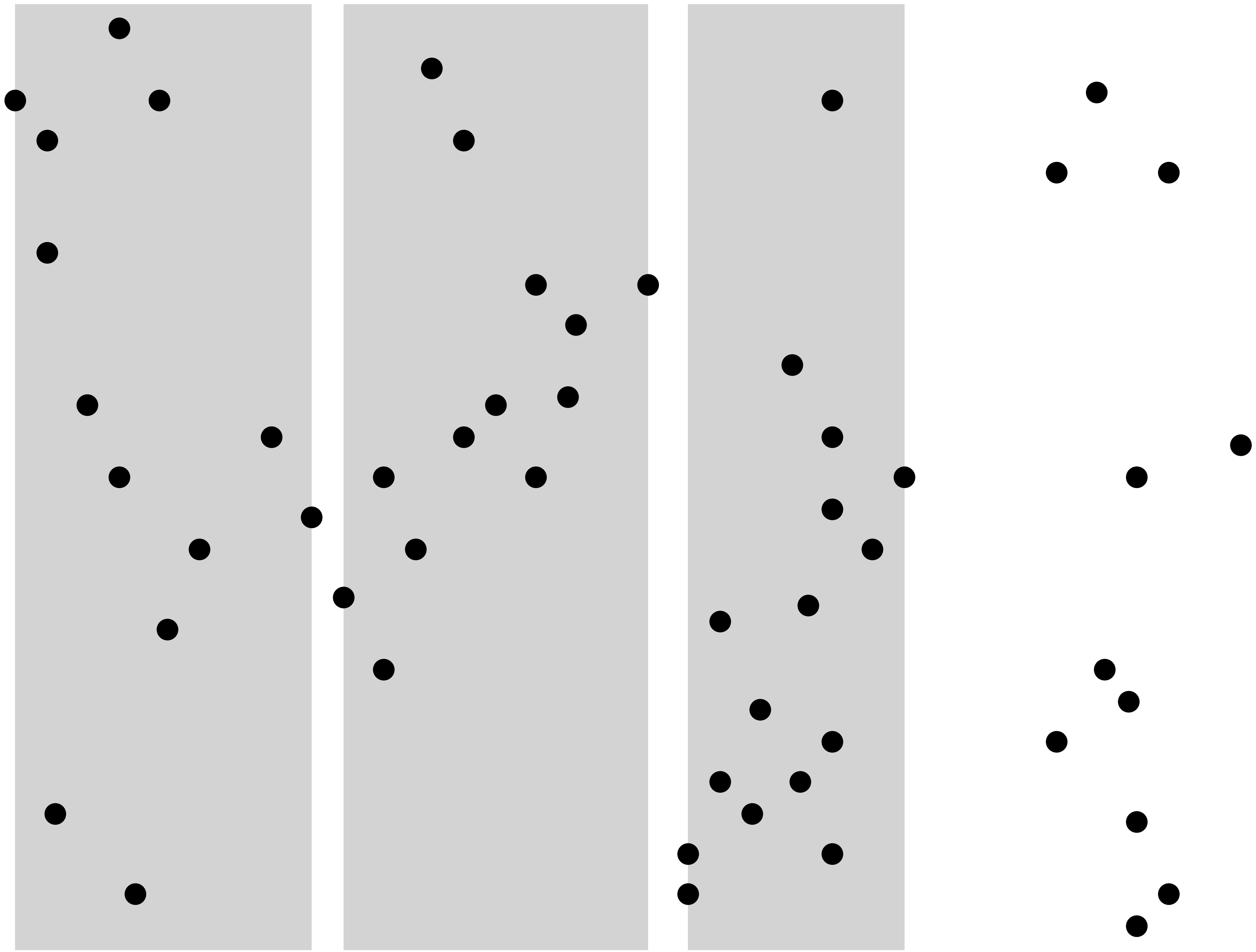
Add points as long as strip width $\leqslant \varepsilon/\sqrt{2}$.



Box graph $\mathcal{G}_{\text{box}}$

ε:

$\varepsilon/\sqrt{2}$:



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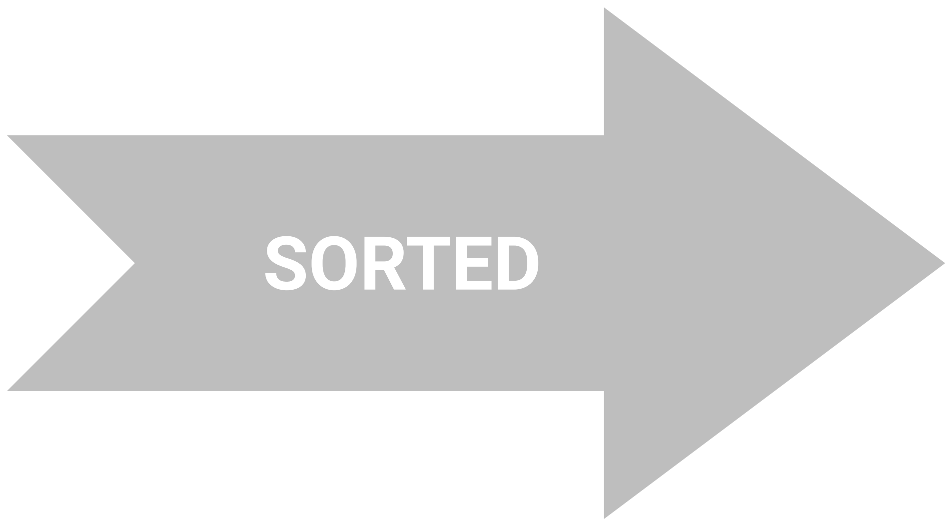

Box graph $\mathcal{G}_{\mathrm{box}}$

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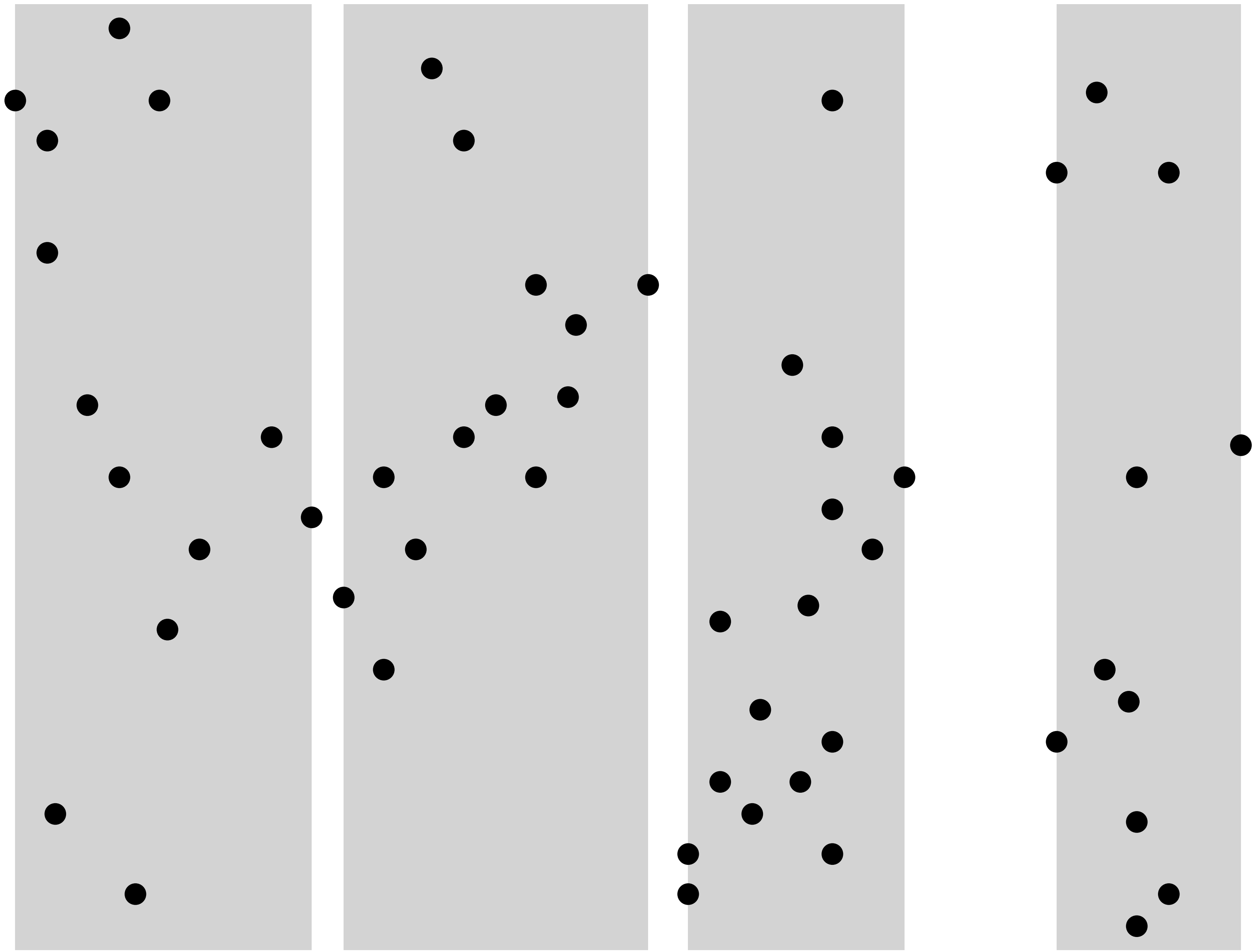
$\varepsilon/\sqrt{2}$:



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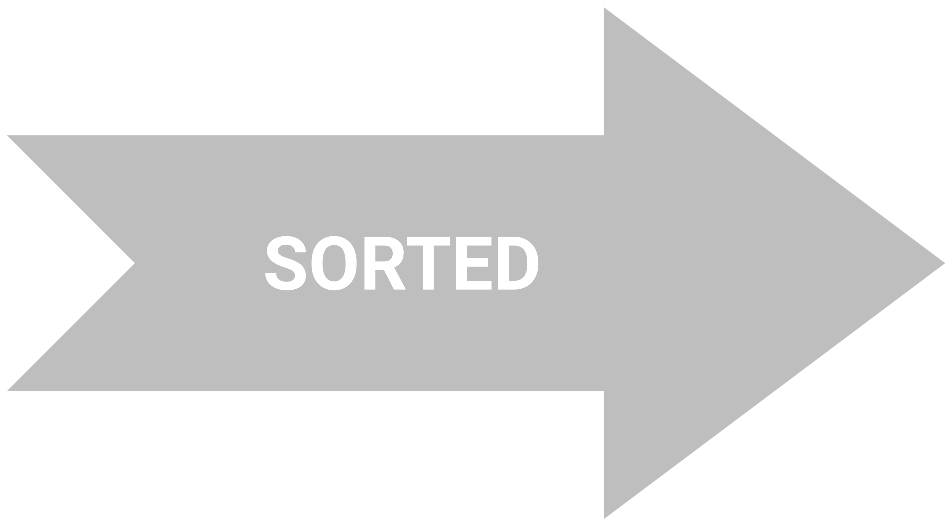
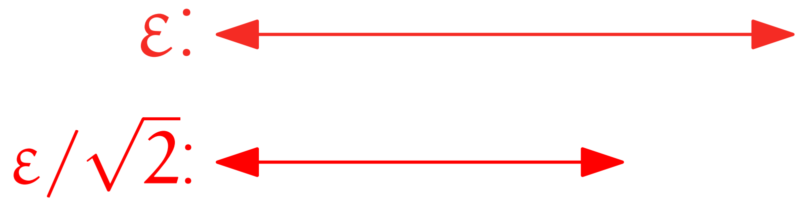
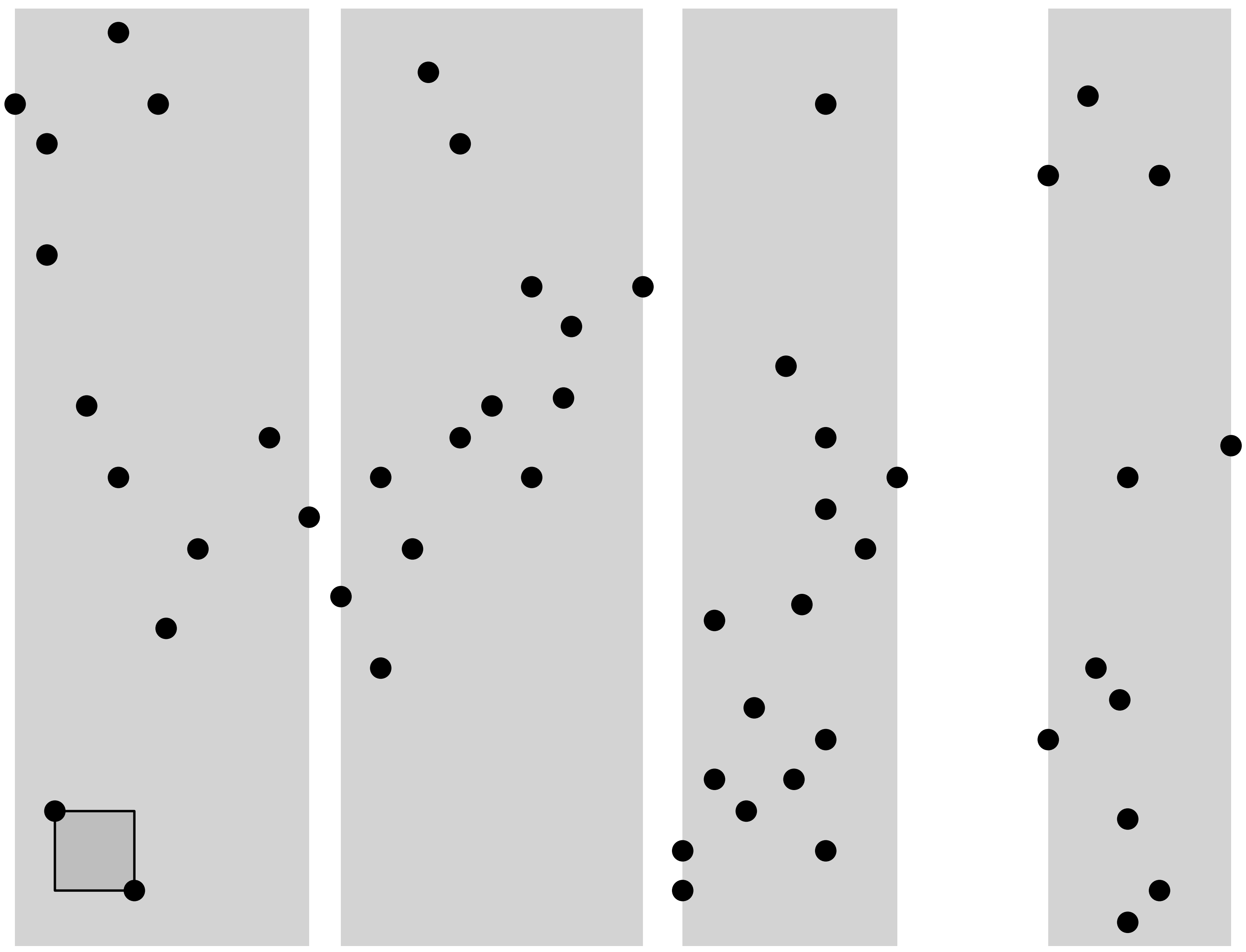


Box graph $\mathcal{G}_{\text{box}}$

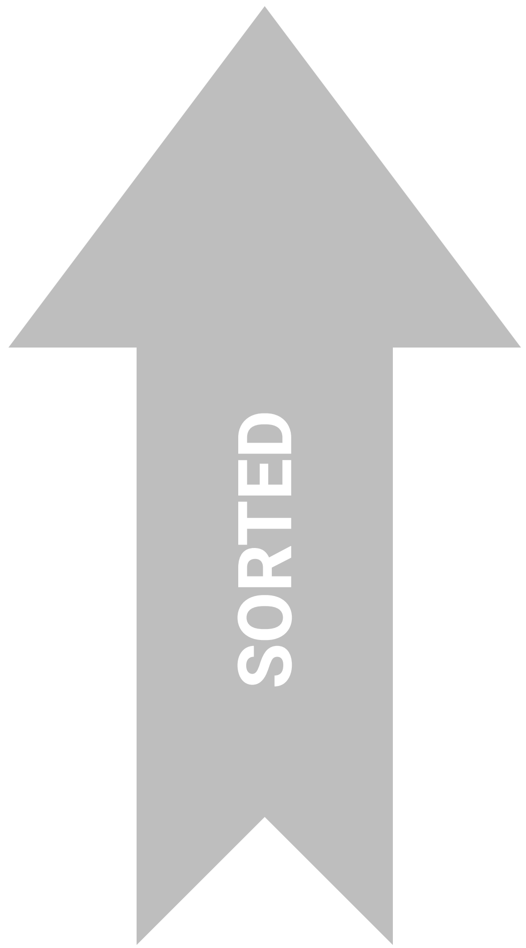




1. Construct boxes

Add points as long as strip width $\leqslant \varepsilon/\sqrt{2}$.

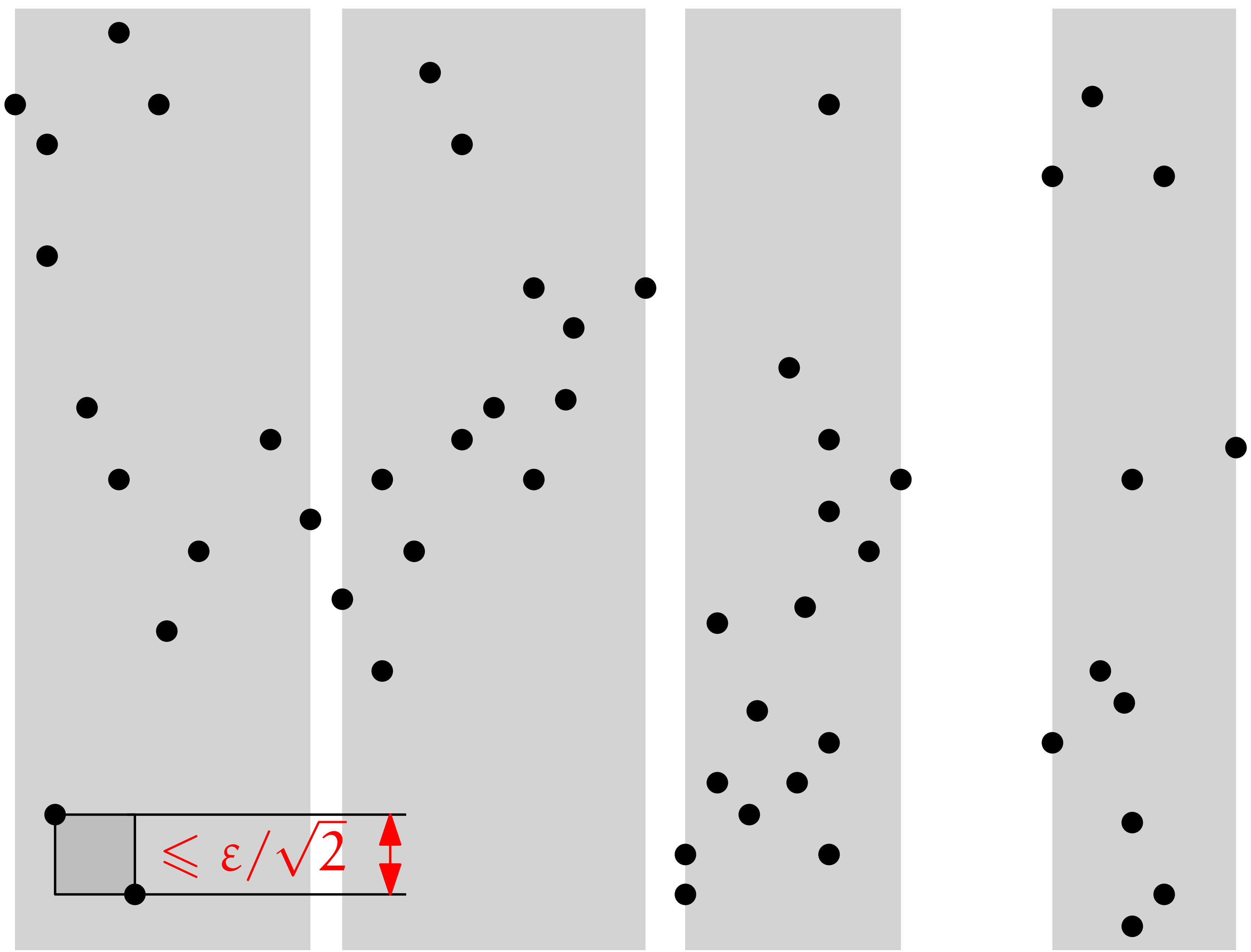
Per strip: add points to box as long as height $\leqslant \varepsilon/\sqrt{2}$.



Box graph $\mathcal{G}_{\text{box}}$

ε: ⟷

$\varepsilon/\sqrt{2}$: ⟷



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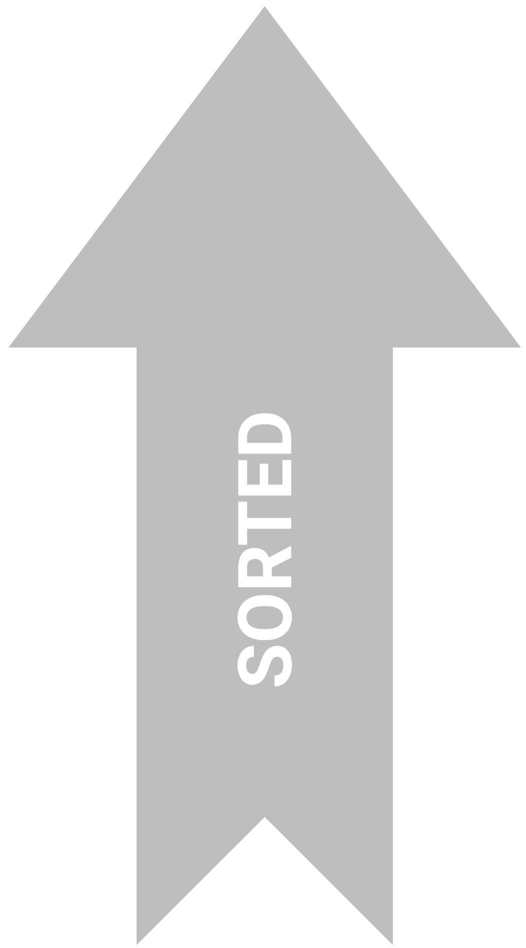
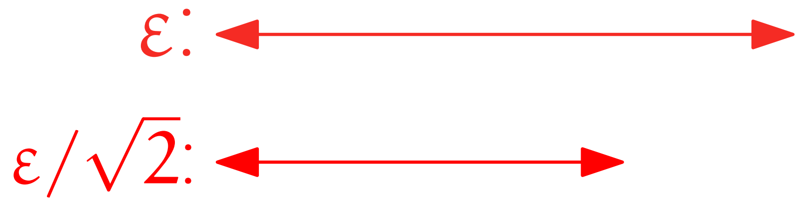
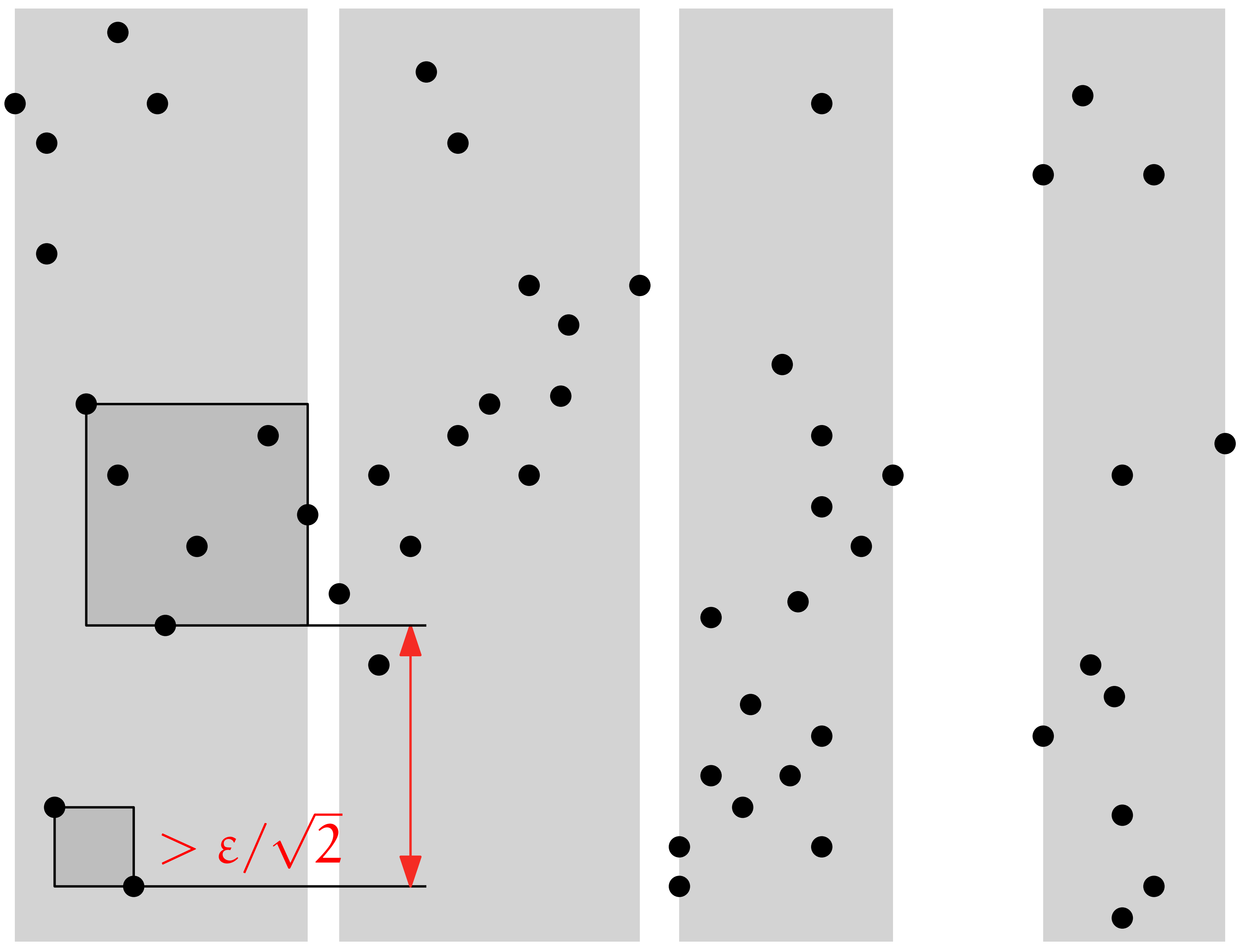
Per strip: add points to box as long as height $\leqslant \varepsilon/\sqrt{2}$.



Box graph $\mathcal{G}_{box}$





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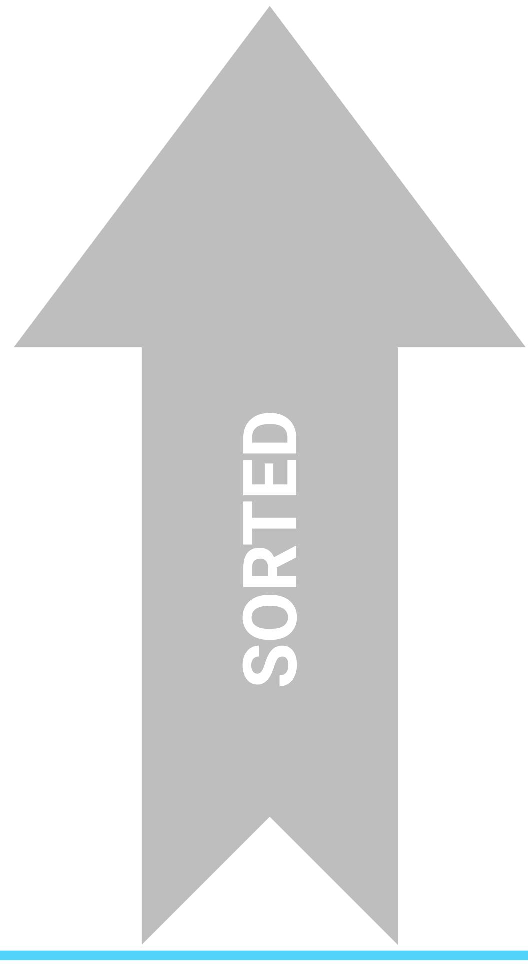
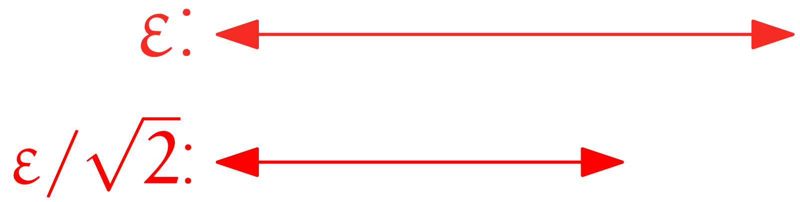
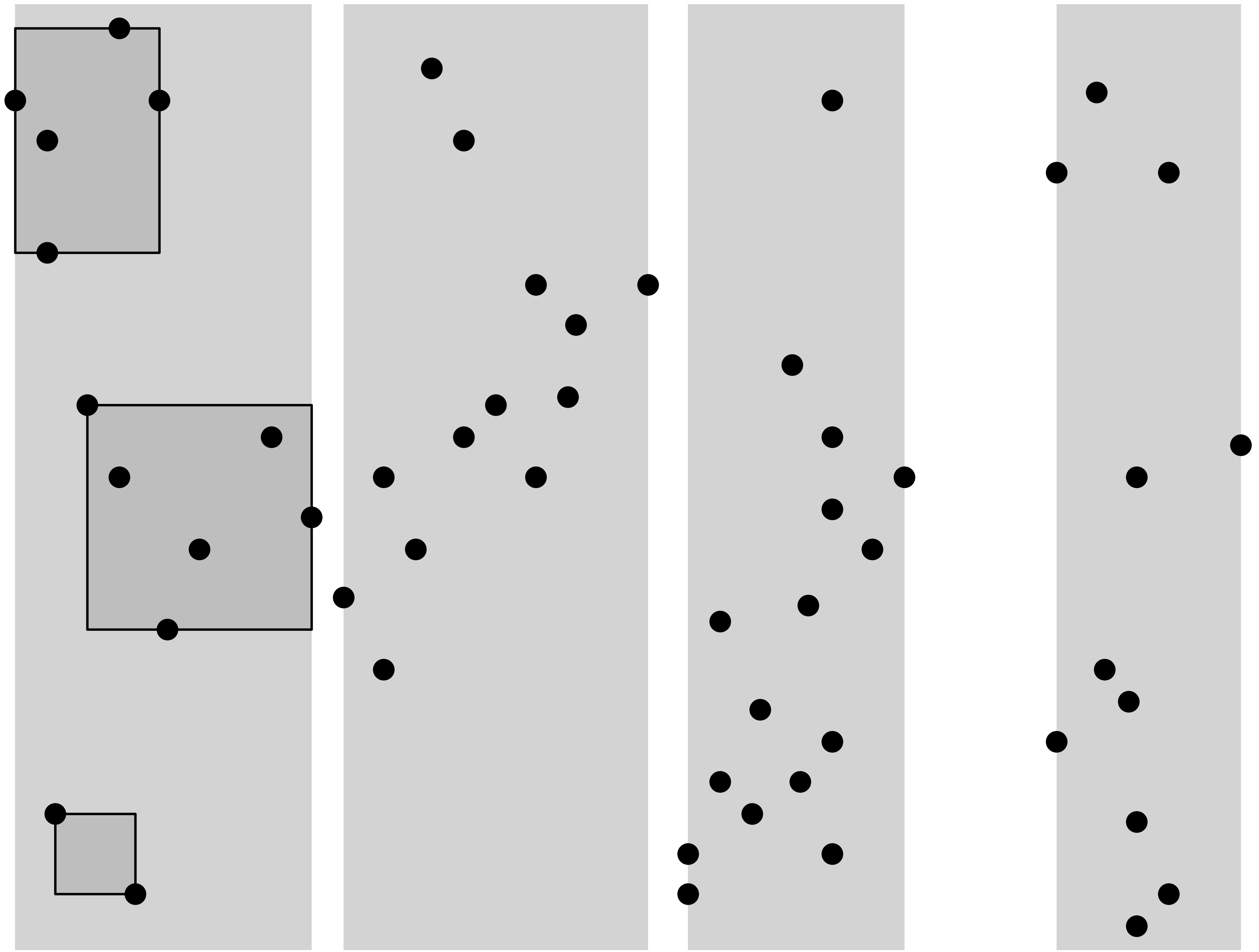


Box graph $\mathcal{G}_{\text{box}}$





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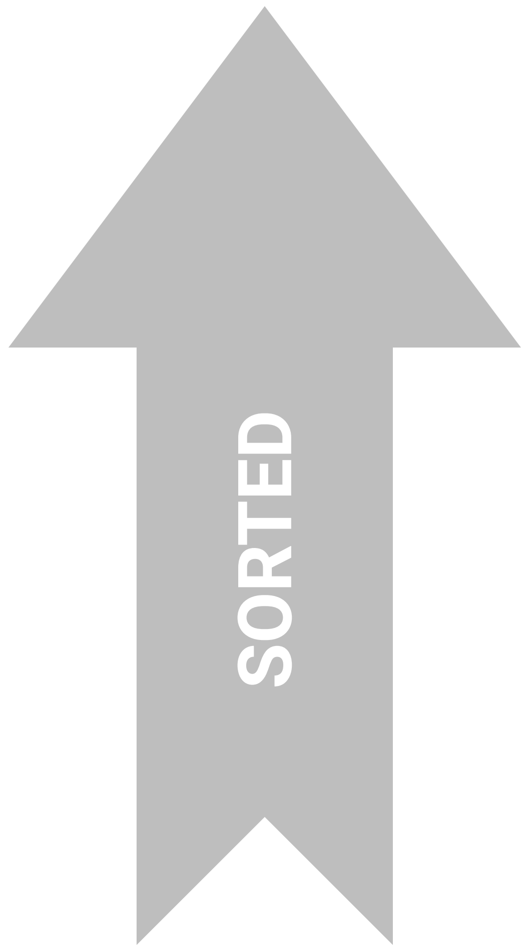
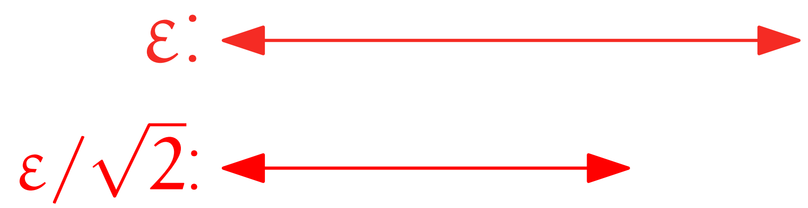
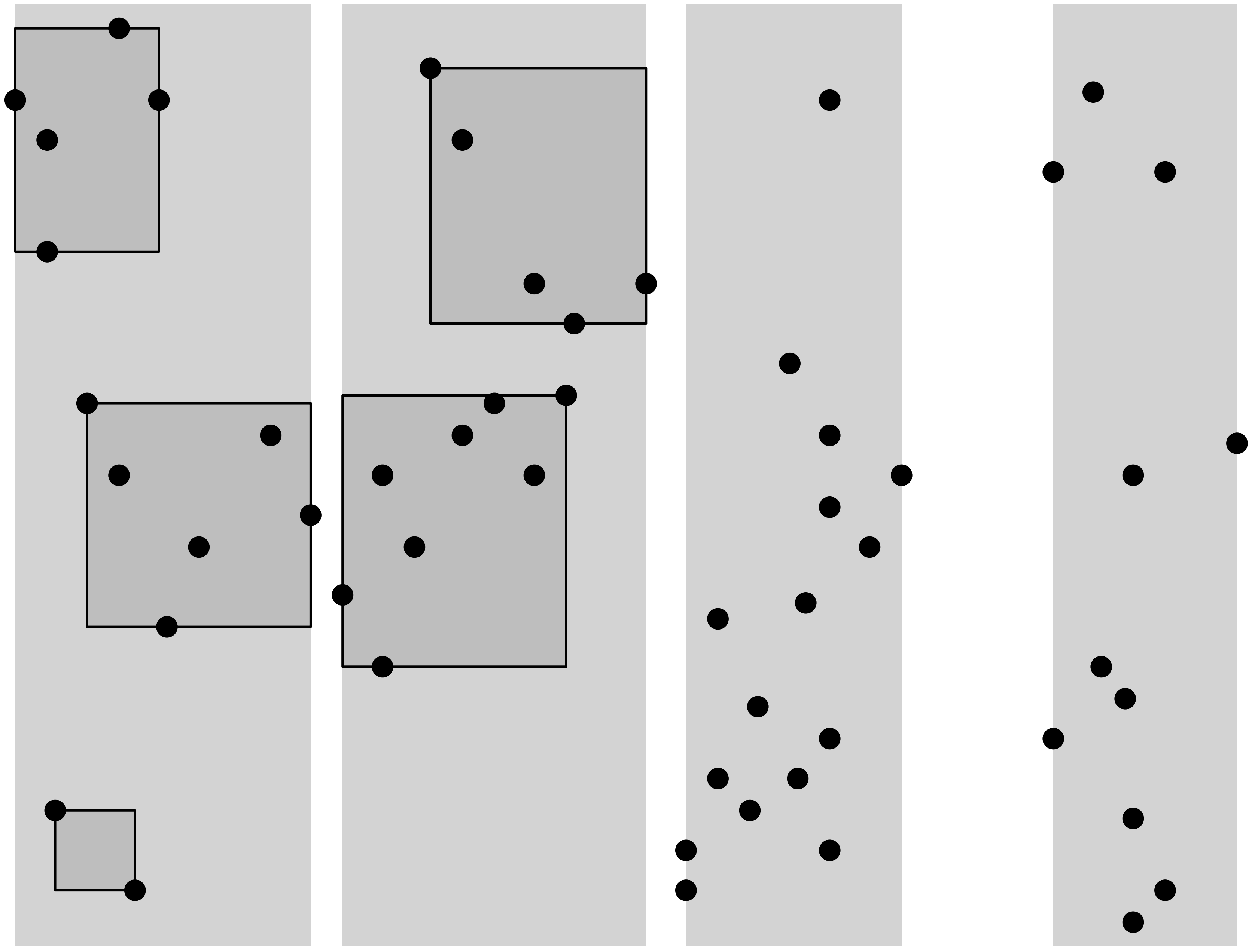




Box graph $\mathcal{G}_{\text{box}}$



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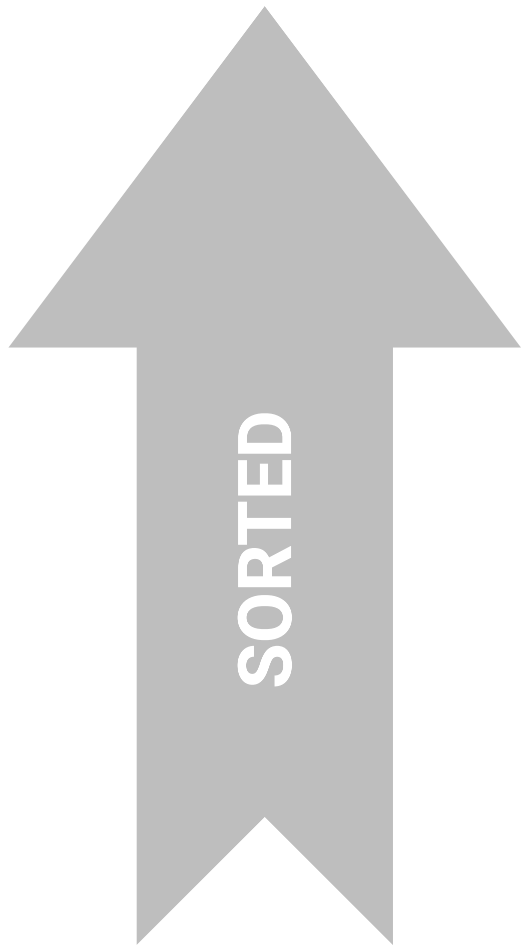
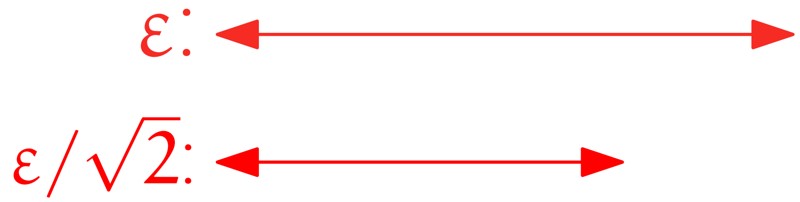
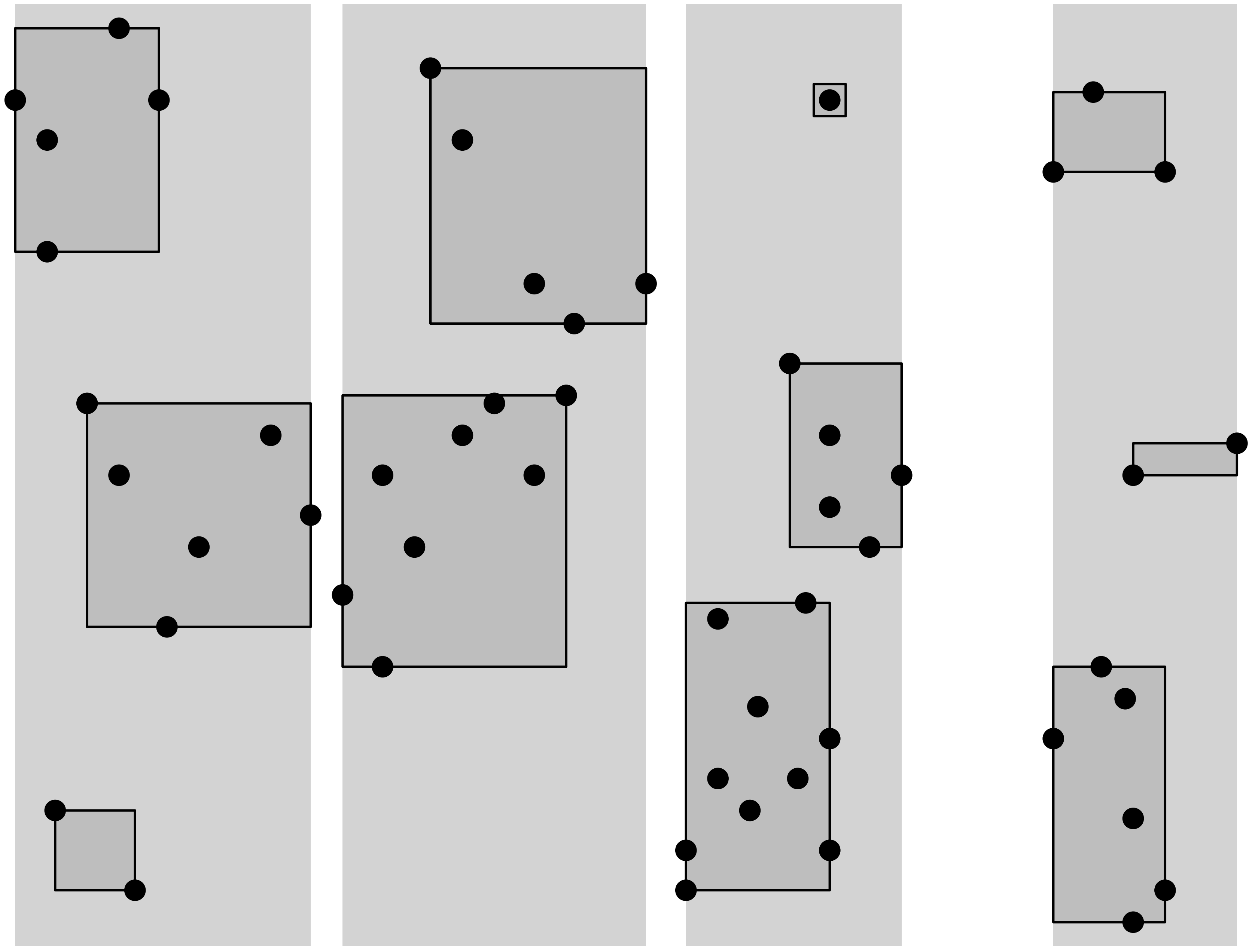


Box graph $\mathcal{G}_{\text{box}}$





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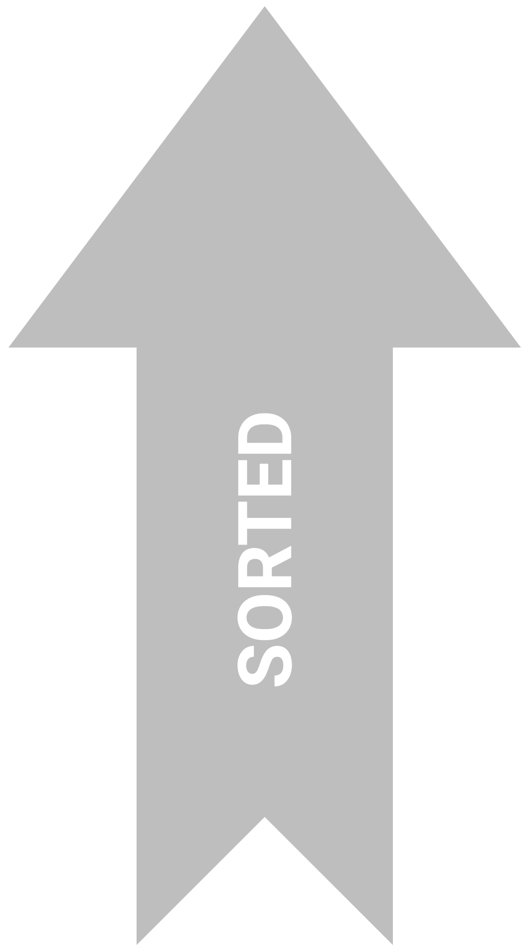
Add points as long as strip width $\leqslant \varepsilon/\sqrt{2}$.

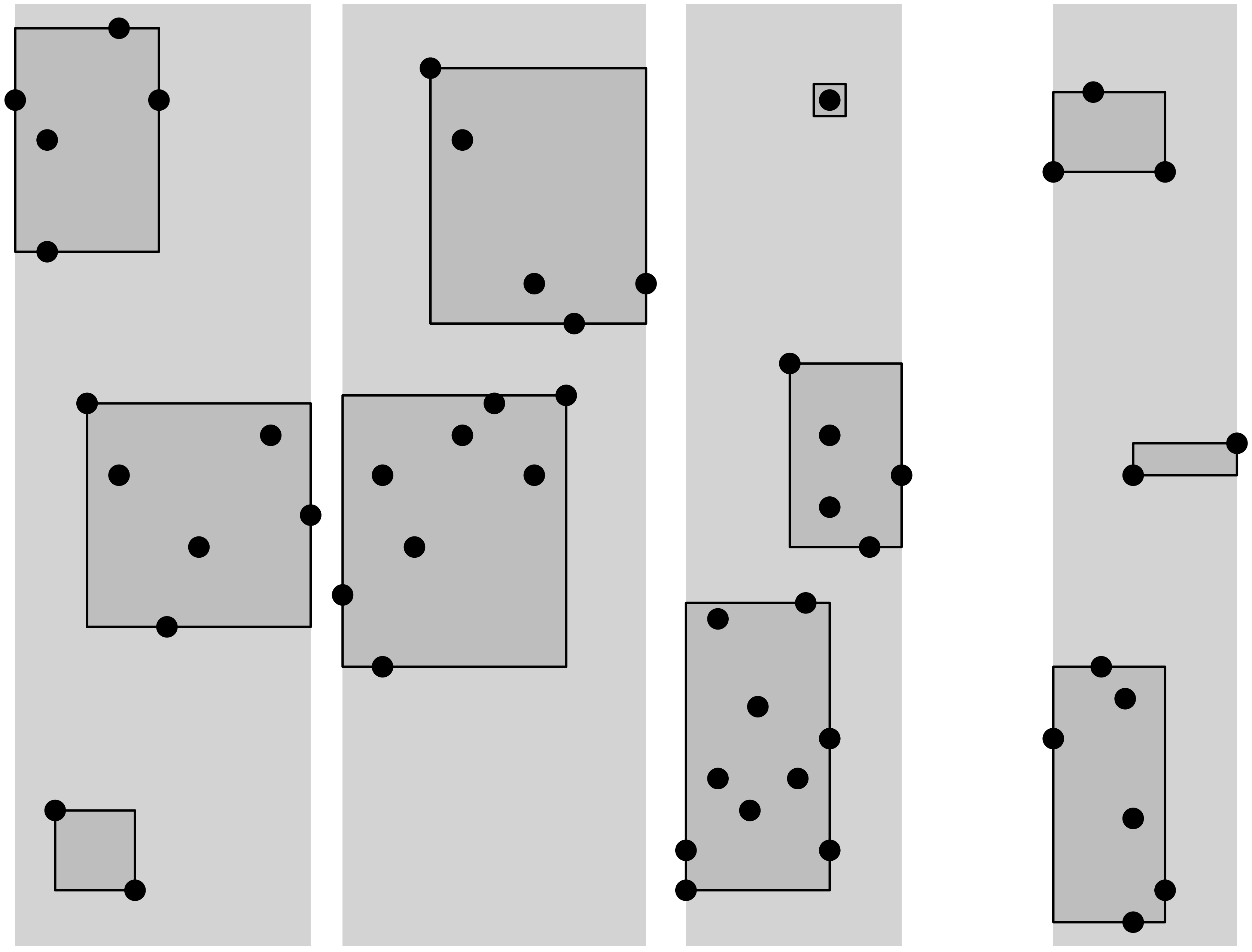
Per strip: add points to box as long as height $\leqslant \varepsilon/\sqrt{2}$.



Box graph $\mathcal{G}_{\text{box}}$

ε:

$\varepsilon/\sqrt{2}$:



1. Construct boxes

Add points as long as strip width $\leqslant \varepsilon/\sqrt{2}$.

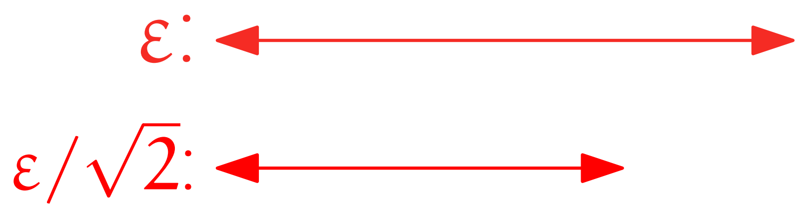
Per strip: add points to box as long as height $\leqslant \varepsilon/\sqrt{2}$.

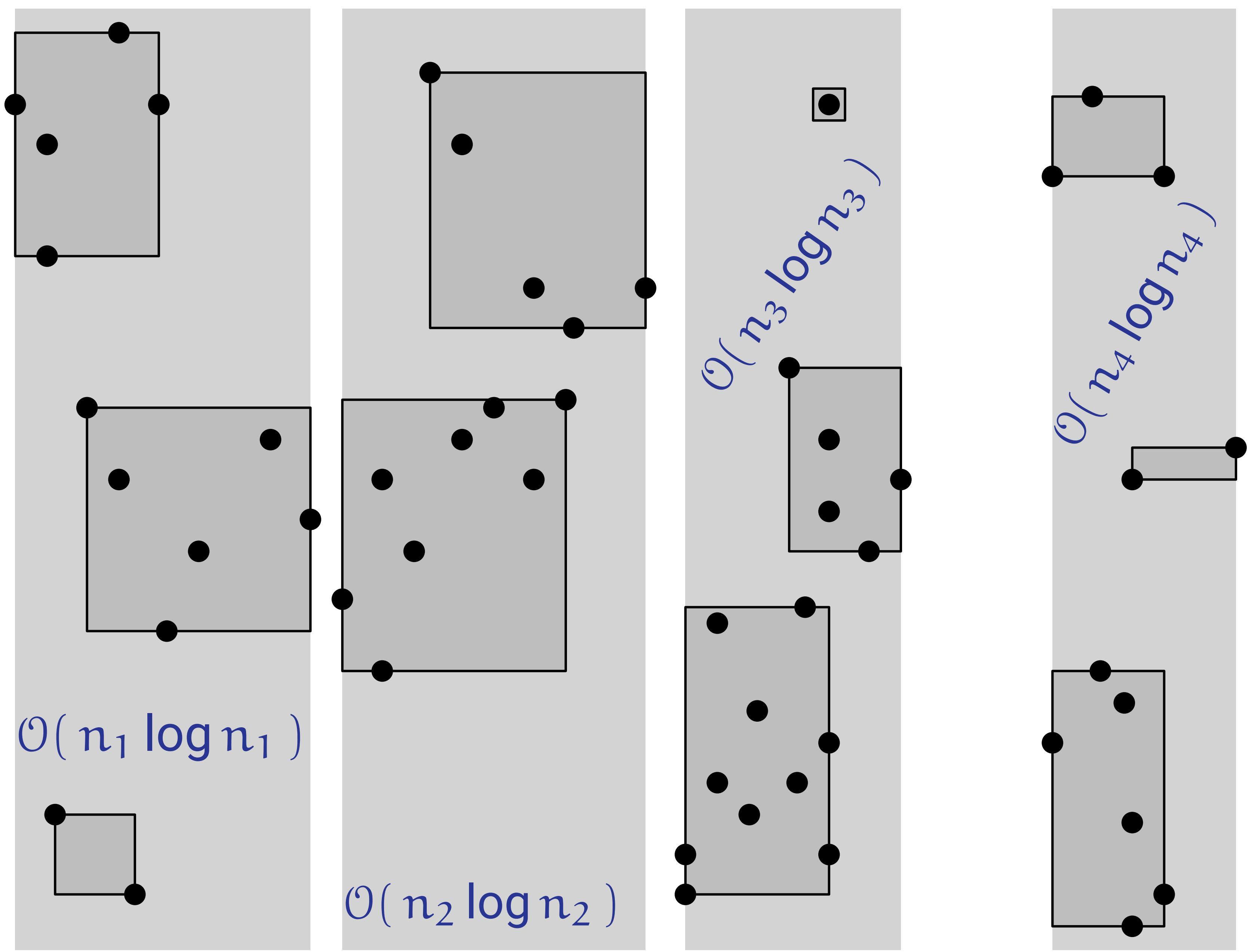
Runtime:

Sort by x

$\mathcal{O}(n \log n)$

Box graph $\mathcal{G}_{\text{box}}$





1. Construct boxes

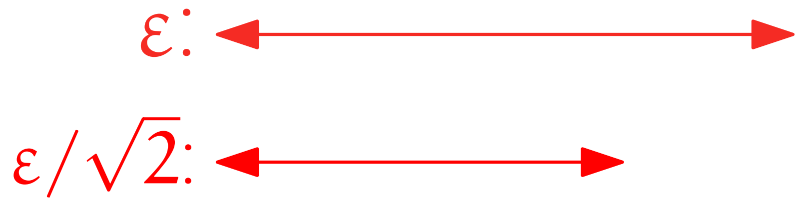
Add points as long as strip width $\leqslant \varepsilon/\sqrt{2}$.

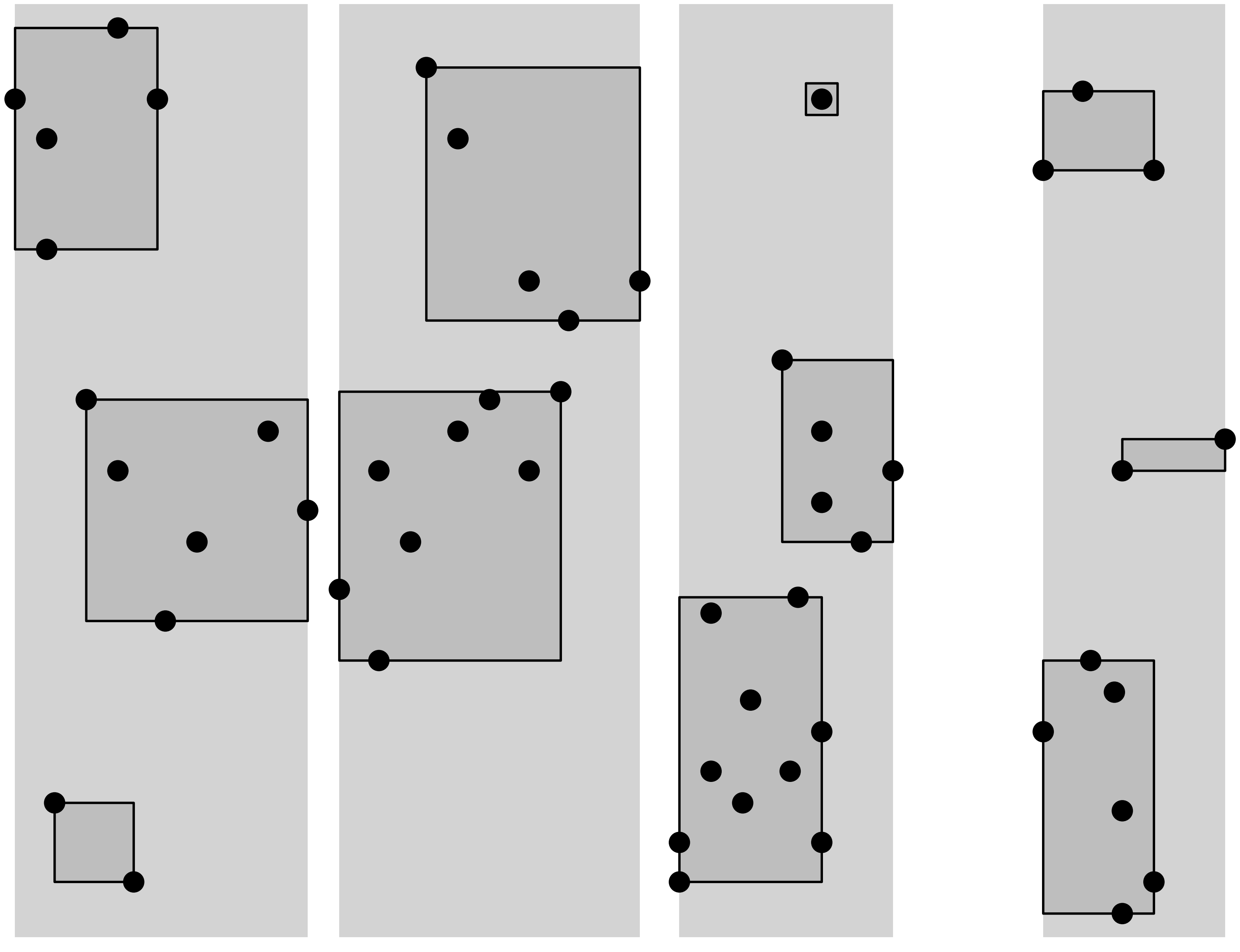
Per strip: add points to box as long as height $\leqslant \varepsilon/\sqrt{2}$.

Runtime:

- Sort by x
  $\mathcal{O}(n \log n)$
- Sort by y per strip
  $\sum_j \mathcal{O}(n_j \log n_j)$
- Total
  $\mathcal{O}(n \log n)$

Box graph $\mathcal{G}_{\text{box}}$

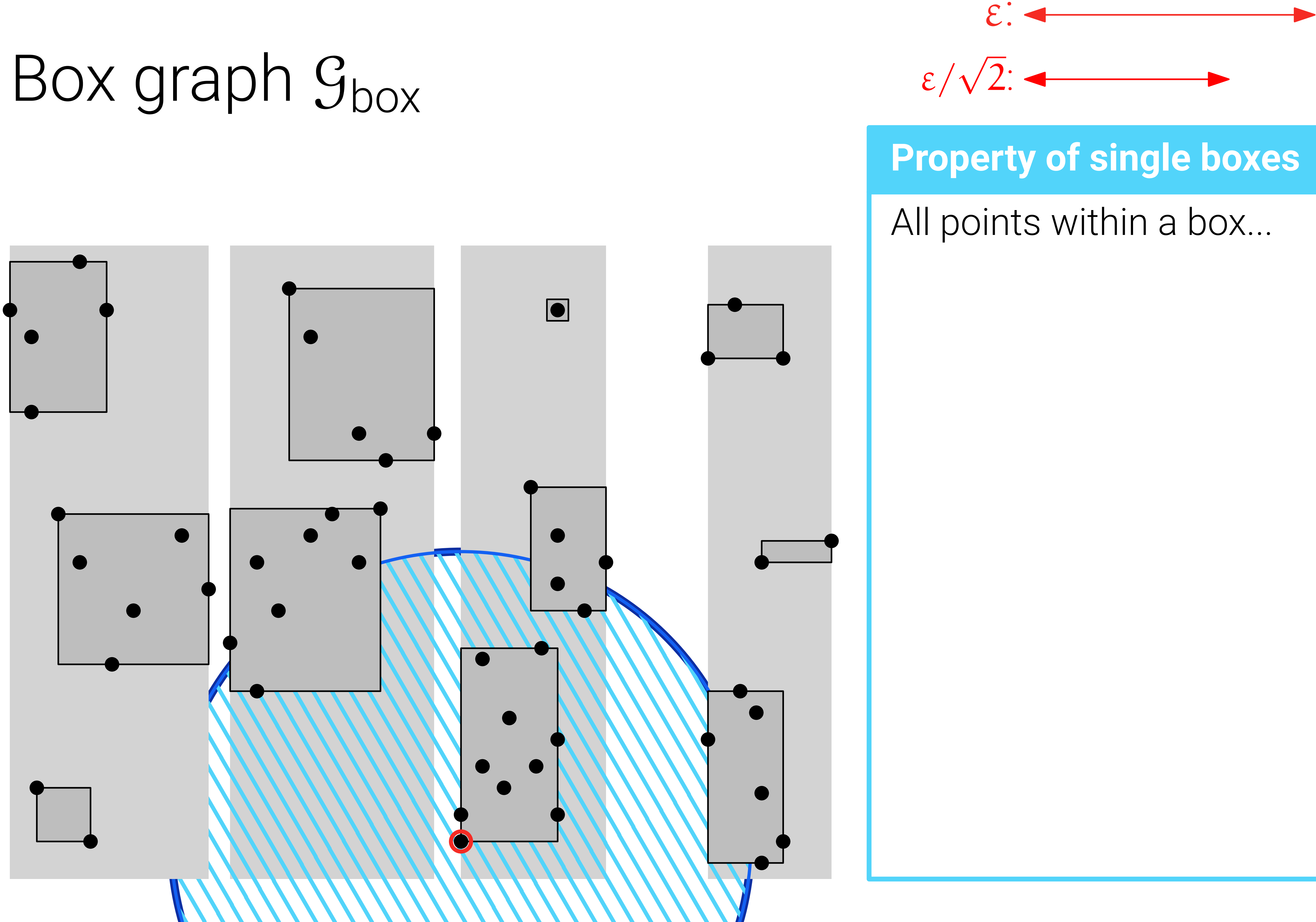




Property of single boxes

All points within a box...

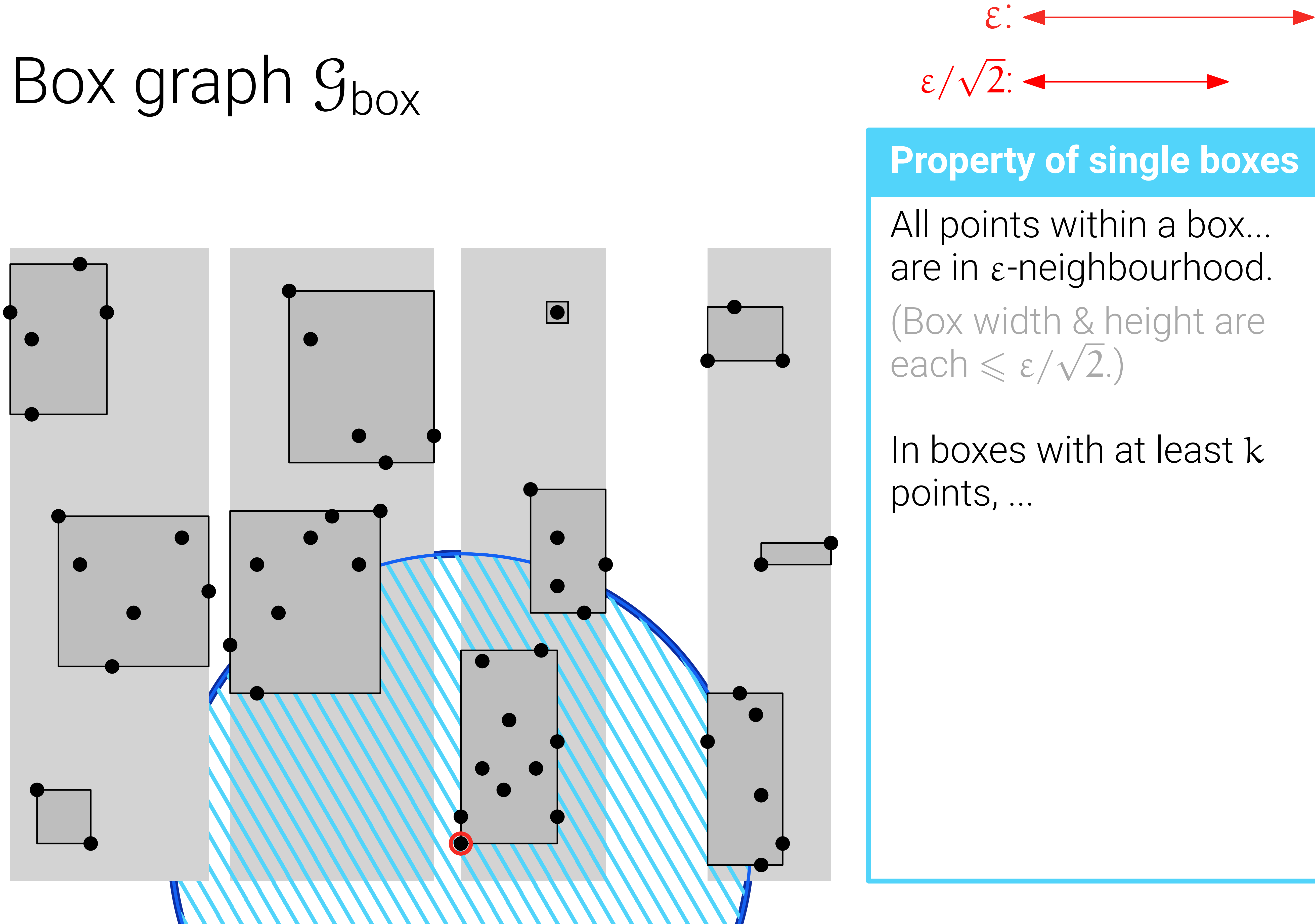
Box graph $\mathcal{G}_{box}$



Property of single boxes

All points within a box...

Box graph $\mathcal{G}_{\text{box}}$



Property of single boxes

All points within a box... are in ε-neighbourhood.

(Box width & height are each $\leqslant \varepsilon/\sqrt{2}$.)

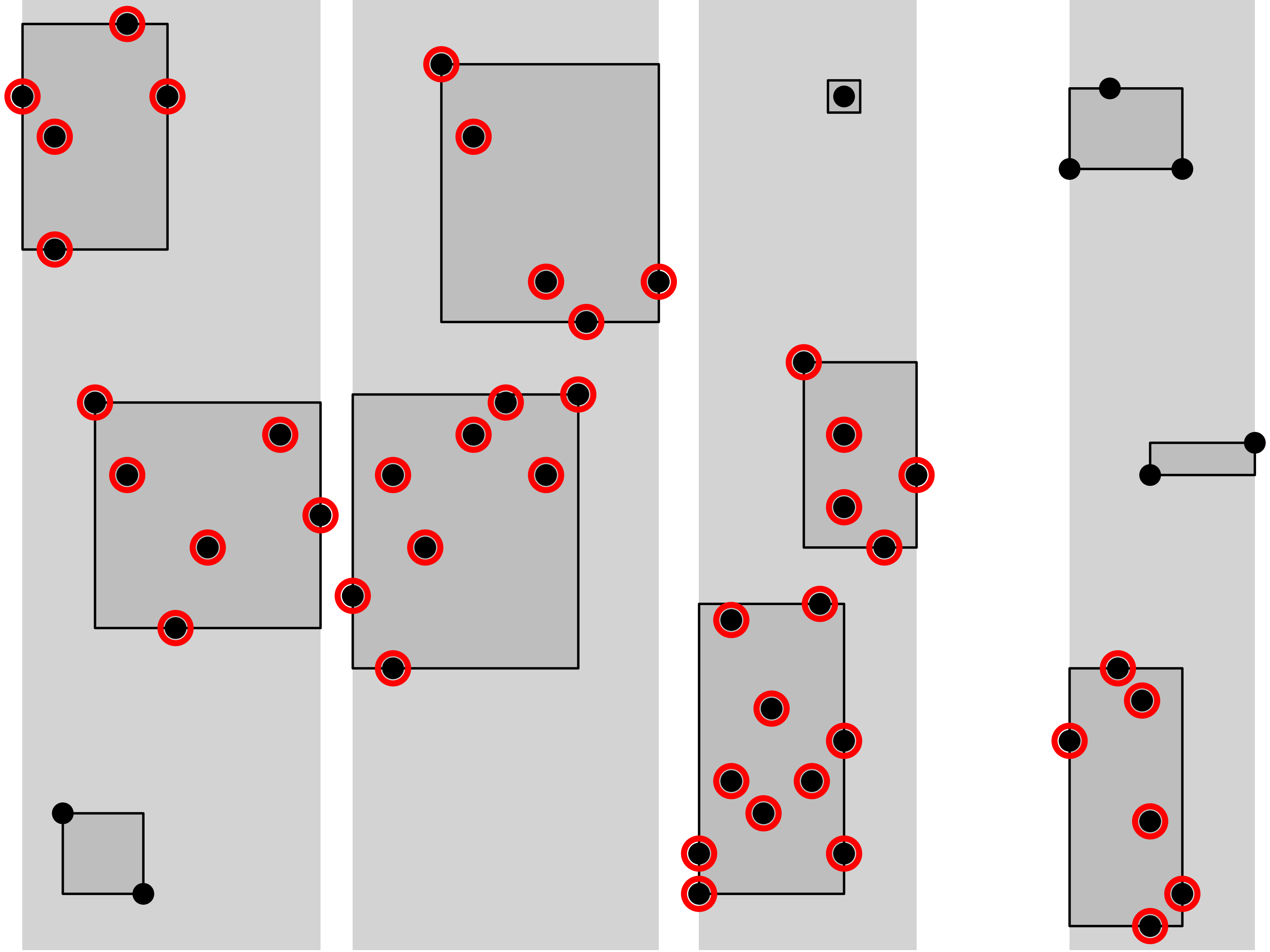
In boxes with at least k points, ...

Box graph $\mathcal{G}_{\text{box}}$

$k = 4$

ε:

$\varepsilon/\sqrt{2}$:



Property of single boxes

All points within a box...
are in ε-neighbourhood.

(Box width & height are each $\leqslant \varepsilon/\sqrt{2}$.)

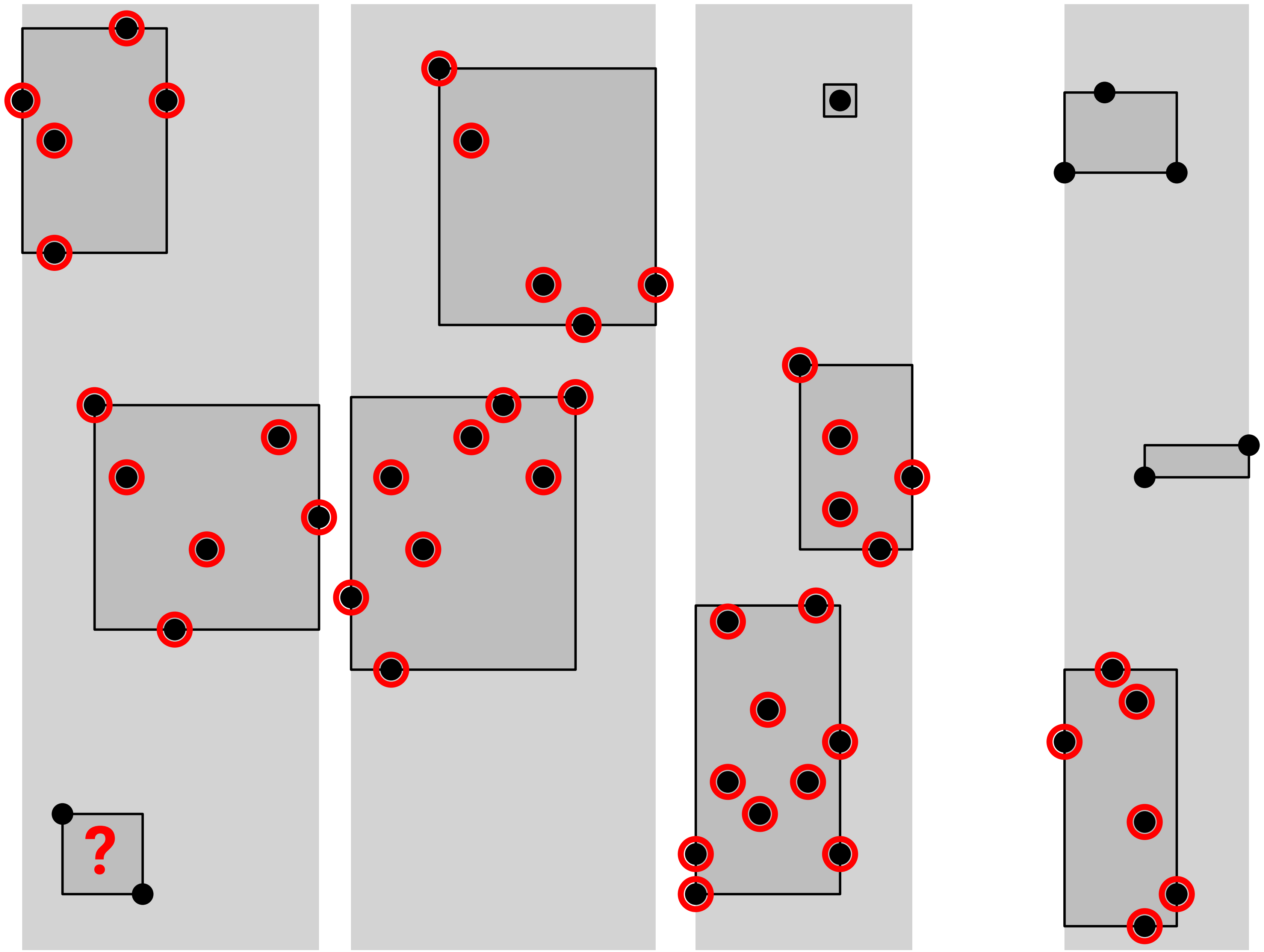
In boxes with at least k points, ...

all points are core points.

$k = 4$ ε: ⟷

$\varepsilon/\sqrt{2}$: ⟷

Box graph $\mathcal{G}_{\text{box}}$



Property of single boxes

All points within a box... are in ε-neighbourhood.

(Box width & height are each $\leqslant \varepsilon/\sqrt{2}$.)

In boxes with at least k points, ...

all points are core points.

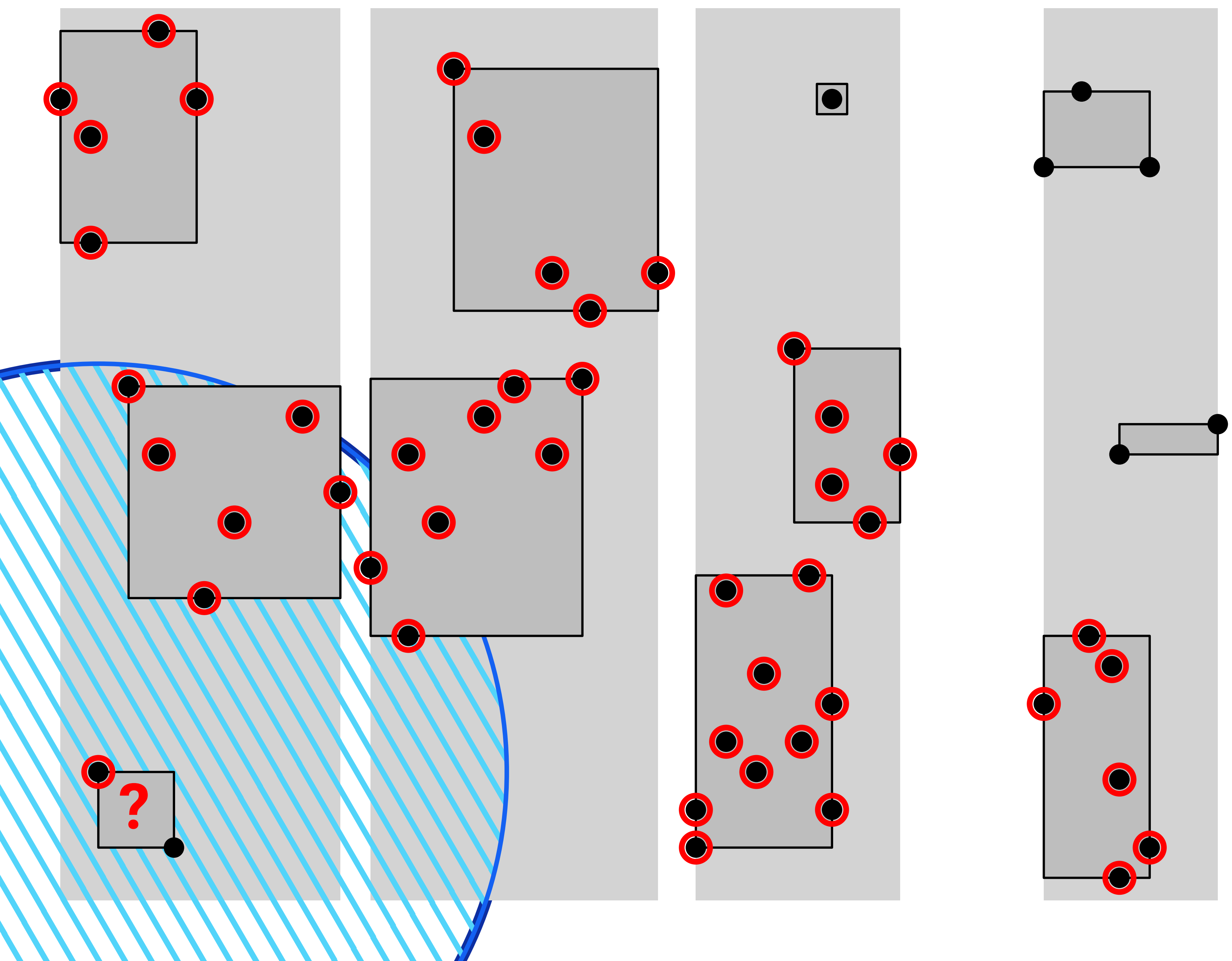
In boxes with fewer than k points, ...

Box graph $\mathcal{G}_{box}$

$k = 4$

ε:

$\varepsilon/\sqrt{2}$:



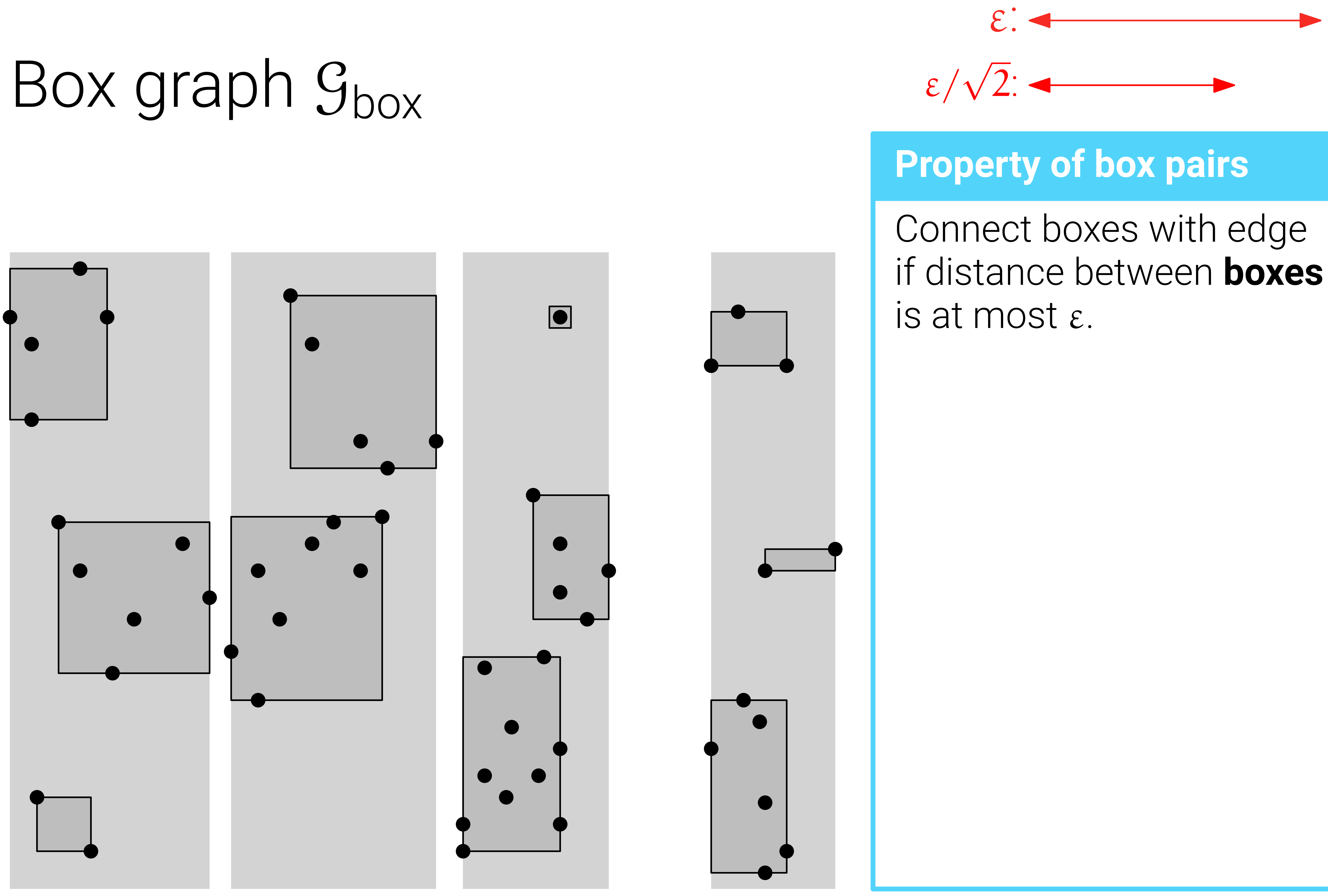
Property of single boxes

All points within a box...
are in ε-neighbourhood.
(Box width & height are each $\leqslant \varepsilon/\sqrt{2}$.)

In boxes with at least k points, ...
all points are core points.

In boxes with fewer than k points, ...
points **can** be core points.

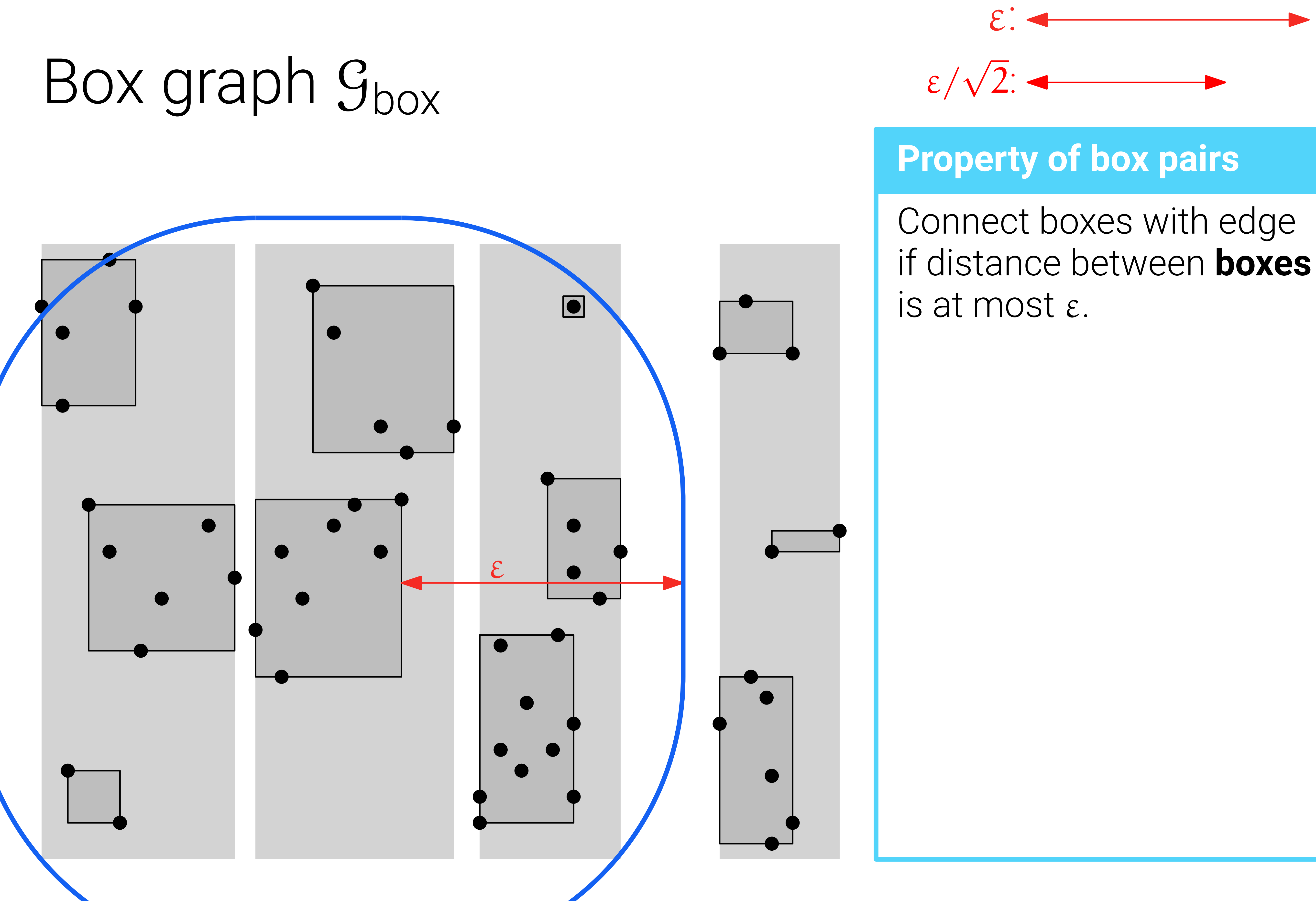
Box graph $\mathcal{G}_{box}$



Property of box pairs

Connect boxes with edge if distance between **boxes** is at most ε.

Box graph $\mathcal{G}_{\text{box}}$



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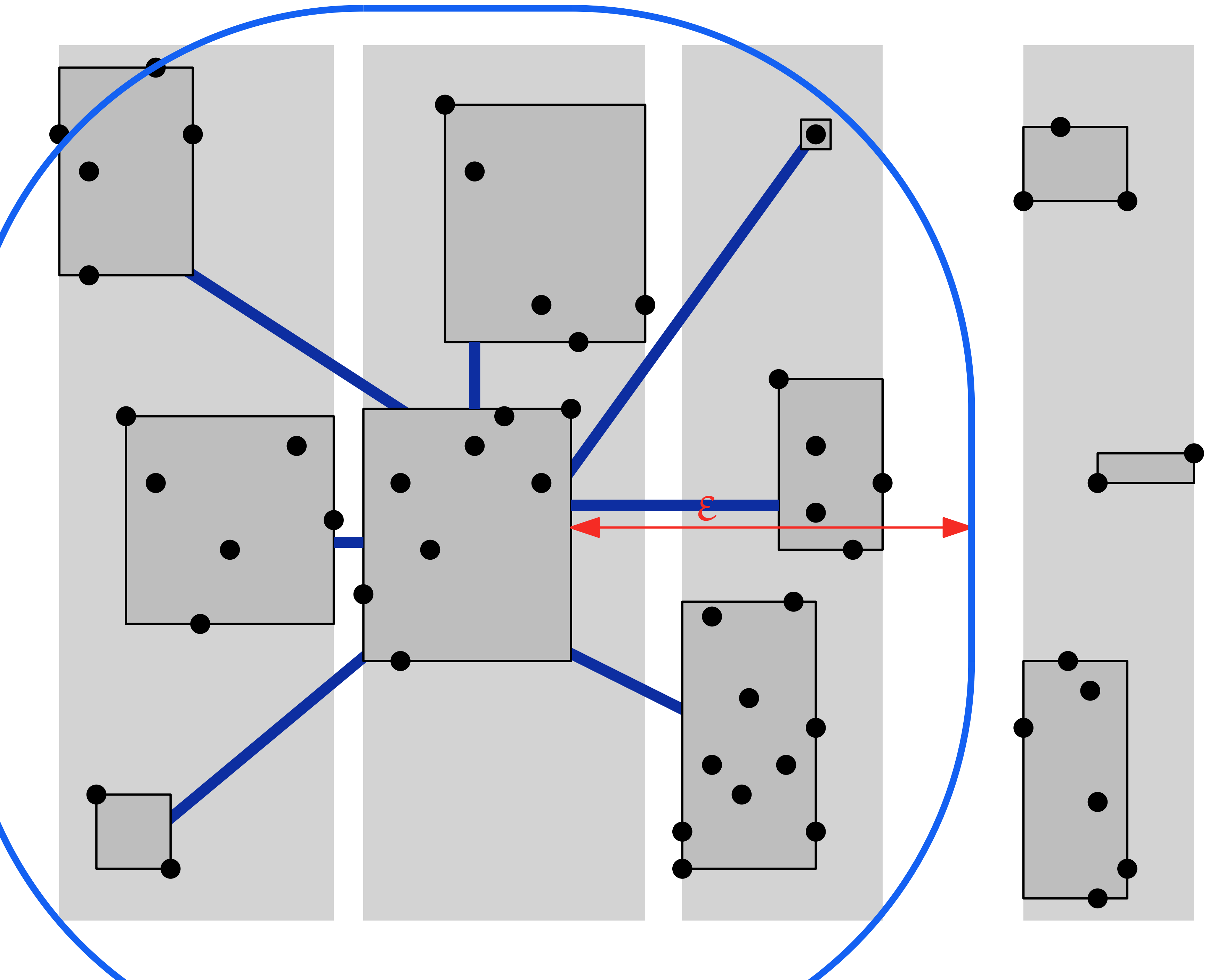
Box graph $\mathcal{G}_{box}$



ε:

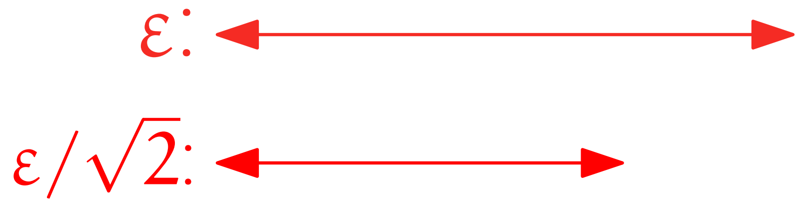
$\varepsilon/\sqrt{2}$:

Property of box pairs

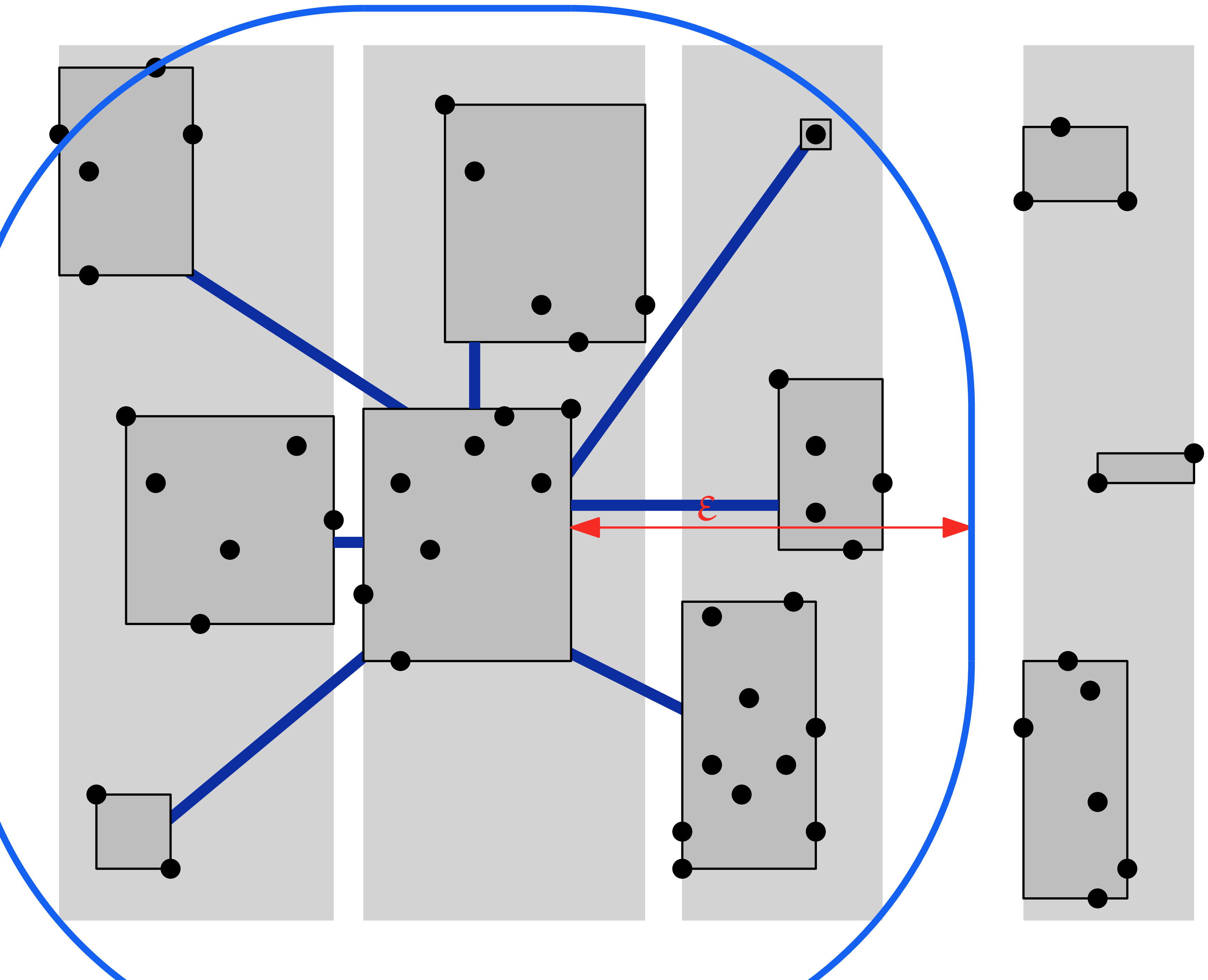
Connect boxes with edge if distance between **boxes** is at most ε.

Nonneighbours in $\mathcal{G}_{box}$:

none of these points are in ε-neighbourhood.



Box graph $\mathcal{G}_{\text{box}}$



Property of box pairs

Connect boxes with edge if distance between **boxes** is at most ε.

Nonneighbours in $\mathcal{G}_{\text{box}}$:

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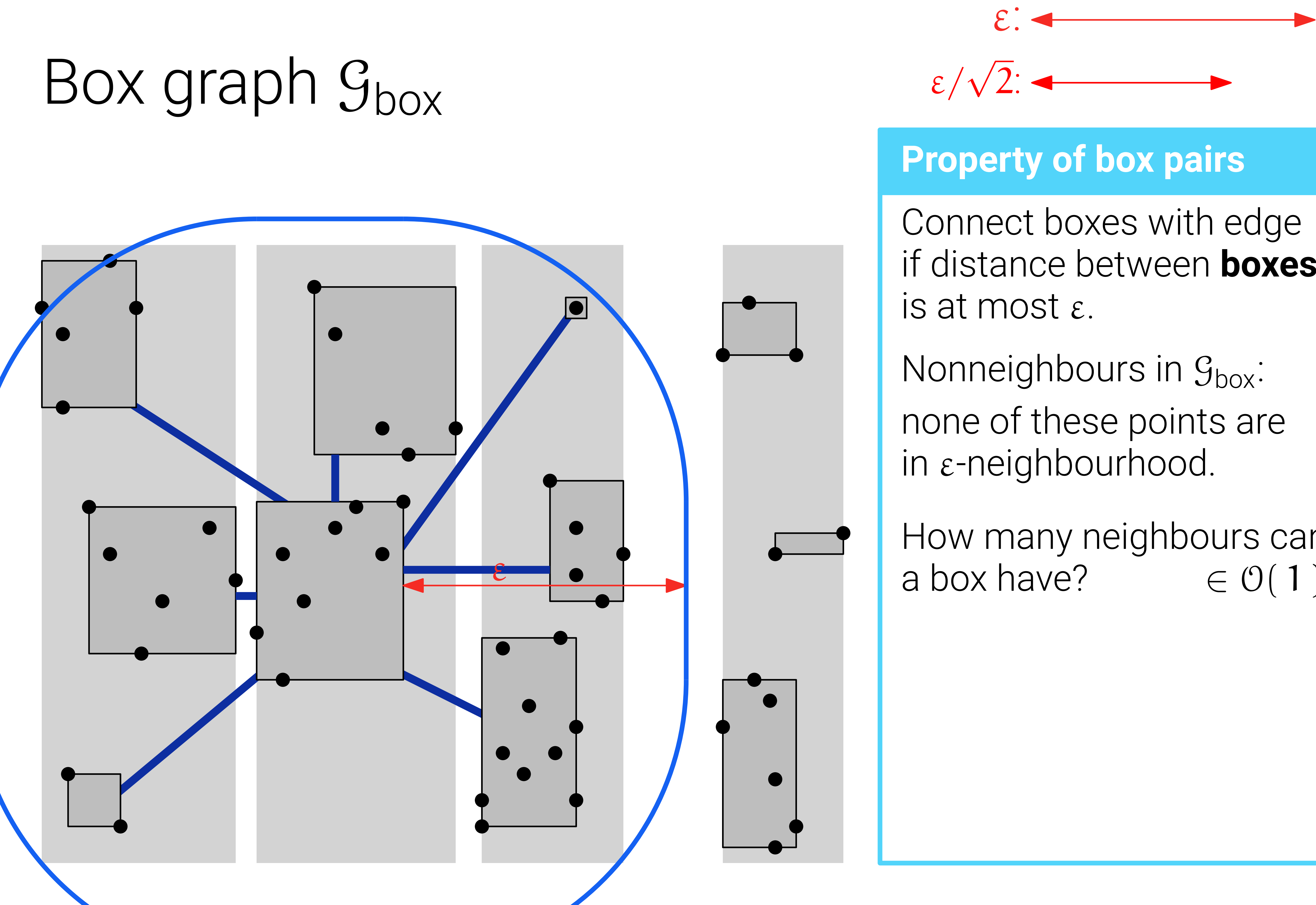
How many neighbours can a box have?

Box graph $\mathcal{G}_{box}$



Property of box pairs

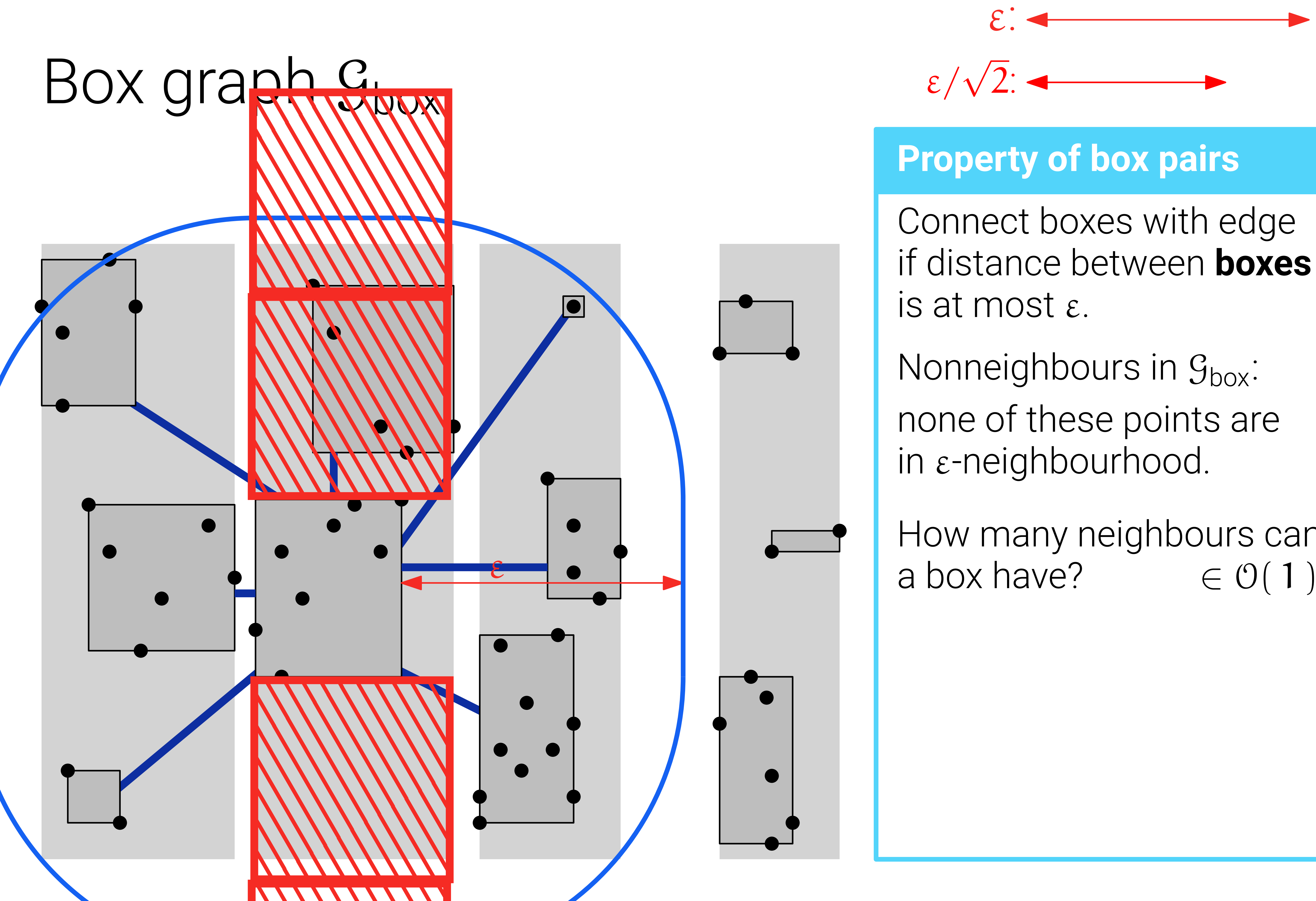
Connect boxes with edge if distance between **boxes** is at most ε.

Nonneighbours in $\mathcal{G}_{box}$:

none of these points are in ε-neighbourhood.

How many neighbours can a box have? $\in \mathcal{O}(1)$

Box graph $\mathcal{G}_{box}$



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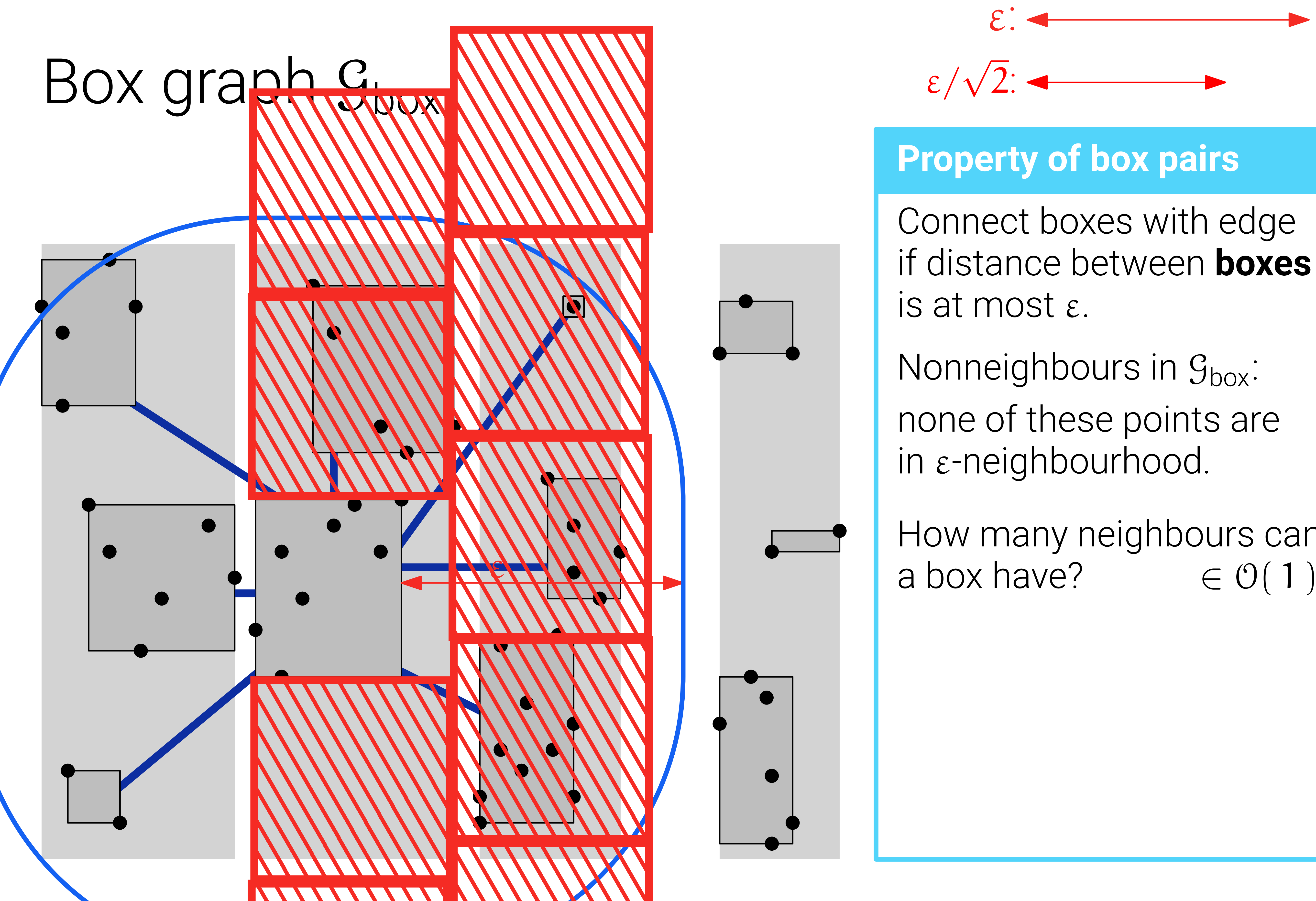

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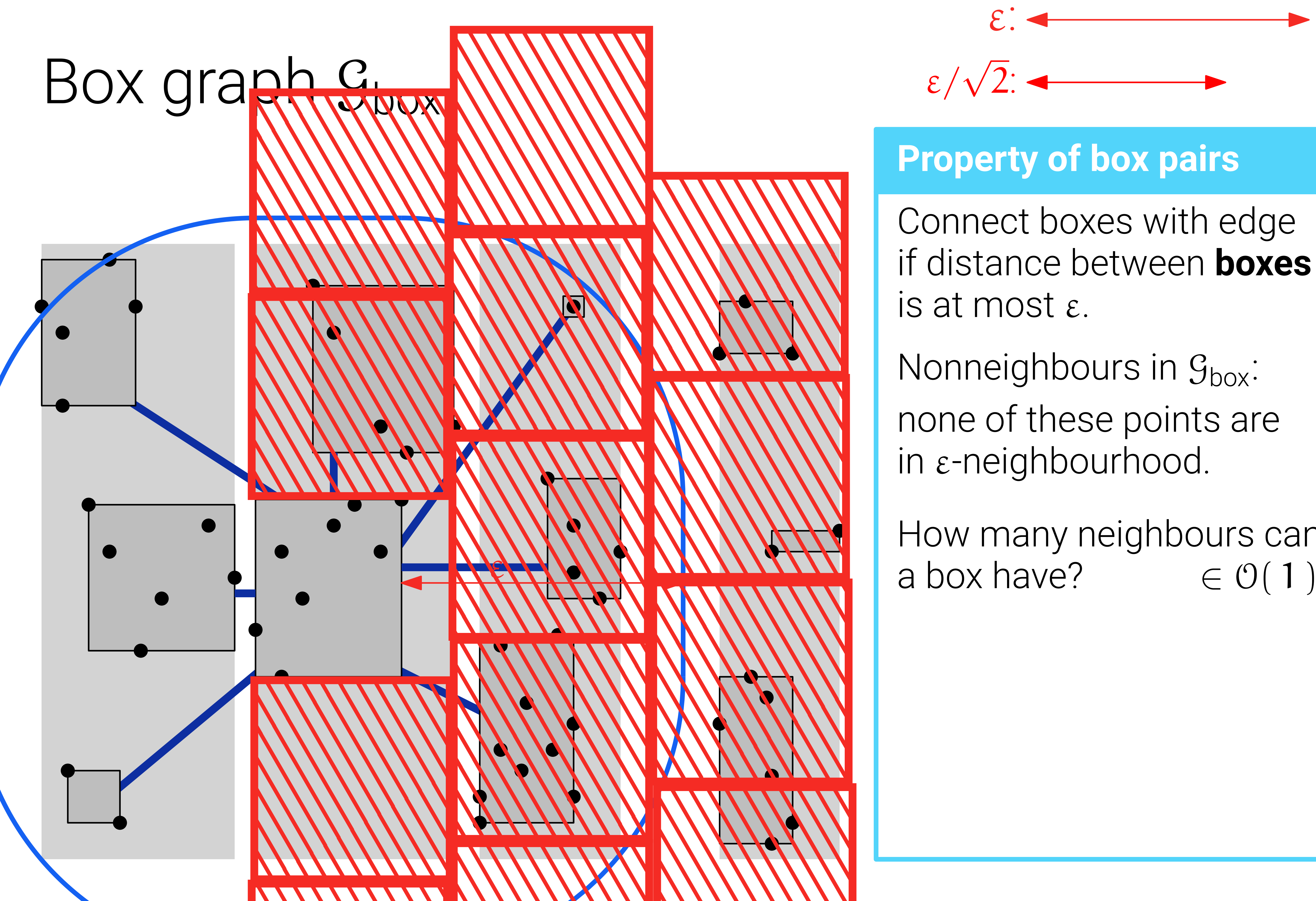

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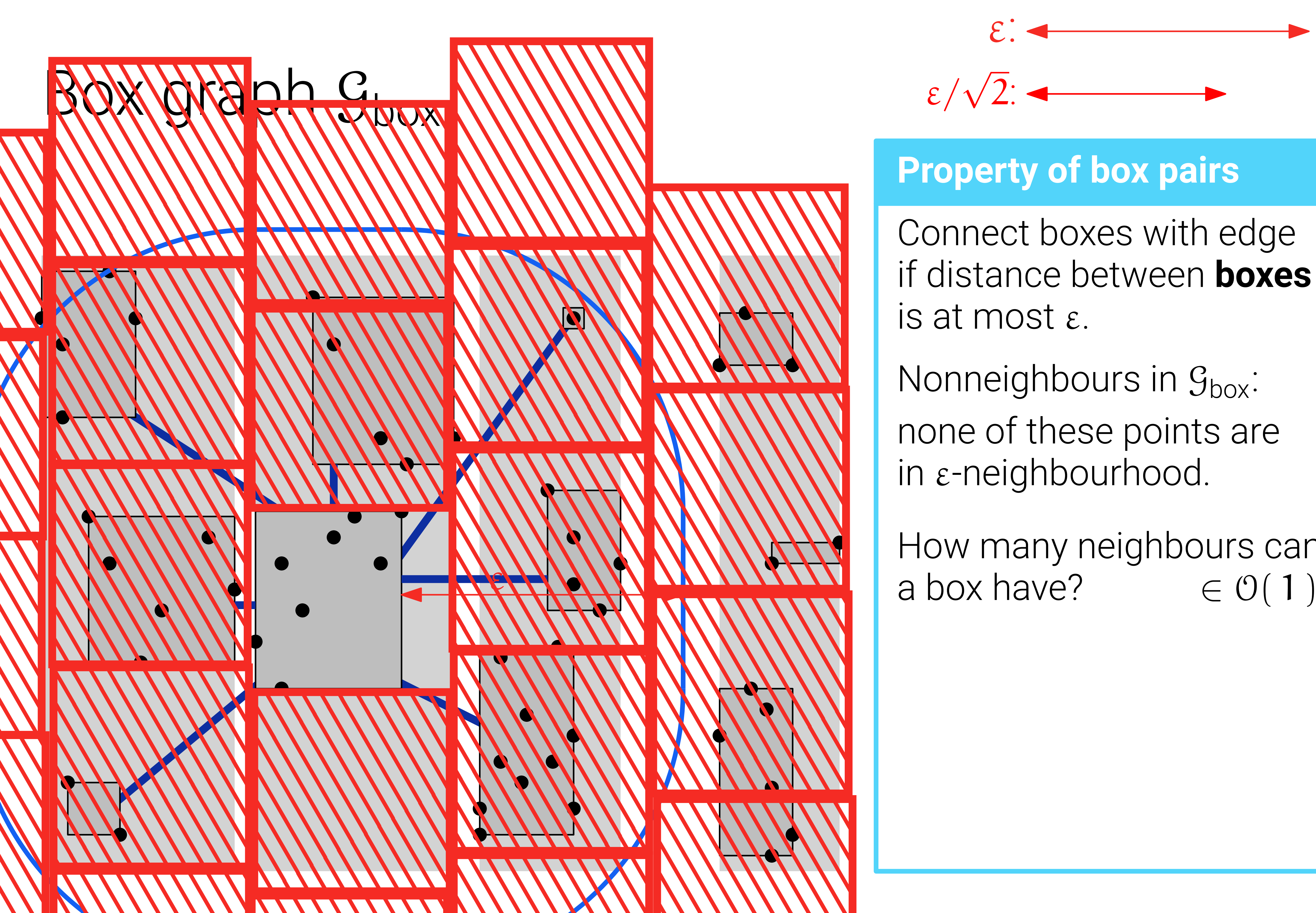

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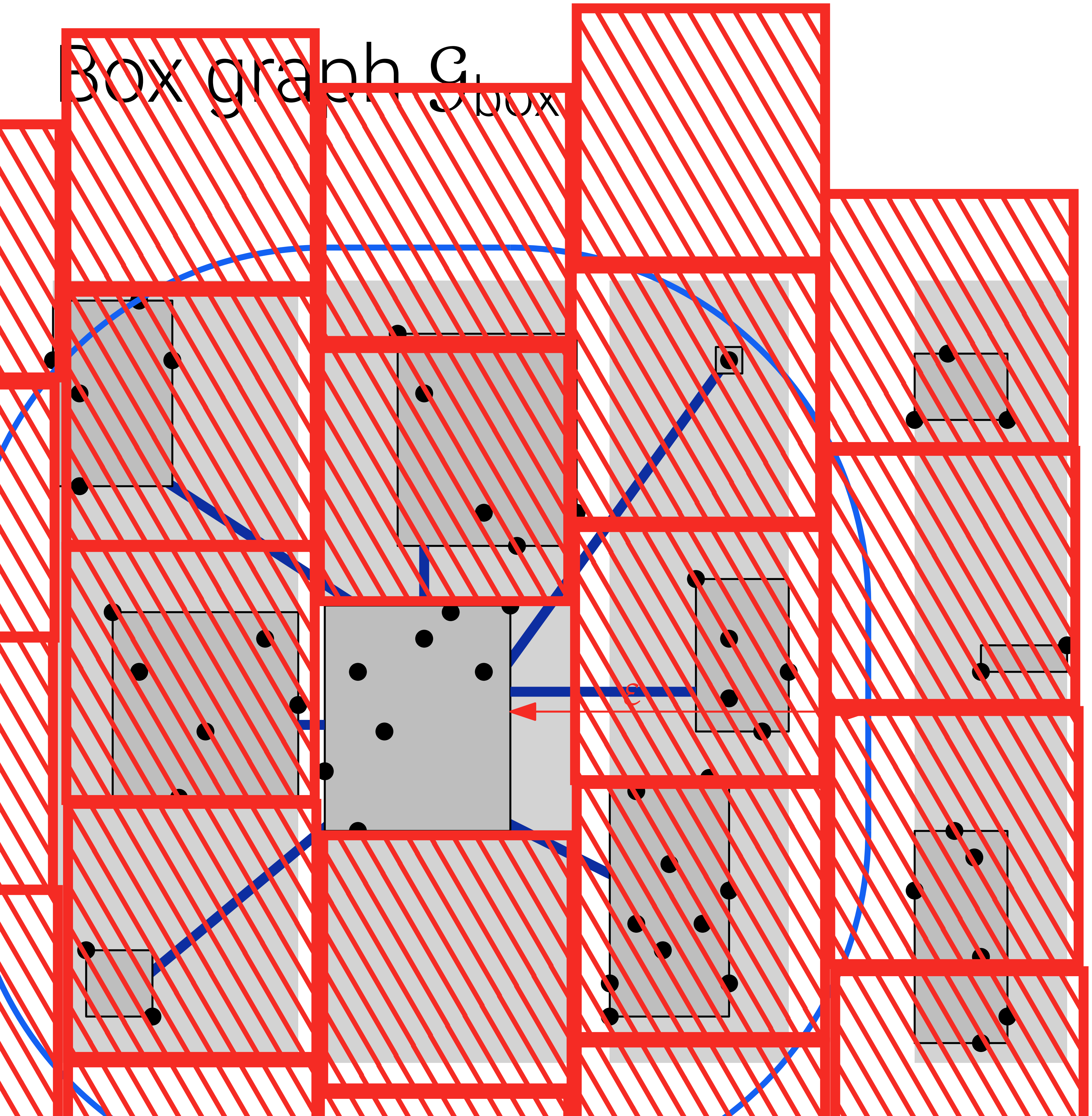
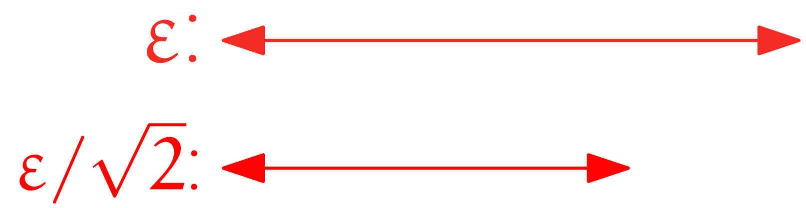
Box graph $\mathcal{G}_{\text{box}}$





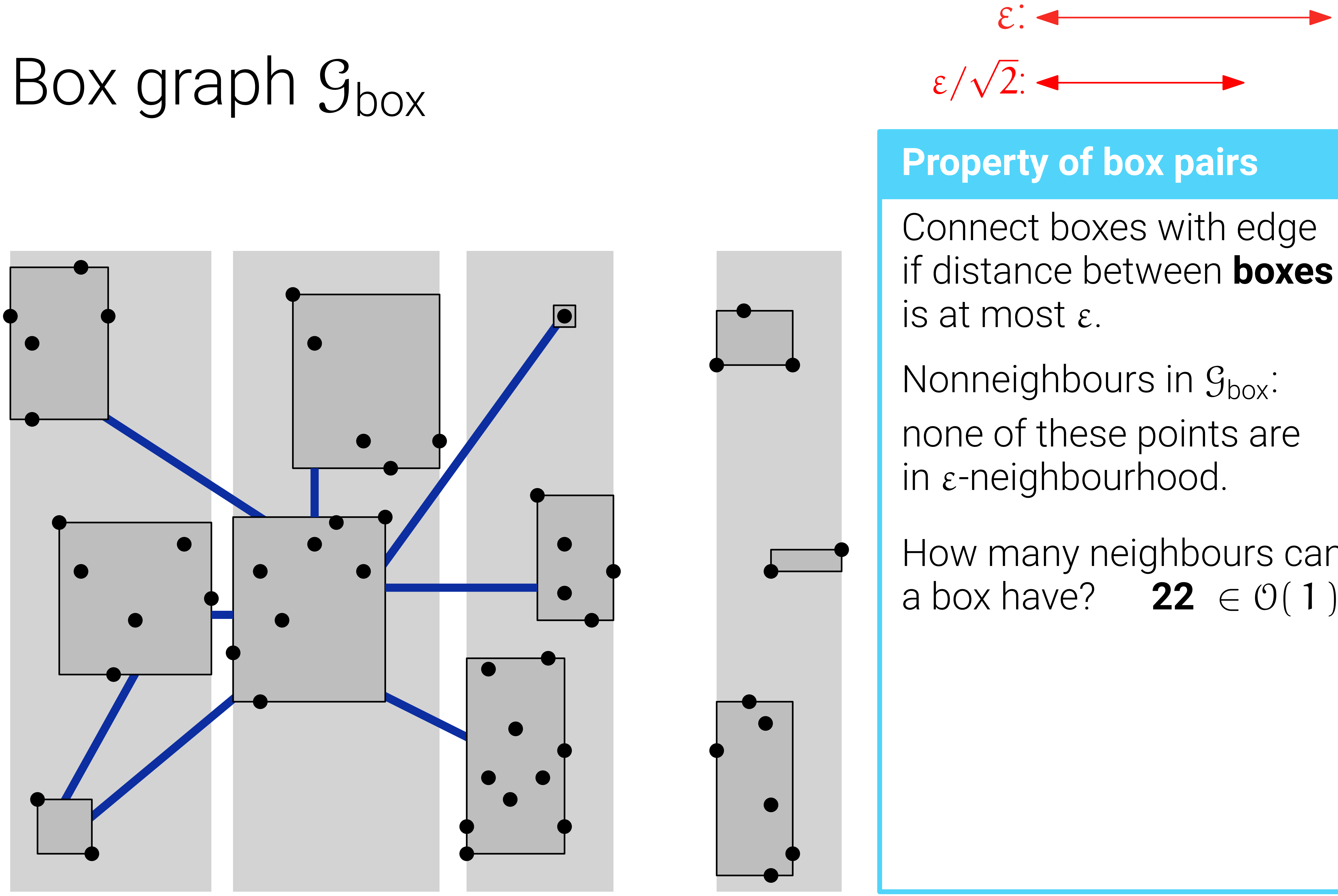
Property of box pairs

Connect boxes with edge if distance between **boxes** is at most ε.

Nonneighbours in $\mathcal{G}_{\text{box}}$: none of these points are in ε-neighbourhood.

How many neighbours can a box have? **22** $\in \mathcal{O}(1)$

Box graph $\mathcal{G}_{box}$



Property of box pairs

Connect boxes with edge if distance between **boxes** is at most ε.

Nonneighbours in $\mathcal{G}_{box}$:

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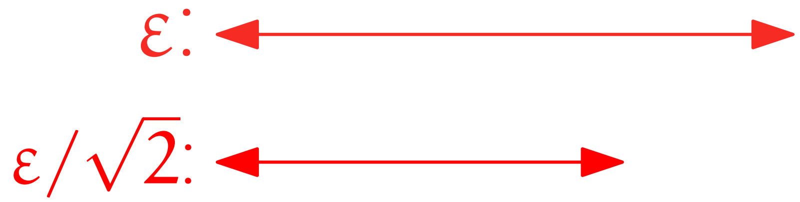
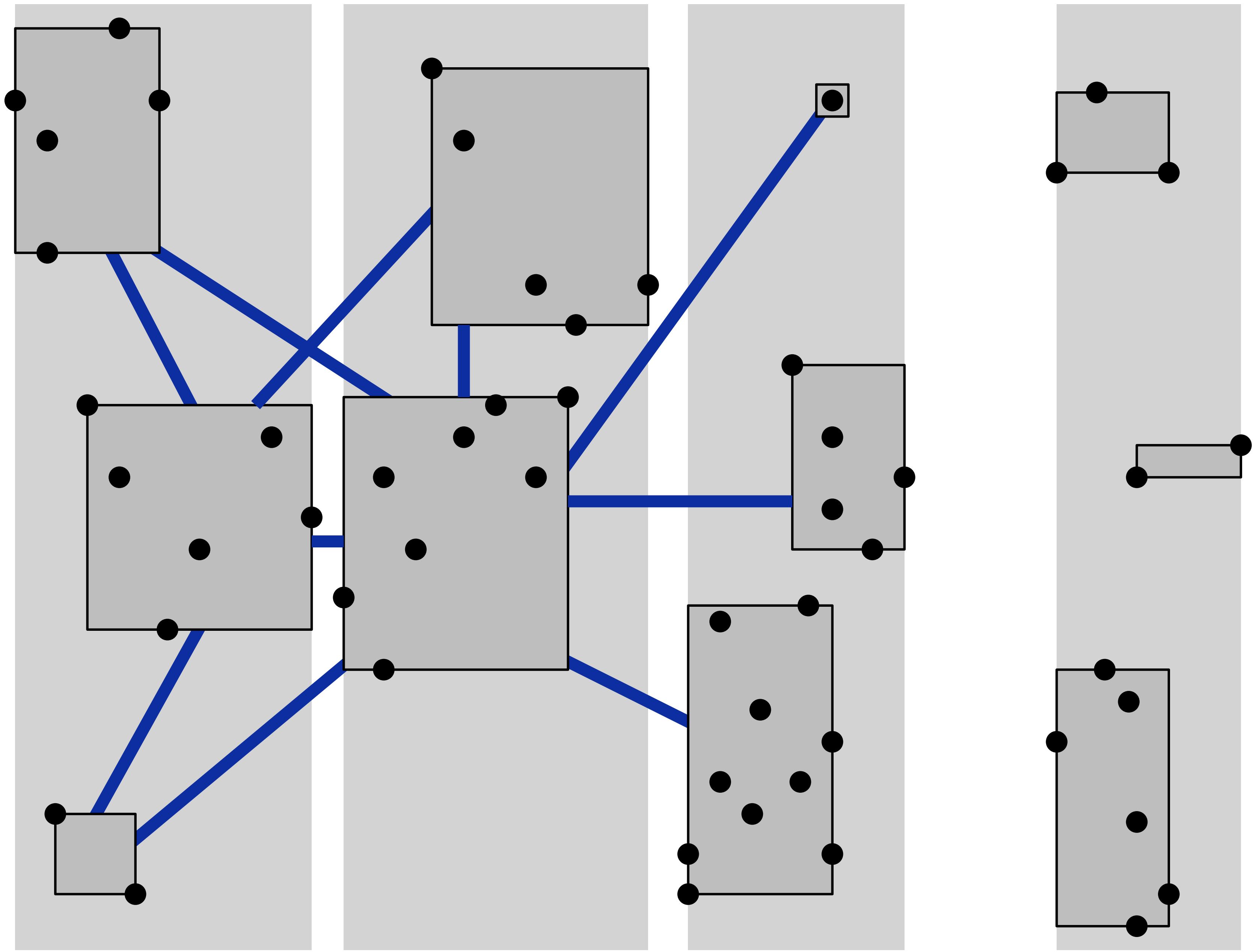
How many neighbours can a box have? **22** $\in \mathcal{O}(1)$

Box graph $\mathcal{G}_{box}$





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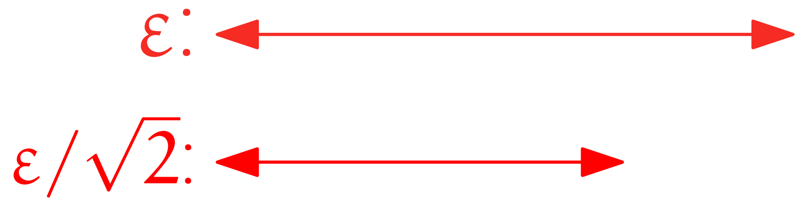
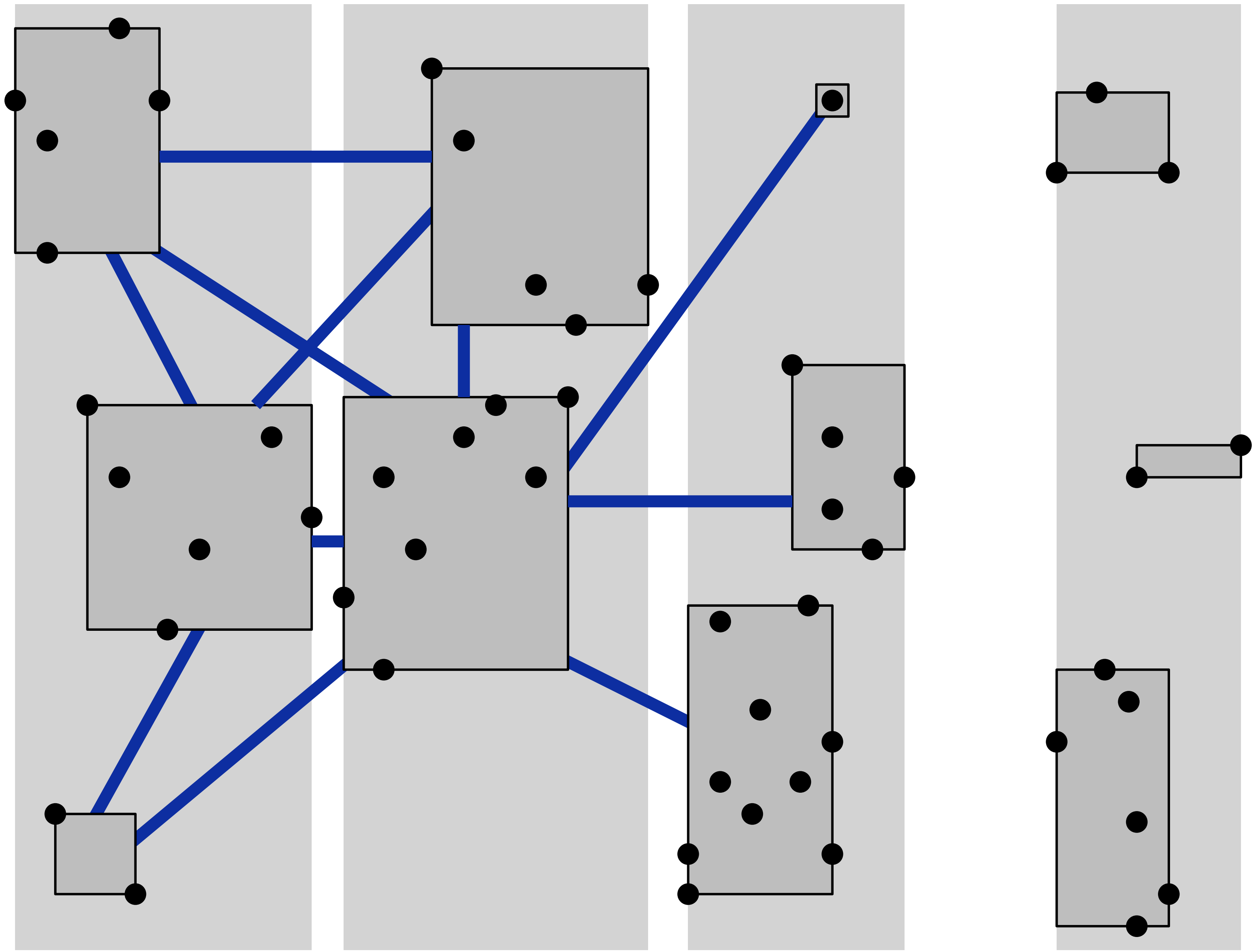
How many neighbours can a box have? **22** $\in \mathcal{O}(1)$

Box graph $\mathcal{G}_{box}$





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Connect boxes with edge if distance between **boxes** is at most ε.

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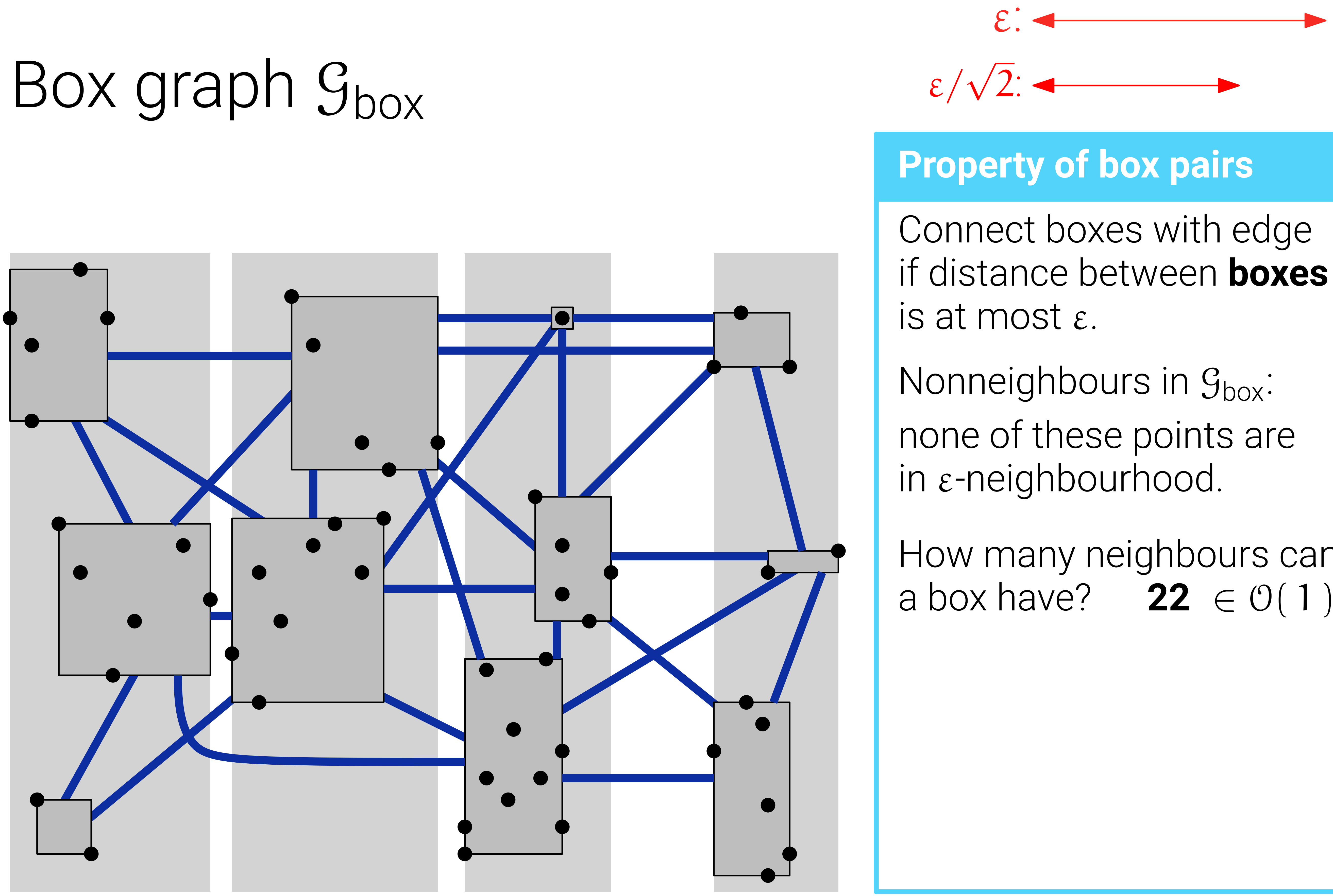
How many neighbours can a box have? **22** $\in \mathcal{O}(1)$

Box graph $\mathcal{G}_{box}$



Property of box pairs

Connect boxes with edge if distance between **boxes** is at most ε.

Nonneighbours in $\mathcal{G}_{box}$: none of these points are in ε-neighbourhood.

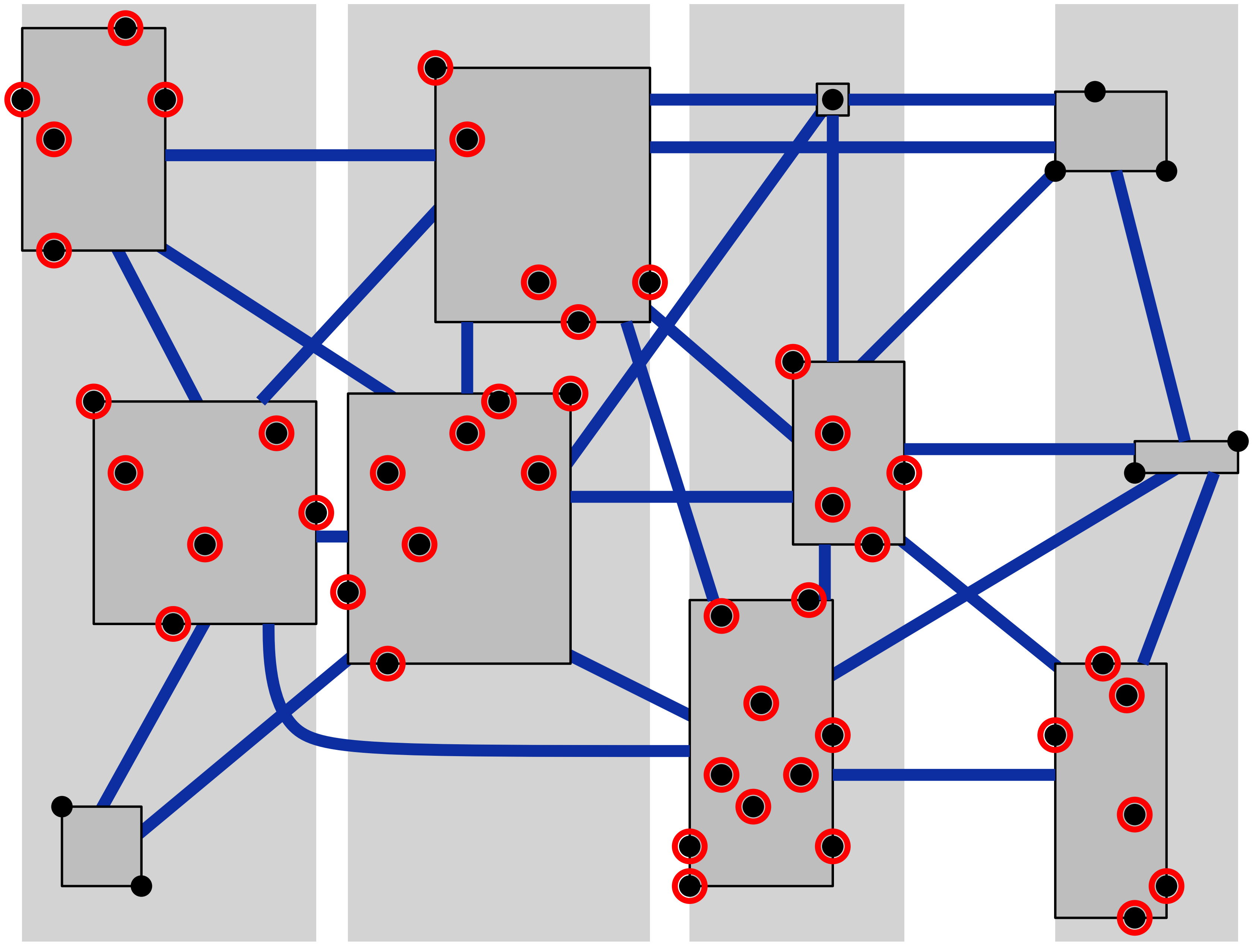
How many neighbours can a box have? **22** $\in \mathcal{O}(1)$

Box graph $\mathcal{G}_{box}$

$k = 4$

ε:

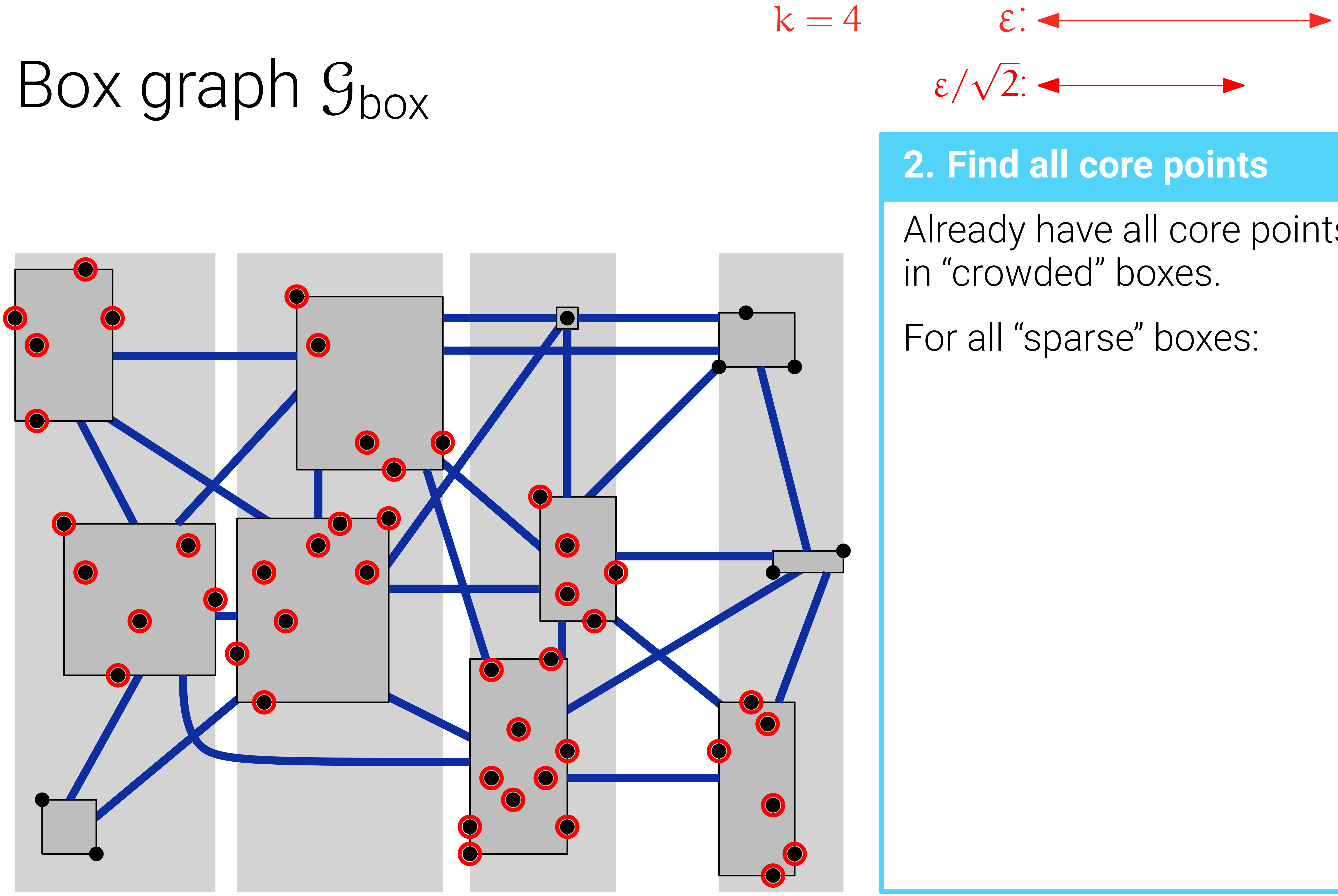
$\varepsilon/\sqrt{2}$:



2. Find all core points

Already have all core points in “crowded” boxes.

Box graph $\mathcal{G}_{box}$

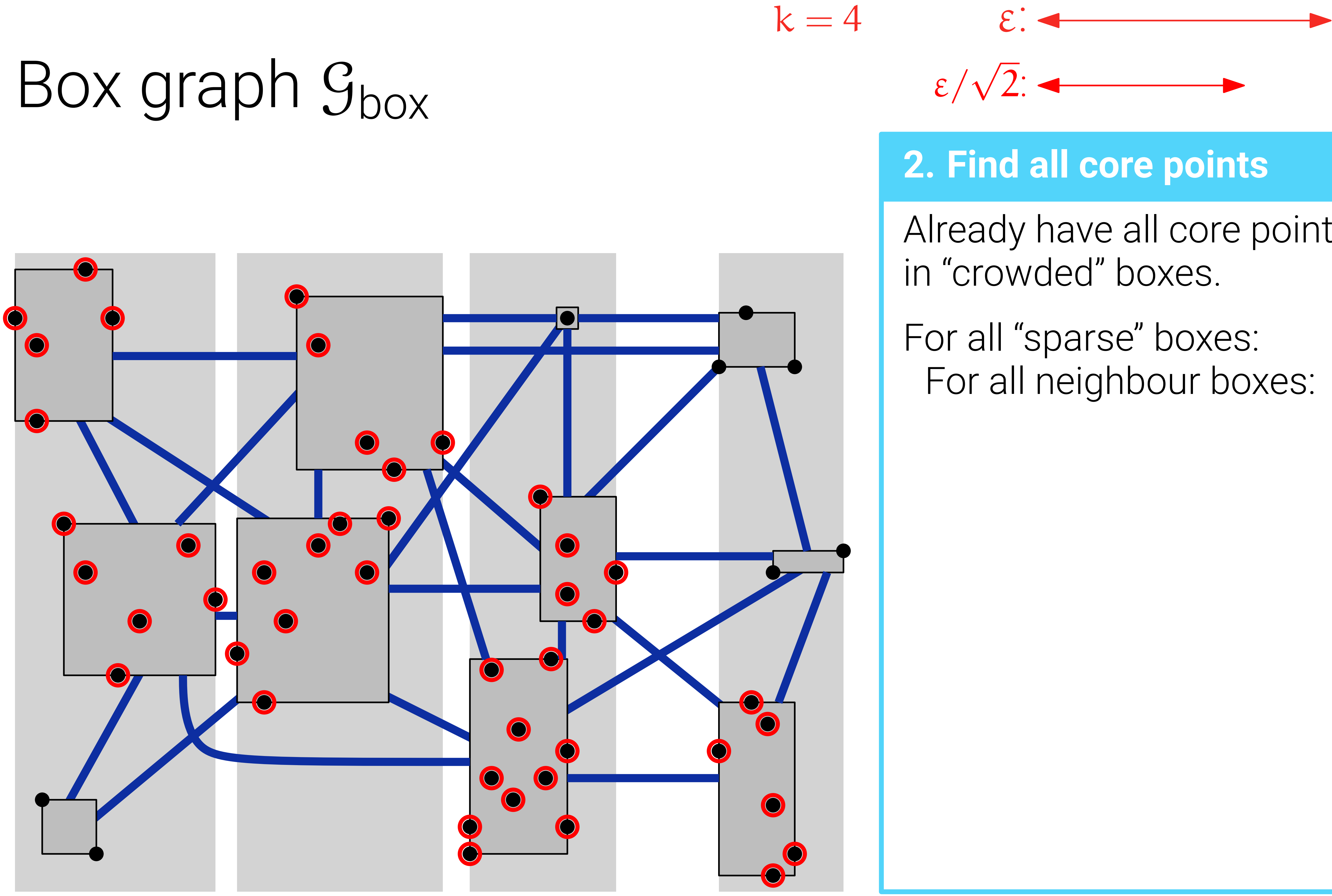


2. Find all core points

Already have all core points in "crowded" boxes.

For all "sparse" boxes:

Box graph $\mathcal{G}_{box}$

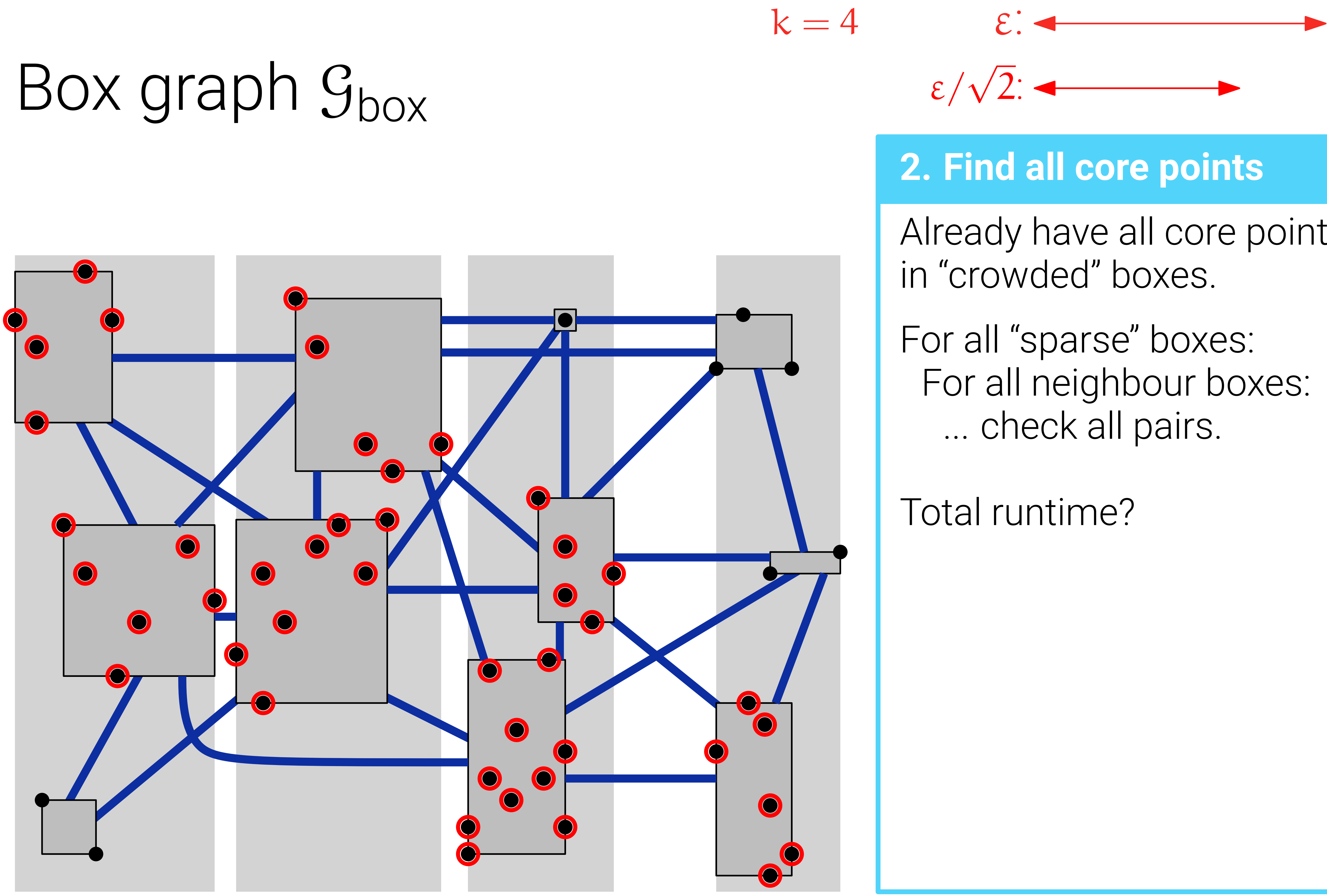


2. Find all core points

Already have all core points in “crowded” boxes.

For all “sparse” boxes:
  For all neighbour boxes:

Box graph $\mathcal{G}_{box}$



2. Find all core points

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Total runtime?

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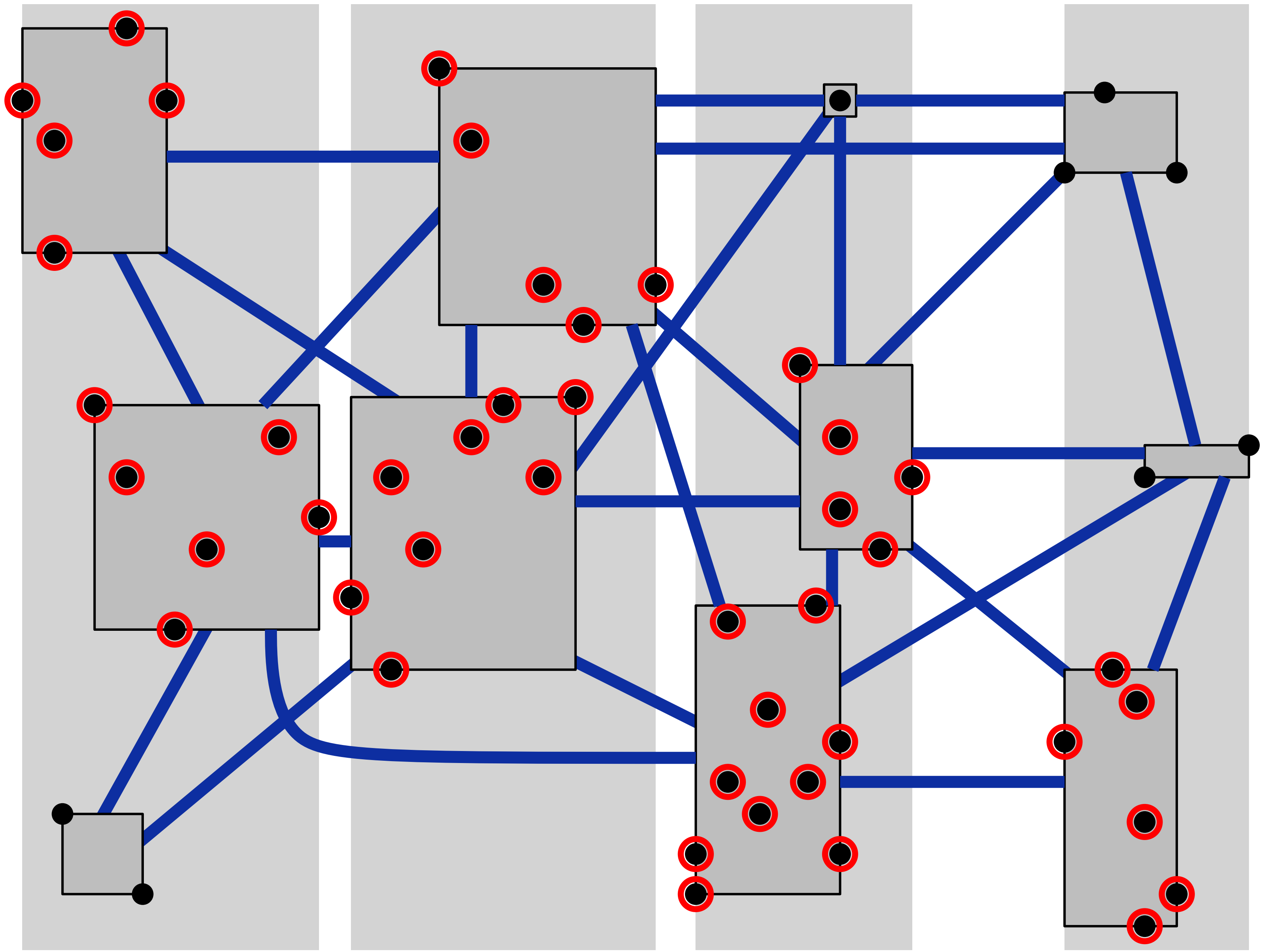

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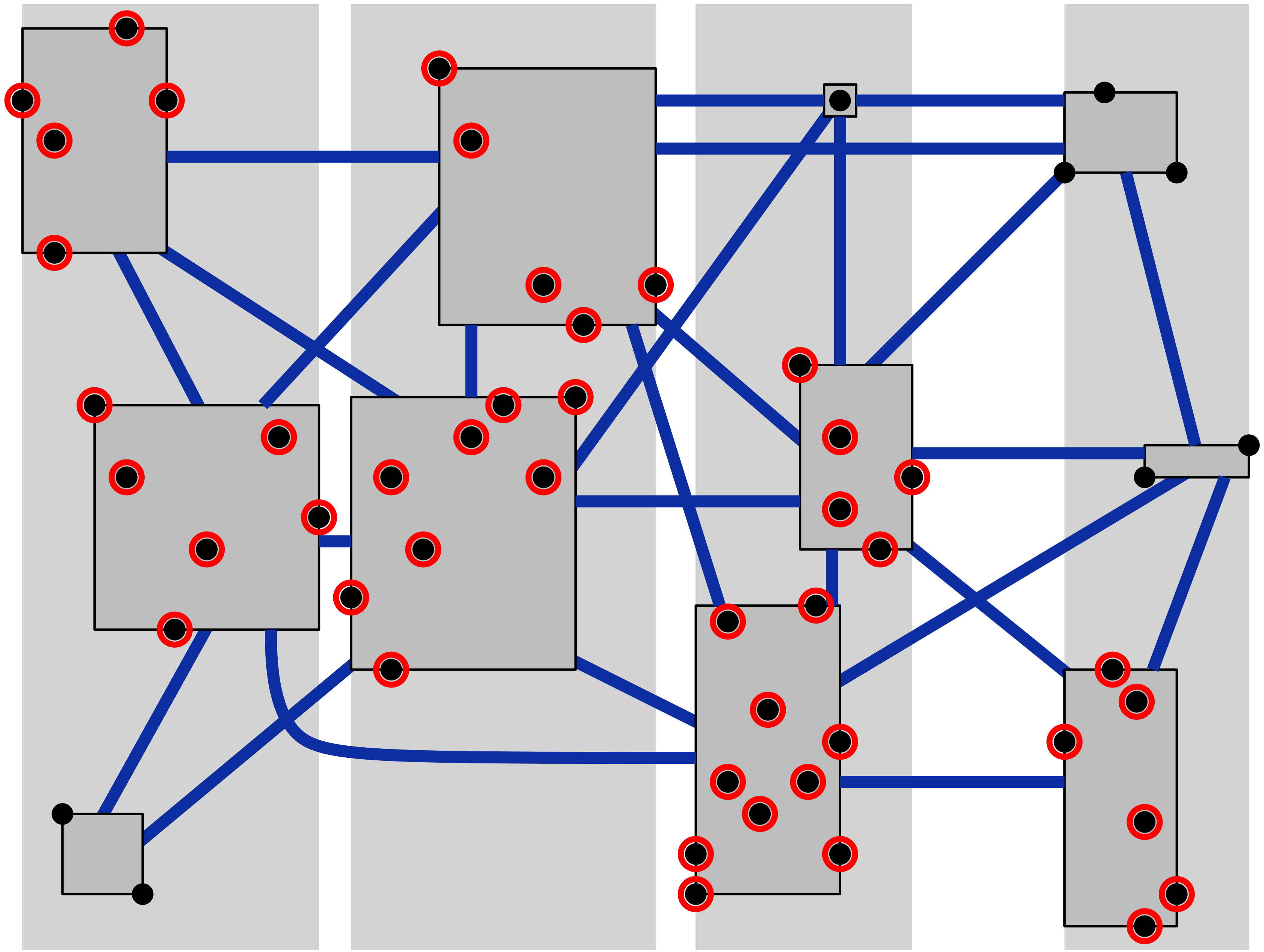

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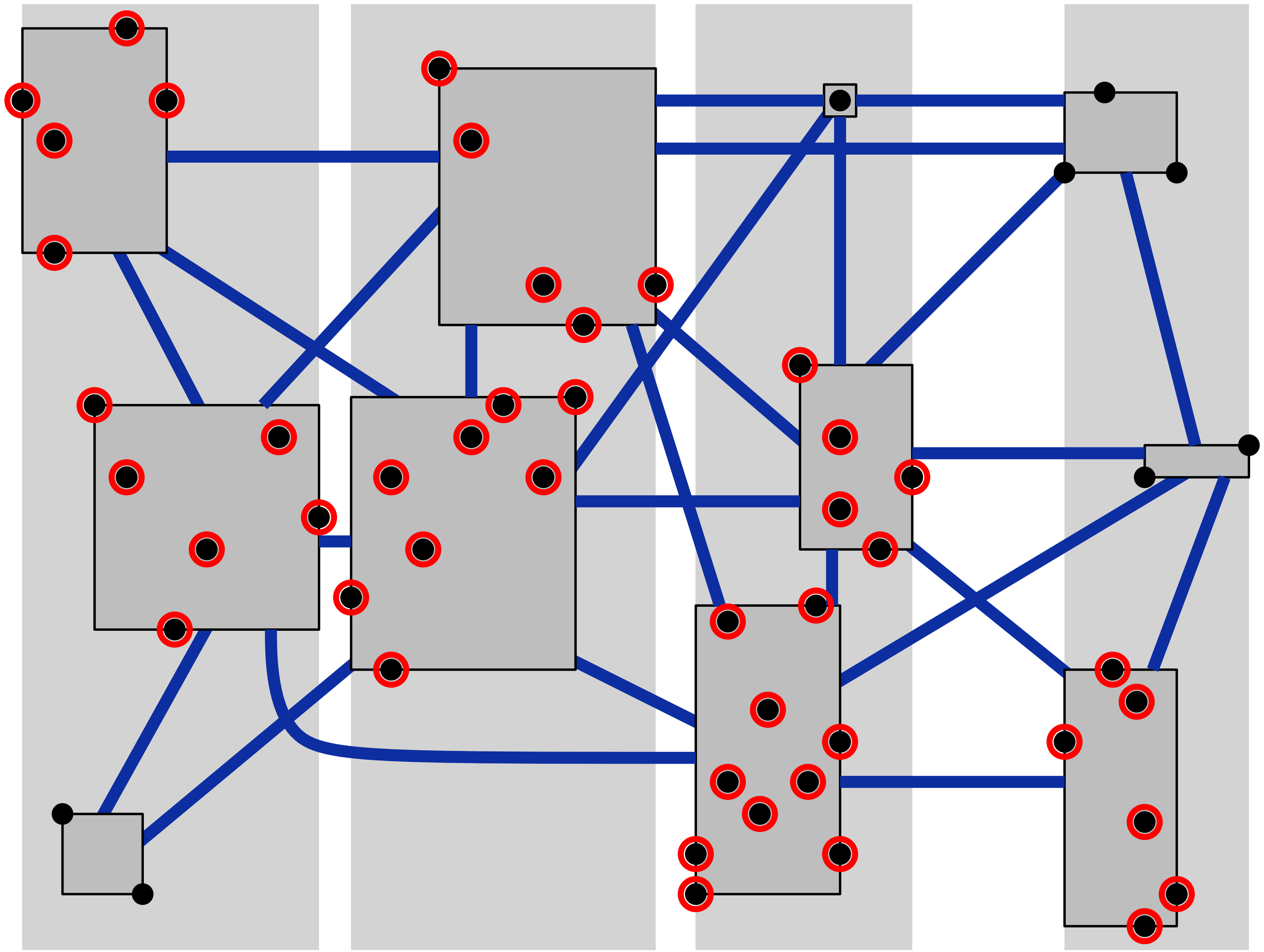

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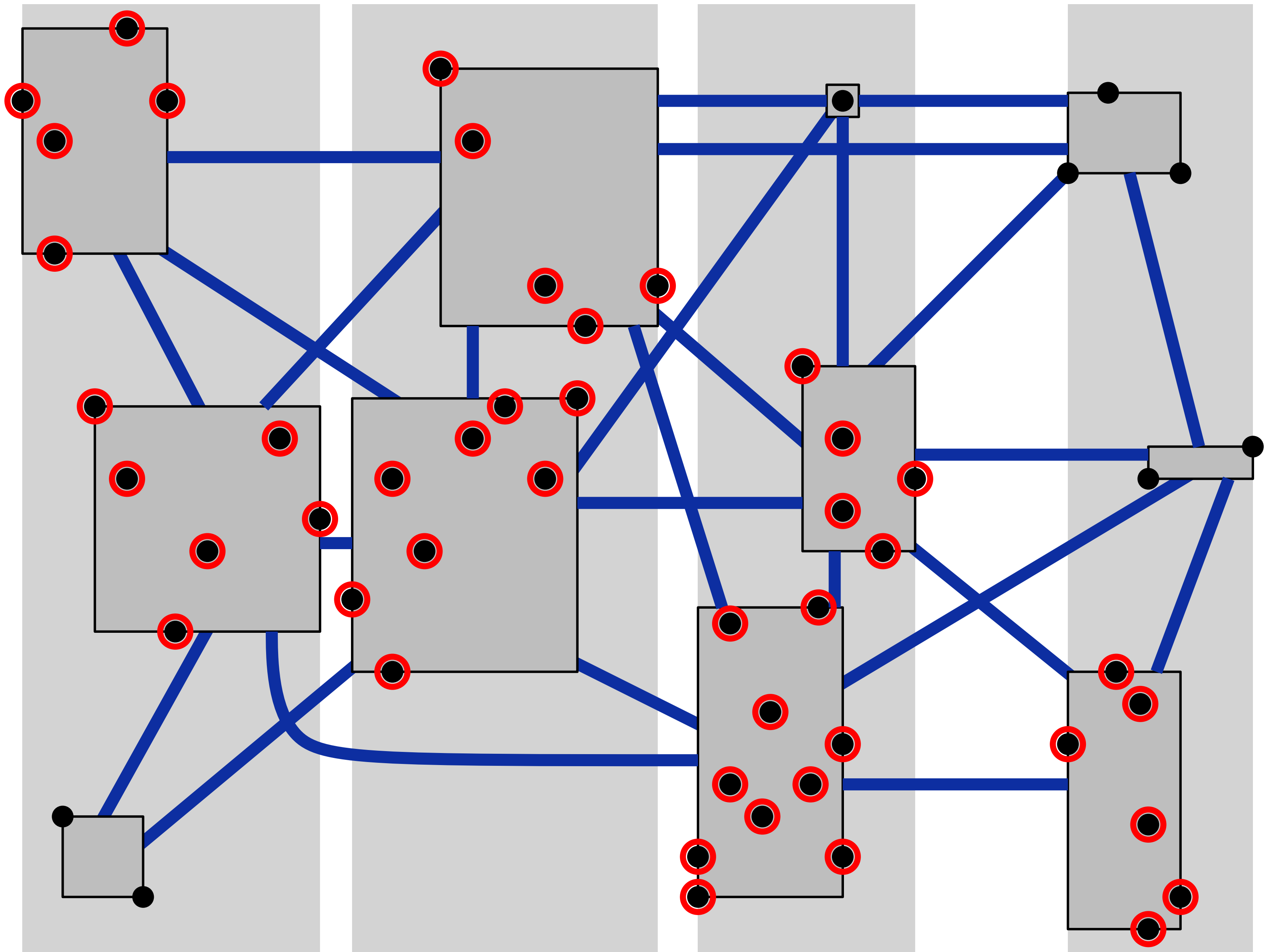

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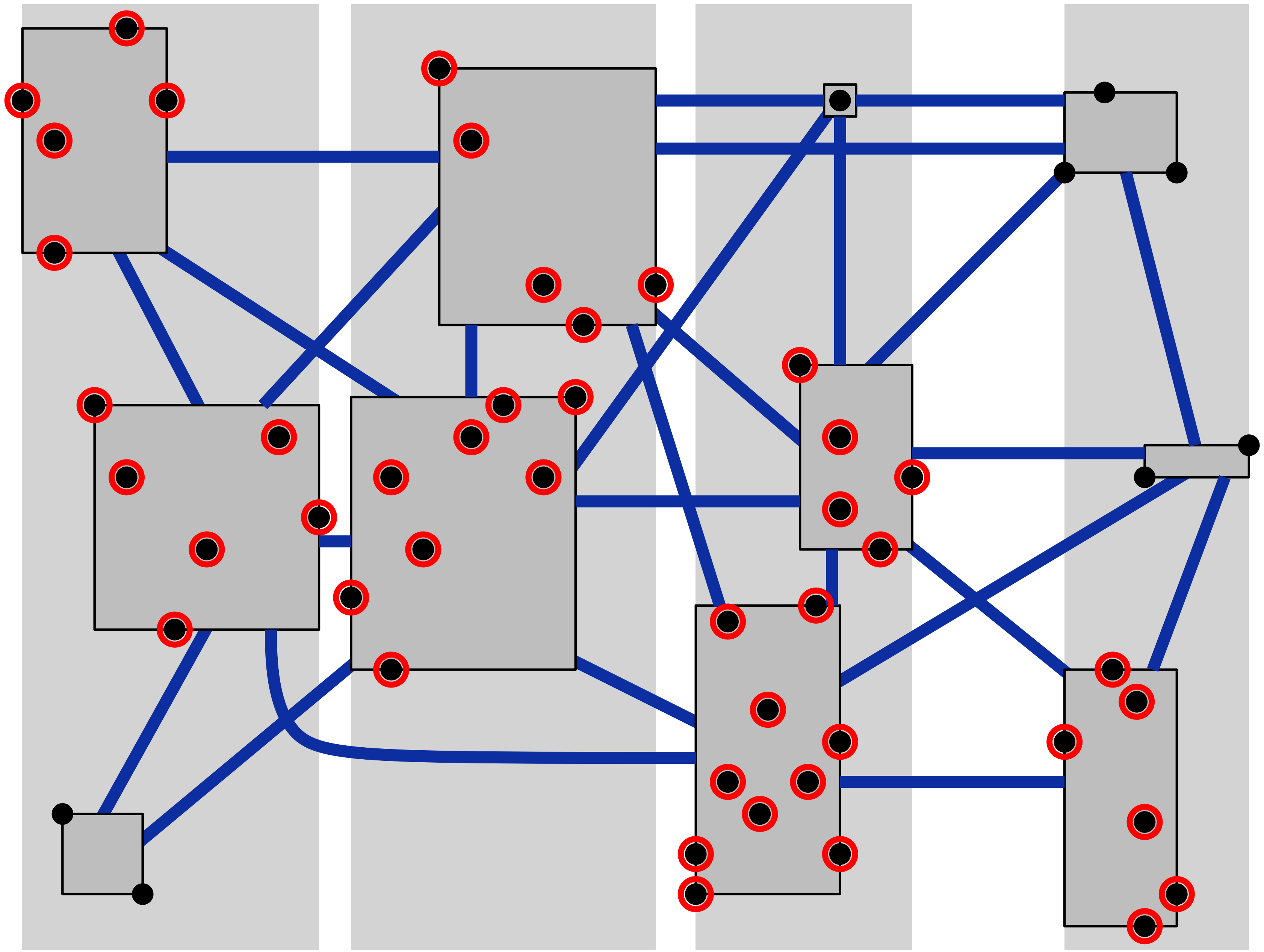

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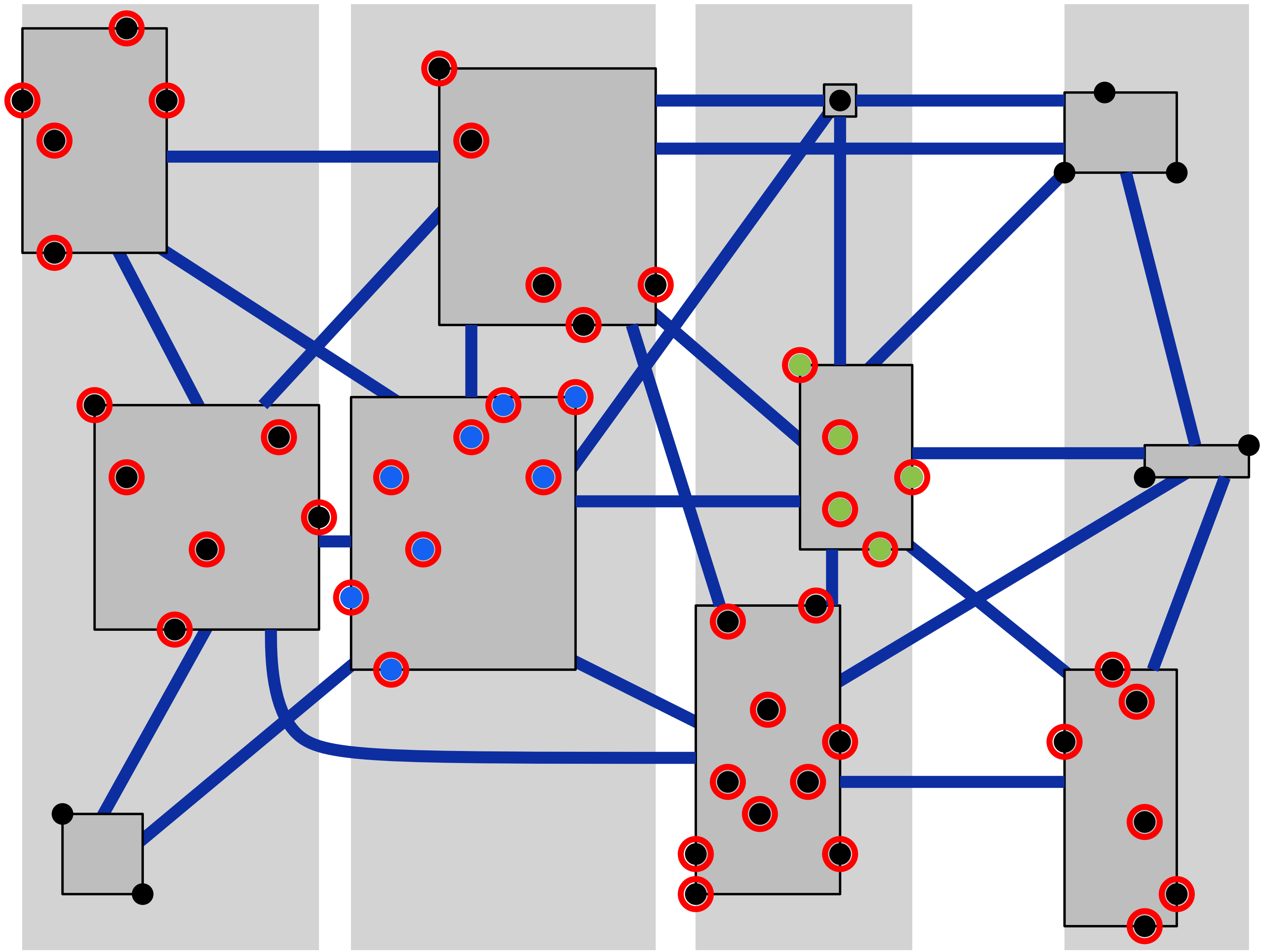

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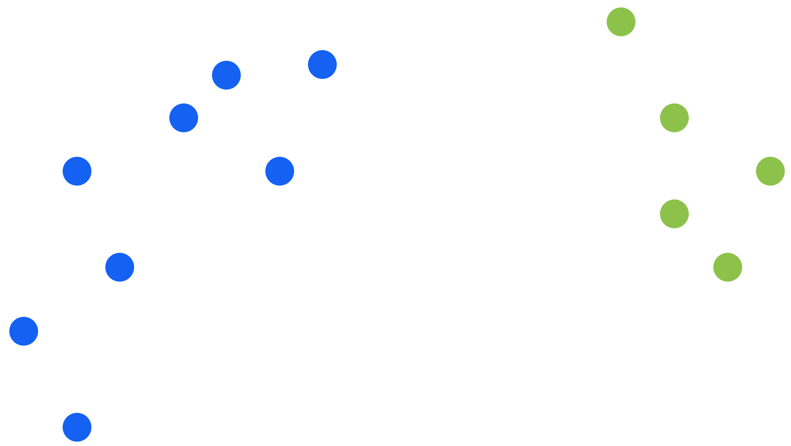

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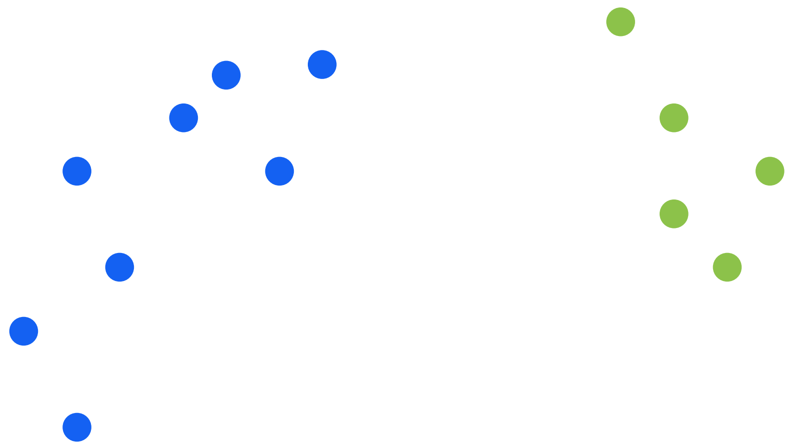

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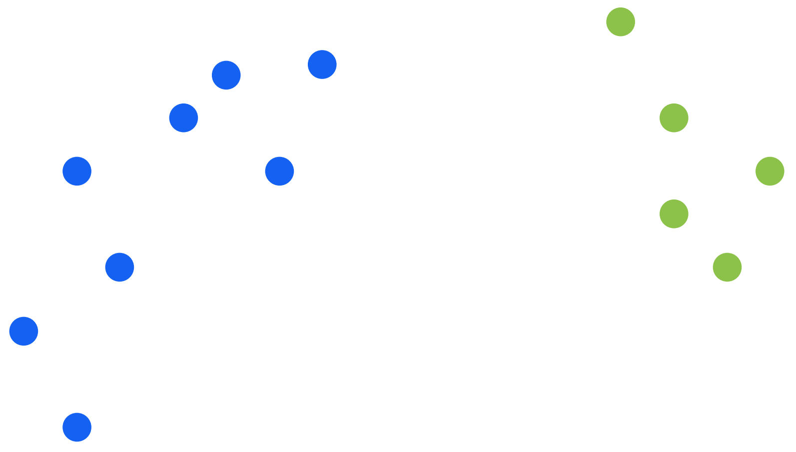

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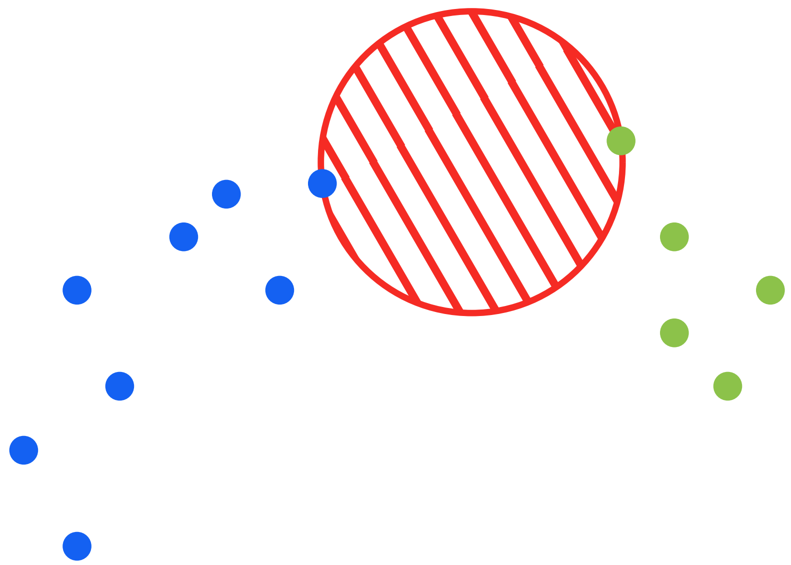

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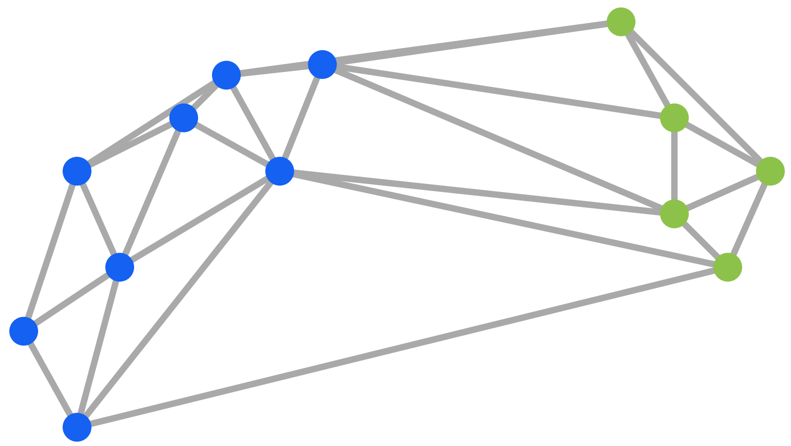

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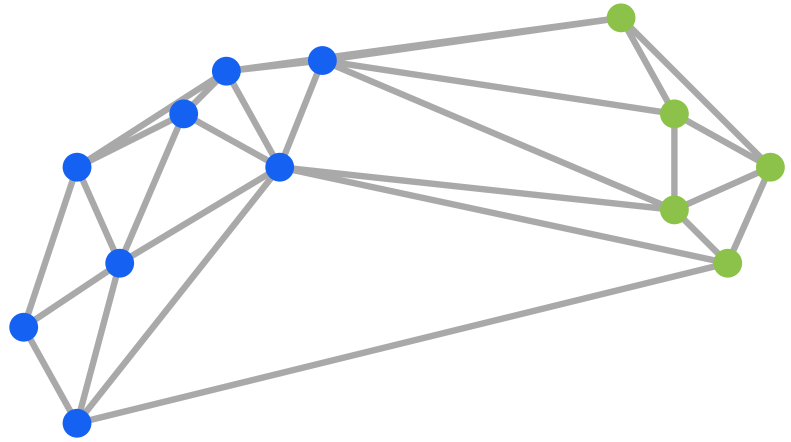

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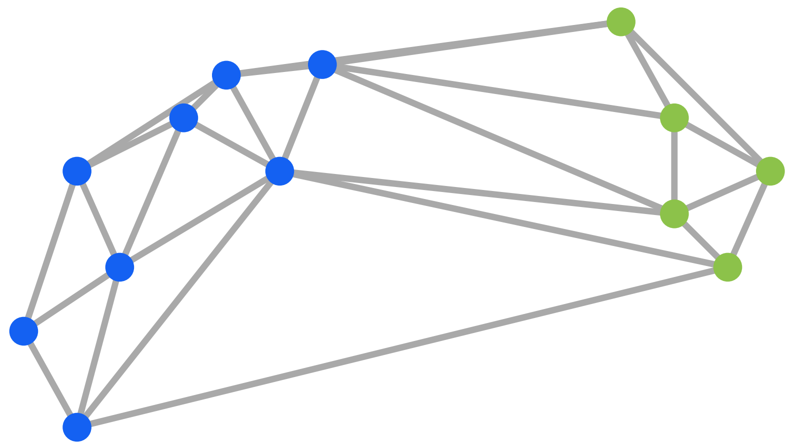

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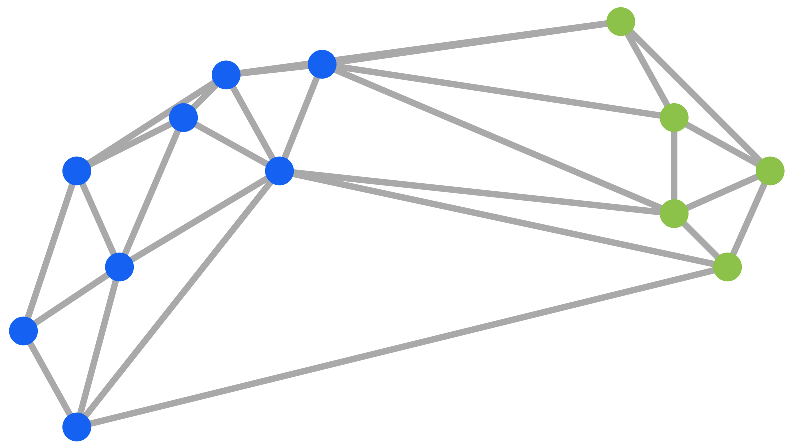

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Everywhere: ε free, k fixed constant, Euclidean distances

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Store this tree structure of cluster creation and merges: HDBSCAN.

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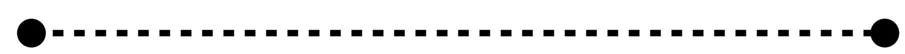

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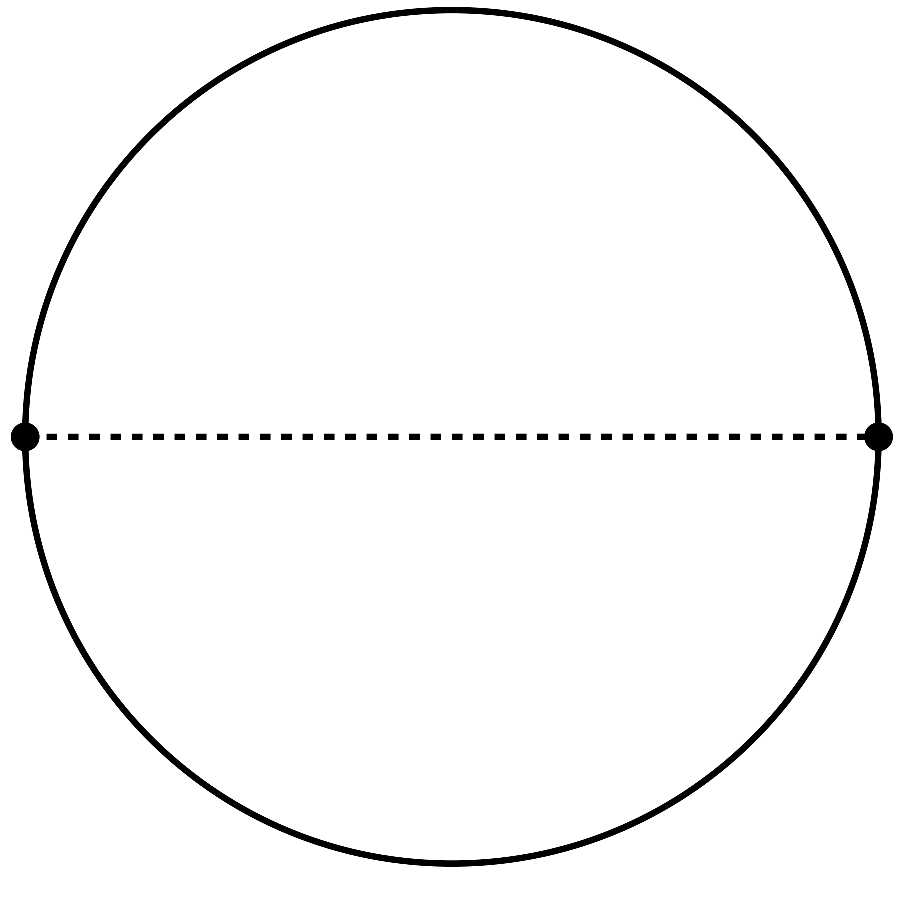

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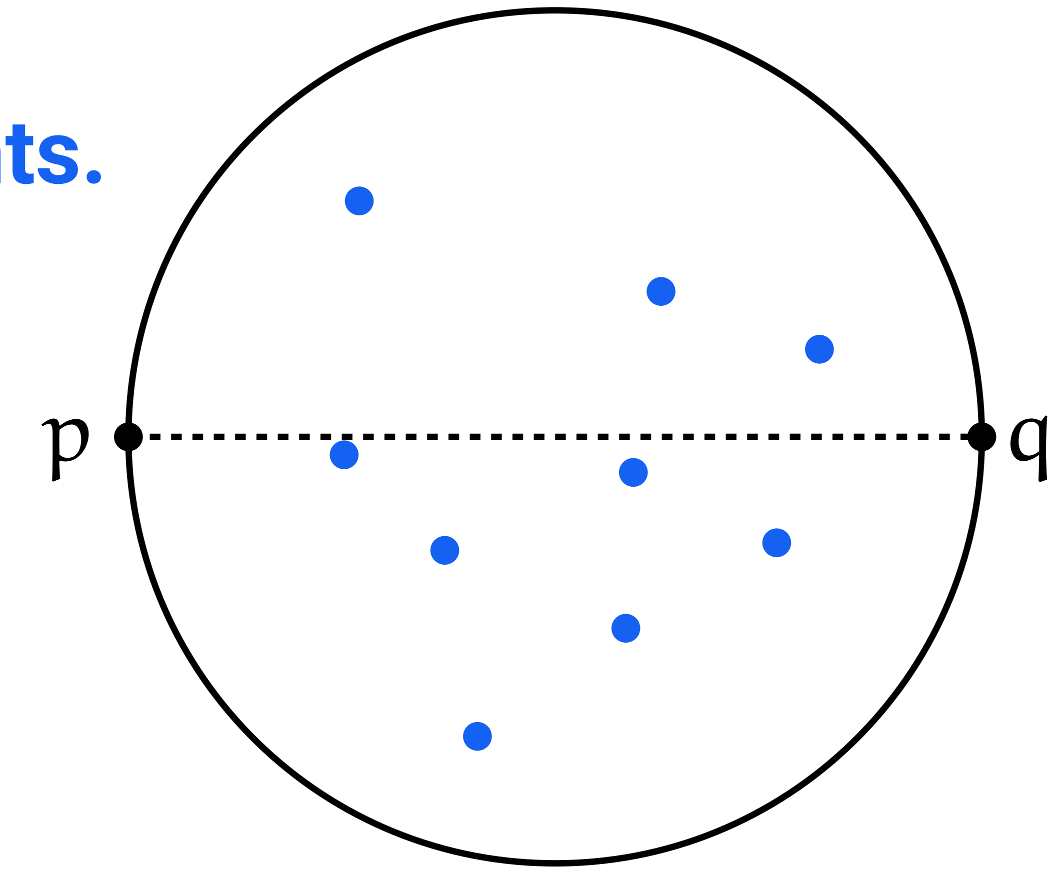

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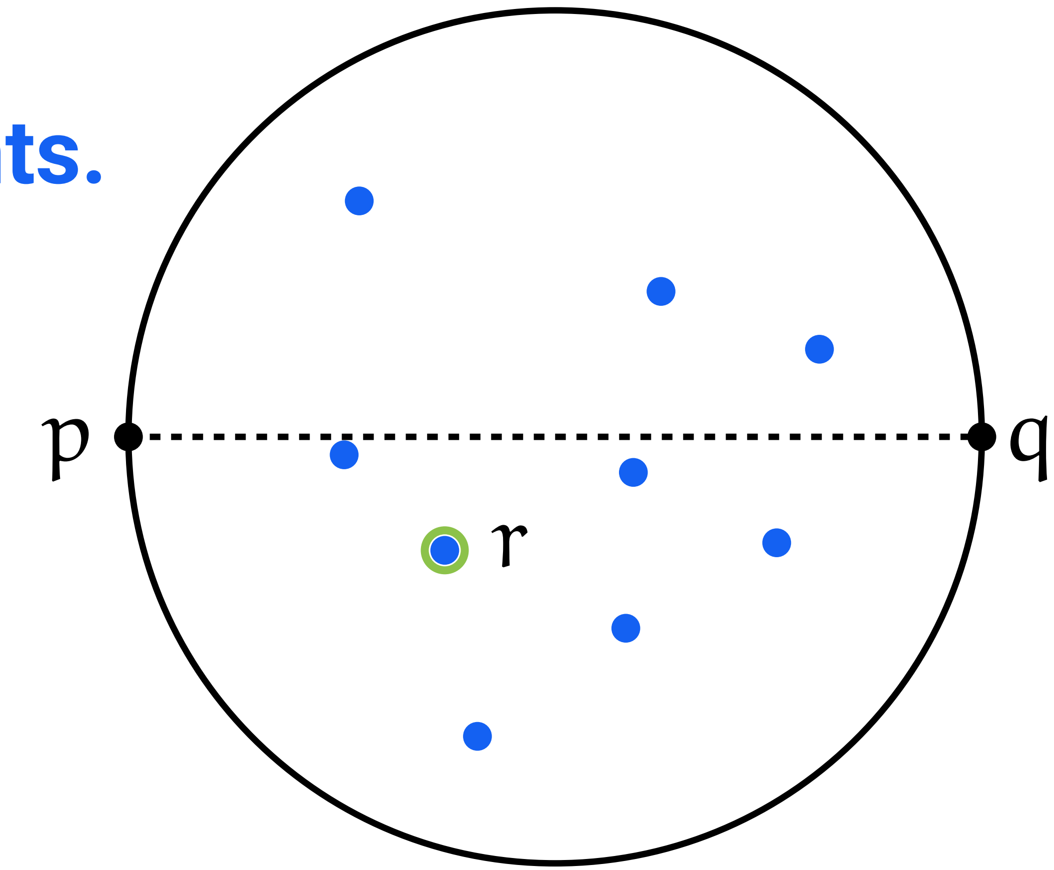

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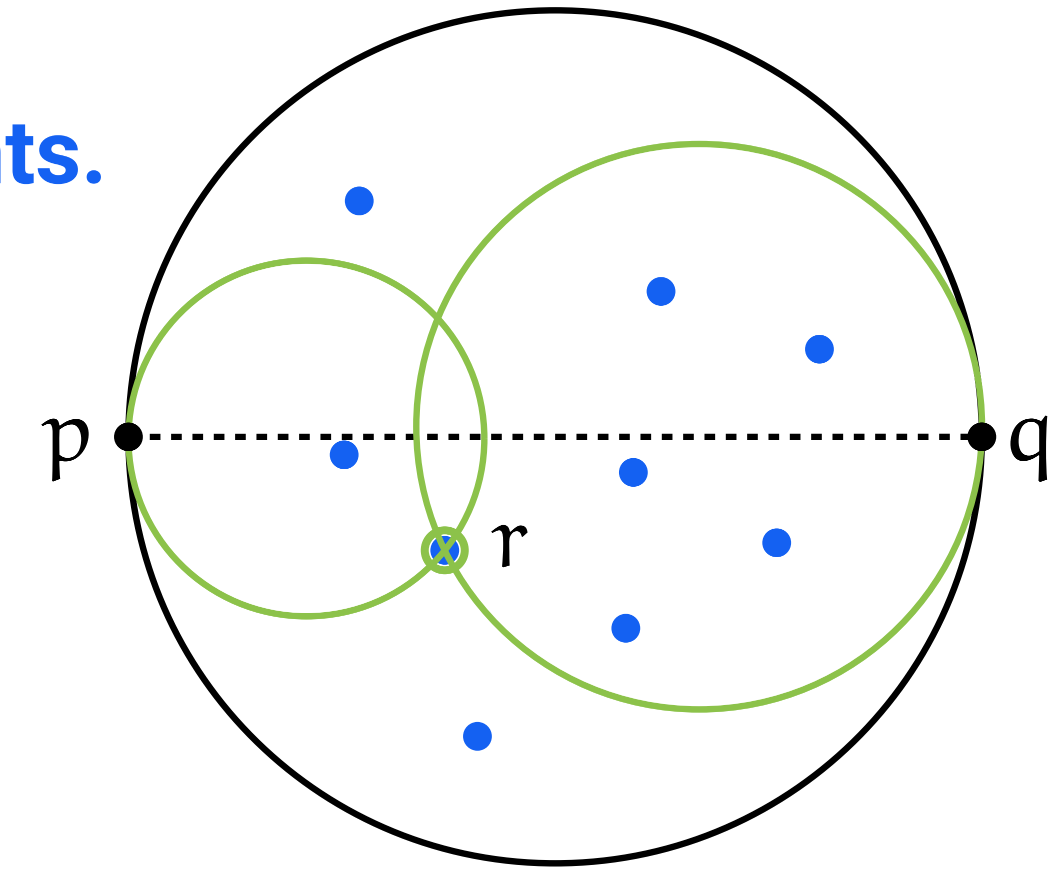

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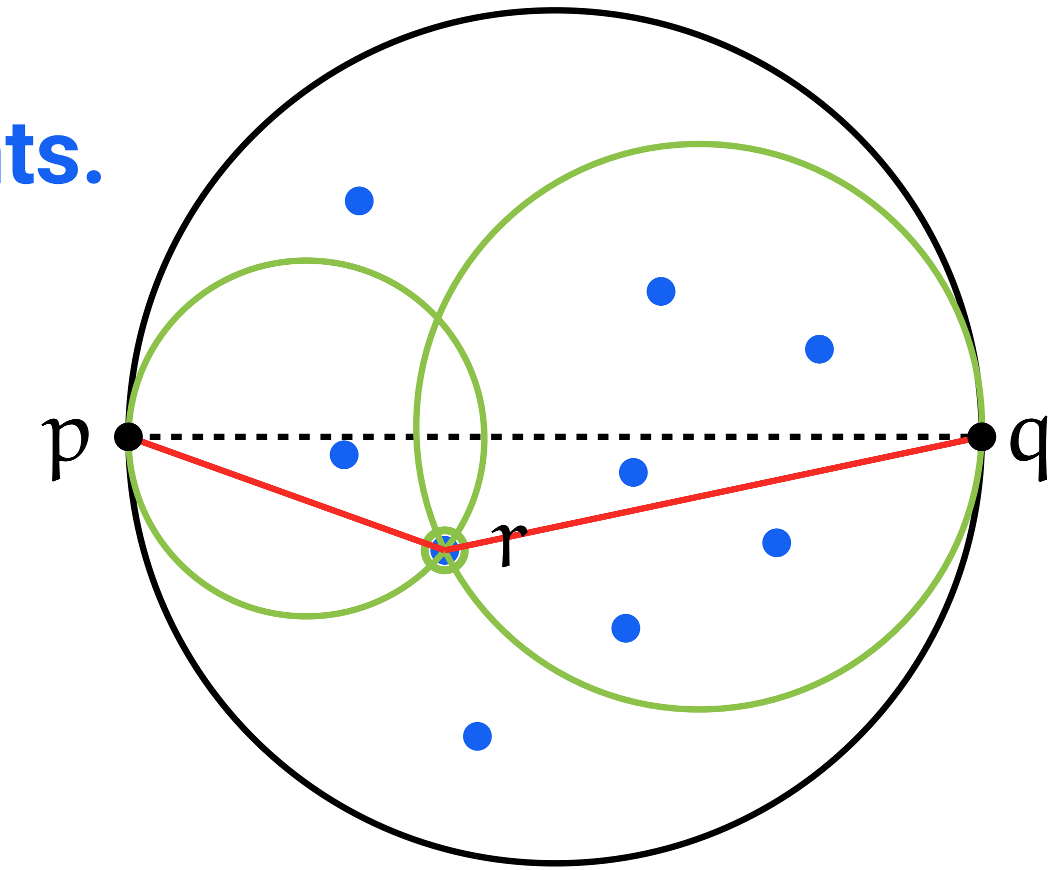

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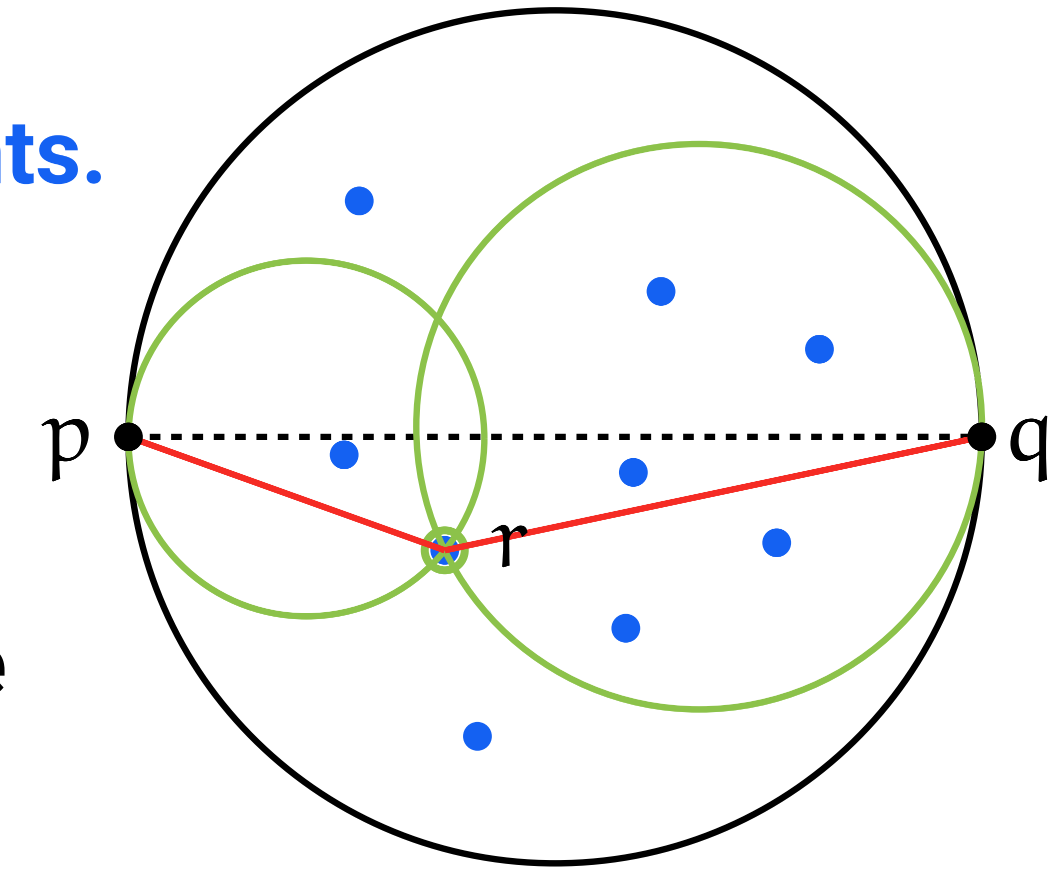
Kruskal has already considered those edges, so p and q already connected.



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