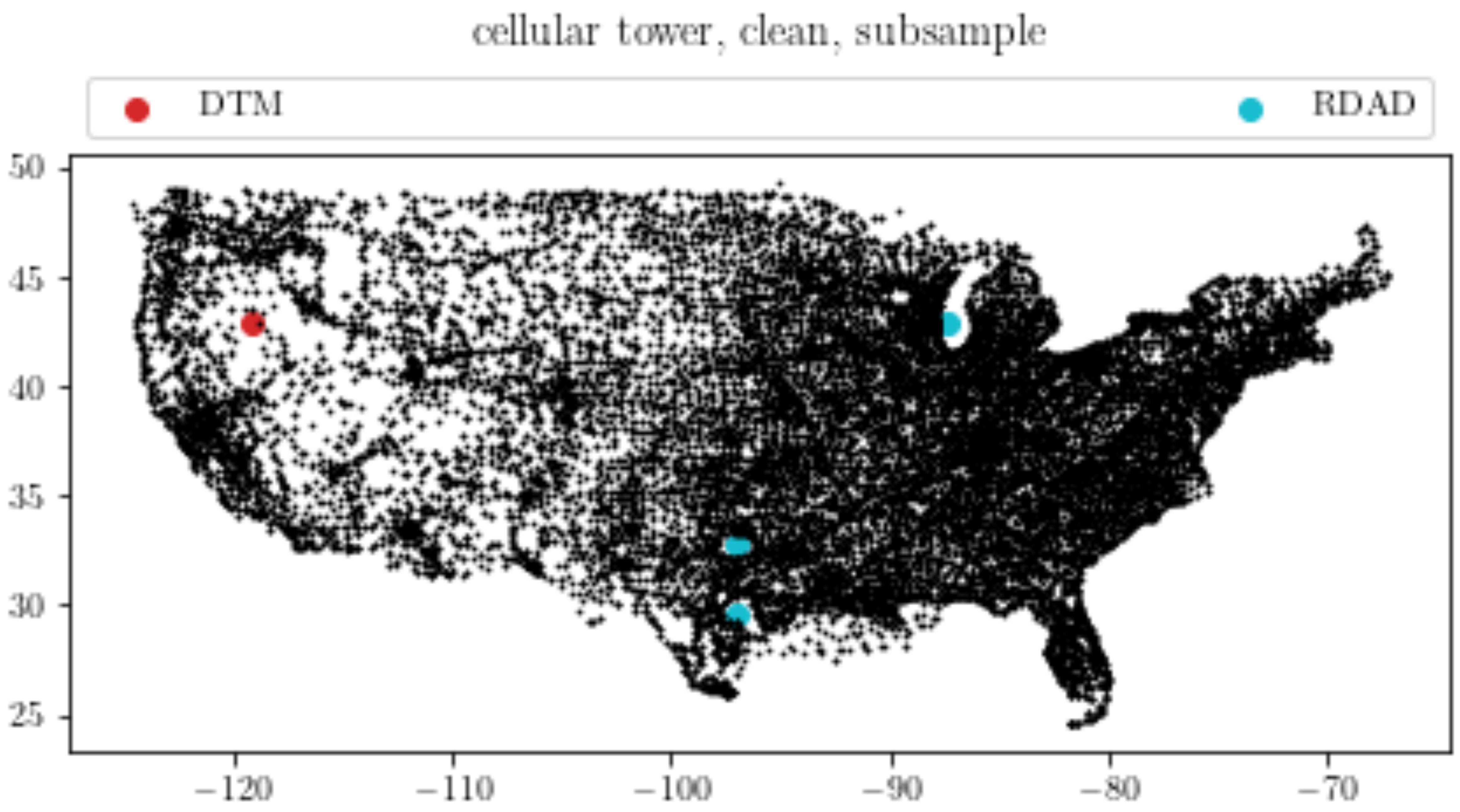
Topological Data Analysis

Small Density Vacuum and How to Find Them Robustly



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In the beginning…

there was the data

Credit: NASA/NCSA, University of Illinois
Visualization by Frank Summers, Space Telescope Science Institute
Simulation by Martin White and Lars Hernquist, Harvard University
https://universe.nasa.gov/resources/89/cosmic-web/

In the beginning…

there was the data

and the data was non-parametric,

Credit: NASA/NCSA, University of Illinois
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https://universe.nasa.gov/resources/89/cosmic-web/

In the beginning…

there was the data

and the data was non-parametric,
and has voids,

Credit: NASA/NCSA, University of Illinois
Visualization by Frank Summers, Space Telescope Science Institute
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https://universe.nasa.gov/resources/89/cosmic-web/

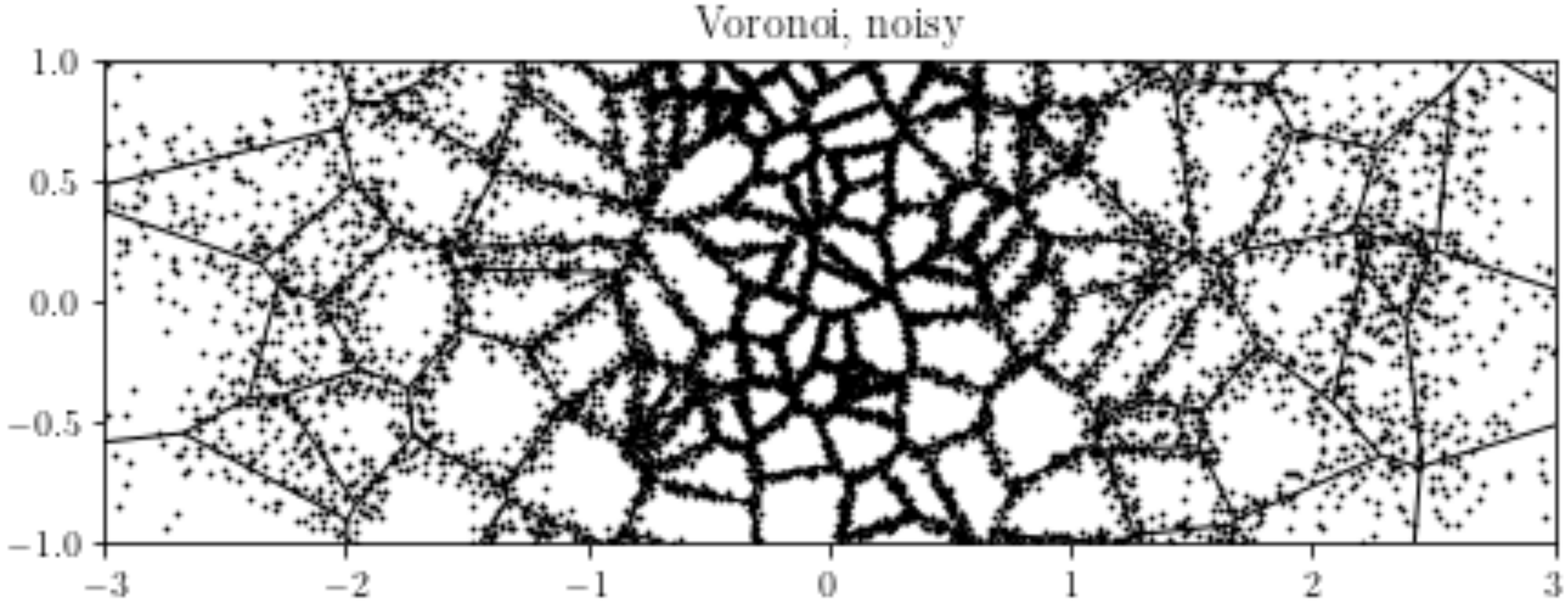
In the beginning…

there was the data

and the data was non-parametric,
and has voids,
and noise is upon the face of the dataset.

Credit: NASA/NCSA, University of Illinois
Visualization by Frank Summers, Space Telescope Science Institute
Simulation by Martin White and Lars Hernquist, Harvard University
https://universe.nasa.gov/resources/89/cosmic-web/

Let there be ground truth



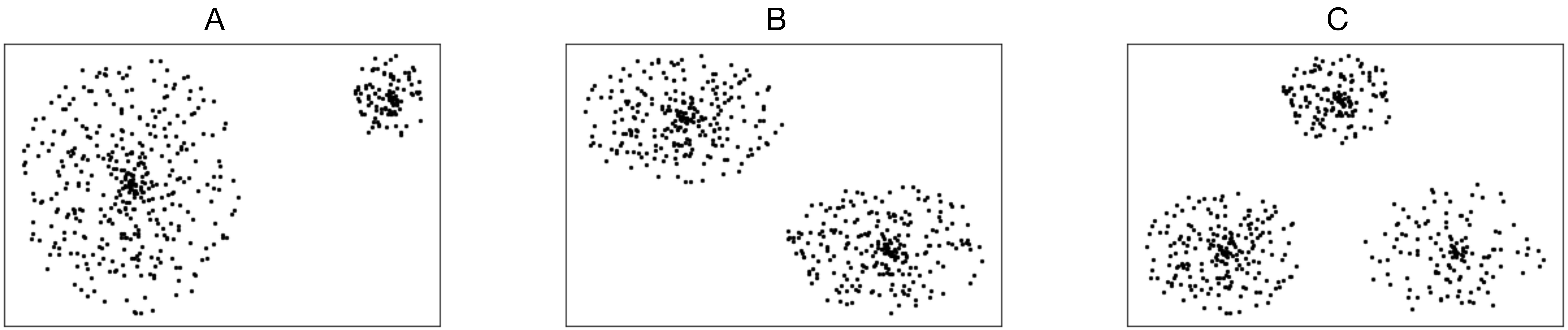
Agenda

- Topological Data Analysis: What and Why
- My Work: the Size, the Noise and the Randomness
- Numerical Simulations

Act I

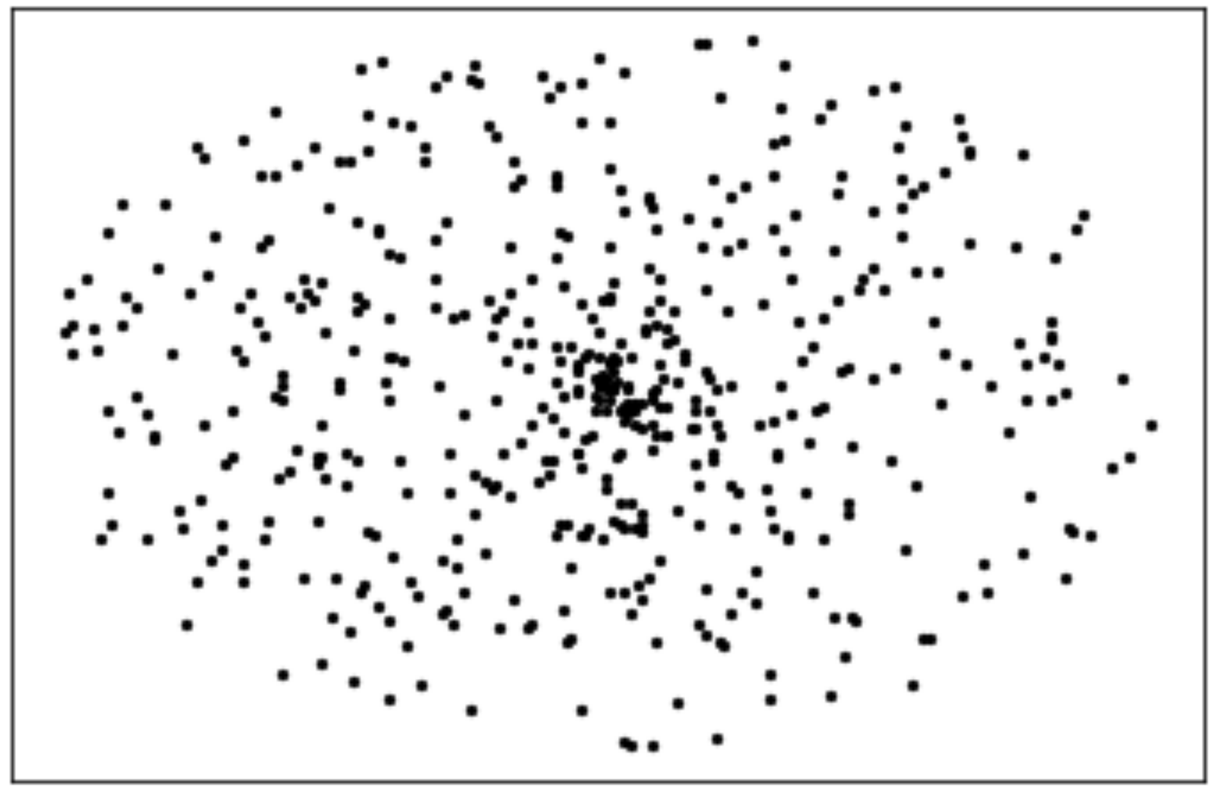
What the Fisher is Topological Data Analysis

Odd One Out

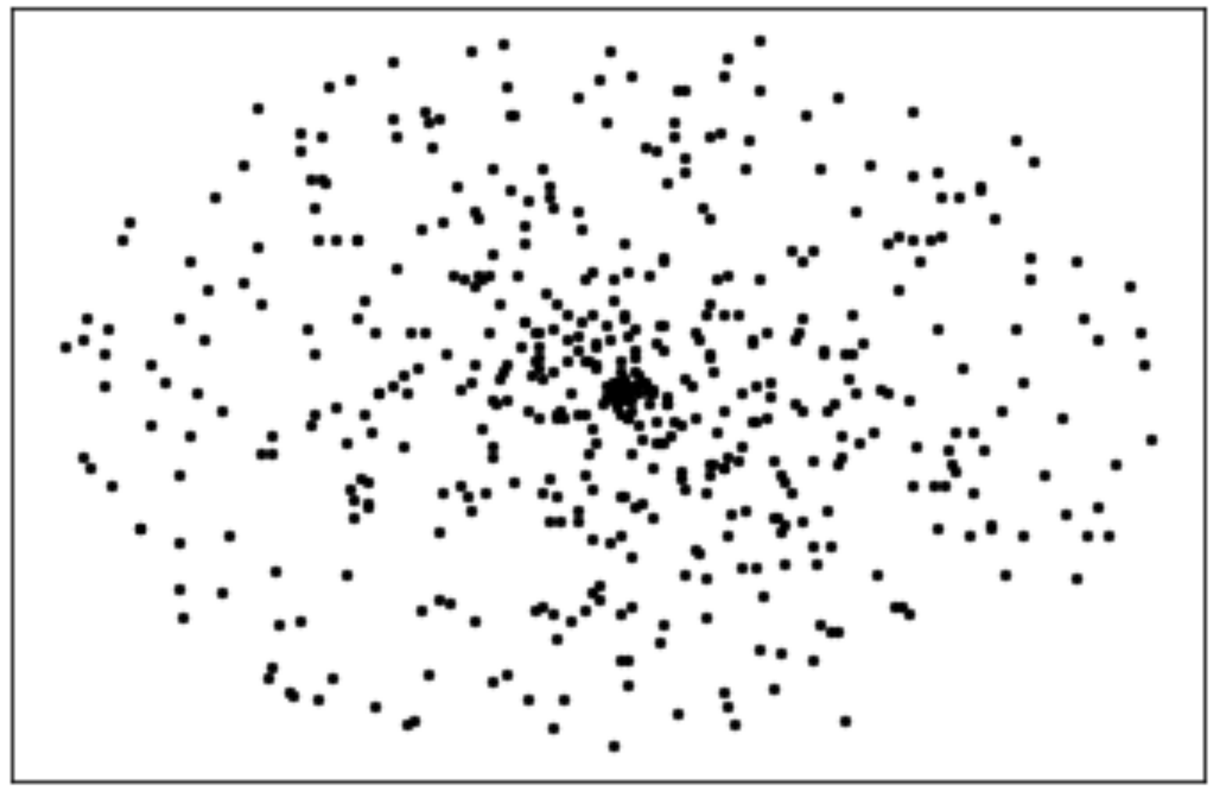


Odd One Out

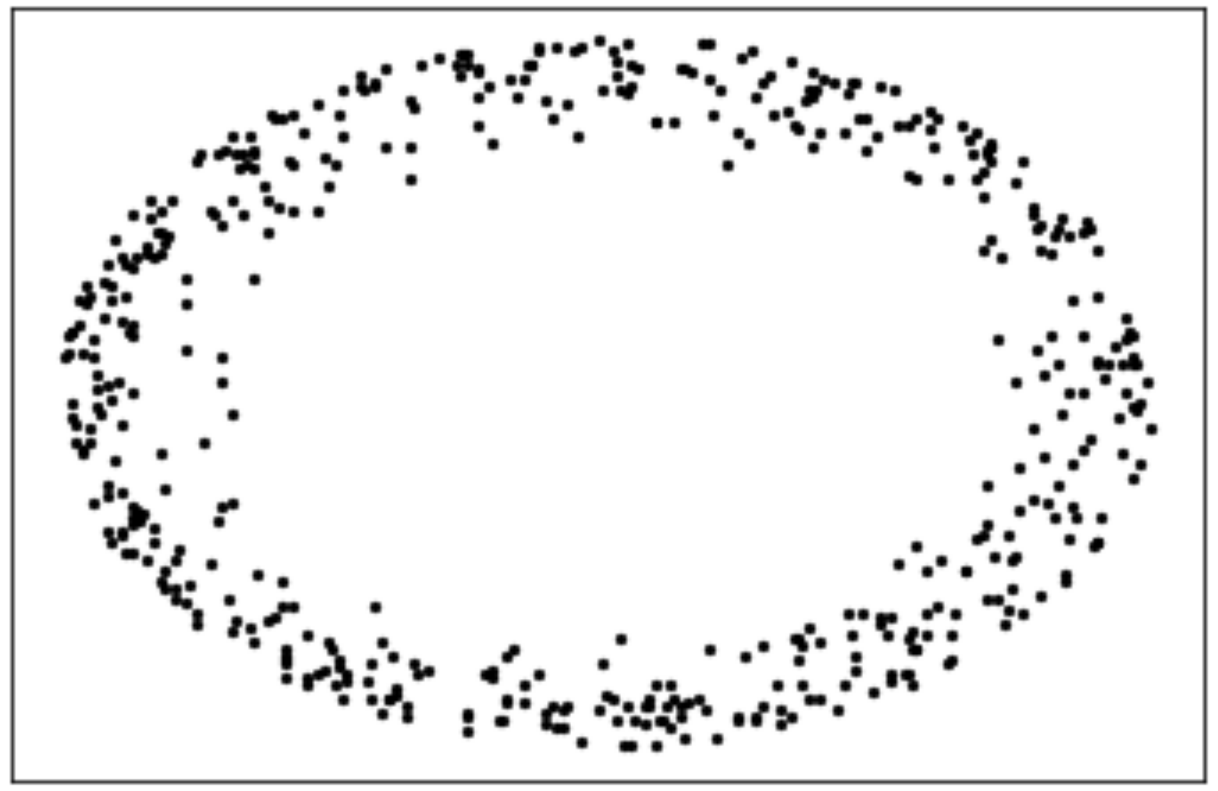
A



B



C



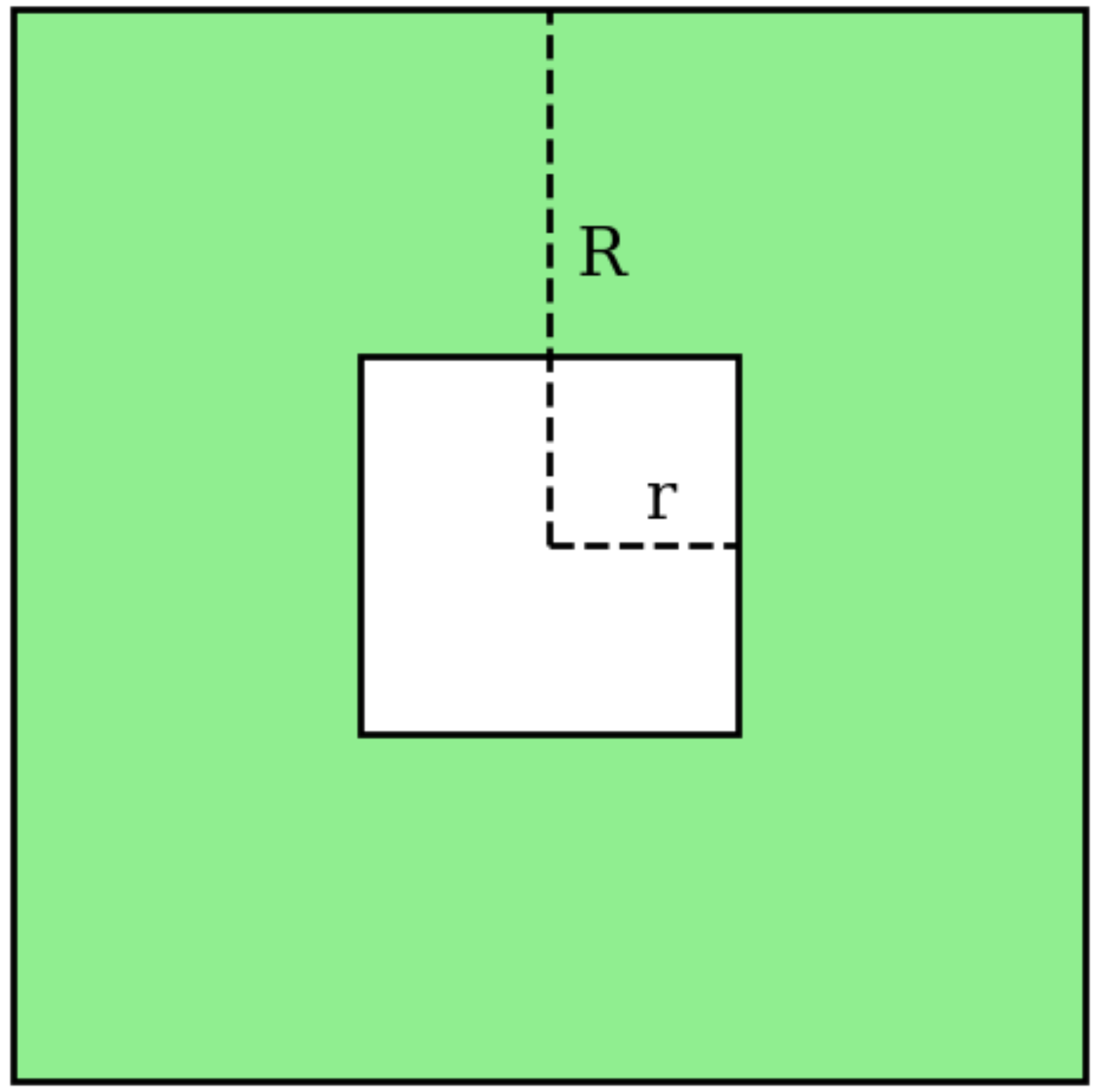
Seriously,
you’re doing this for a PhD?

0 training data
0 parameters
100% accuracy

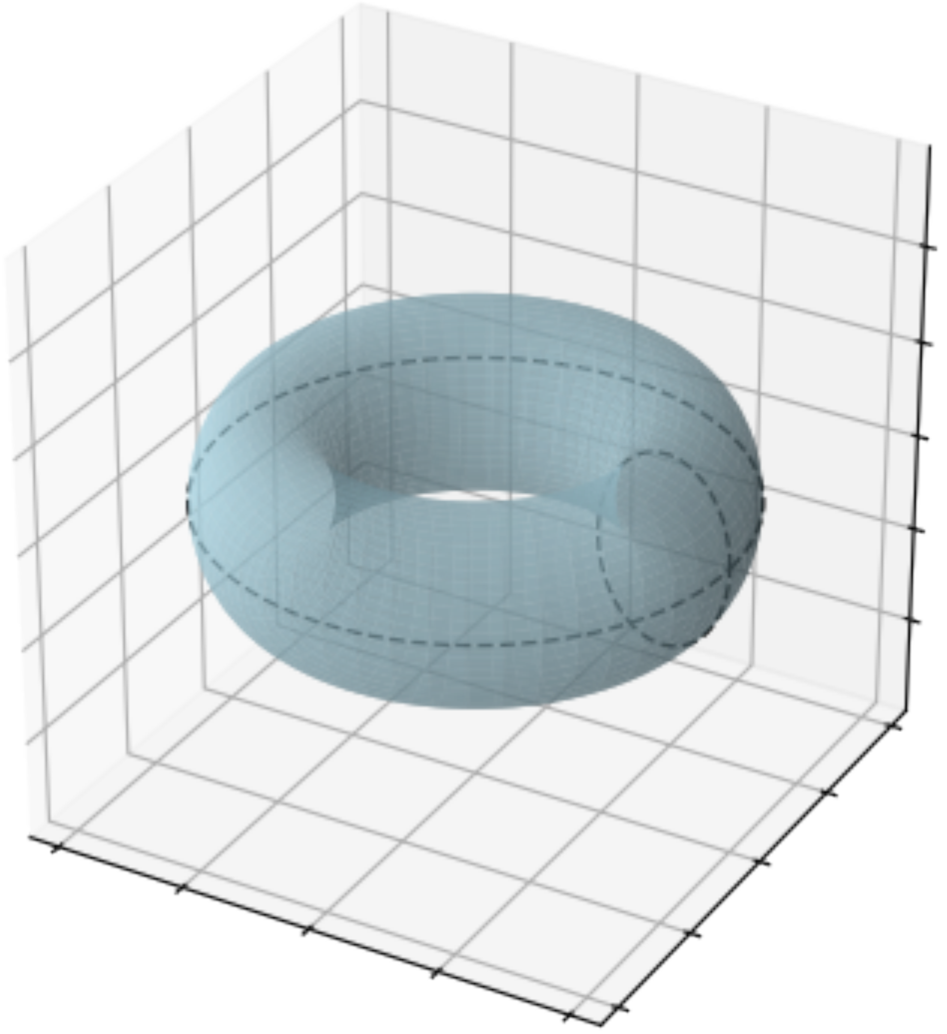
(for simple datasets)

Topological Features
of the Support of the Density

- i.e. components, loops, cavities and higher-dimensional holes



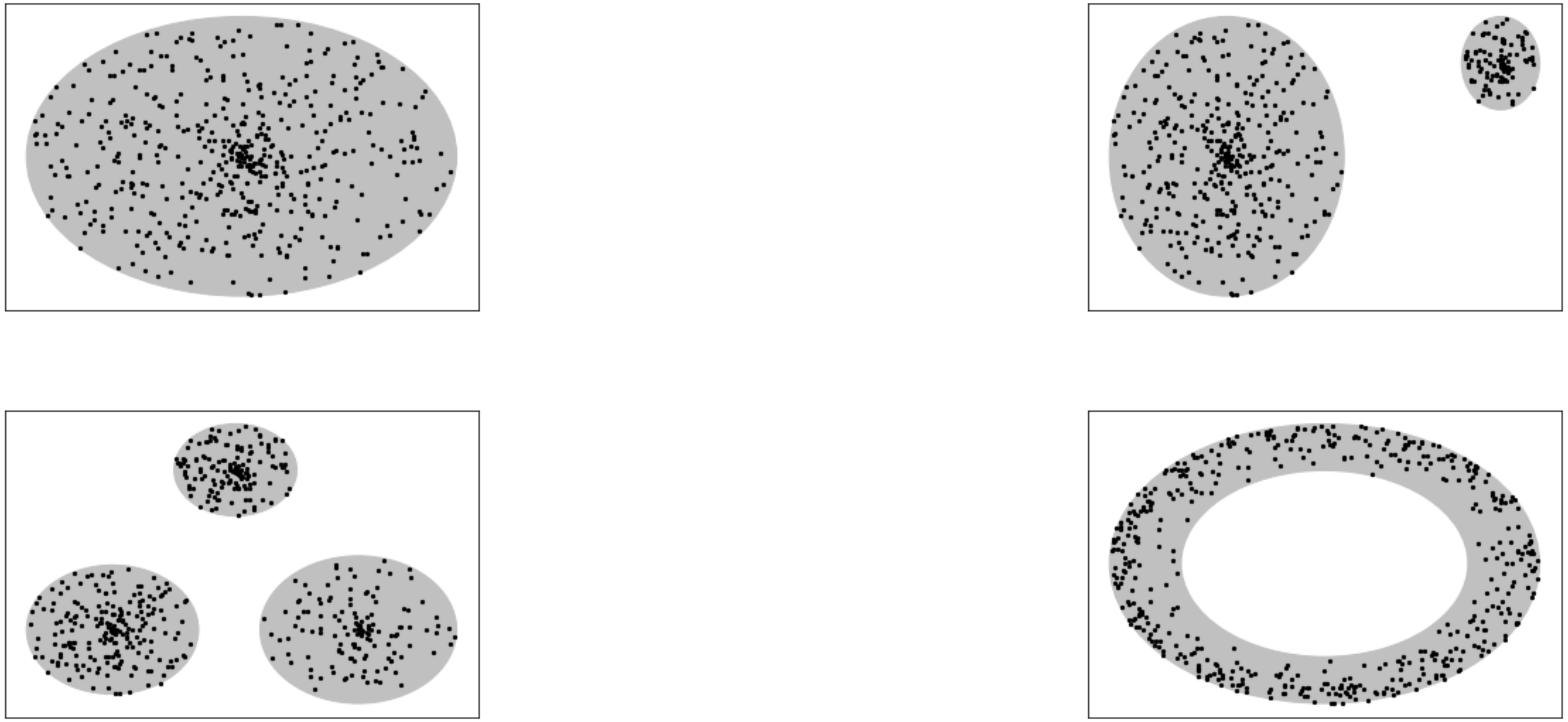
one component
one loop



one component
two loops
one cavity

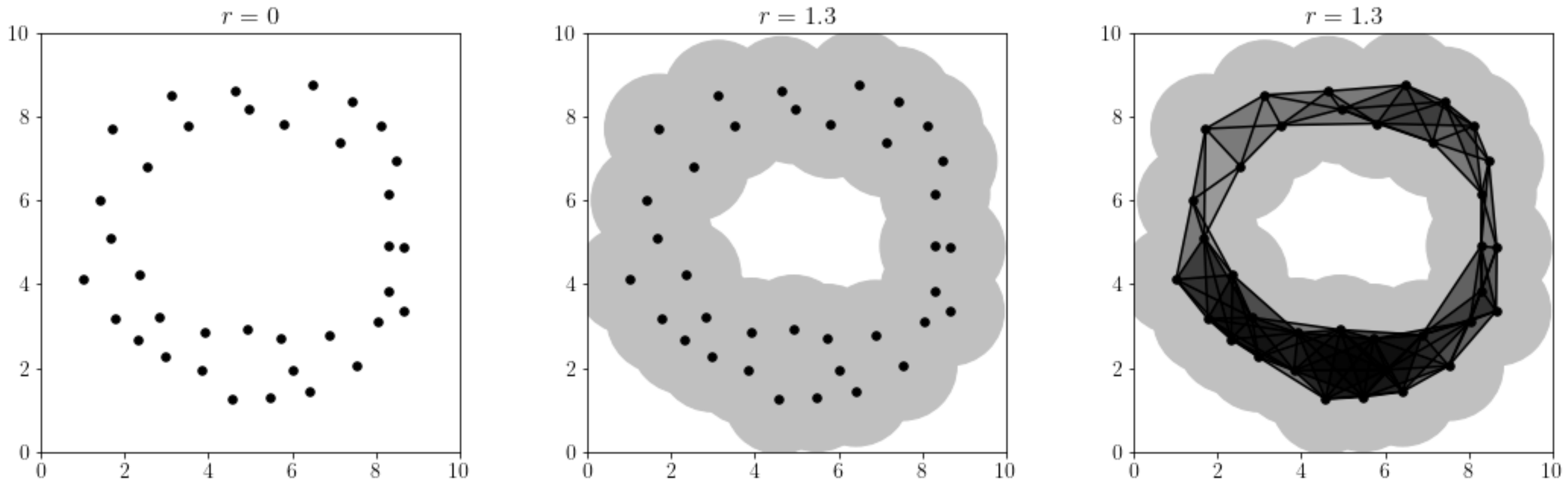
Topological Features

of the Support of the Density

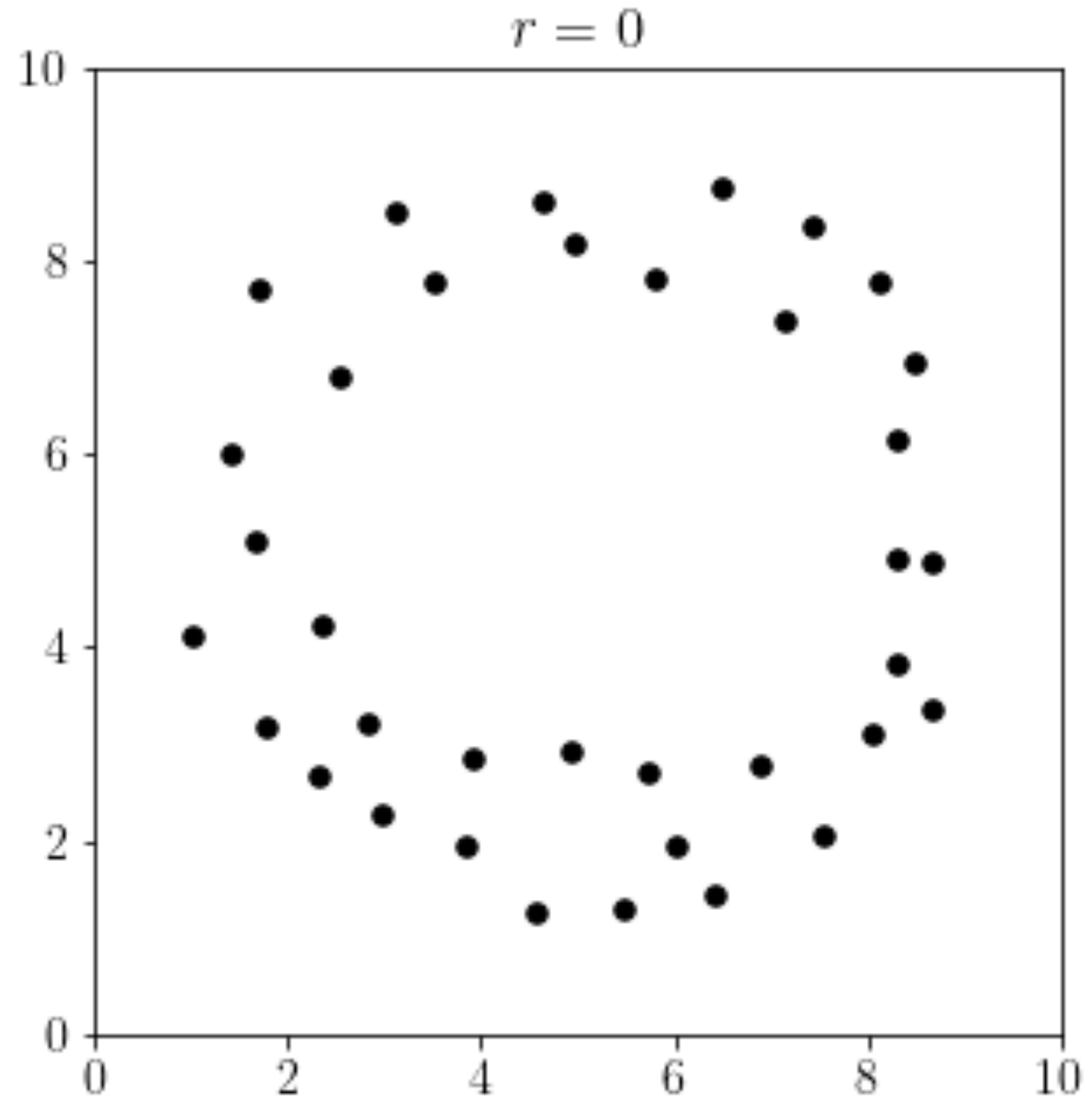


Estimator?
Mathematical Algorithm?

Yes!



Pitfall



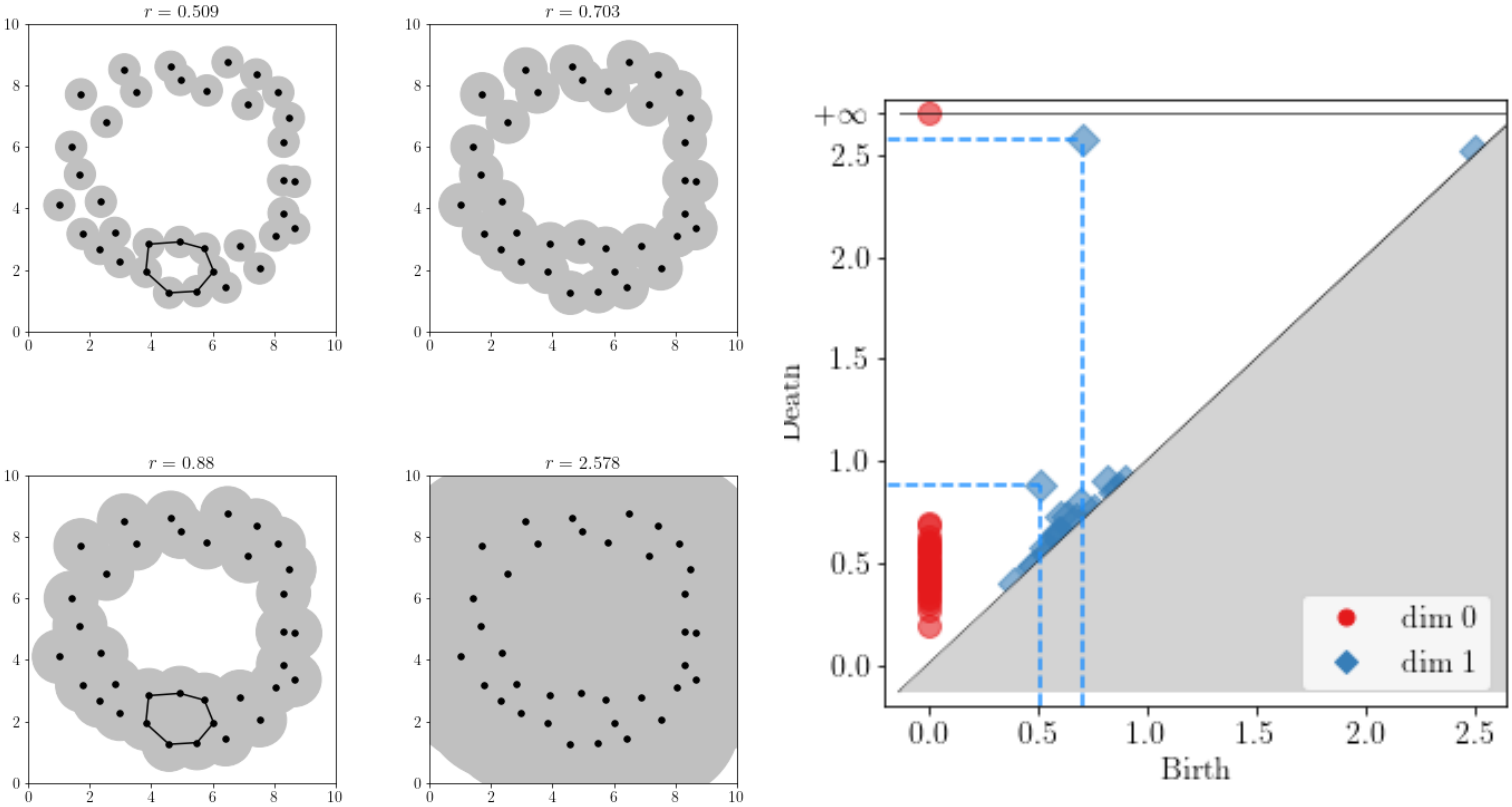


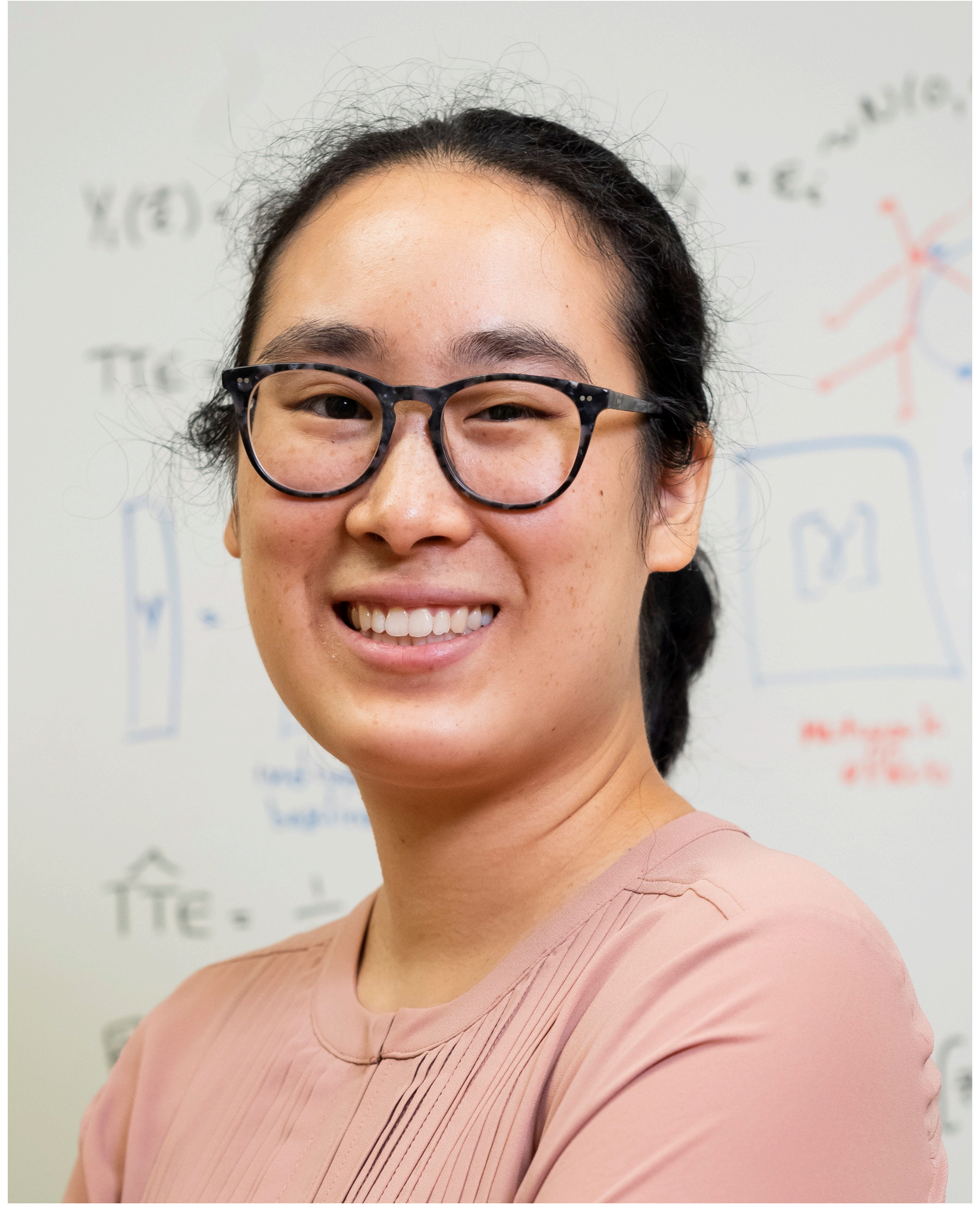
diagram credit: Andrey Yao

Act II

Small Density Vacuum and How to Find Them Robustly

My Lovely Collaborators

Gennady Samorodnitsky

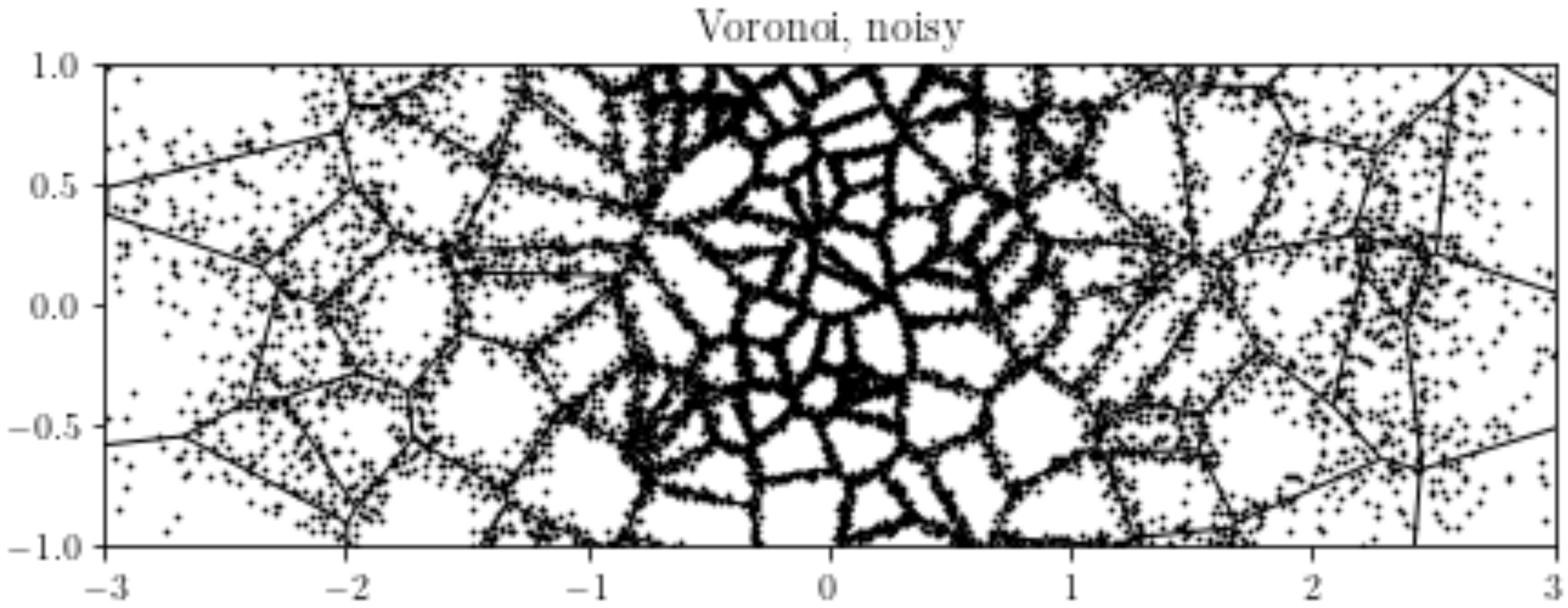


Christina Lee Yu

Andrey Yao

Two problems

- Size
- Noise



Two Problems

- Size
- Noise

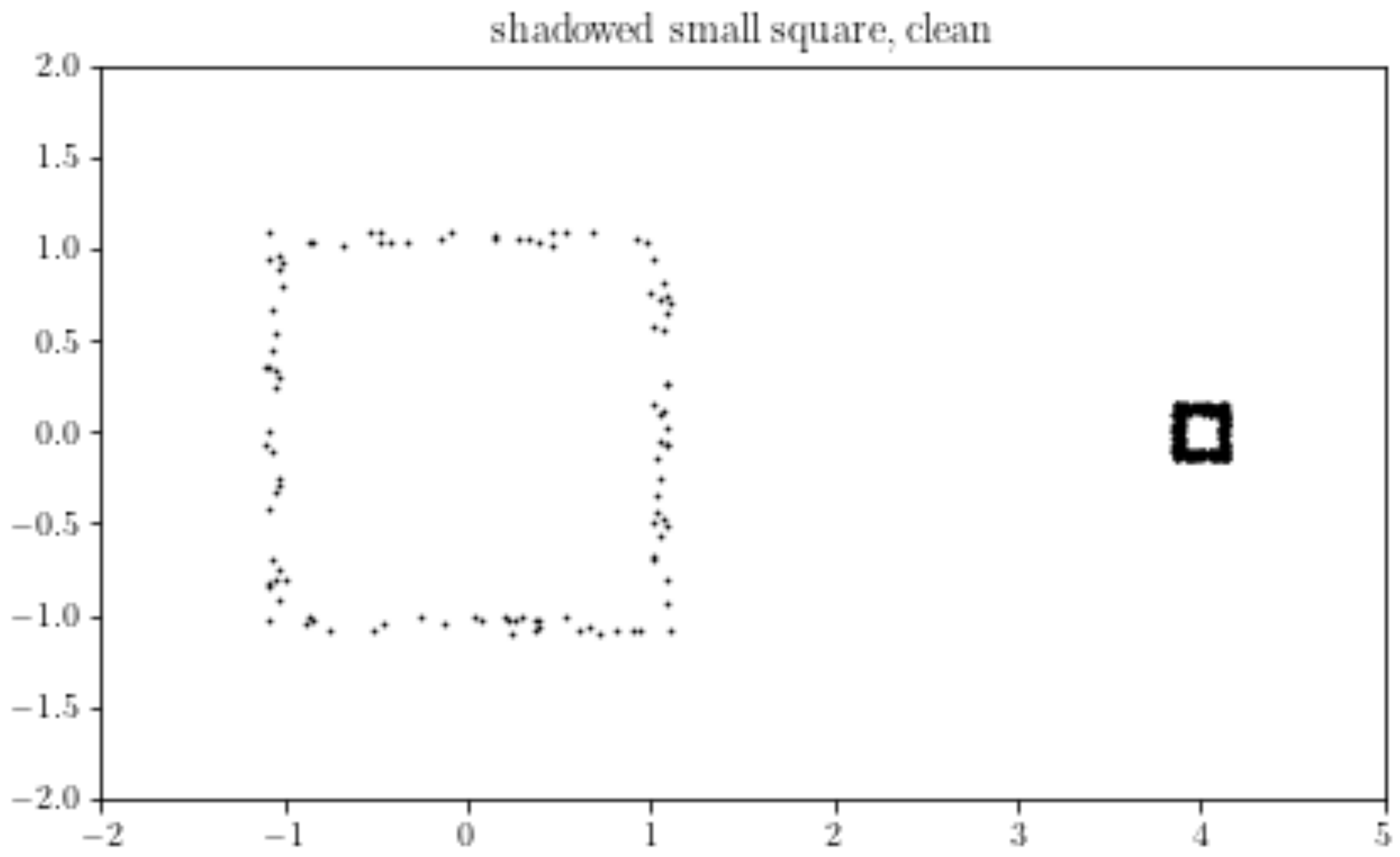
- Related works
    - Hickok (2022)
    - Berry and Sauer (2019)
    - Moon et al (2018)
    - Carlsson and Zomorodian (2009)
    - etc…

One solution

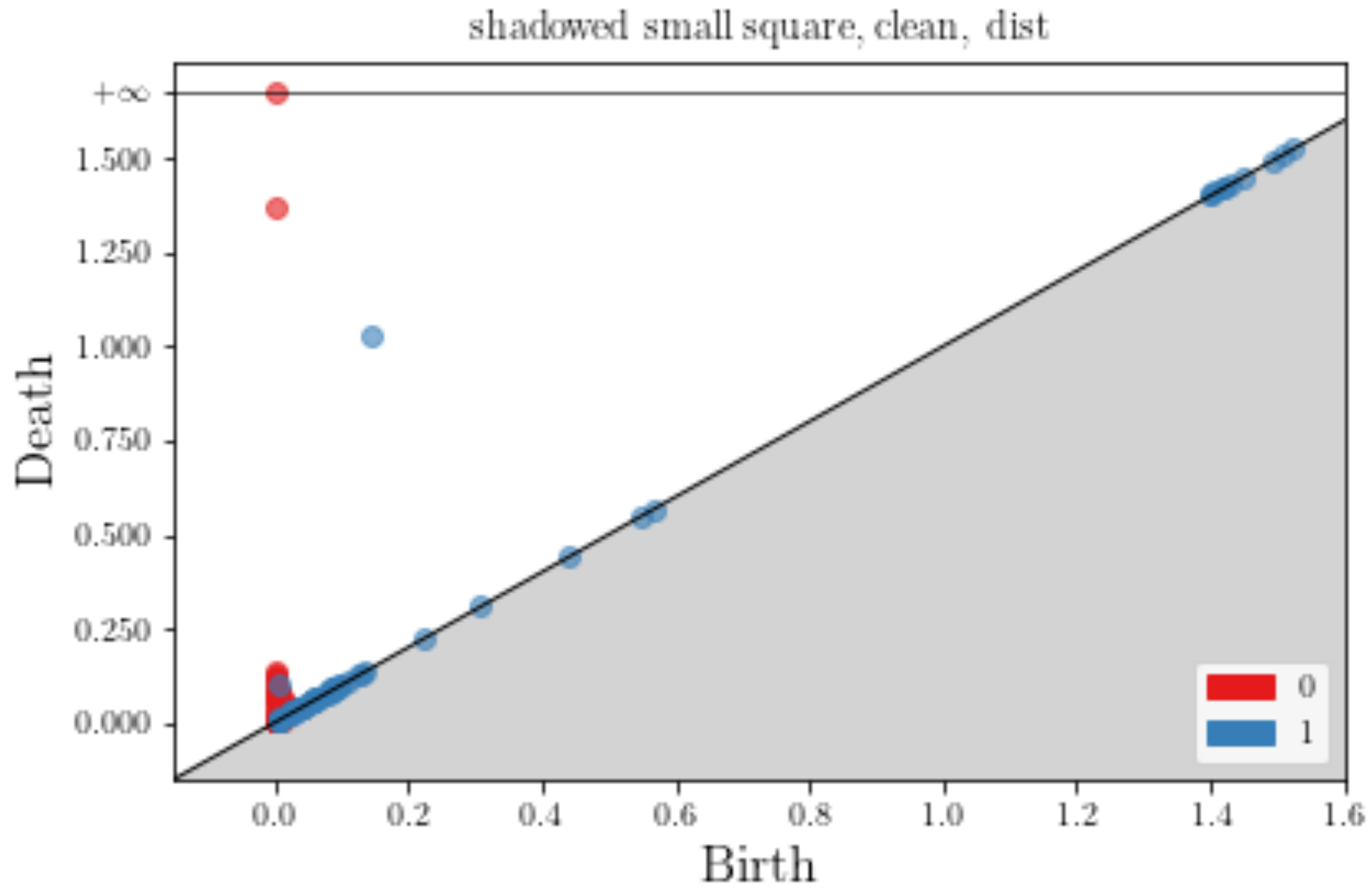
- Size
- Noise

- statistical model that highlights small features
- with a provably robust estimator

Size



shadowed small square, clean
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2
−1
0
1
2
3
4
5



shadowed small square, clean, dist
+∞
1.500
1.250
1.000
0.750
0.500
0.250
0.000
Death
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
Birth
0
1

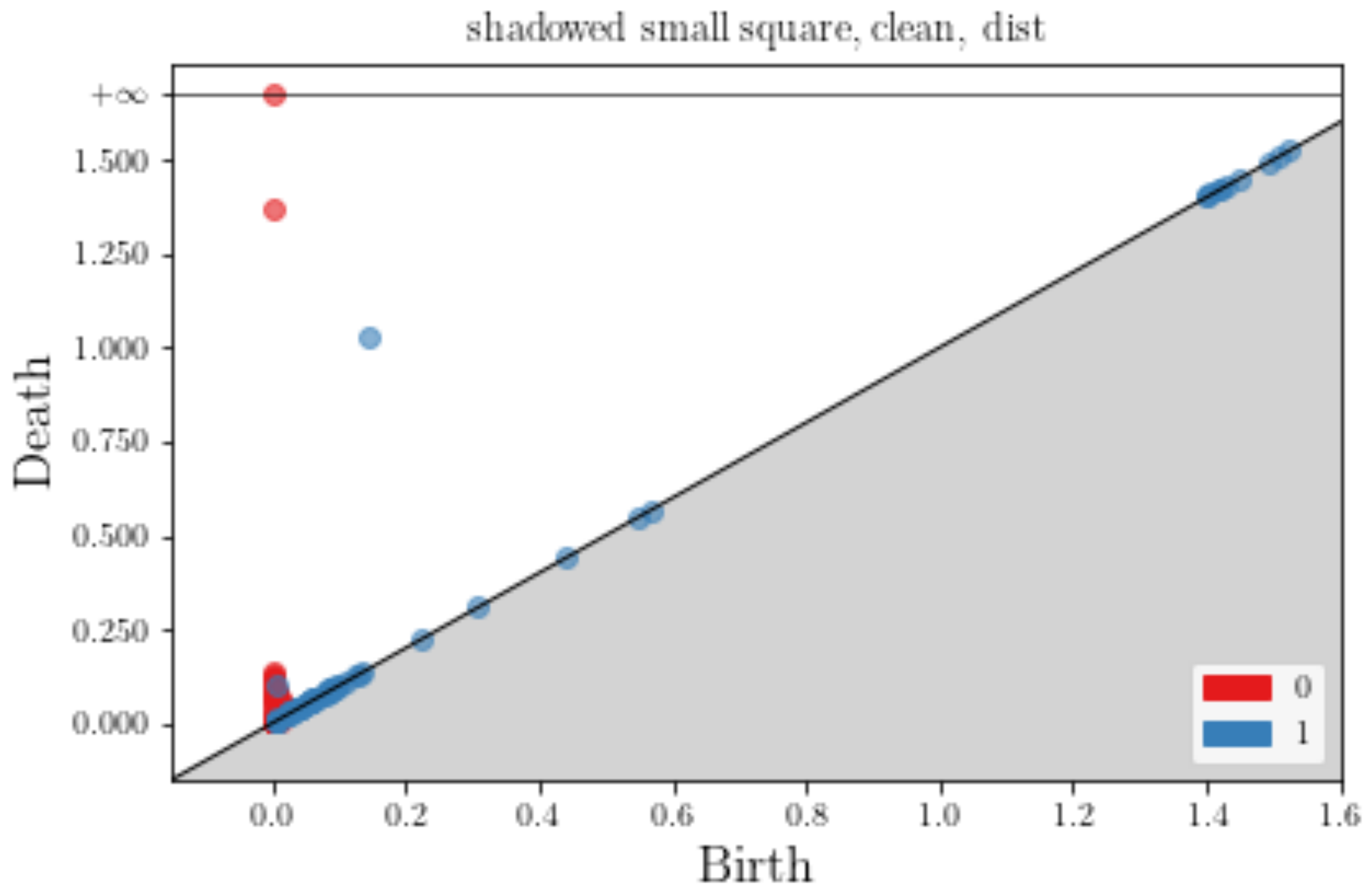
Grow Balls Sloooooooooooooooooooowly
on the smaller square

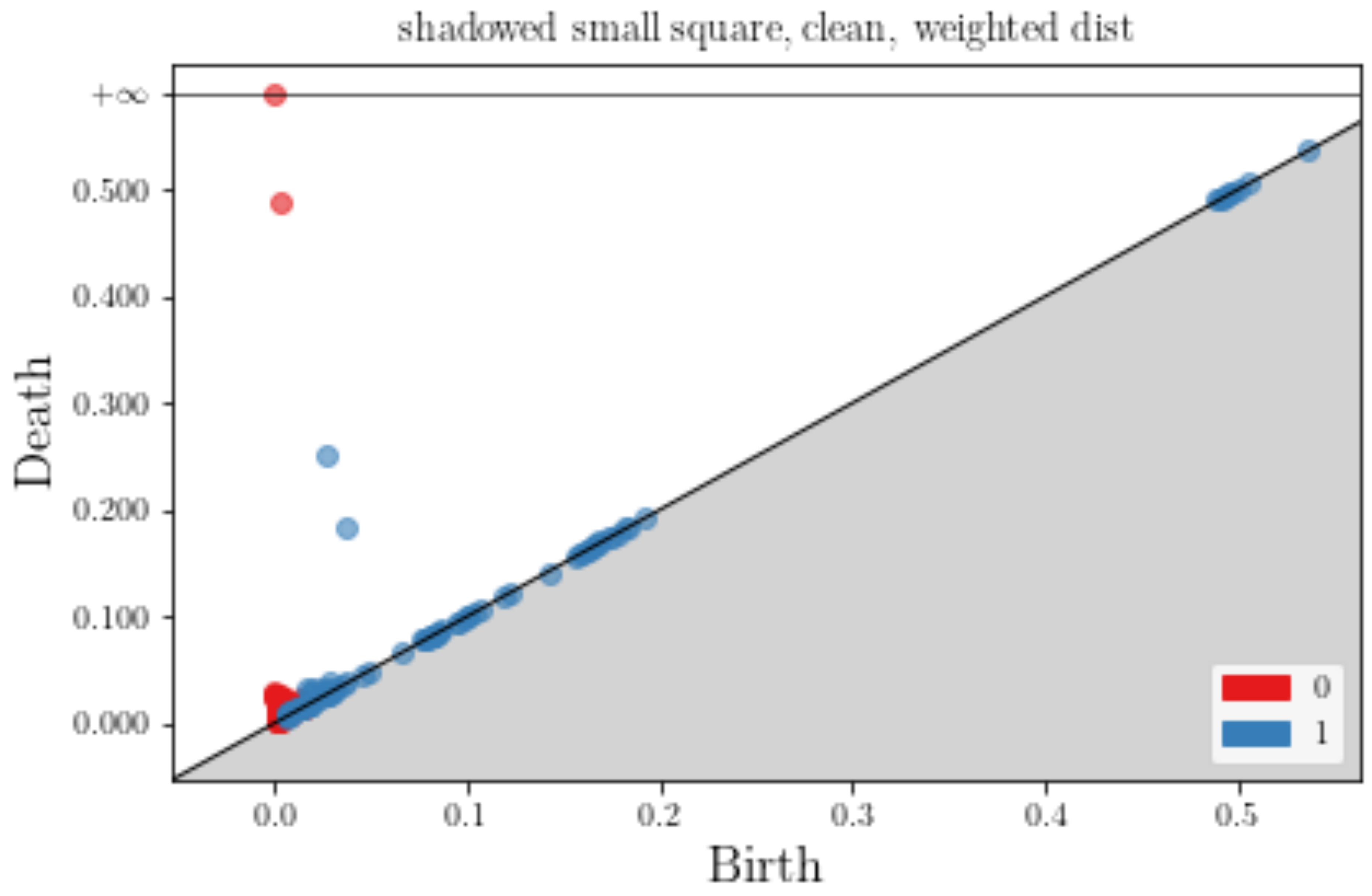
- Bell et al, 2019: growing balls at customized rates

Grow Balls Sloooooooooooooooooowly

on the smaller square

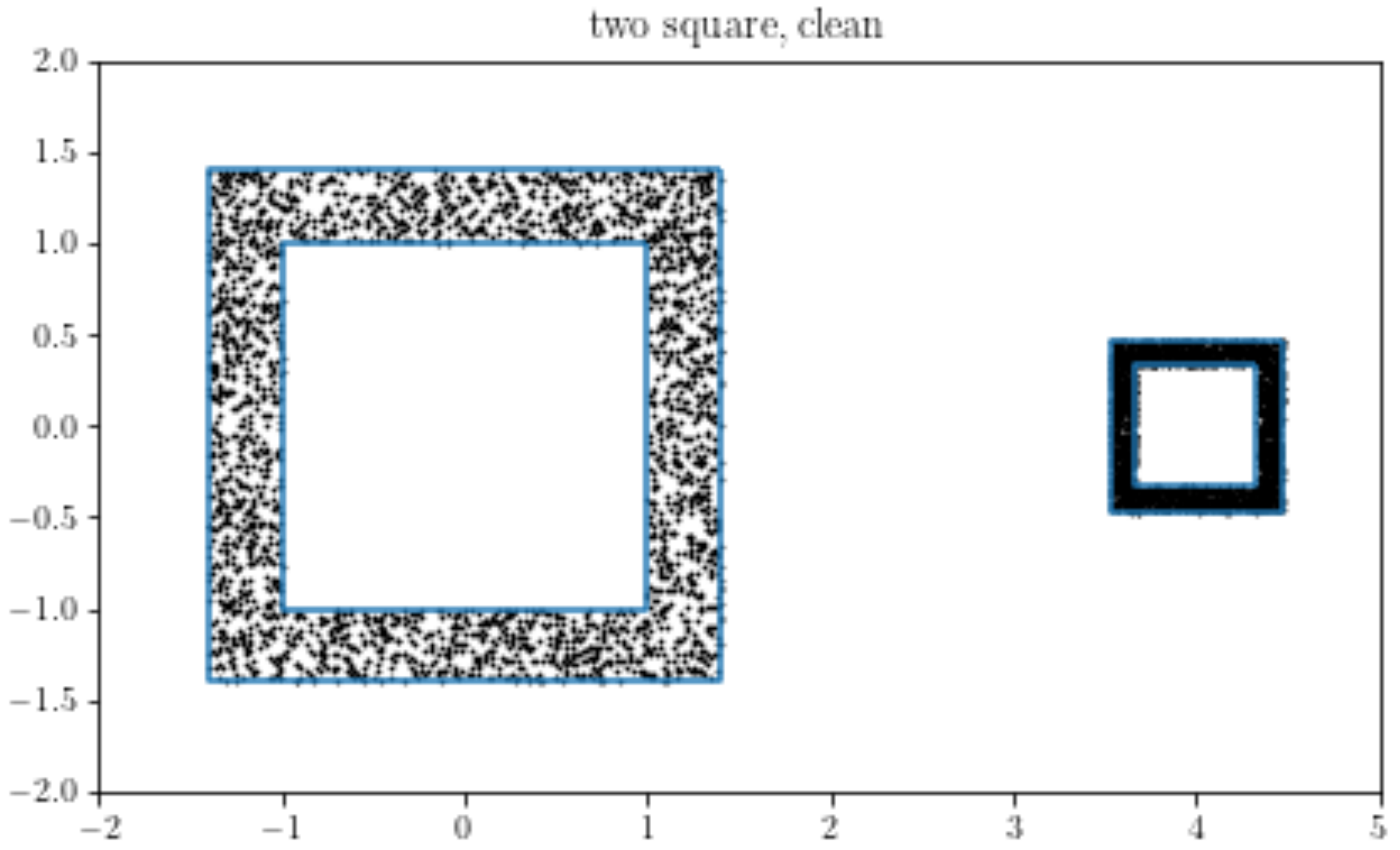
- rate = 1/density$^{1/D}$

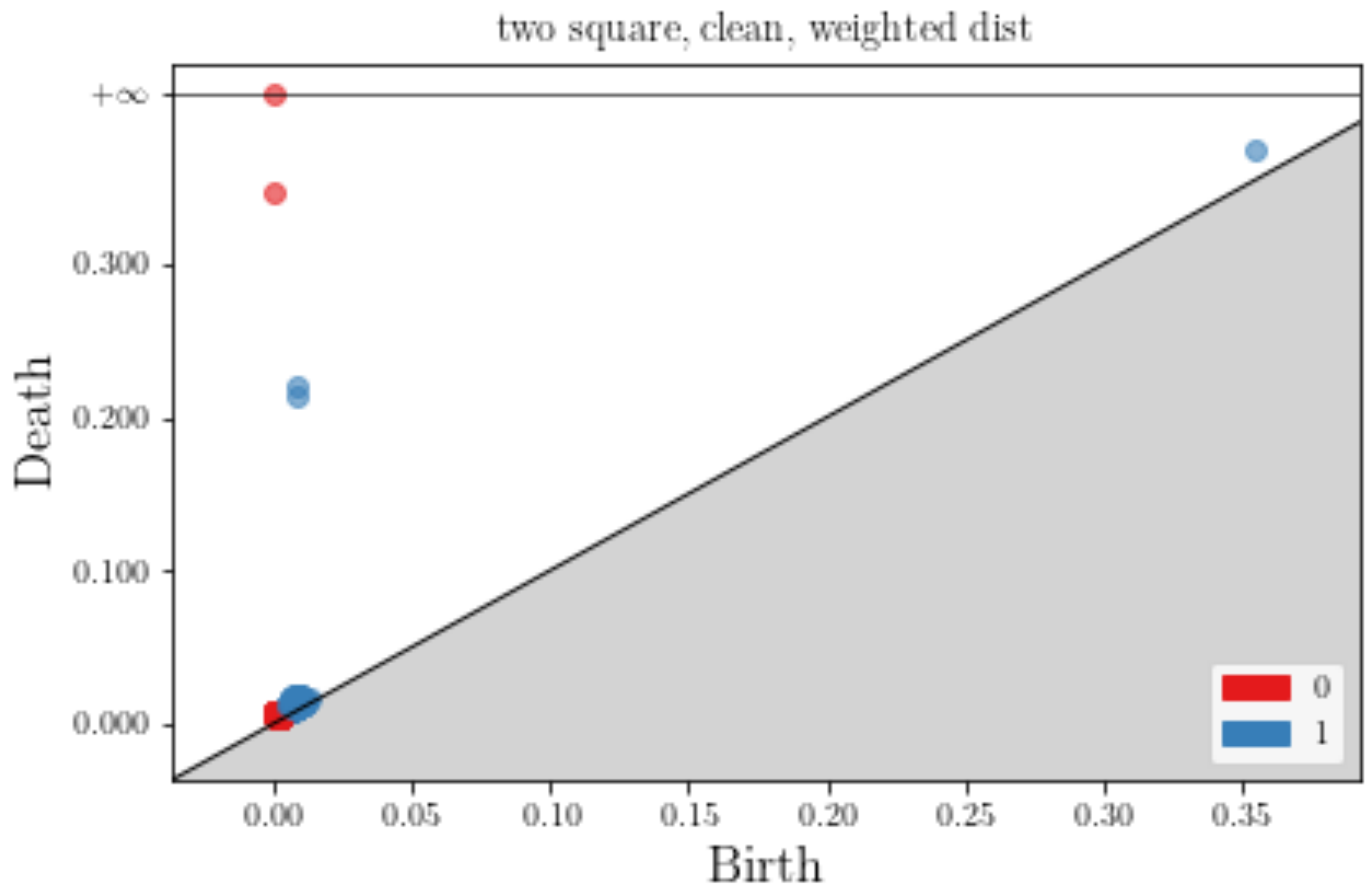




Scale invariance

- uniform scaling —> same persistence diagrams



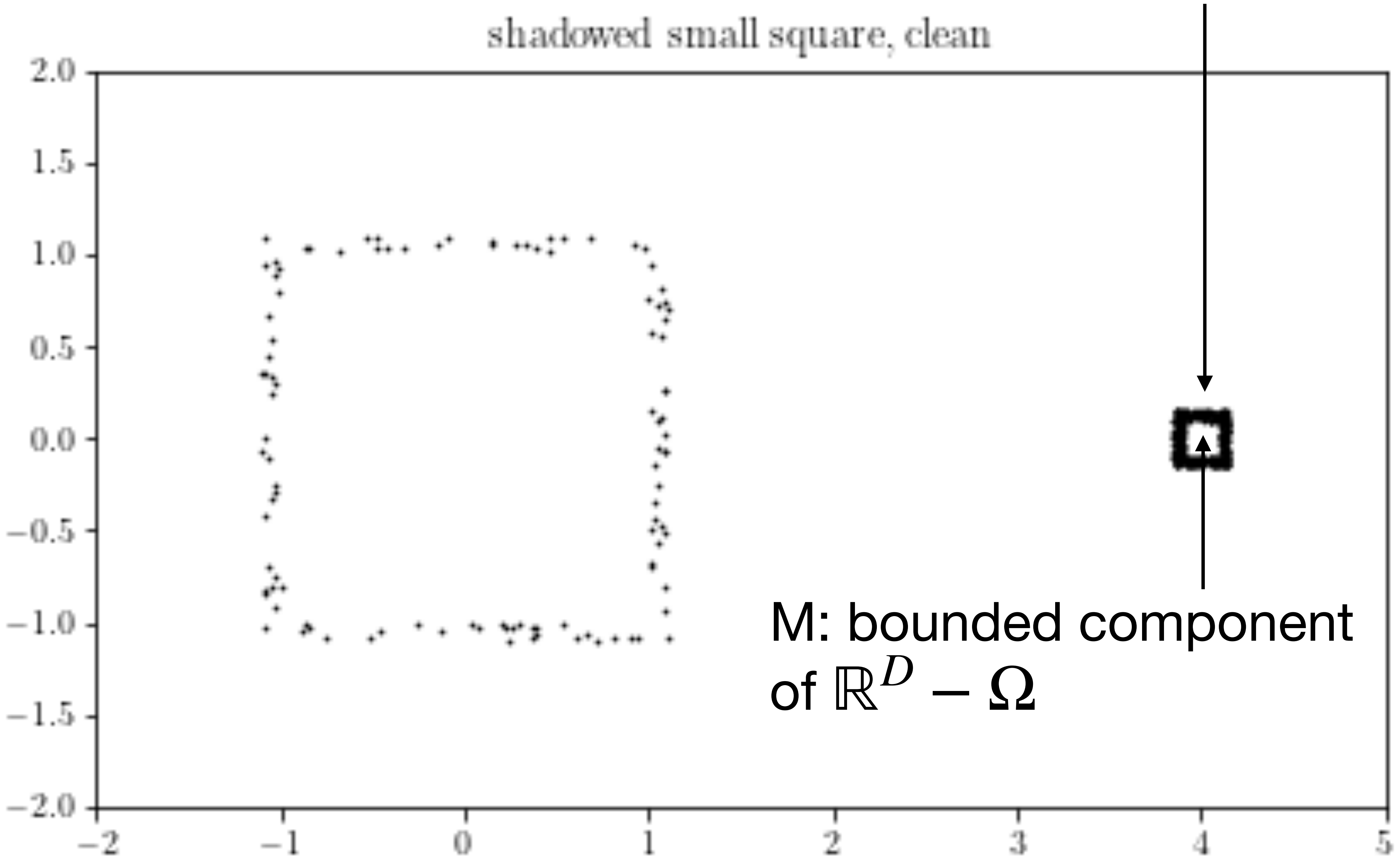


Theorem

TLDR: Small holes of high-density regions are far from diagonal.

- Let t be a density threshold.
- As in the figure, let M be a "hole" of a high-density region Ω with size $r = \max_{x \in M} d(x, \partial M)$.
- Under nice assumptions,
  M induces a (D − 1)-dimensional homology class
  with persistence at least $\frac{1}{\sqrt{2}} t^{1/D} r - O(m^{1/D})$

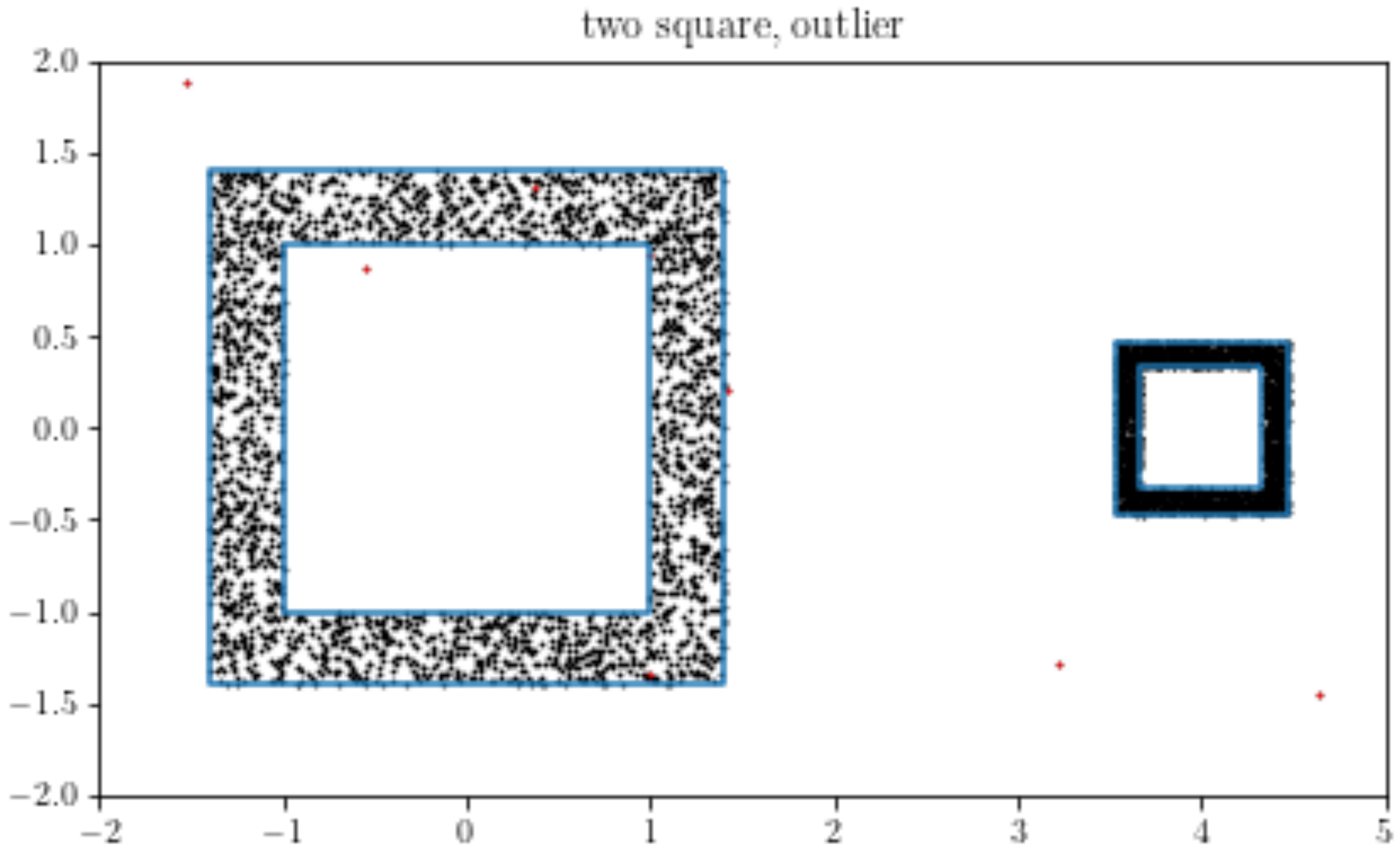
Ω: component of the the high-density region $\{\xi : f(\xi) \geq t\}$

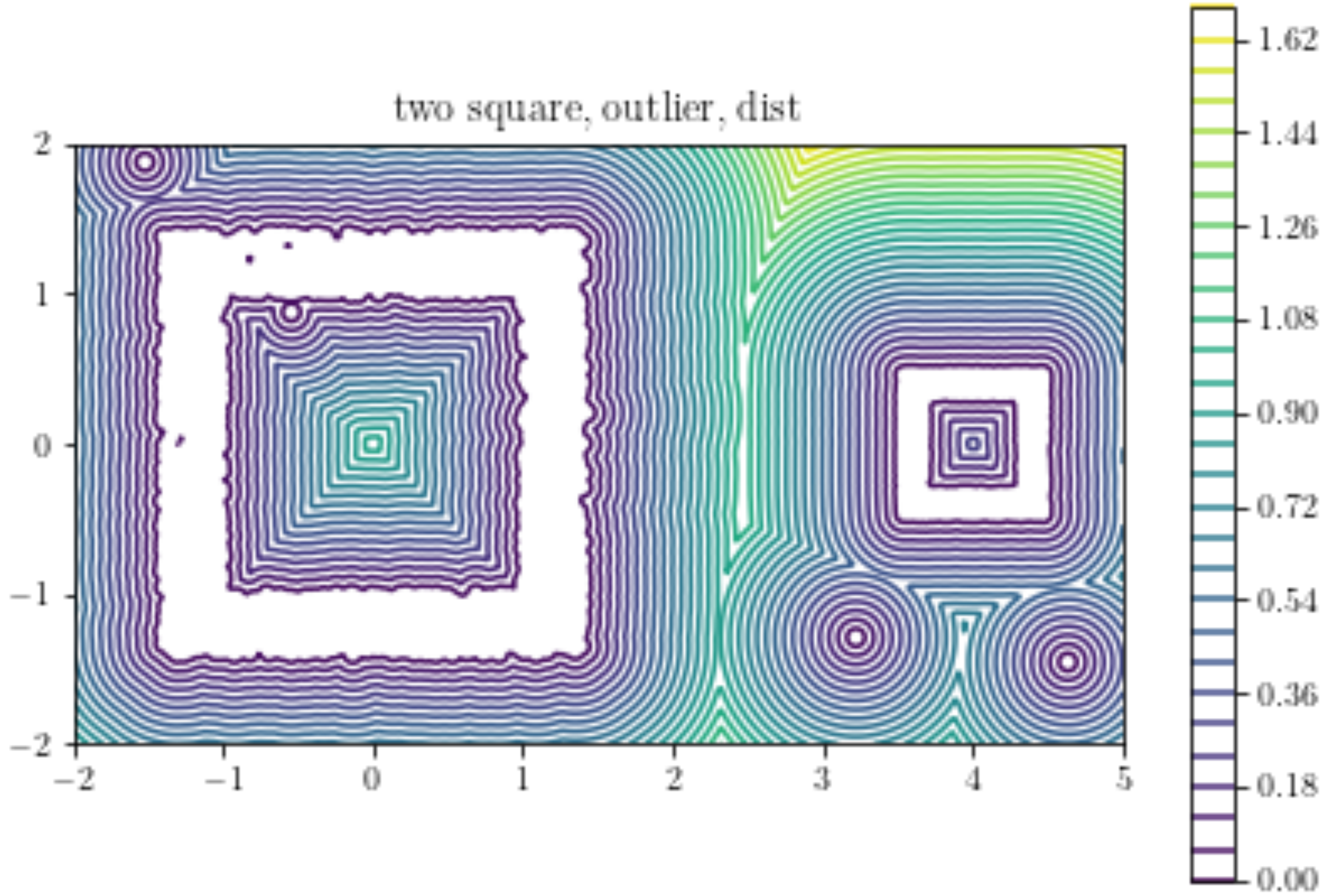


M: bounded component of $\mathbb{R}^D - \Omega$

Noise

Outliers


two square, outlier
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2
−1
0
1
2
3
4
5


two square, outlier, dist
2
1
0
−1
−2
−2
−1
0
1
2
3
4
5
1.62
1.44
1.26
1.08
0.90
0.72
0.54
0.36
0.18
0.00

Known Problem, Known Solution

- solution: distance-to-measure
  - wait for more balls, and take average
  - can leverage empirical process theory
  - Chazal et al (2011), Chazal et al (2018)

Robust Density-Aware Distance
(RDAD)

Robust Density-Aware Distance function

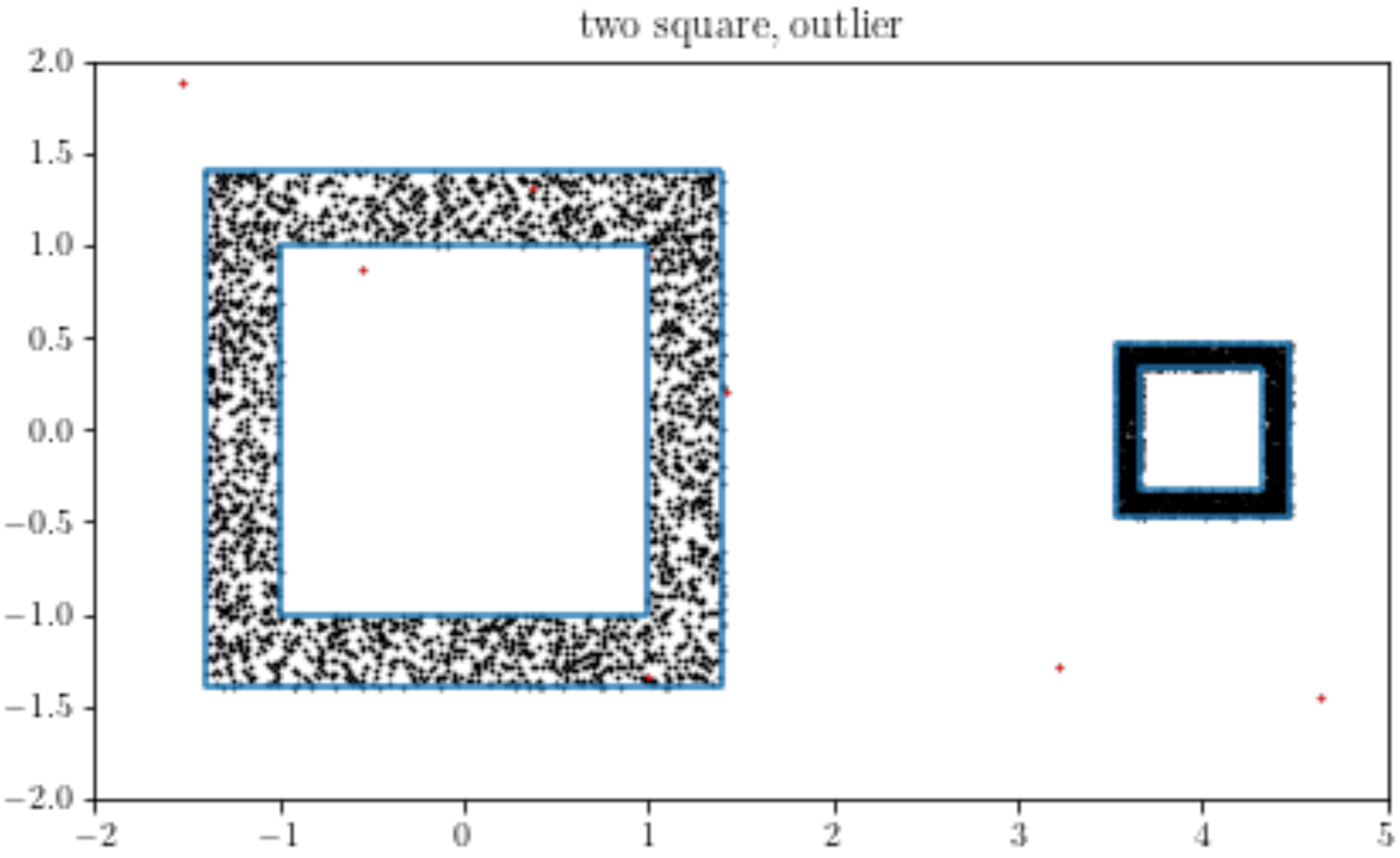
$$DTM(x) = \sqrt{\frac{1}{m}\int_0^m G_x^{-1}(q)^2 dq}$$

$$G_x(r) = P\{d(x, X) \leq r\}$$

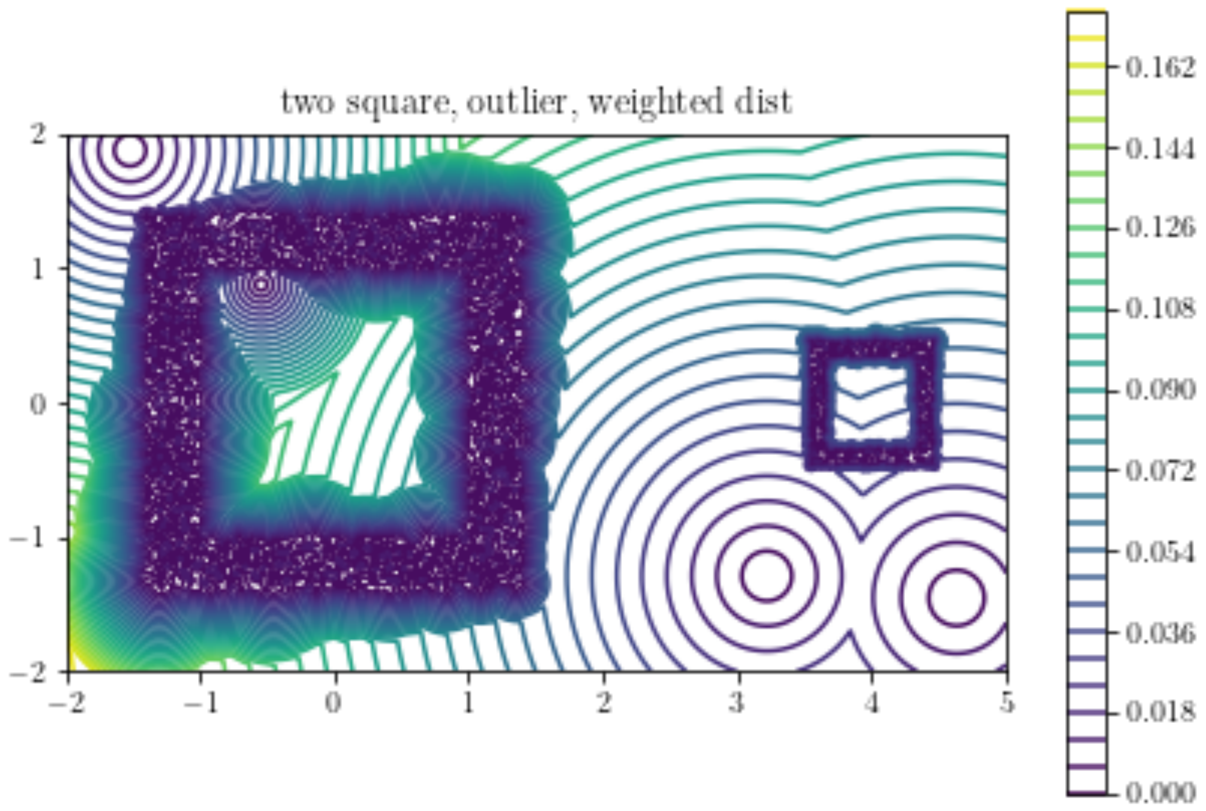
$$RDAD(x) = \sqrt{\frac{1}{m}\int_0^m F_x^{-1}(q)^2 dq}$$

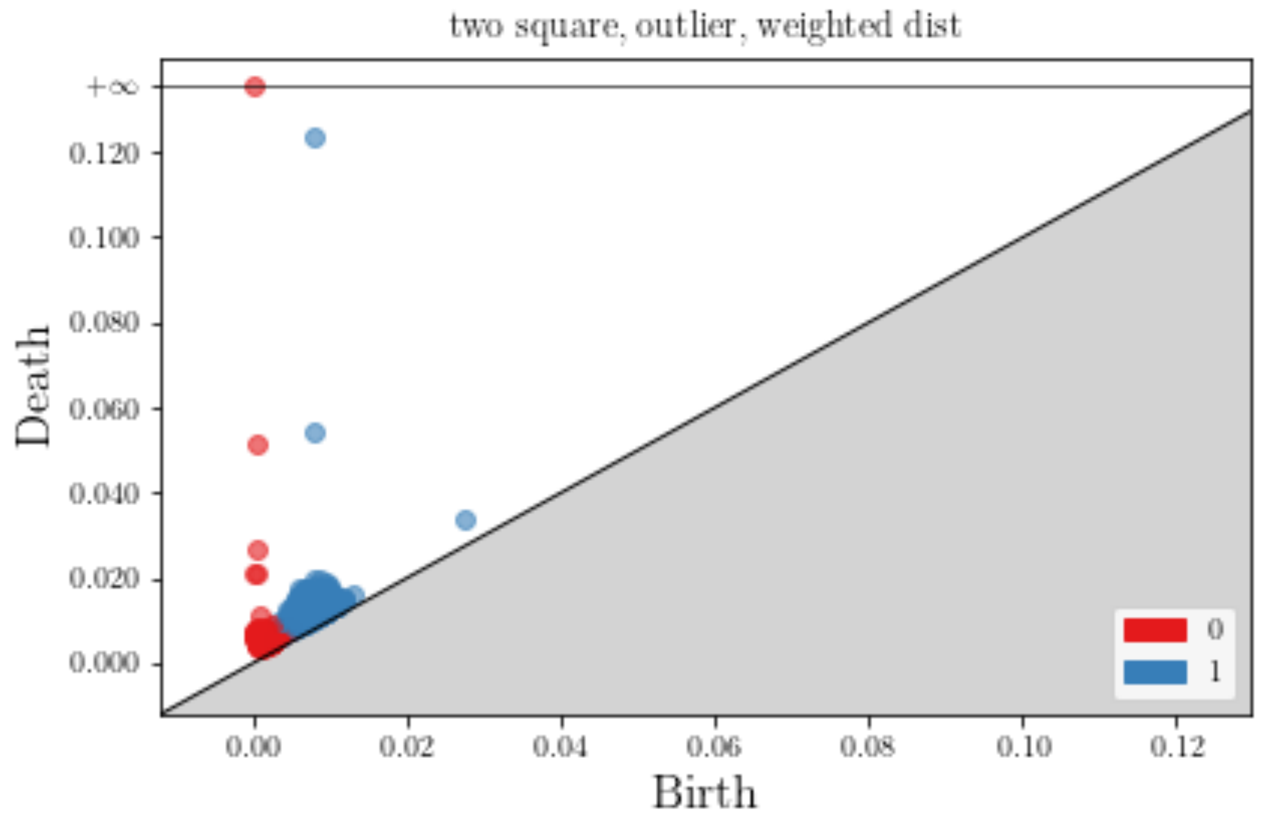
$$F_x(r) = P\{d(x, X)f(X)^{1/D} \leq r\}$$

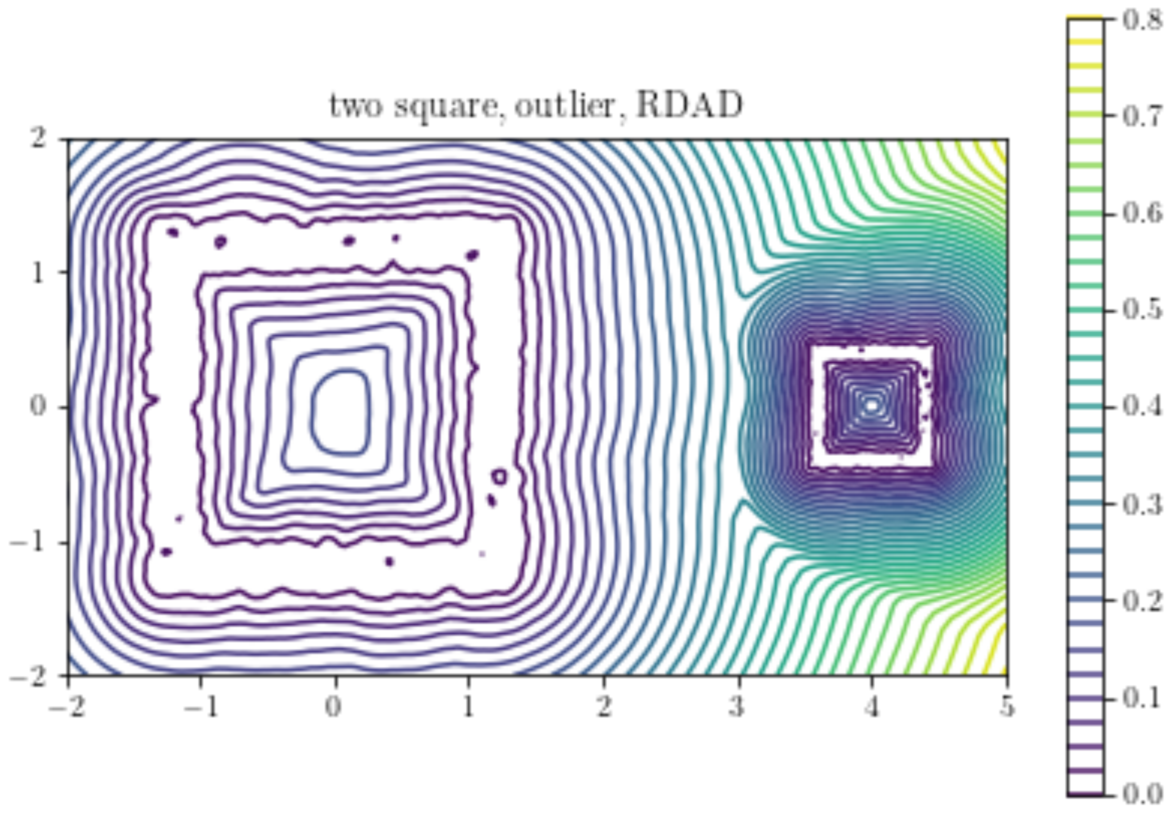
Outlier

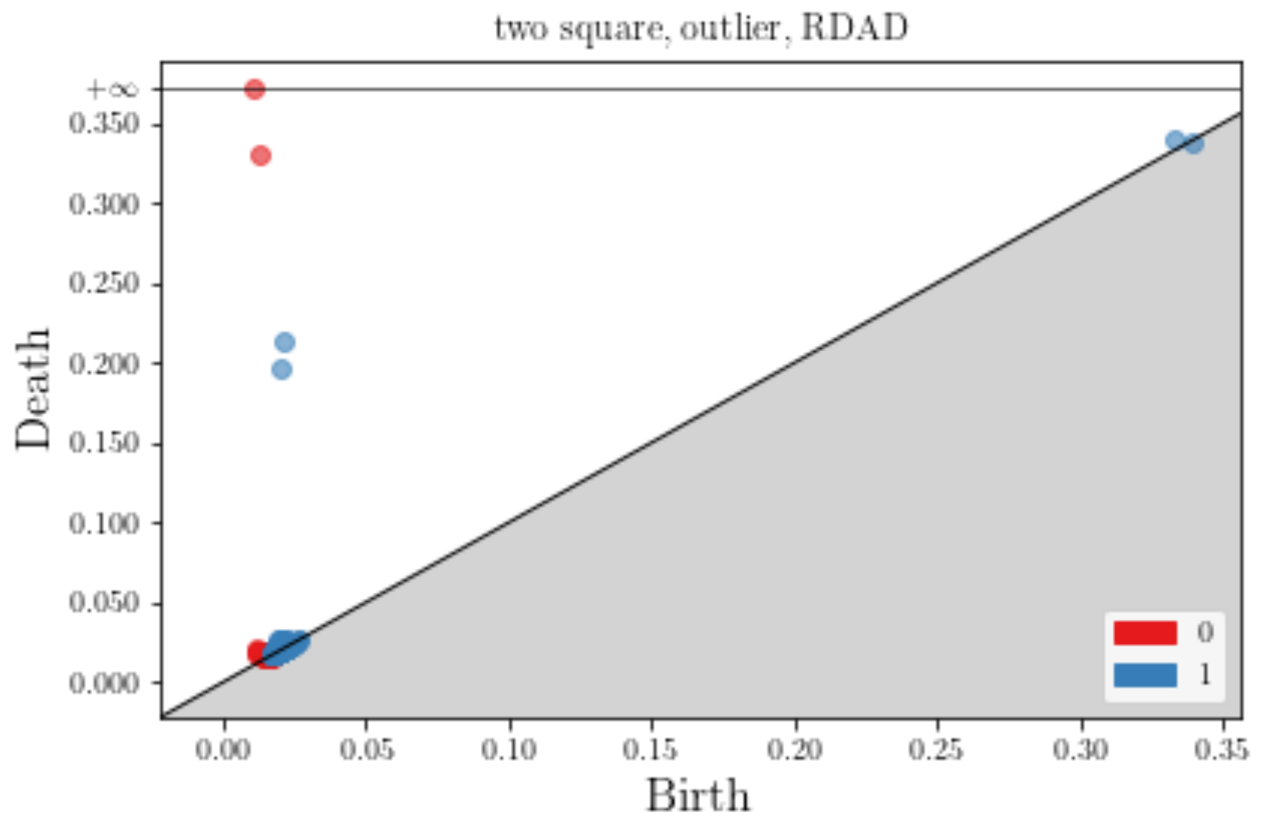


Weighted distance v.s. RDAD









Theorem

- Let f and $\tilde{f}$ be two densities.
- Under nice condition, the persistence diagrams of $RDAD_f$ and $RDAD_{\tilde{f}}$ on a compact set *K* have bottleneck distance bounded by

$$O(W_p(f, \tilde{f}) + \|f - \tilde{f}\|_\infty)$$

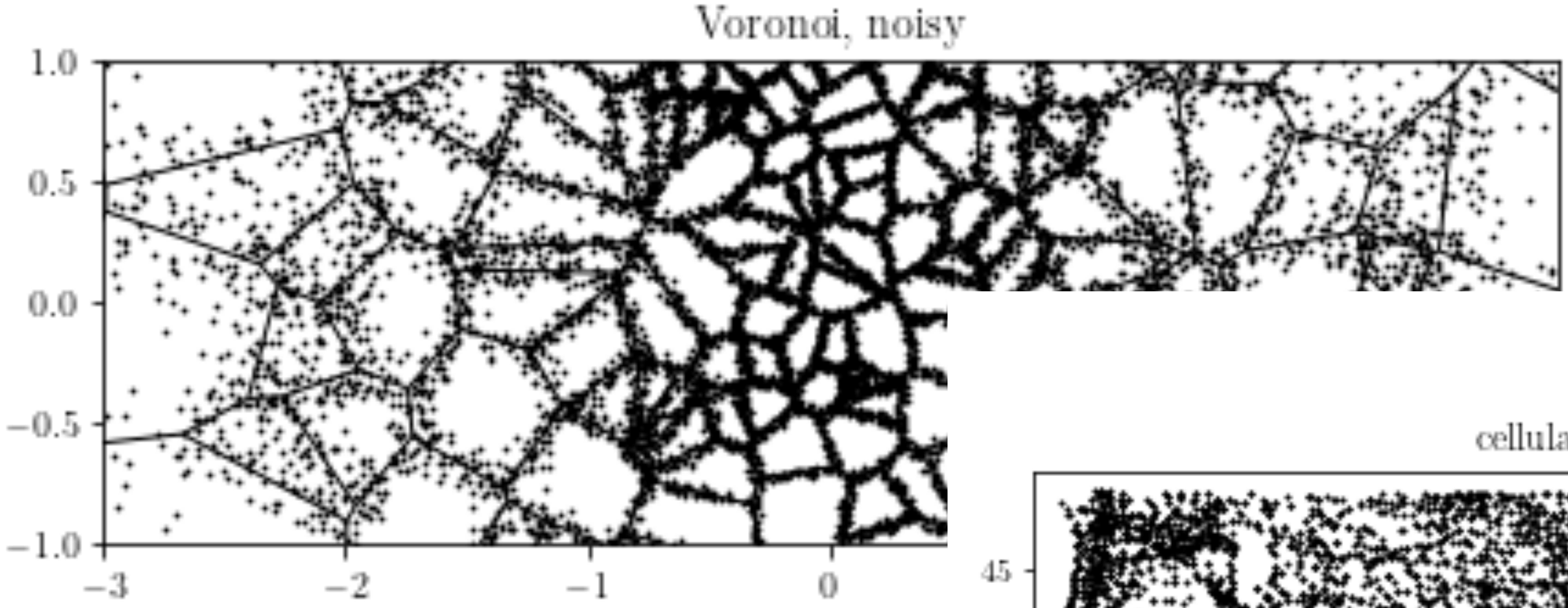
Statistical Convergence?

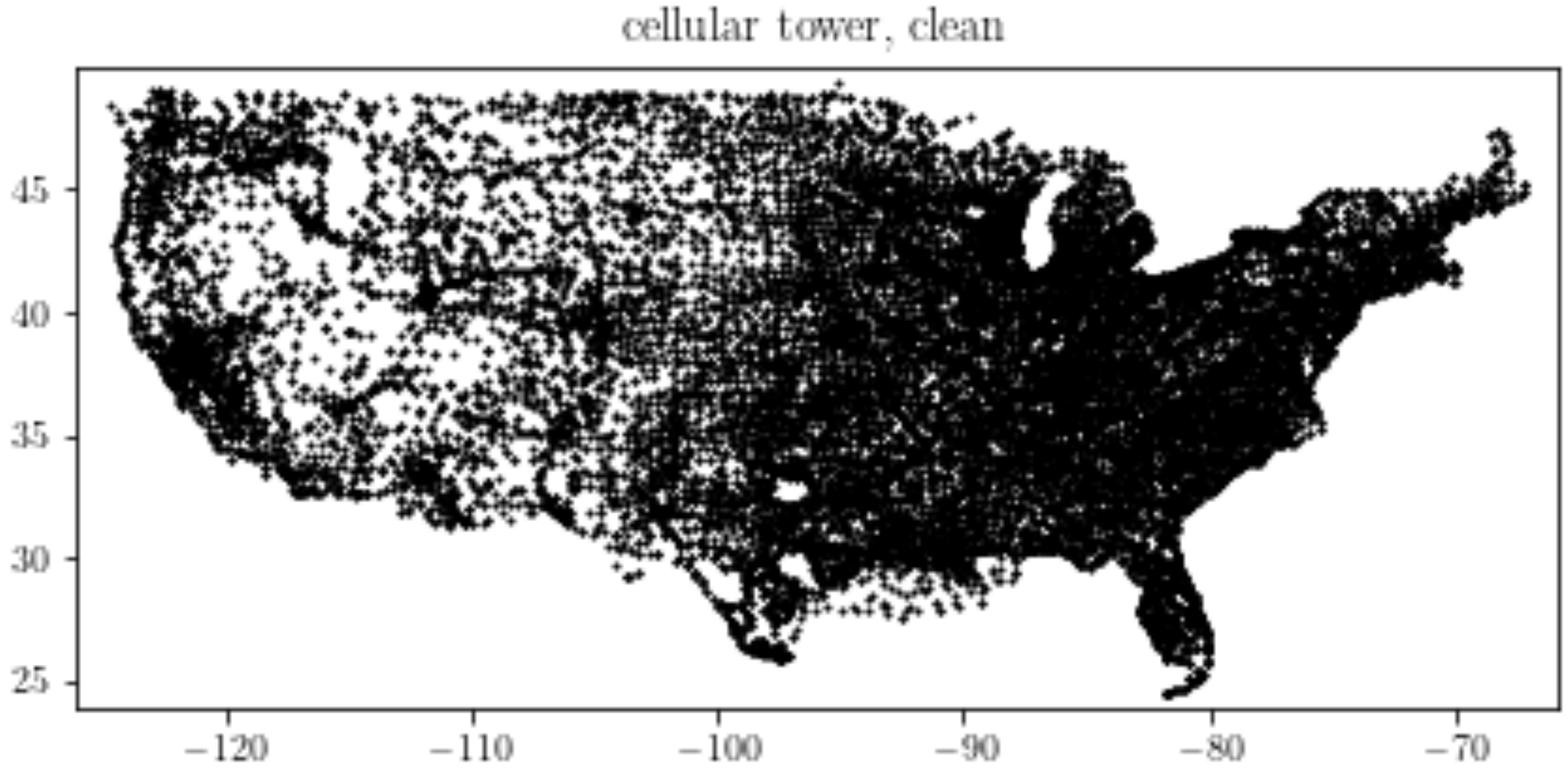
Theorem

- Let $X_1, \ldots, X_N$ be iid points sampled from a nice density.
- Then on every compact set *K*,

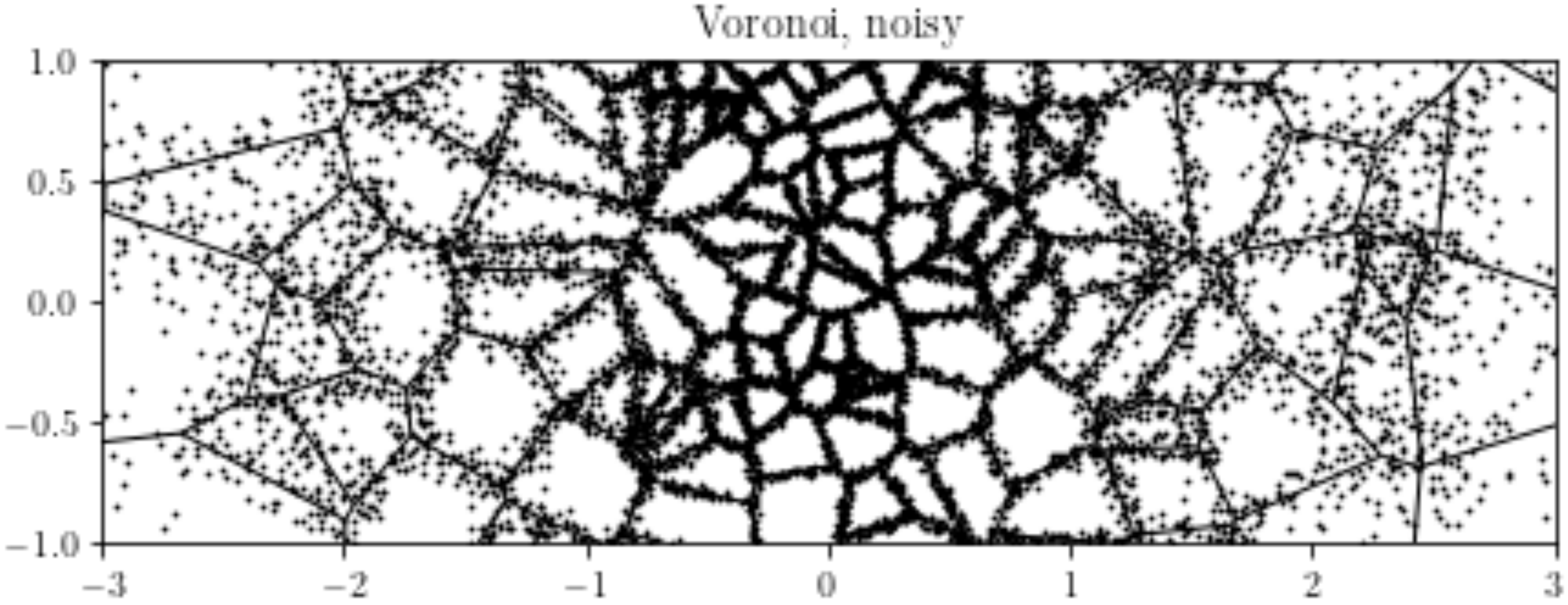
$$\sqrt{N}(\widehat{RDAD}^2 - RDAD^2) \xrightarrow{\text{weakly in } L^\infty(K)} \text{a centered Gaussian process}$$

Simulations

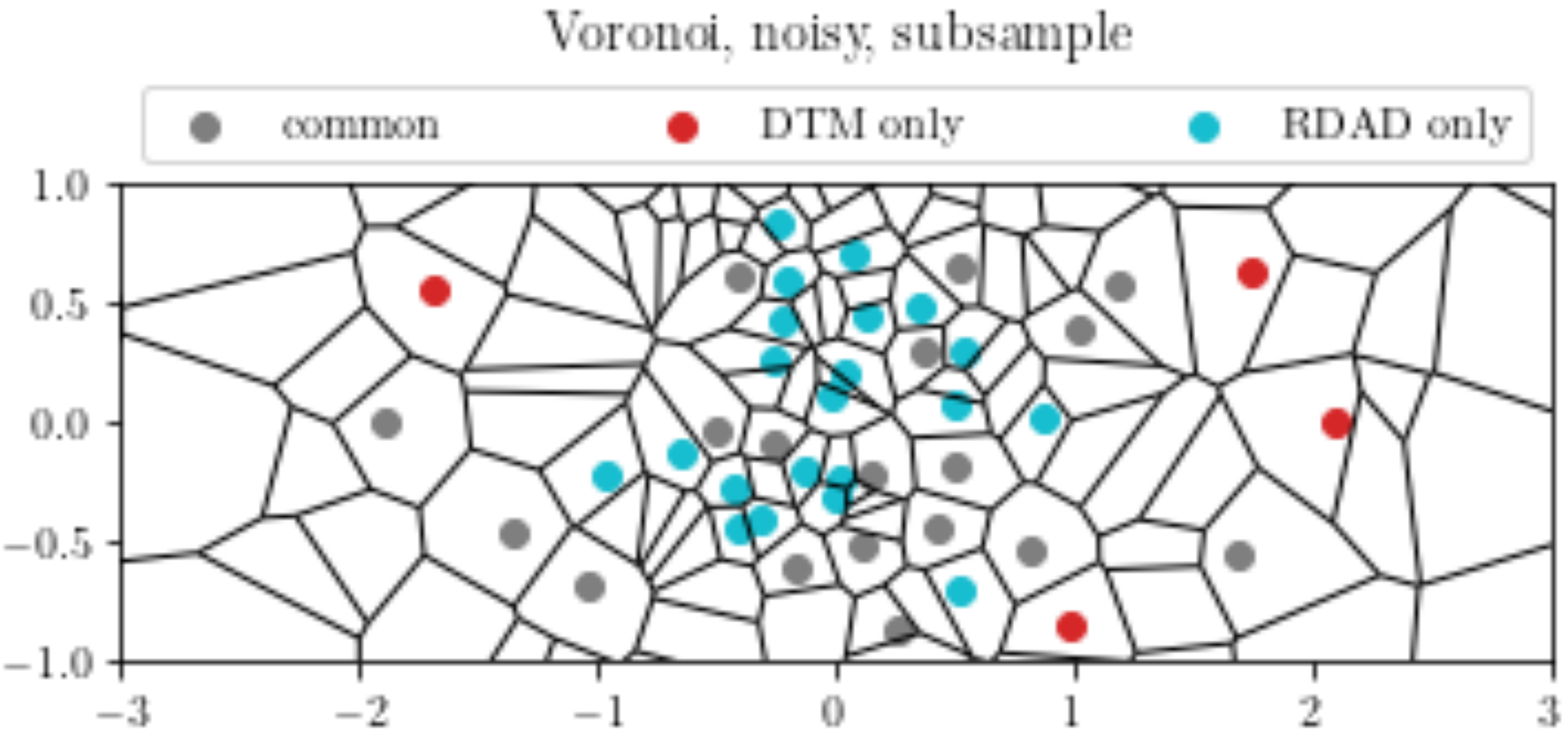

Voronoi, noisy
1.0
0.5
0.0
−0.5
−1.0
−3
−2
−1
0


cellular tower, clean
45
40
35
30
25
−120
−110
−100
−90
−80
−70

Noisy Voronoi

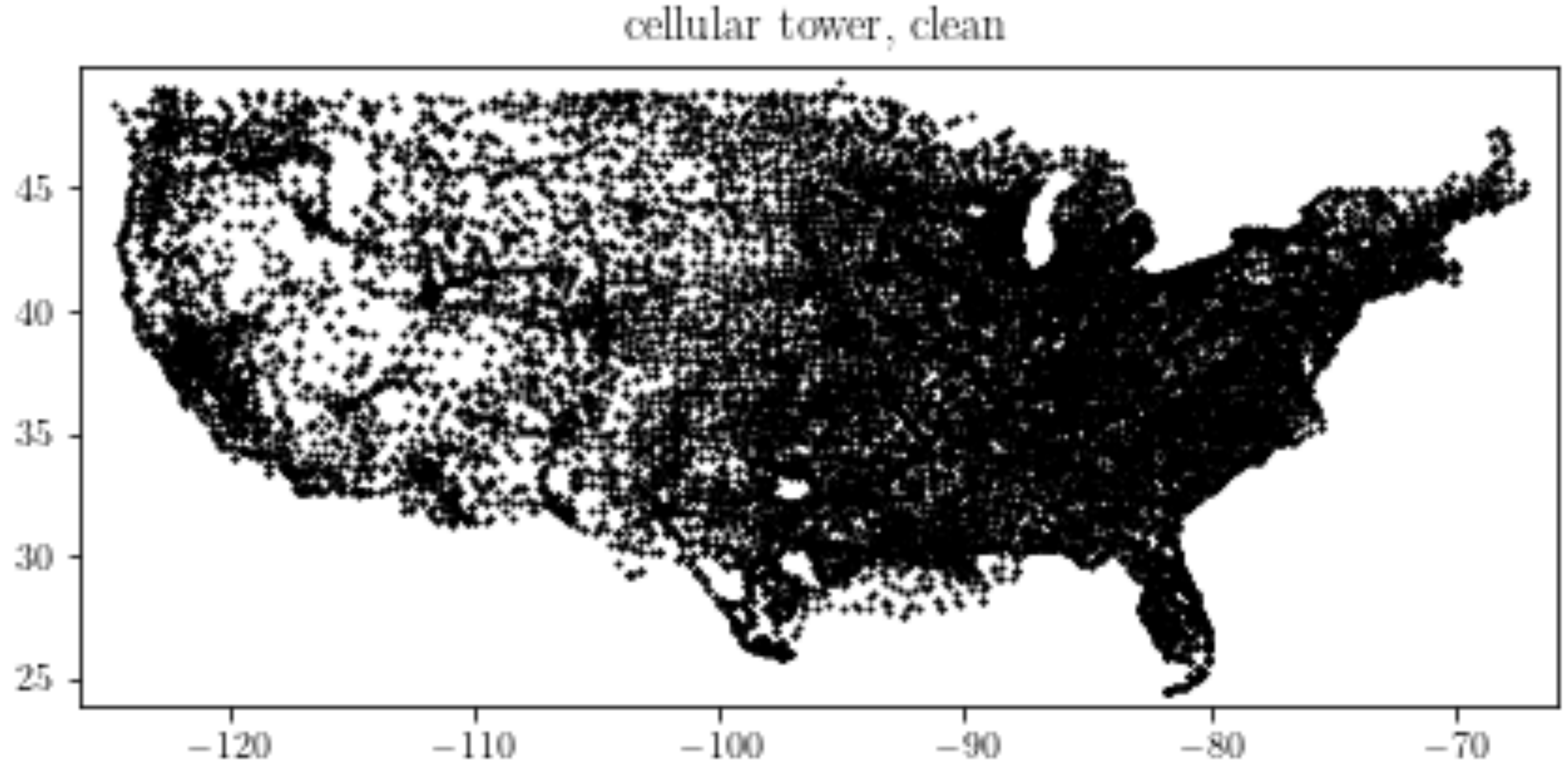


DTM and RDAD

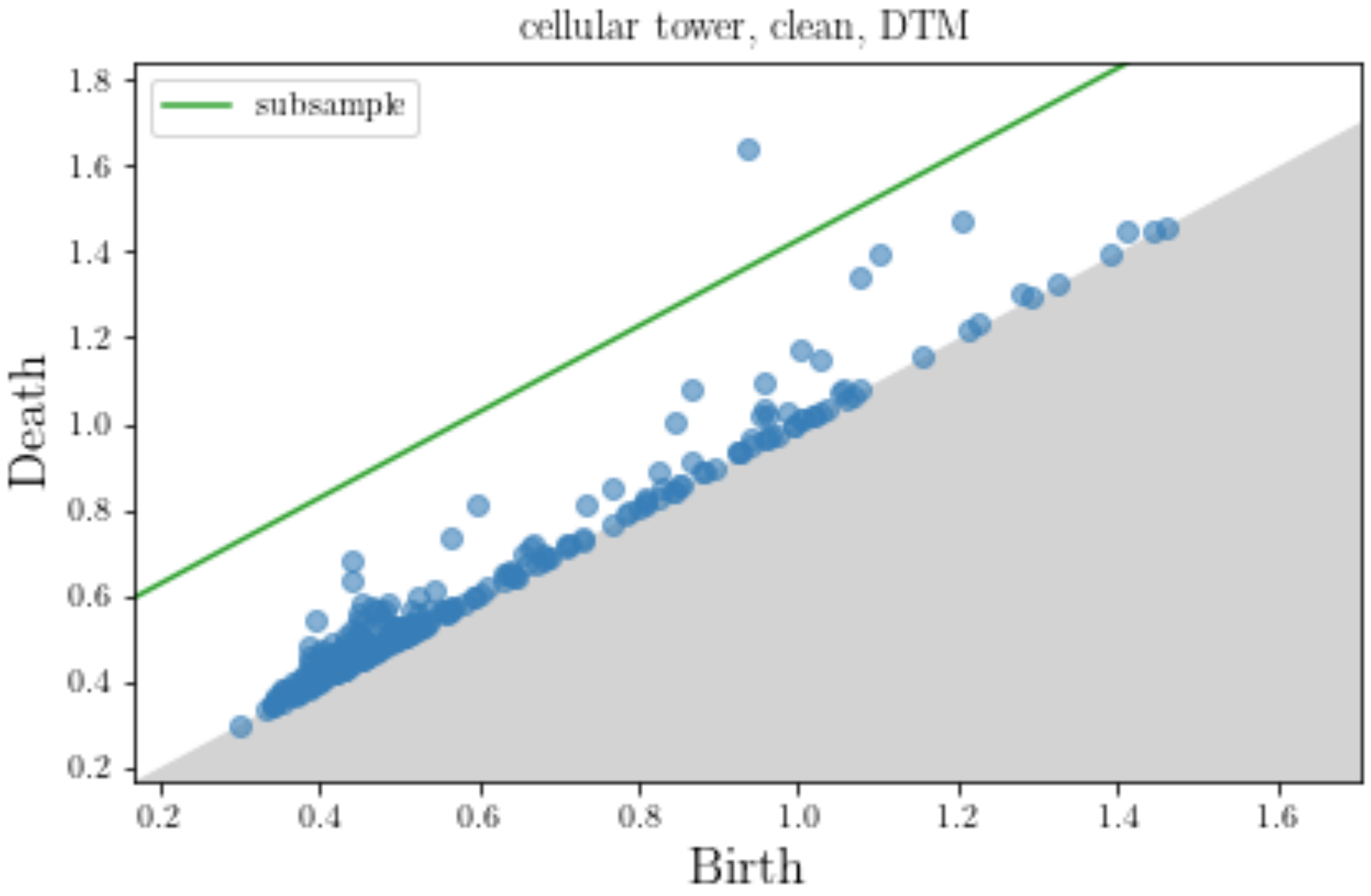

Voronoi, noisy, subsample
common
DTM only
RDAD only
1.0
0.5
0.0
−0.5
−1.0
−3
−2
−1
0
1
2
3

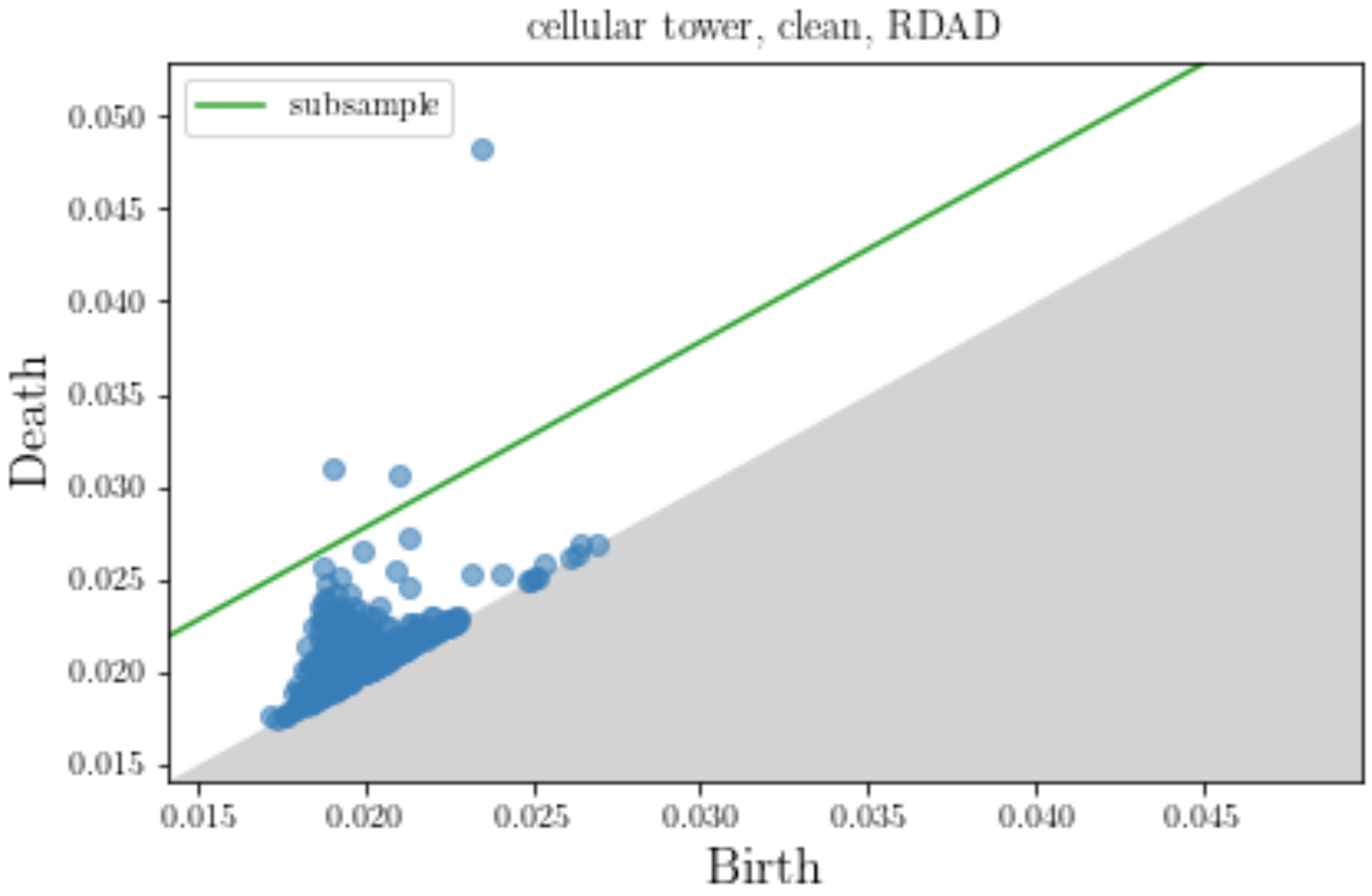
Cellular Towers

Cellular Towers
(HIFLD, 2021)

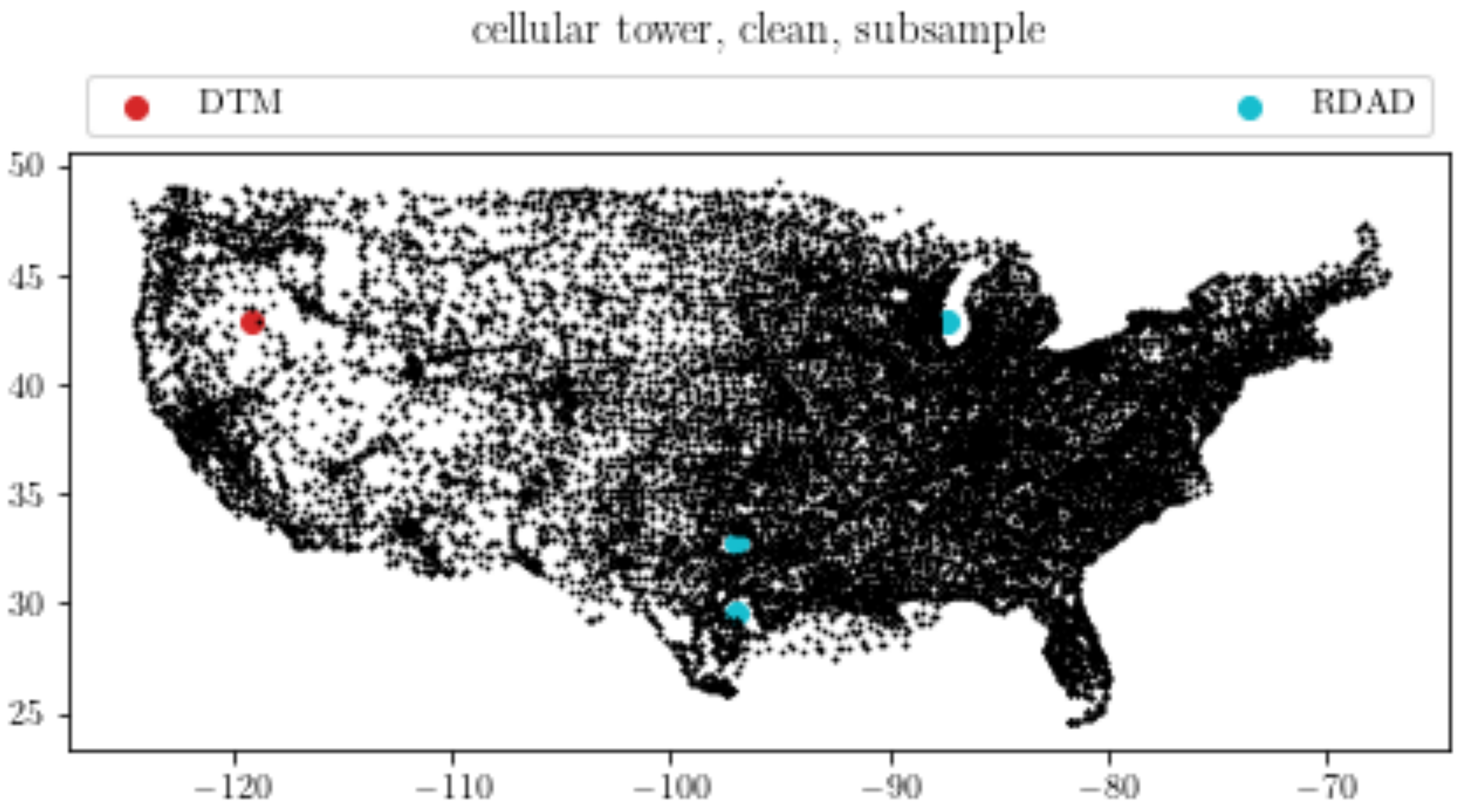


DTM and RDAD


cellular tower, clean, DTM
subsample
Death
Birth
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8


cellular tower, clean, RDAD
subsample
Death
Birth
0.015
0.020
0.025
0.030
0.035
0.040
0.045
0.050

Cellular Towers



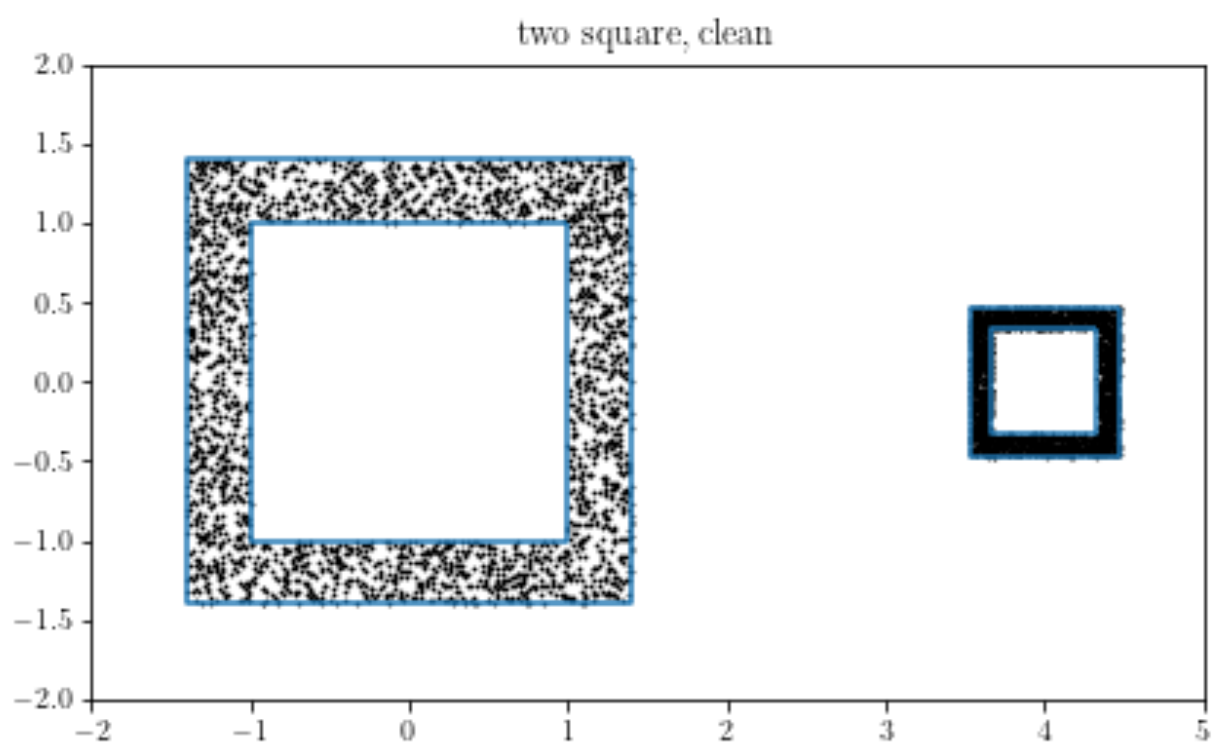
Epilogue:
The End of the Beginning

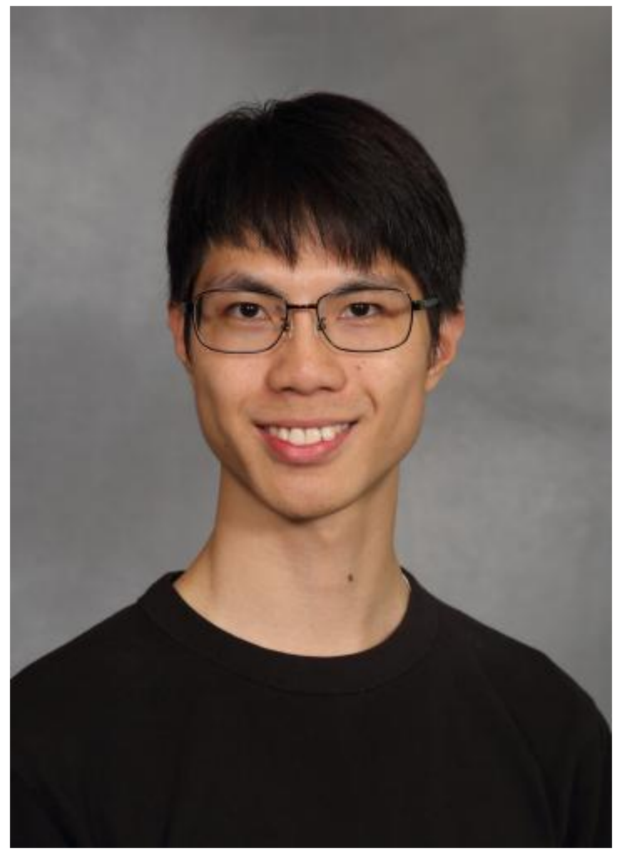
Ongoing / Future Works

- Bootstrapping properties of RDAD?
- Inference of Cosmological Parameters?
- Organic combination of topology and statistics???

Thank you!

- Chunyin Siu (Alex)
- Cornell University
- cs2323@cornell.edu





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