SUPER*TREE LEARNERS:

a new metalearner for local data science

LEVI JOHN WOLF levi.john.wolf@bristol.ac.uk

WHY DO WE NEED THIS?

GEOGRAPHICAL CLUSTER-REG

UNDERSTANDING QUADTREES

APPLYING QUADTREE REGRESSION

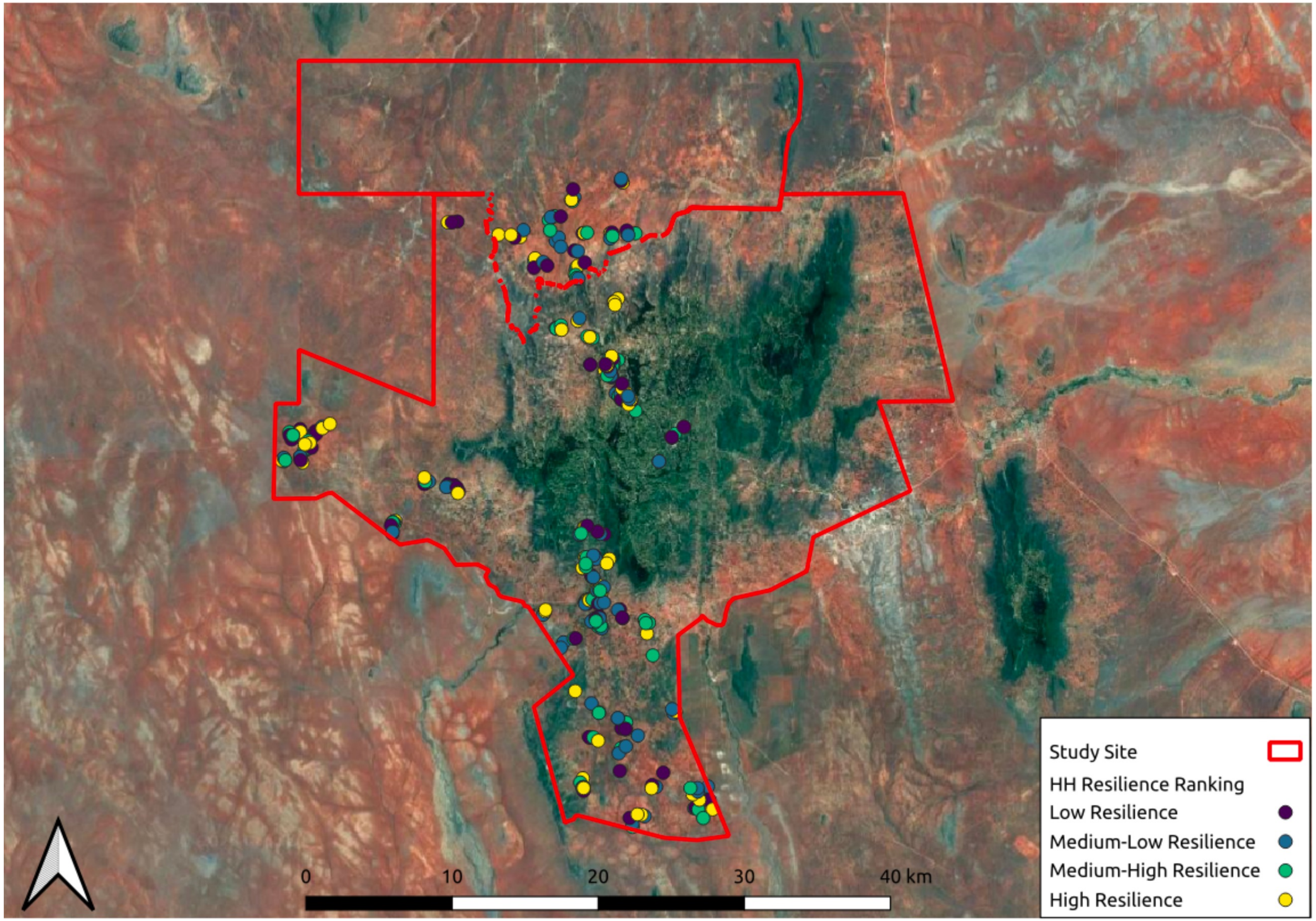
WHY DO WE NEED THIS?

place is not always so obvious

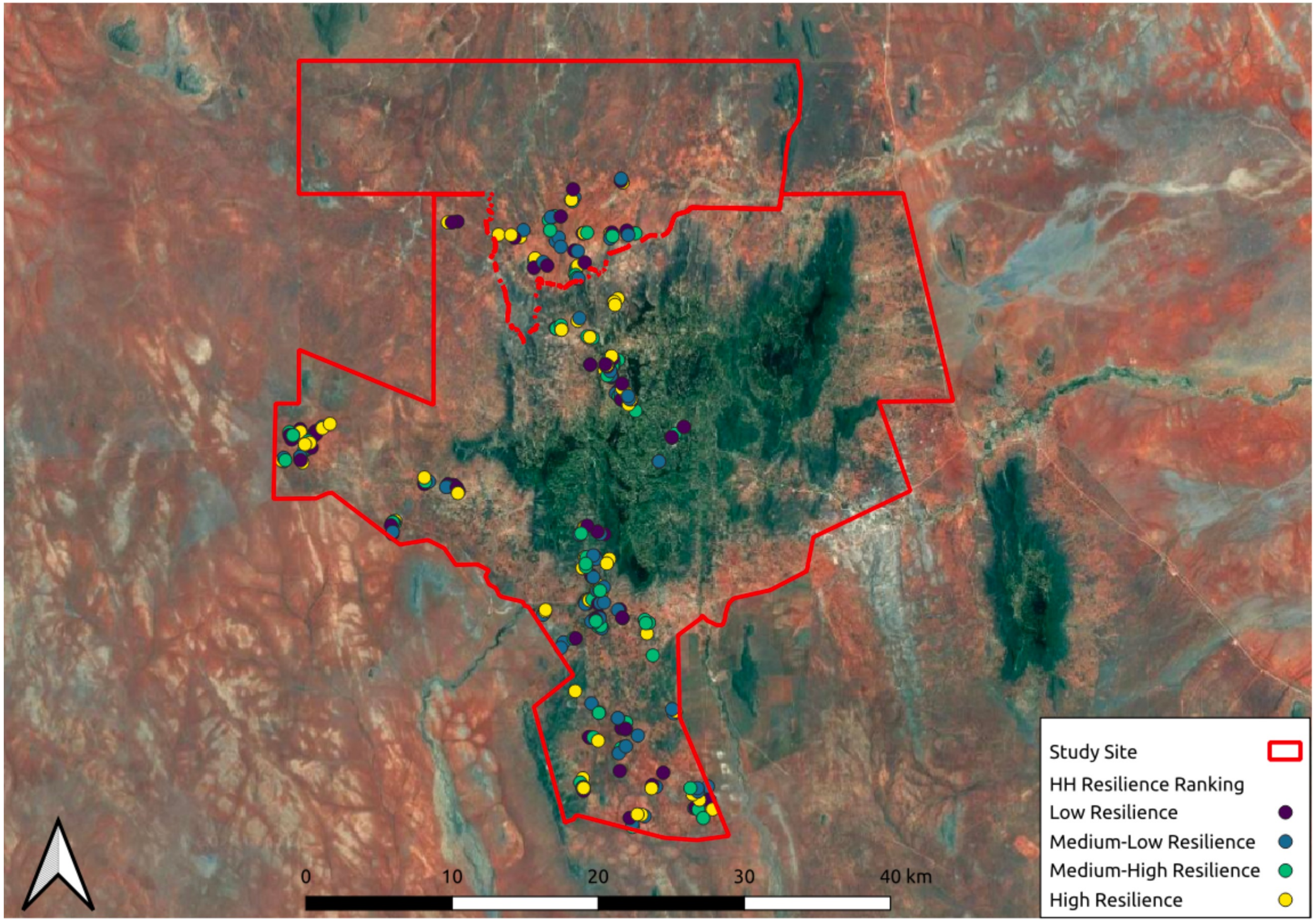
GEOGRAPHICAL CLUSTER-REG

UNDERSTANDING QUADTREES

APPLYING QUADTREE REGRESSION



WHAT IS CLUSTERING REGRESSION



Different clusters differ:
- What is “food”?
- Do we farm or herd?
- How do we do that?
- Is water held in common?
- Is there a community safety net?

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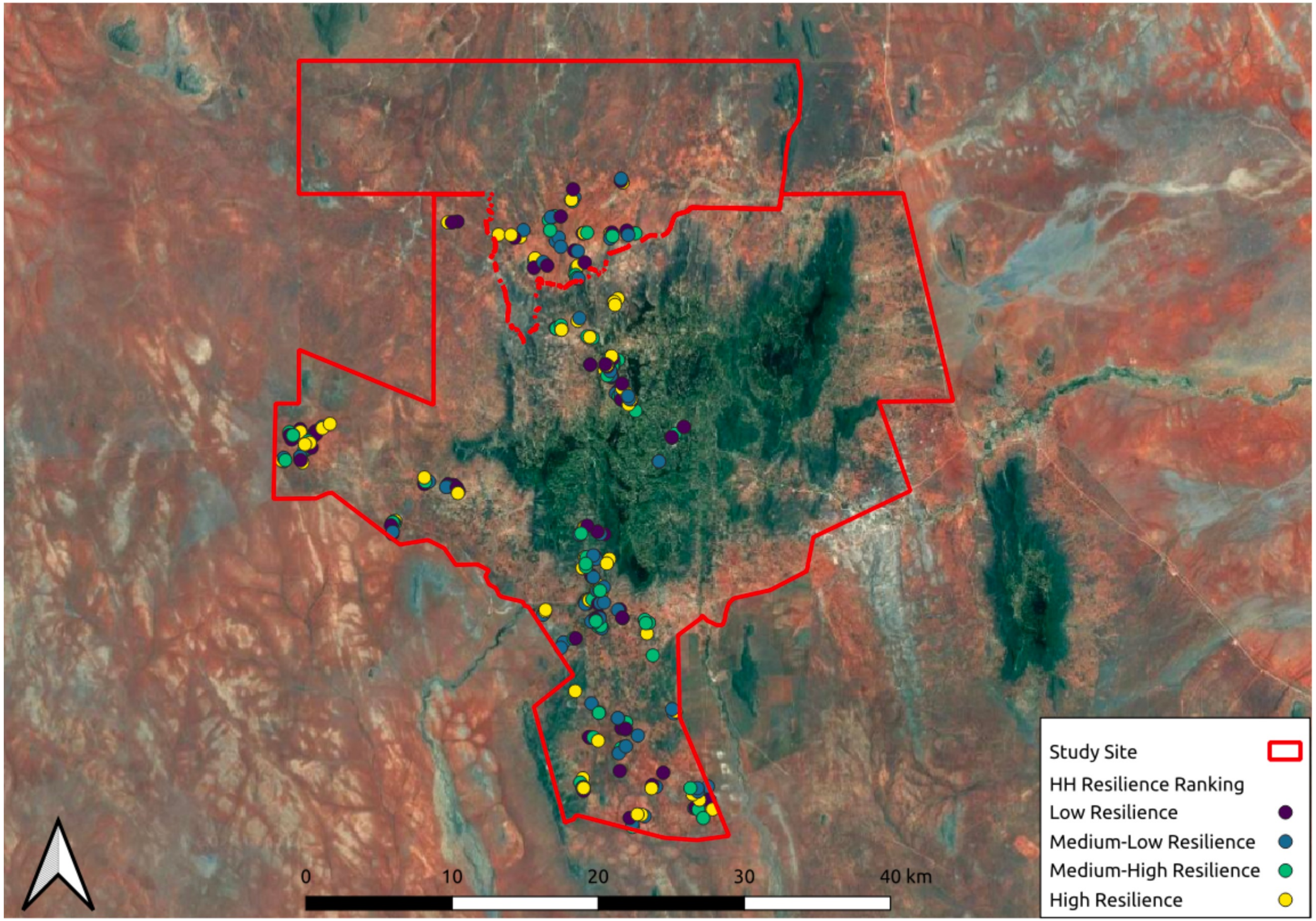

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Nearby households are more similar …

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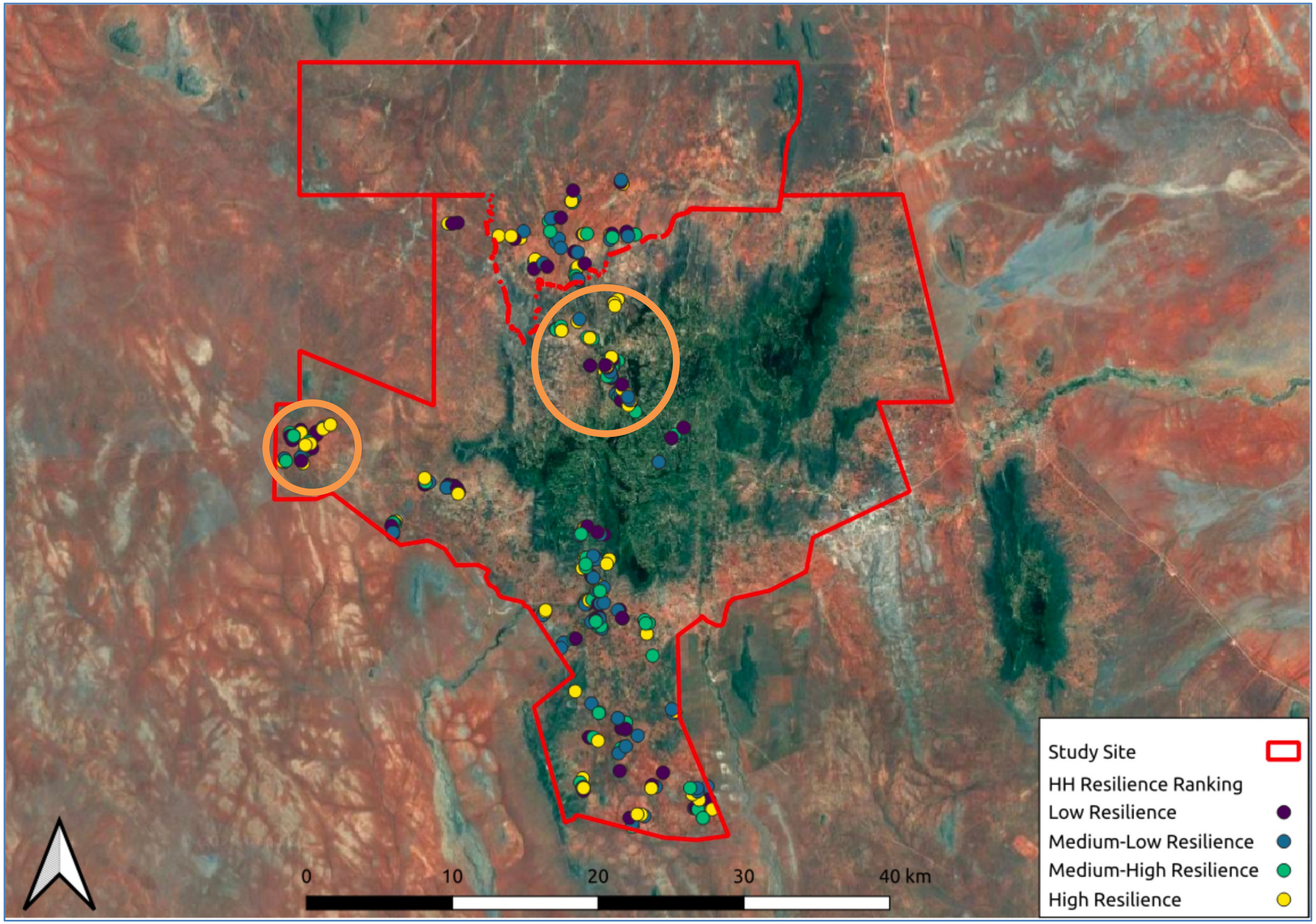

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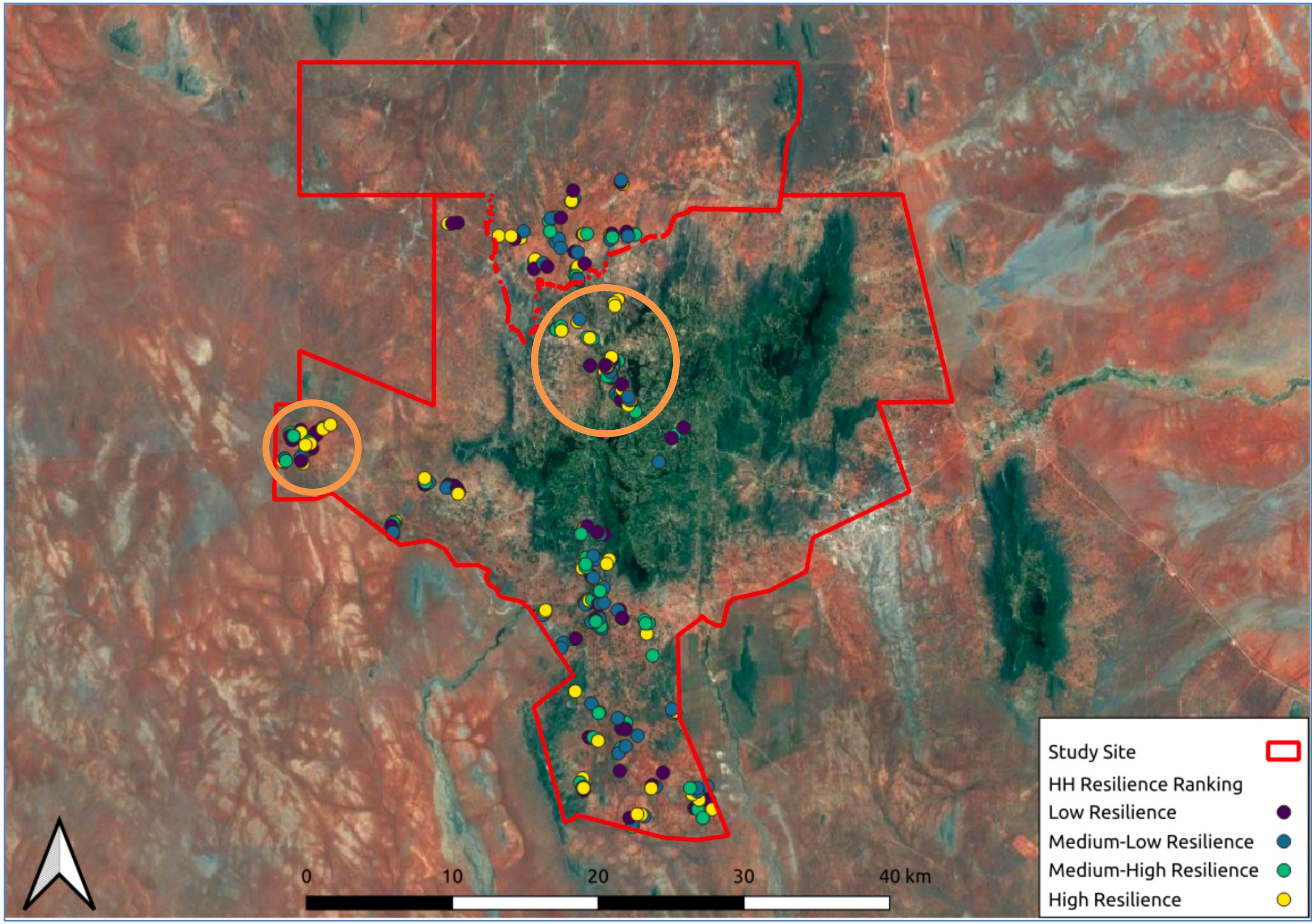
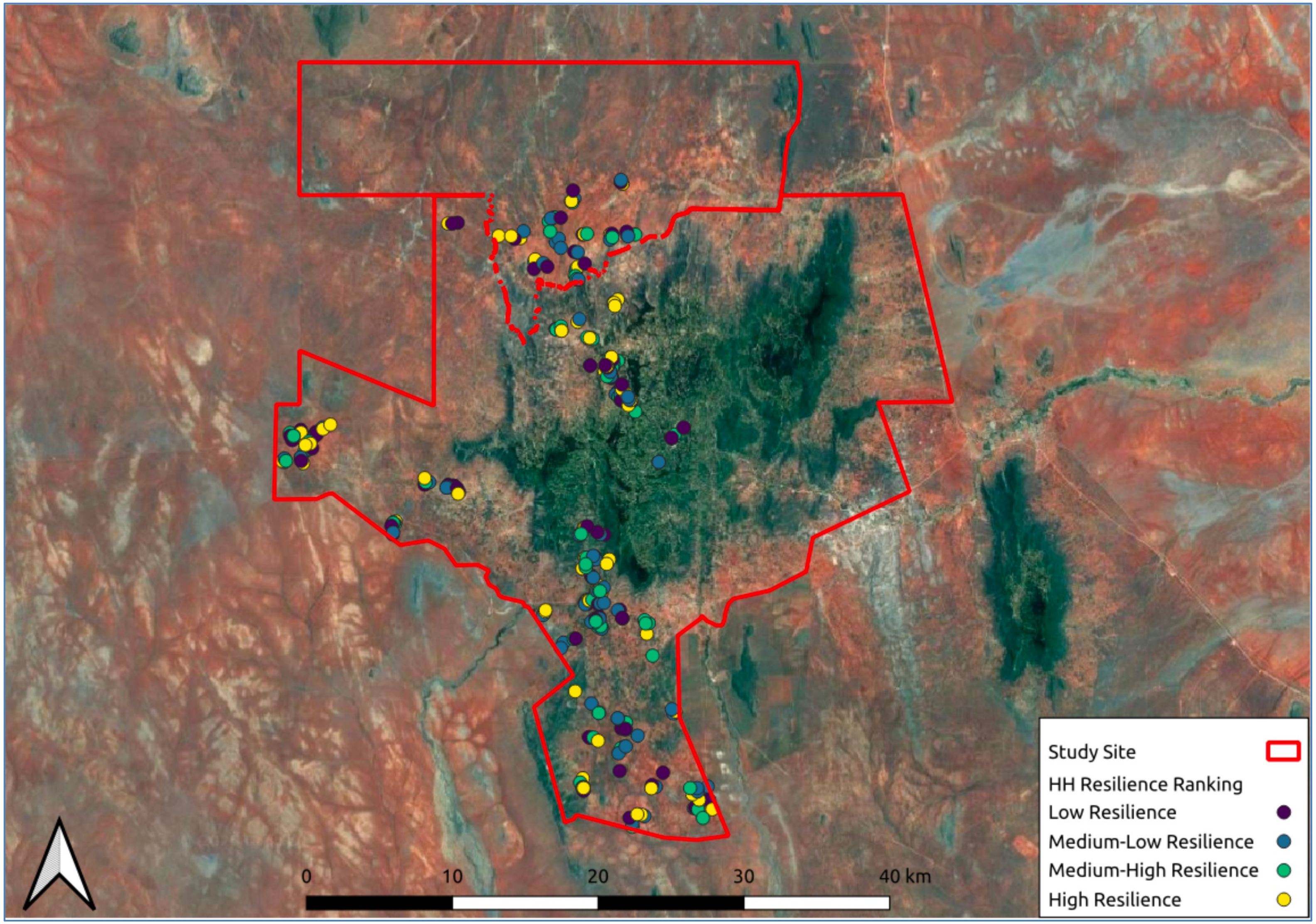


Often, separation is poor!

Nearby households are more similar …

Geographically Weighted Regression

WHAT IS CLUSTERING REGRESSION



Instead, let's find who's similar in y~X and group'em!

Nearby households are more similar …

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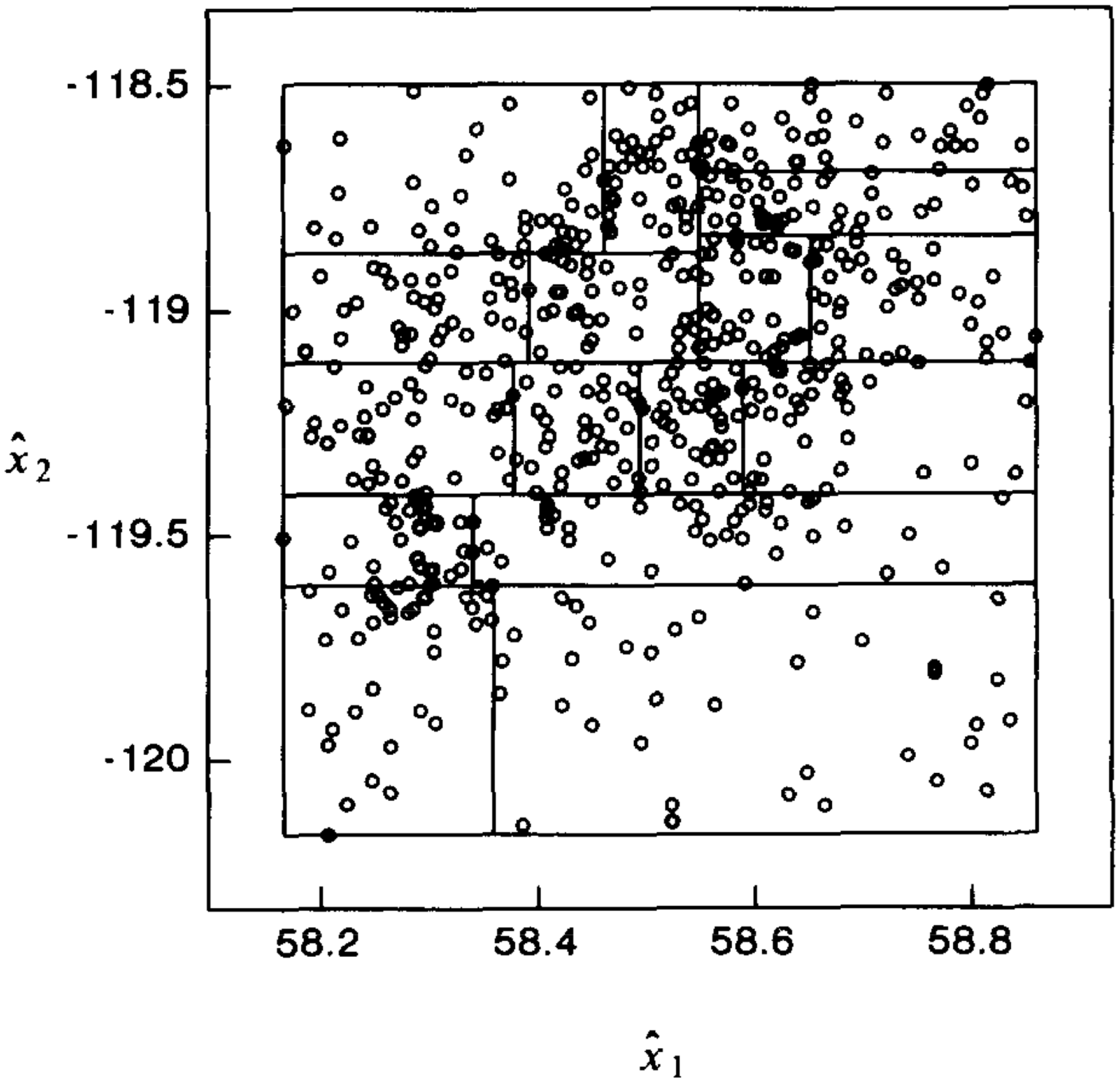

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REGRESSION BY LOCAL FITTING
Methods, Properties, and Computational Algorithms

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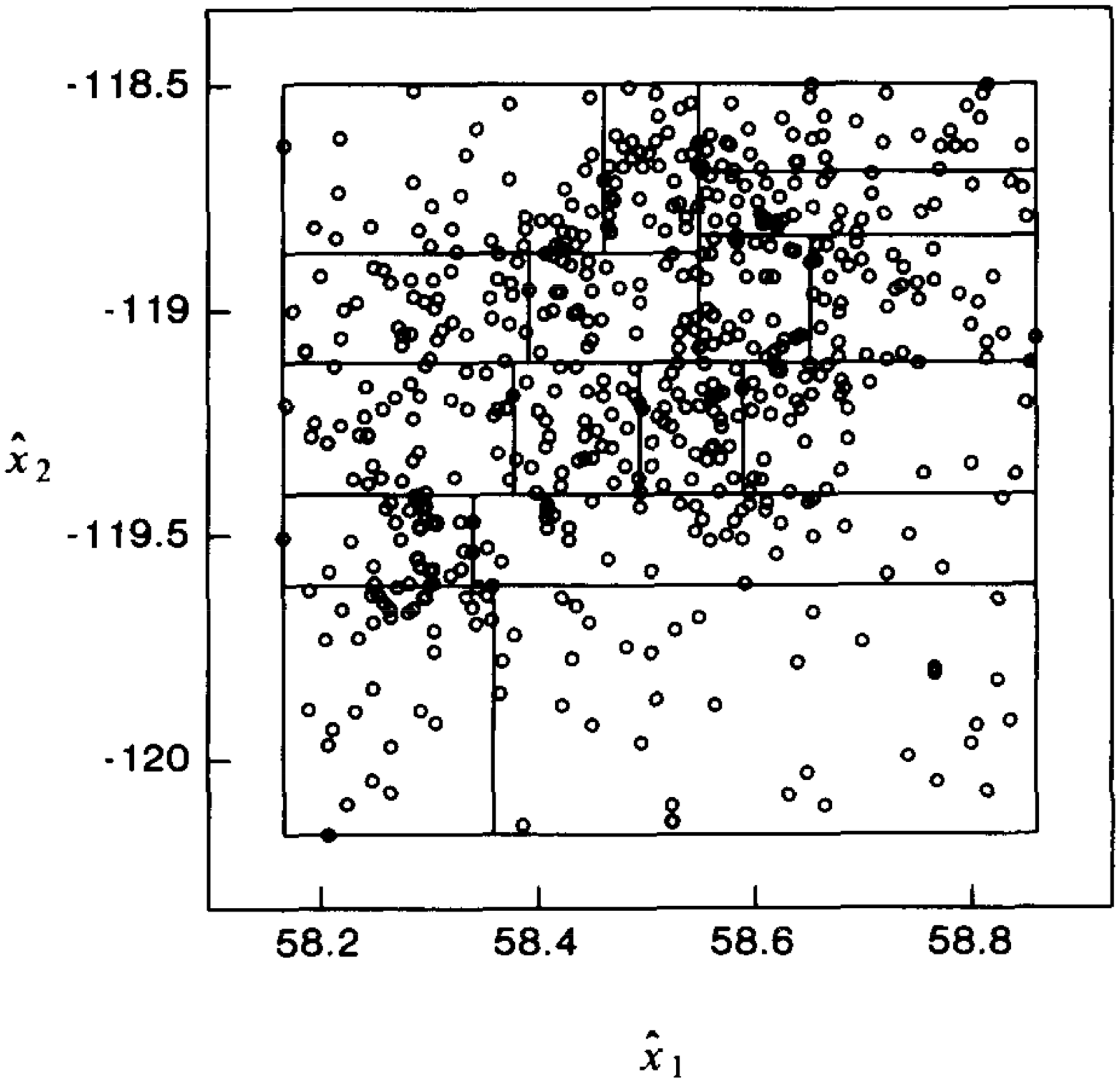

LOWESS Idea:
Fit a spatial tree on feature data
Estimate separately for each leaf
Smooth between nearby leaves

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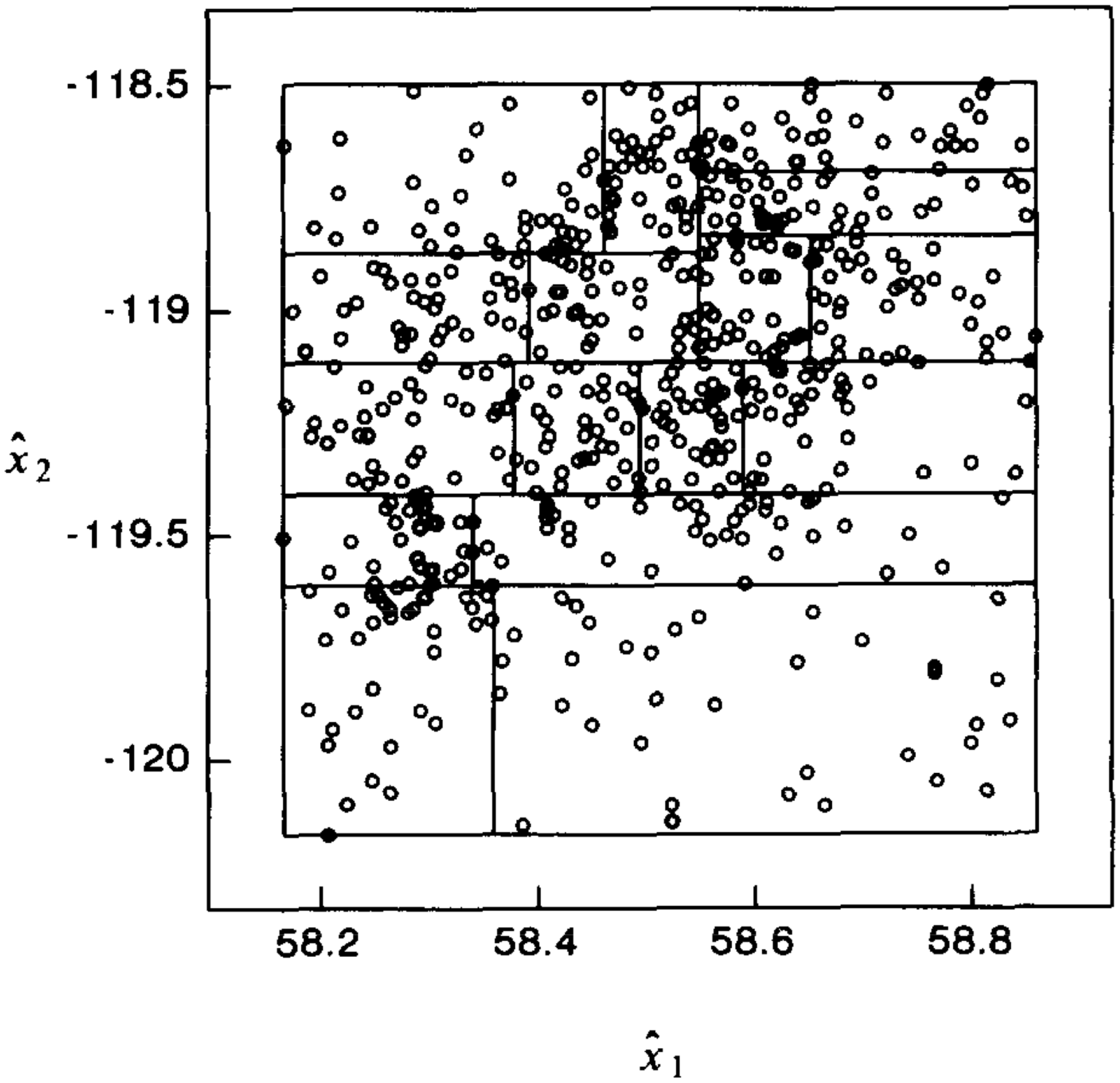

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"Cluster" on X alone

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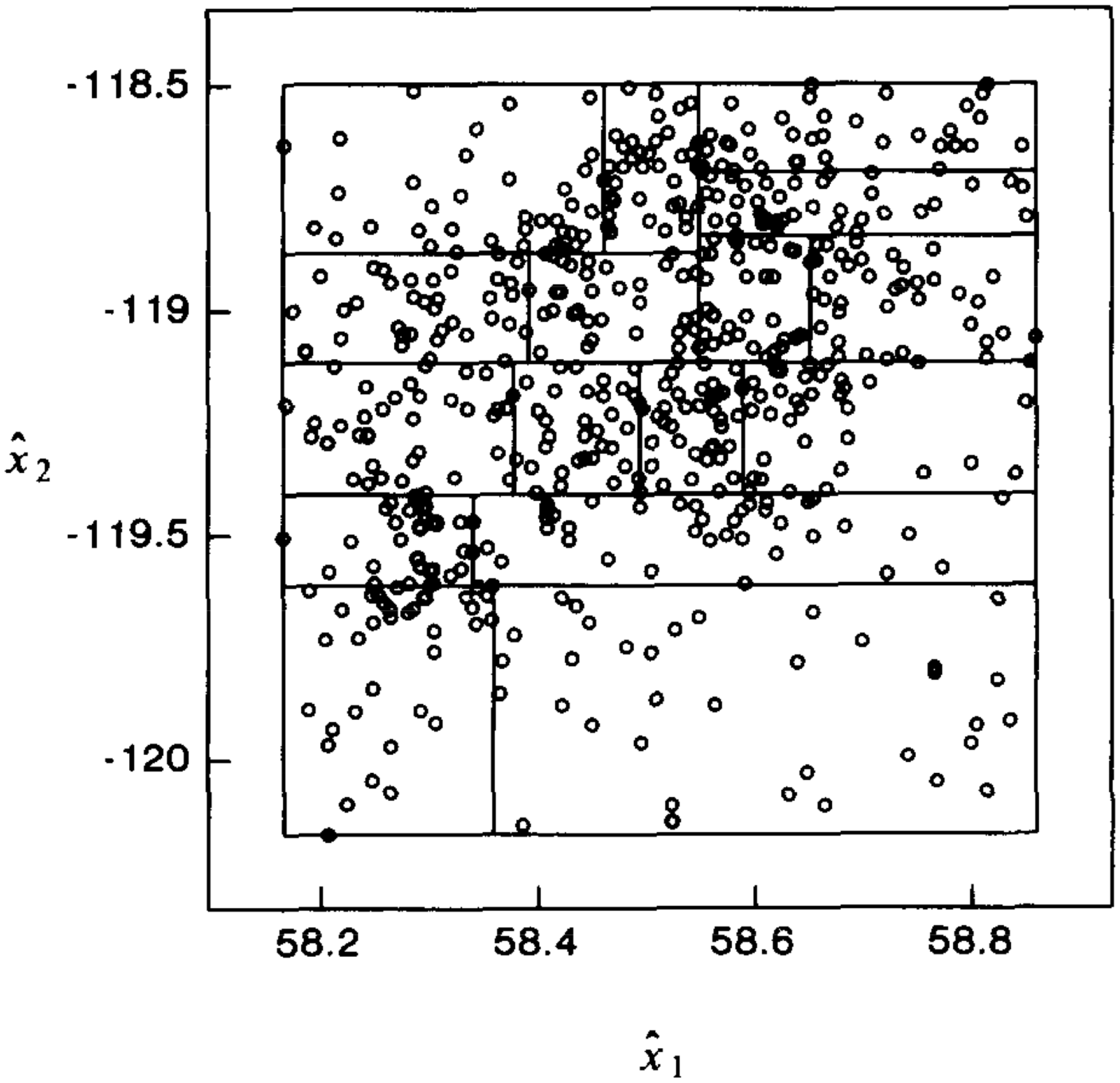

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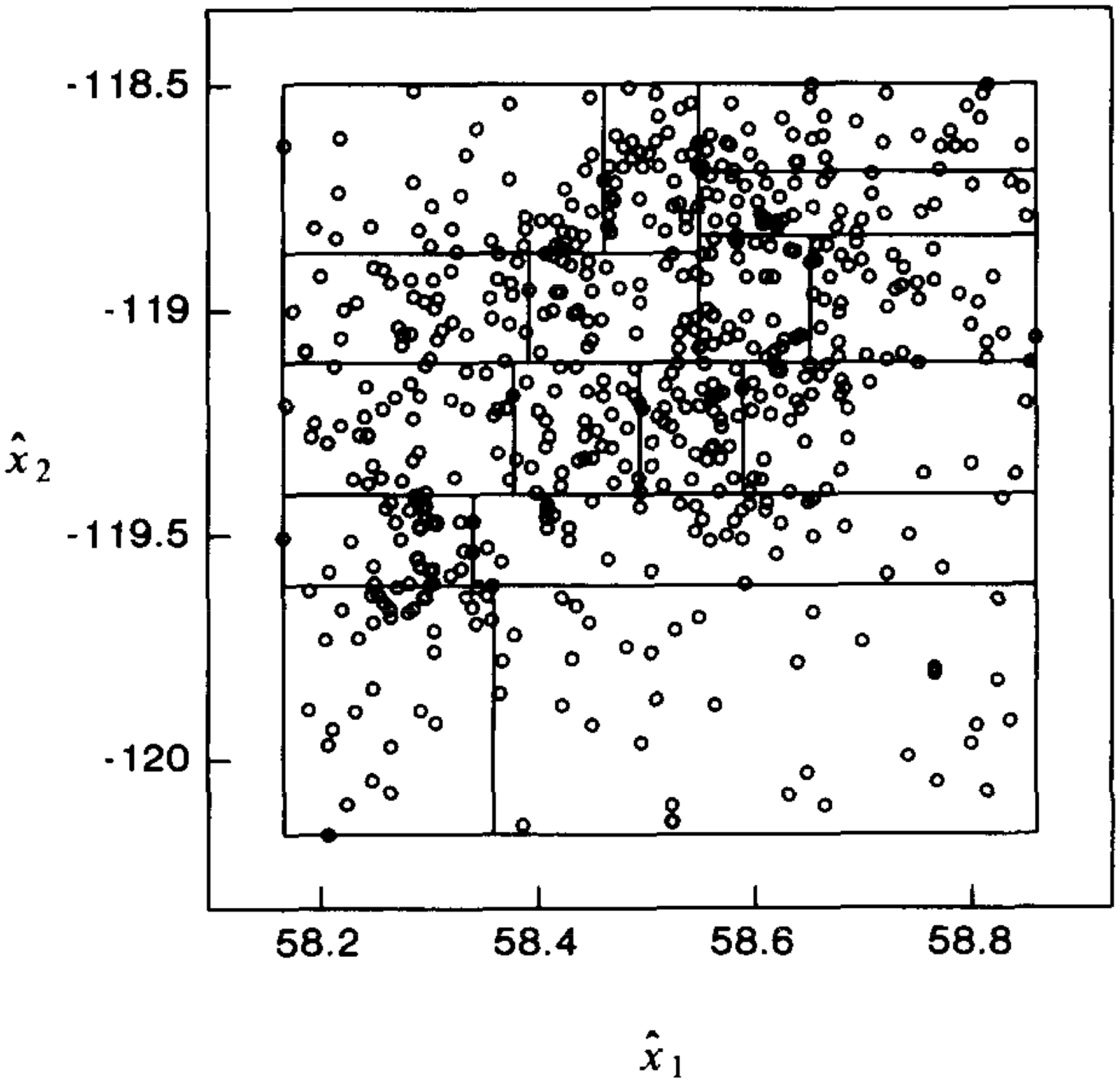

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Tree uses location, not regression loss

Can we do better?

WHAT IS CLUSTERING REGRESSION

CLUSTERING REGRESSION

jointly solving clustering and regression

(GEO)CLUSTERING REGRESSION

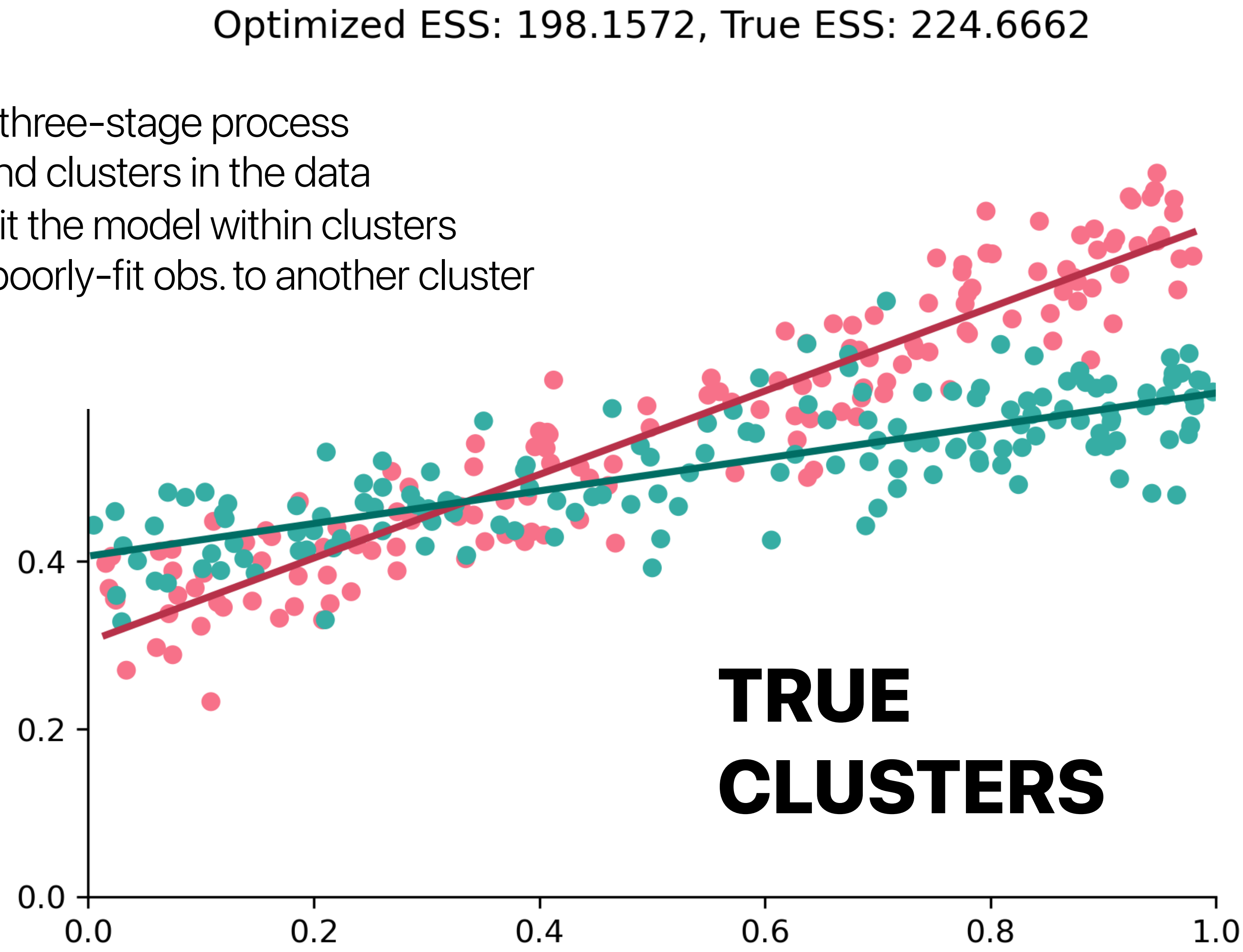
long-studied, quite recently revived

UNDERSTANDING QUADTREES

APPLYING QUADTREE REGRESSION

THE SUPERVISED QUADTREE

Späth (1979)'s three-stage process
- **CLUSTER:** find clusters in the data
- **ESTIMATE:** fit the model within clusters
- **REFINE:** flip poorly-fit obs. to another cluster



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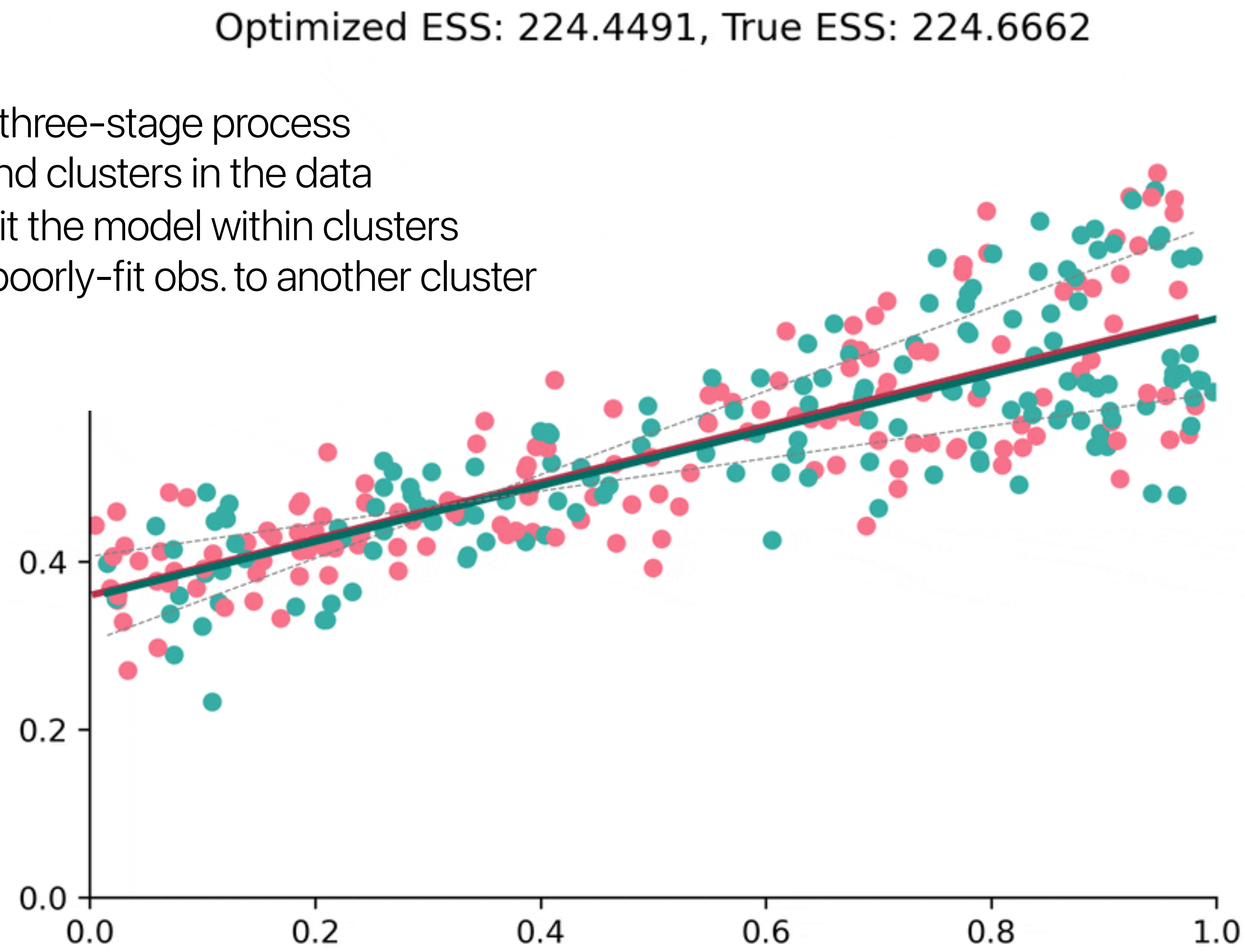

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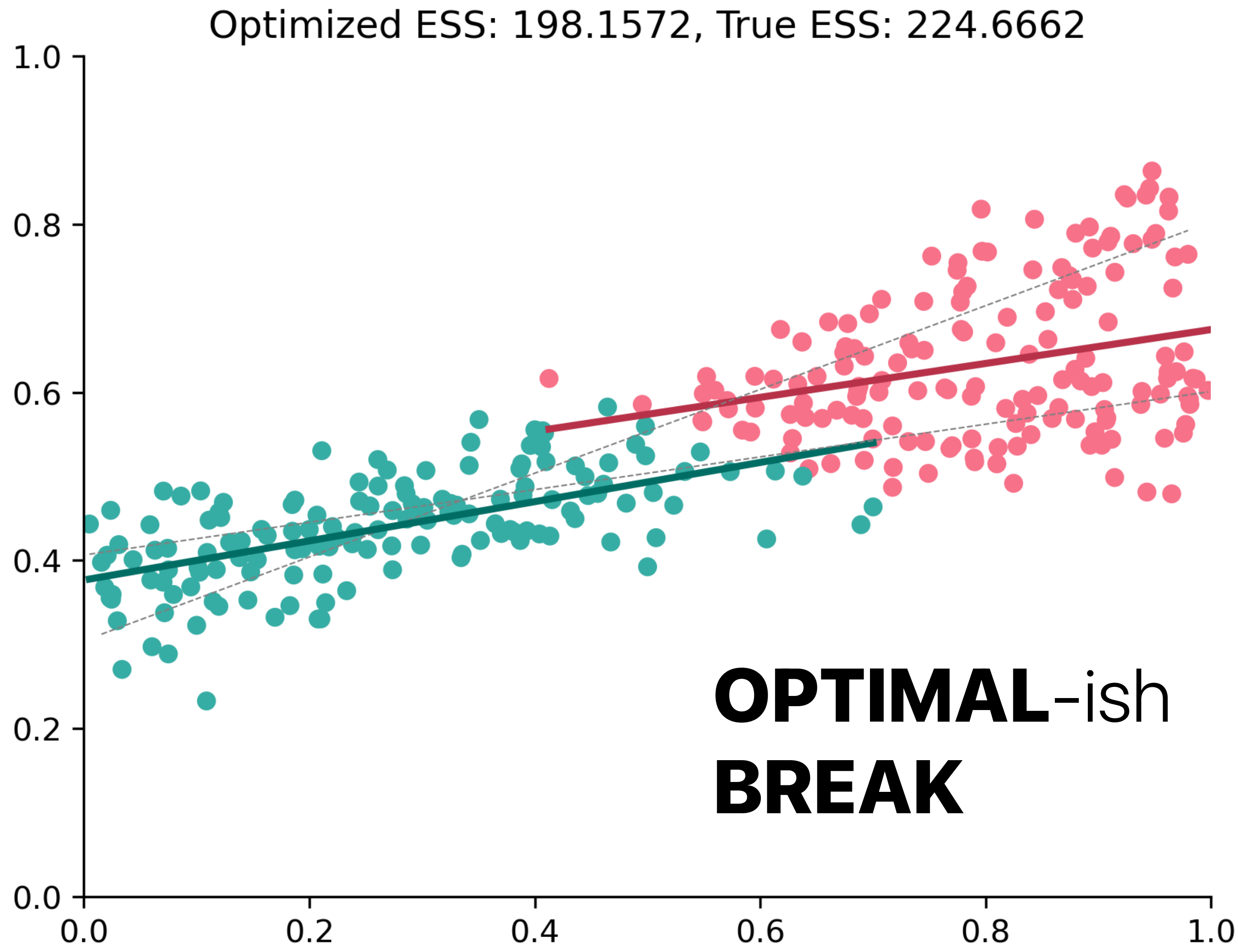

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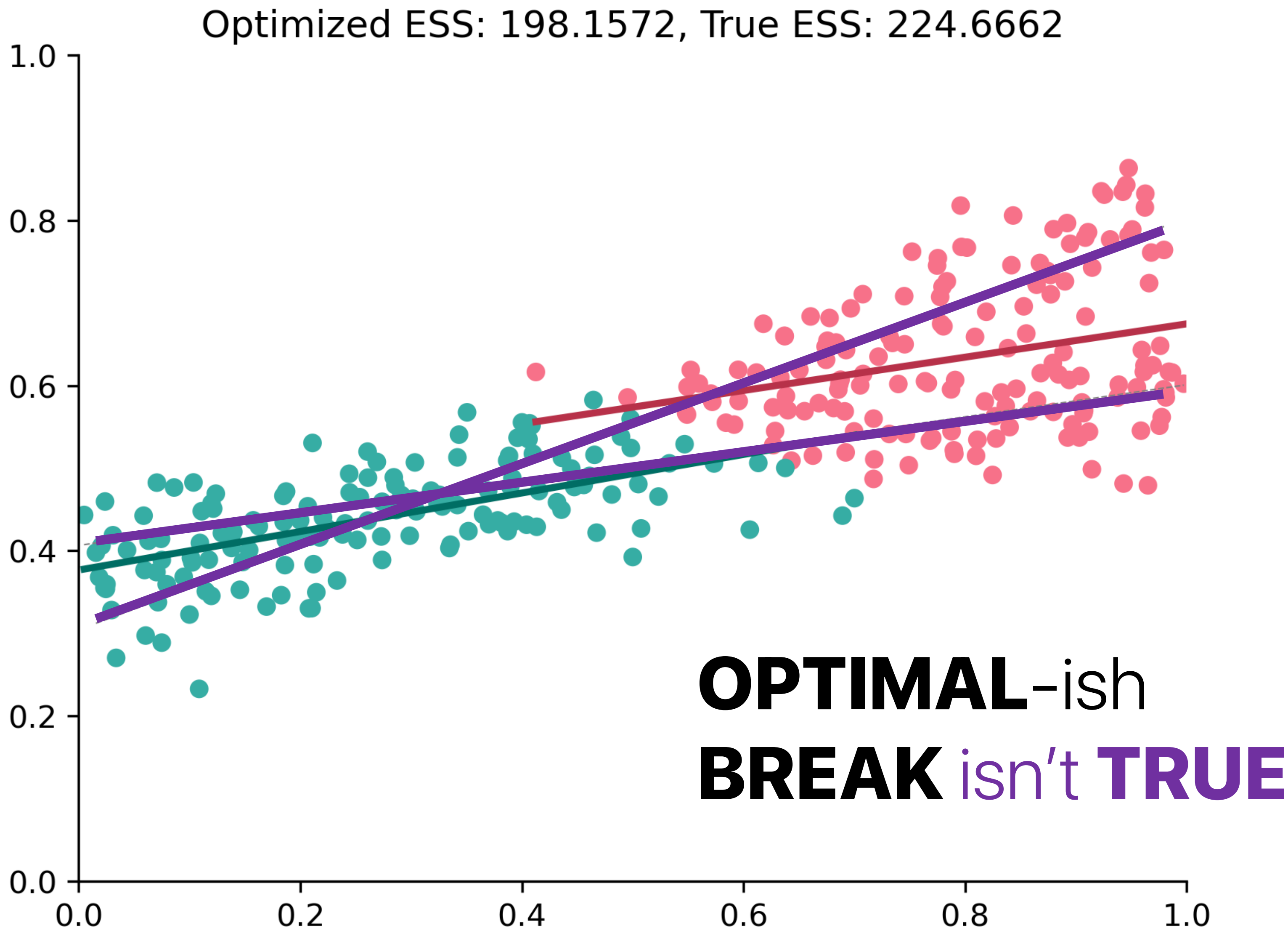

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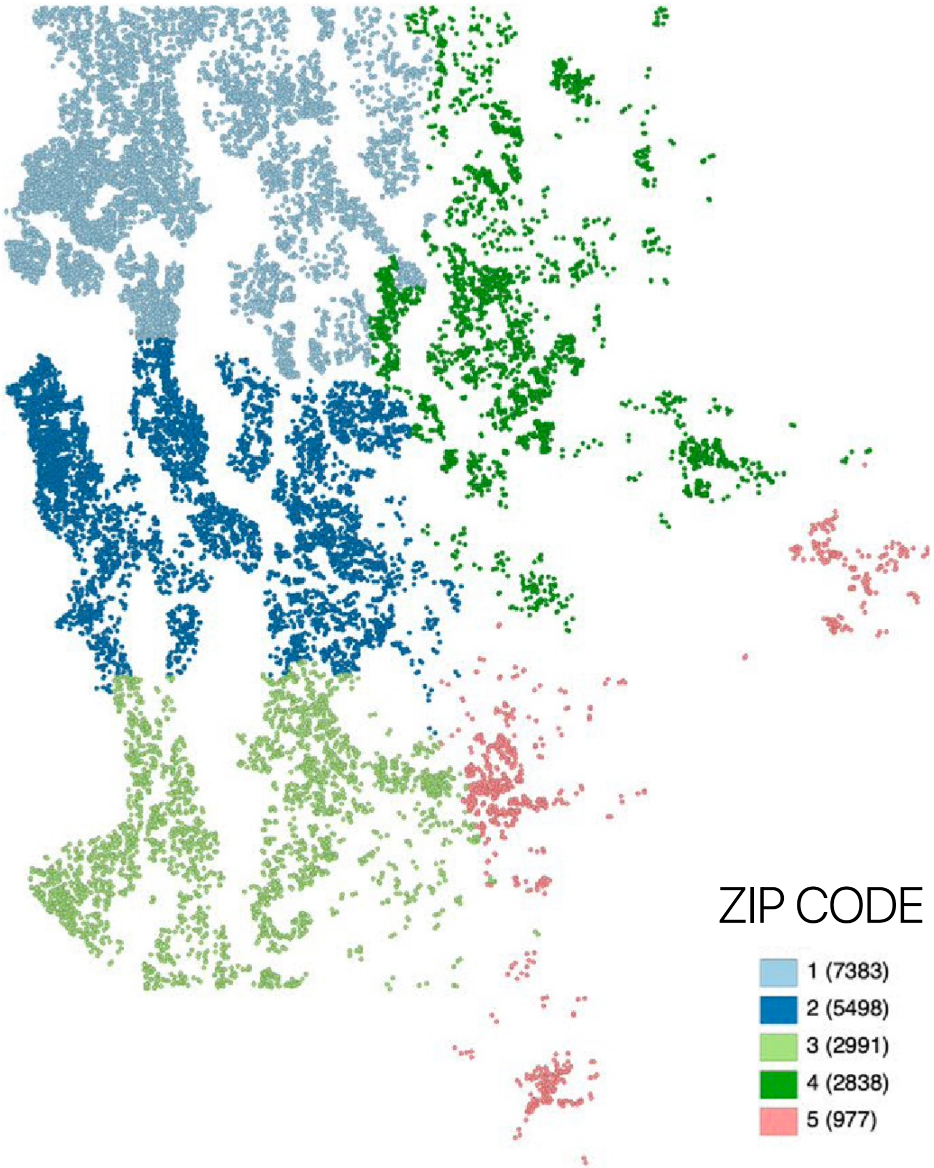
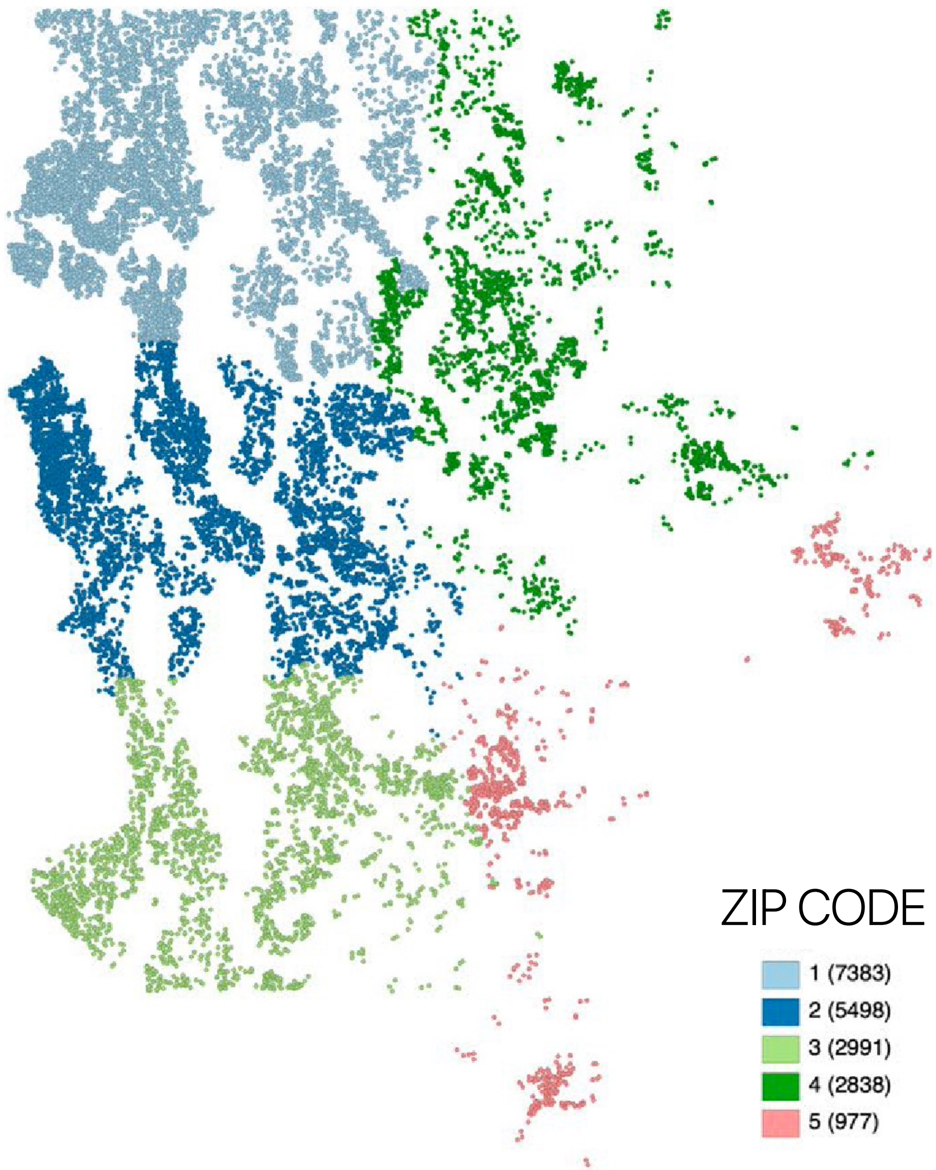
Heuristic (i.e. not optimal), slow+computationally intensive, even in the seriously improved spatial variant provided by Sugasawa and Murakami (2021)
No uncertainty for checking assignment, hence no guarantee of recovering the true classes

BEFORE THE SUPER*TREE LEARNER



Spatial SUR Models

WHAT IS CLUSTERING REGRESSION



Spatial SUR Models

Stack each group's y~X model together

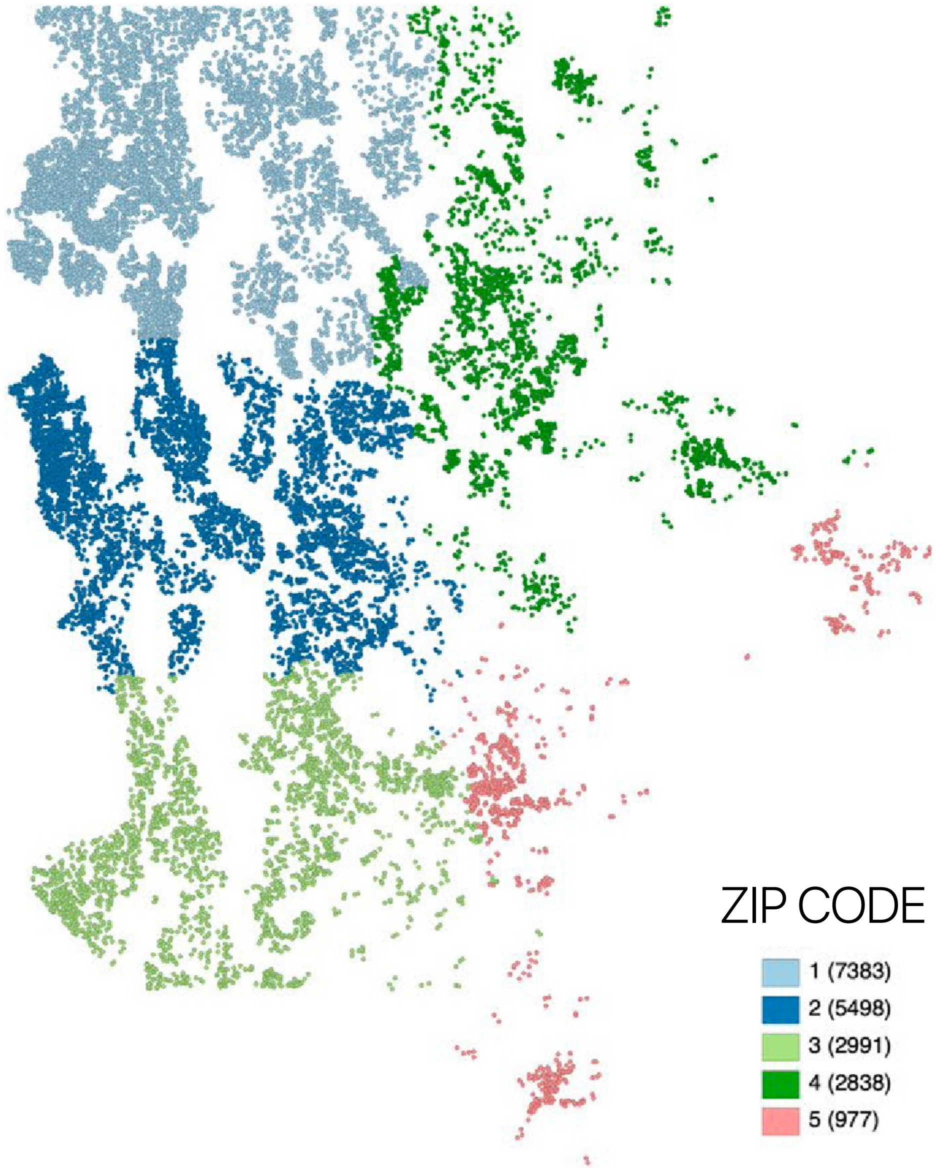
JOURNAL OF REGIONAL SCIENCE, VOL. 30, NO. 2, 1990, pp. 185–207

SPATIAL DEPENDENCE AND SPATIAL STRUCTURAL INSTABILITY IN APPLIED REGRESSION ANALYSIS*

Luc Anselin†

Test to check if separate models are needed!

WHAT IS CLUSTERING REGRESSION



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Can we integrate *that* test during fitting?

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Anselin & Amaral (2023)
- **COMBINE:** Combine spatial and feature similarity
- **SPAN:** compute a MST over the combined affinity matrix
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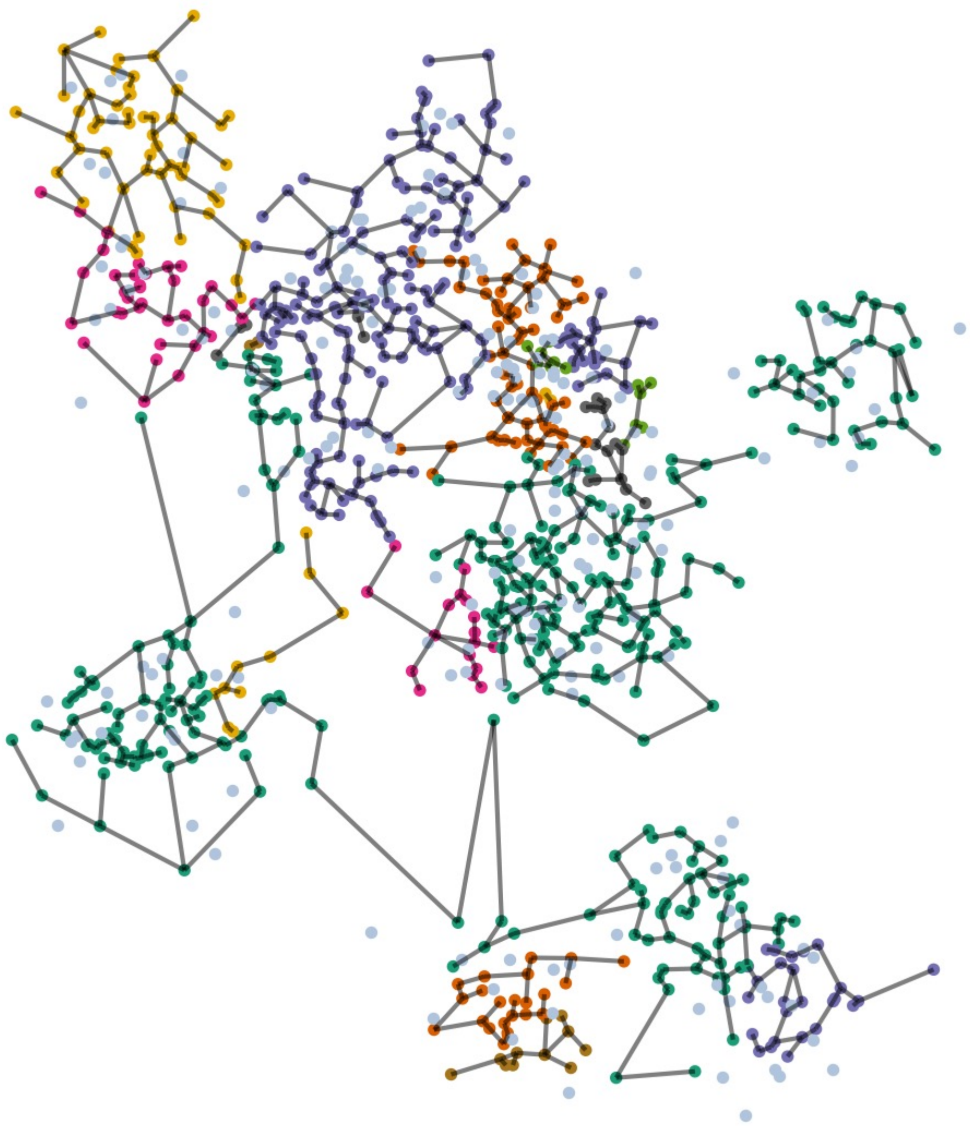
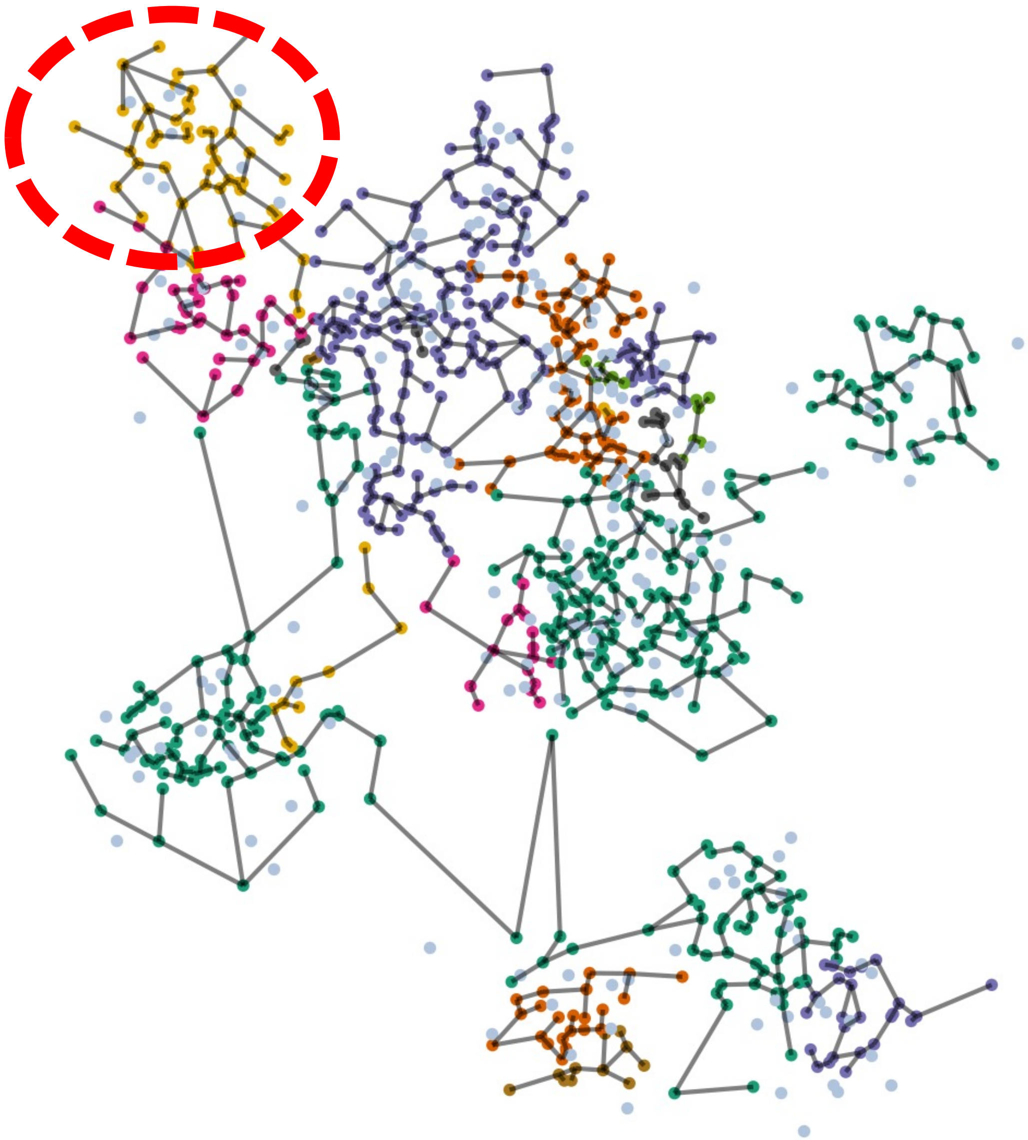
BEFORE THE SUPER*TREE



SKATER REGRESSION

each cluster gets
one regression

Clusters are subtrees
with good regressions.



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Sui Zhang[*1], Wei Zheng[†1] and Cecilia Wong[‡1]

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GISRUK 2025

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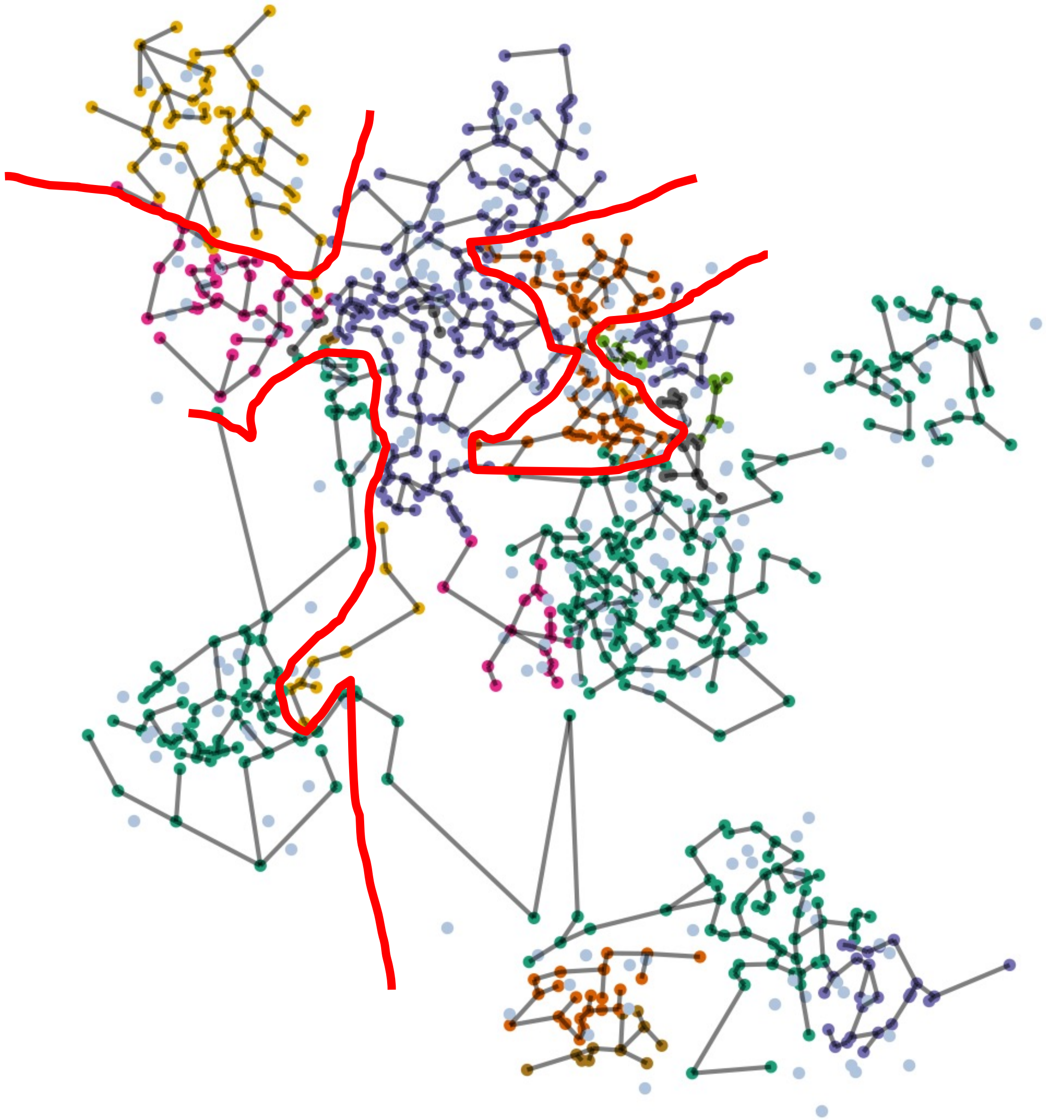
BEFORE THE SUPERVISED QUADTREE

each cluster gets
one ~~regression~~
dummy term

stack these into a
dummy matrix, $\mathbf{D}$

Regression becomes
$y \sim \mathbf{D} + \mathbf{DX}$

clusters are regions
where interaction term
improves model fit

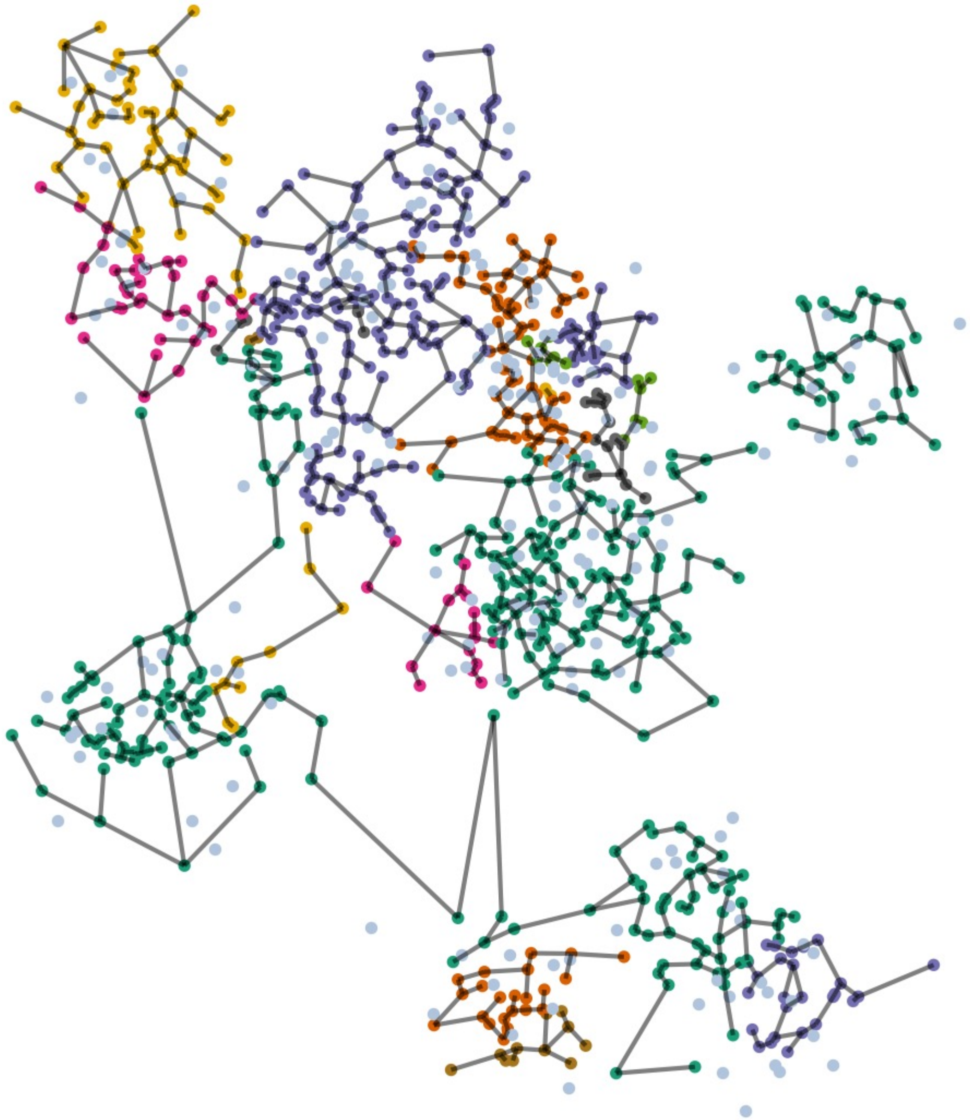


SKATER REGRESSION

Strengths:

Judicious use of degrees of freedom

Uses LRT to find good clusters



SKATER REGRESSION IN PRINCIPLE

Strengths:

Judicious use of degrees of freedom

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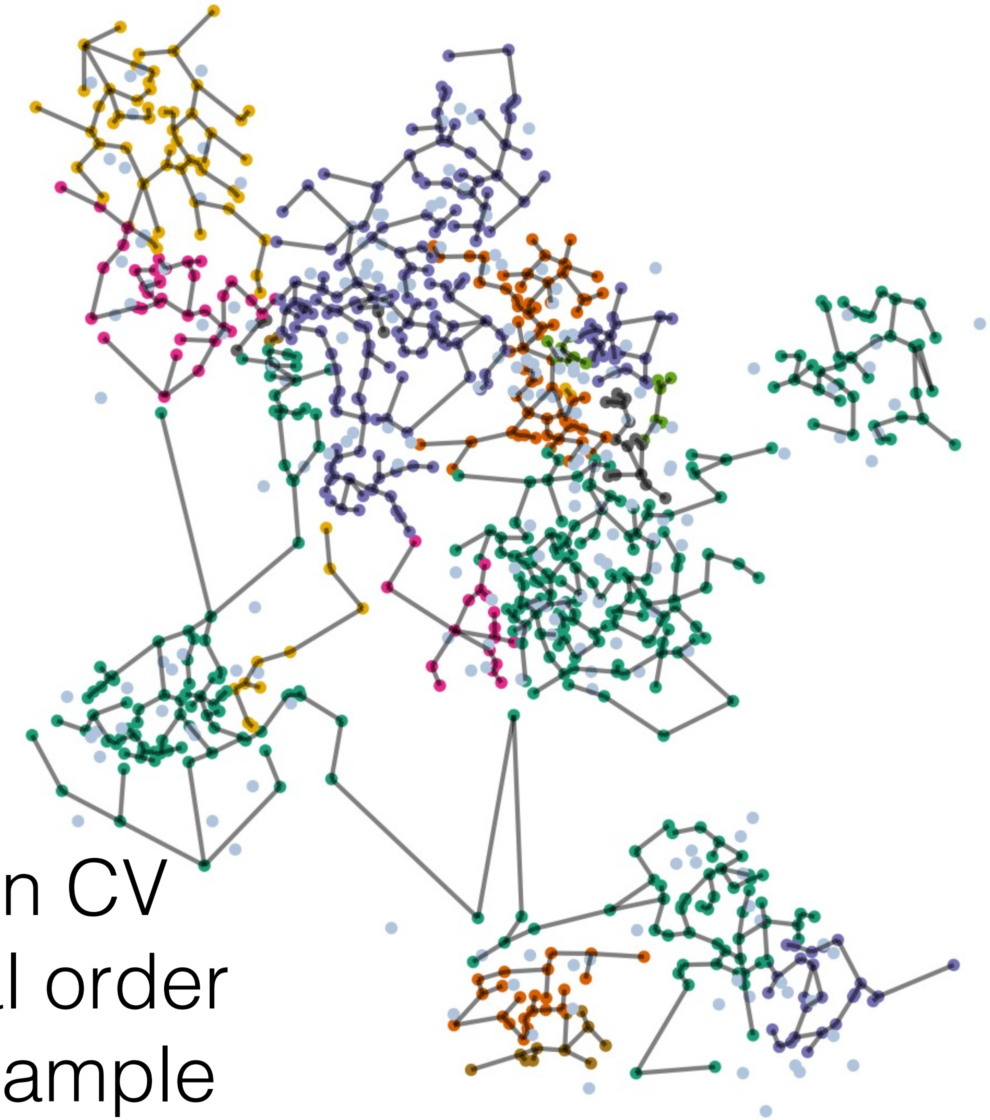
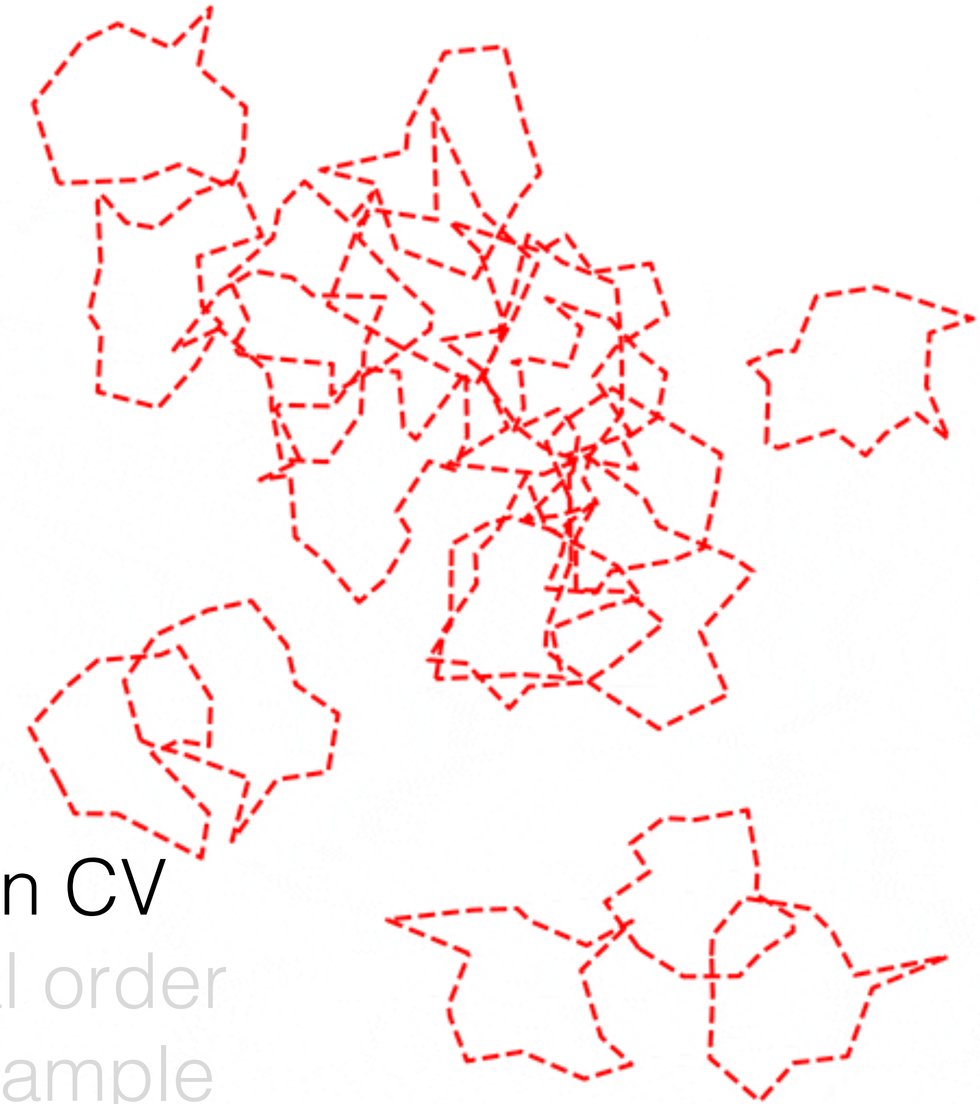


Weaknesses:

- MST is finnicky in CV
- MST has no total order
- can't do out of sample

SKATER REGRESSION IN PRINCIPLE



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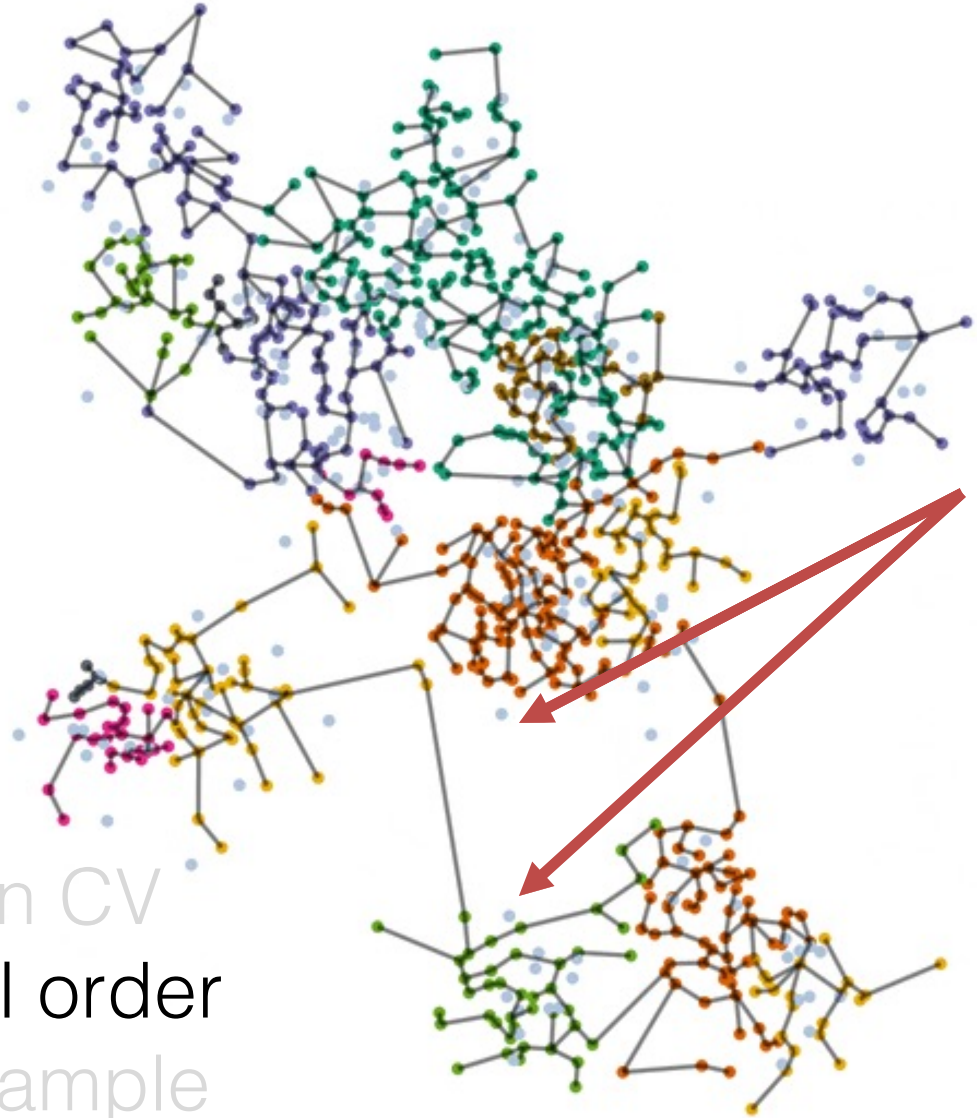
MSTs ARE VERY SENSITIVE OBJECTS



Very distant in some splits, neighbors in others!

Weaknesses:

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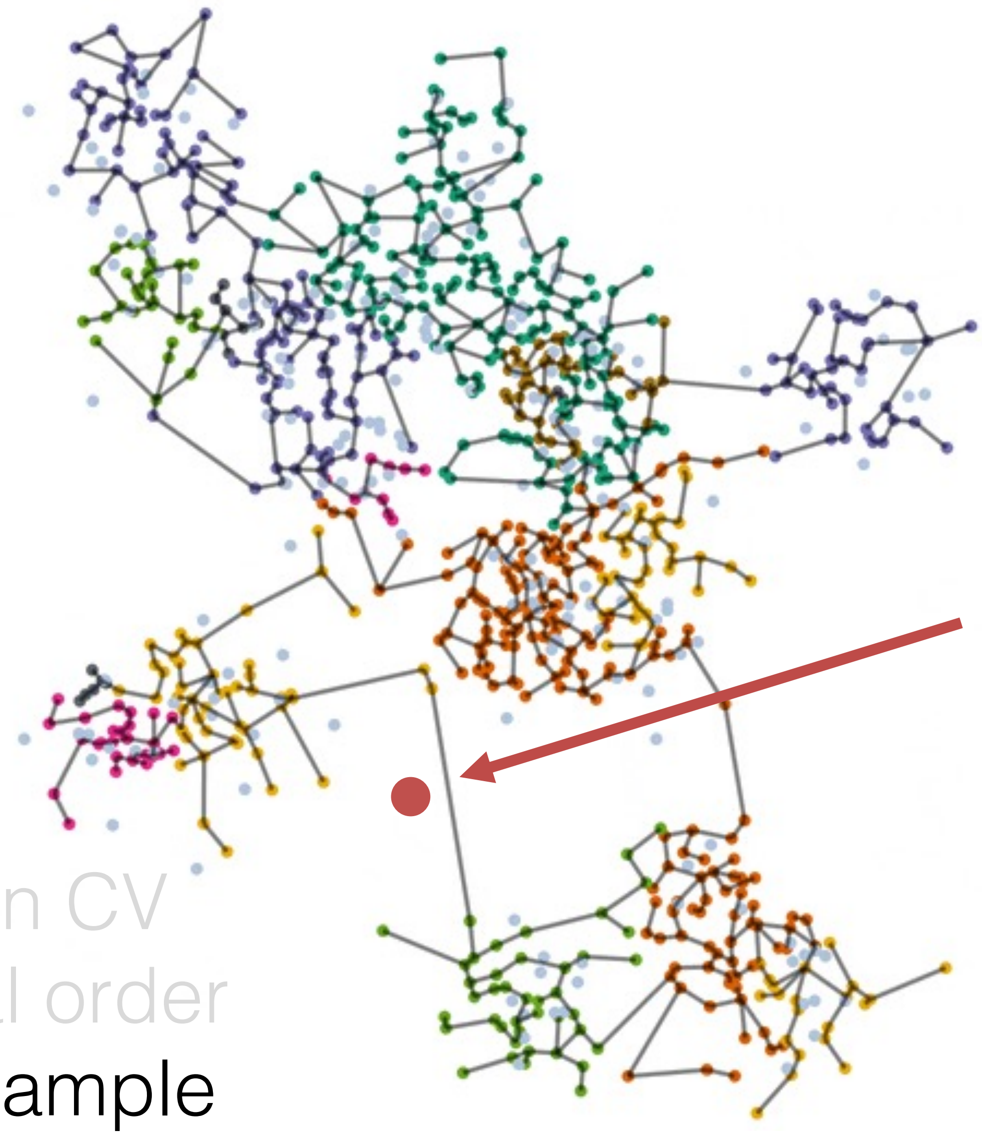
- MST has no total order
- can't do out of sample

TREE ADJACENCY IS NOT SIMILARITY



How should this connect?

Nearest leaf?
Nearest node?
Re-tree everybody?

Weaknesses:

- MST is finnicky in CV
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- can’t do out of sample

NEW POINTS BREAK MST STRUCTURE

CLUSTERING REGRESSION

jointly solving clustering and regression

GEOGRAPHICAL CLUSTER-REG

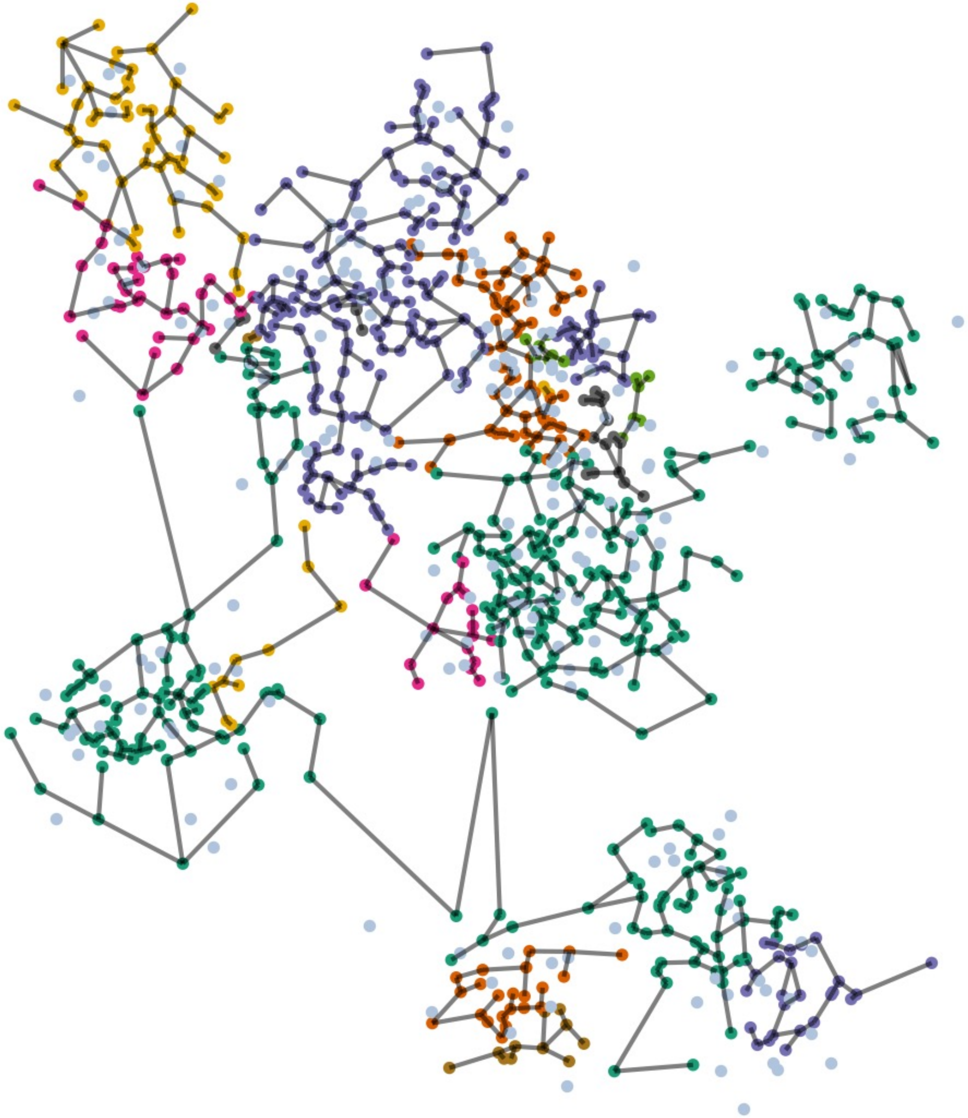
jointly solving clustering and regression

UNDERSTANDING SUPER*TREES

spatial splits for spatial fits

APPLYING QUADTREE REGRESSION

Build a Minimum Spanning Tree
Split tree when it improves predictions
Aggregate subtrees to make predictions



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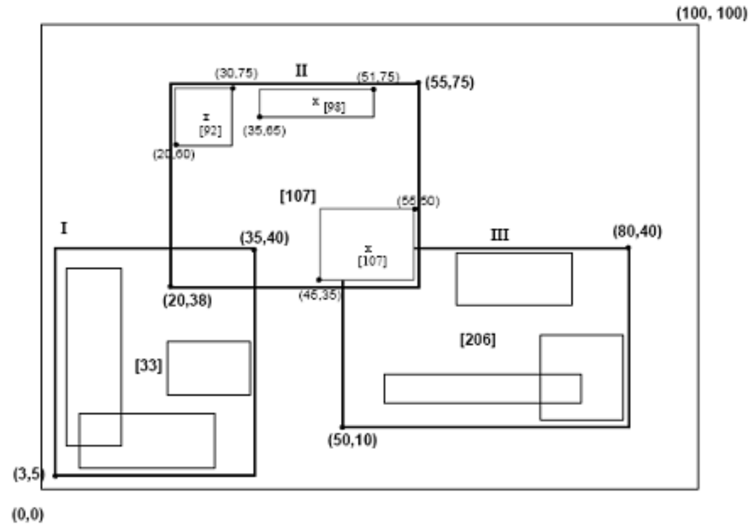
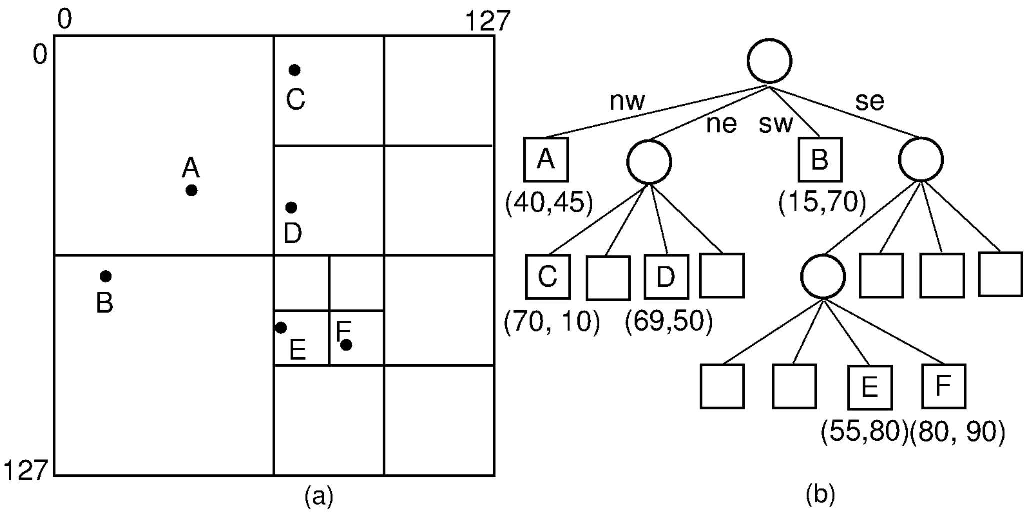
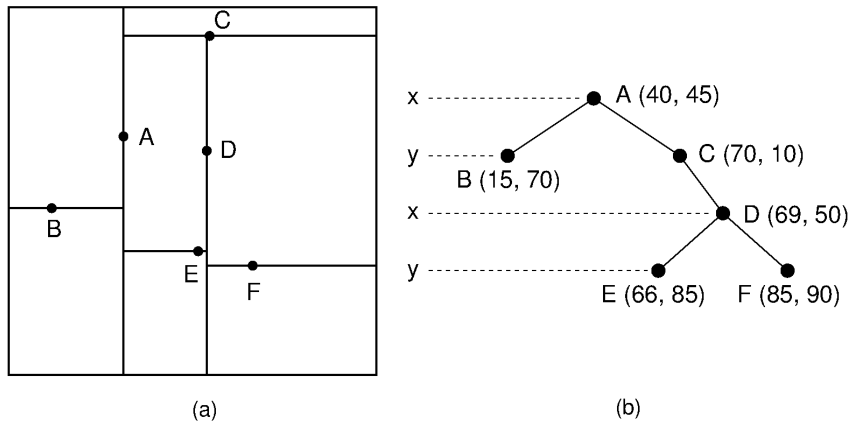


Hilbert R-Tree



QuadTree



kd-Tree

THE SUPER*TREE

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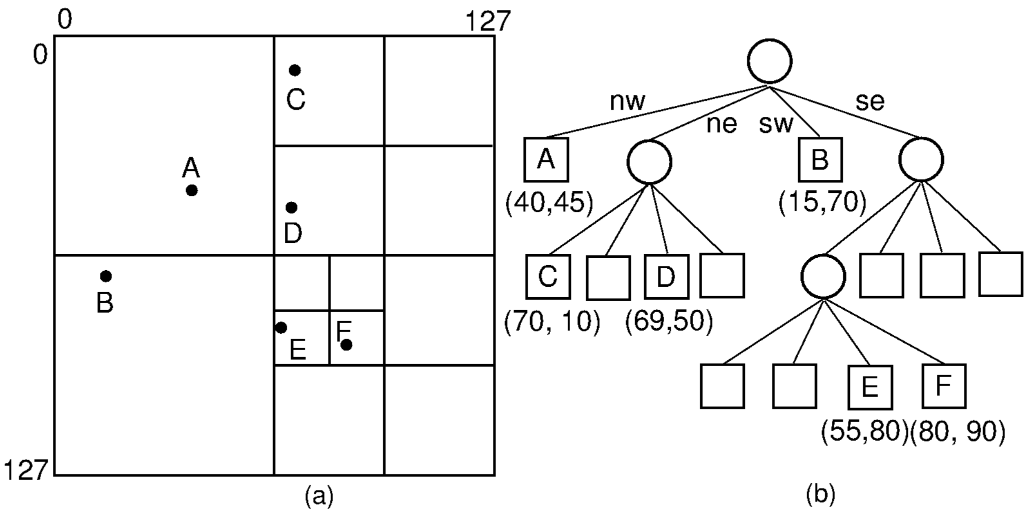

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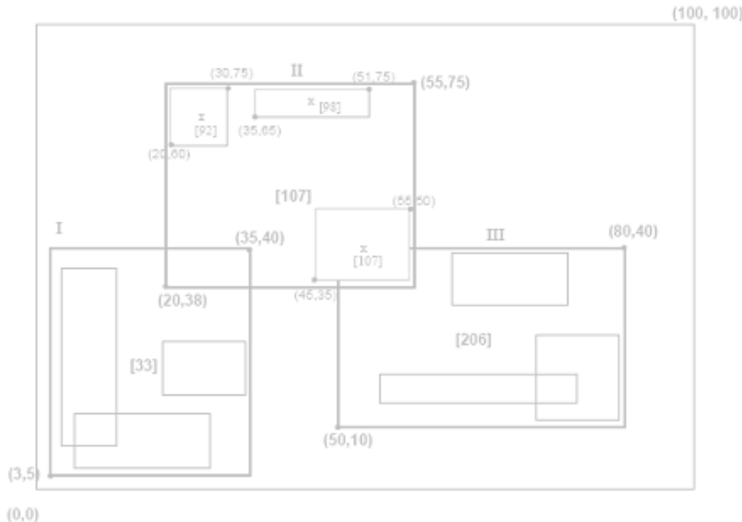

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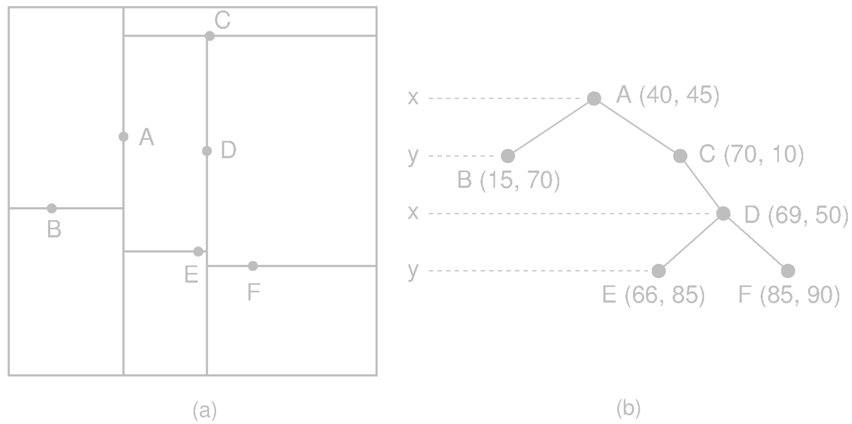
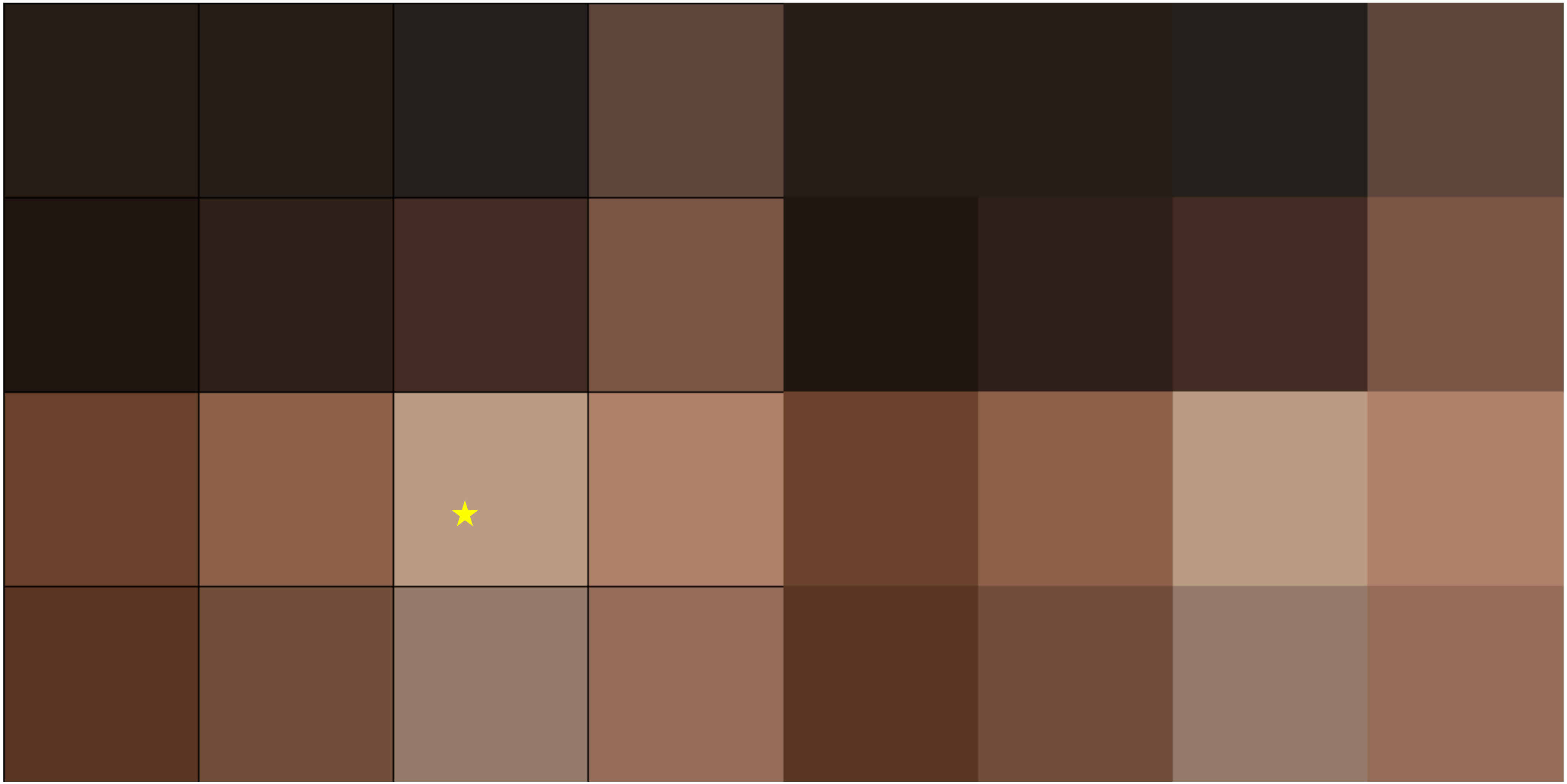


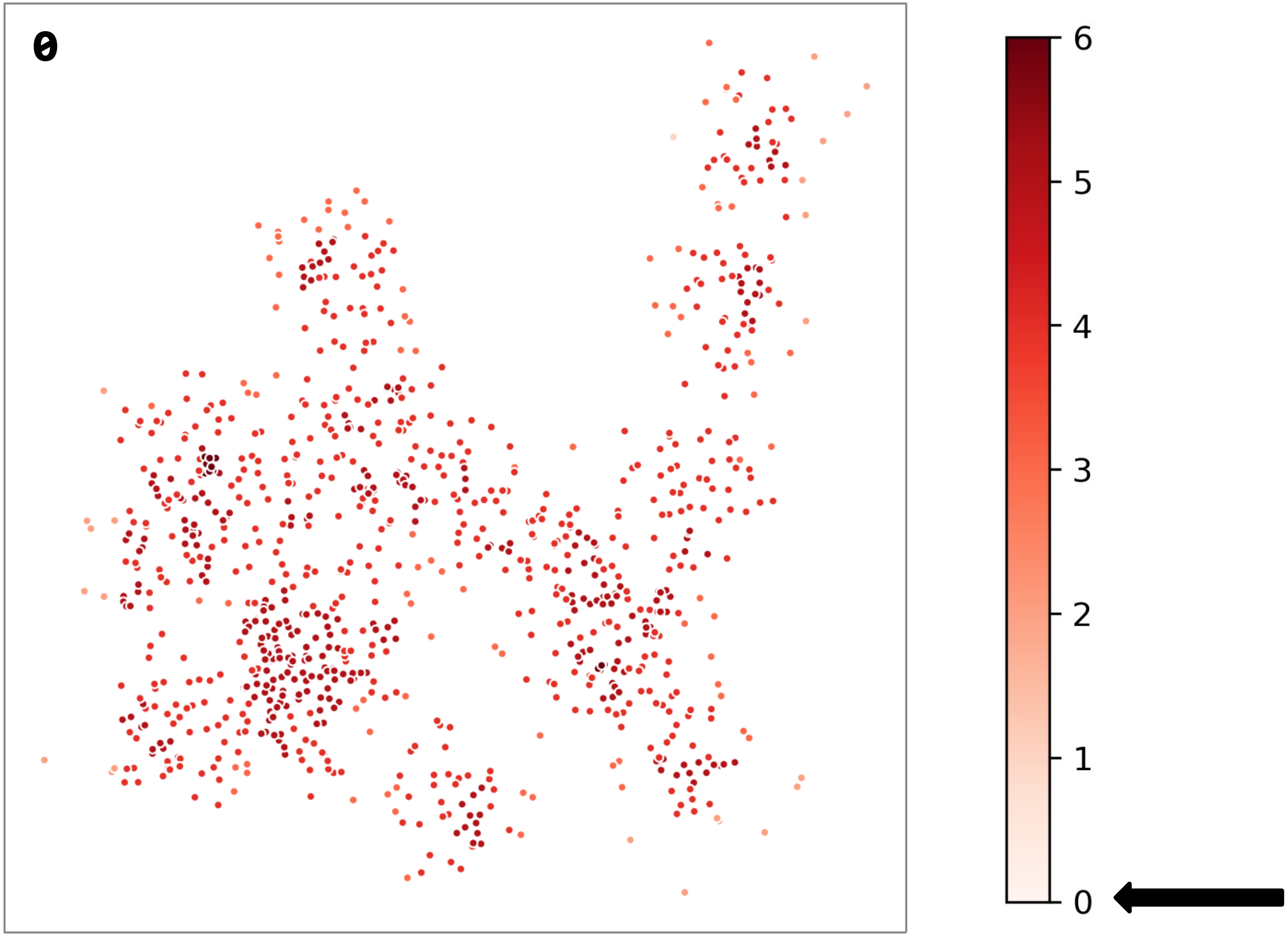
kd-Tree

THE SUPER QUADTREE (SUPERQT)

QUADTREES IN IMAGE COMPRESSION

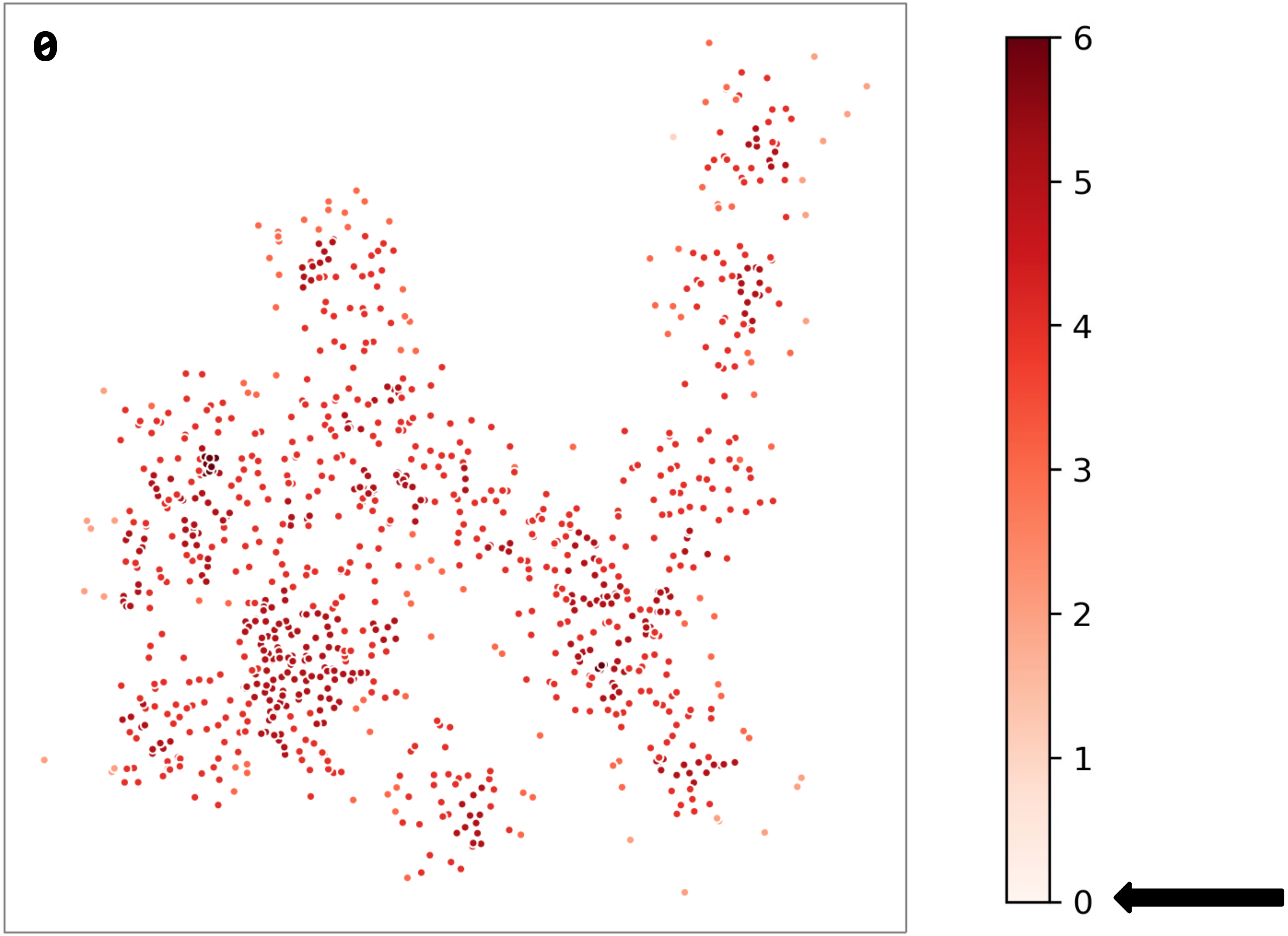


SPEND DETAIL WHERE ITS NEEDED MOST



WALK DOWN THE DEPTH LADDER

c	x_1
1	x_{11}
1	x_{12}
1	x_{13}
1	x_{14}
1	x_{15}
...	...
1	x_{1n}



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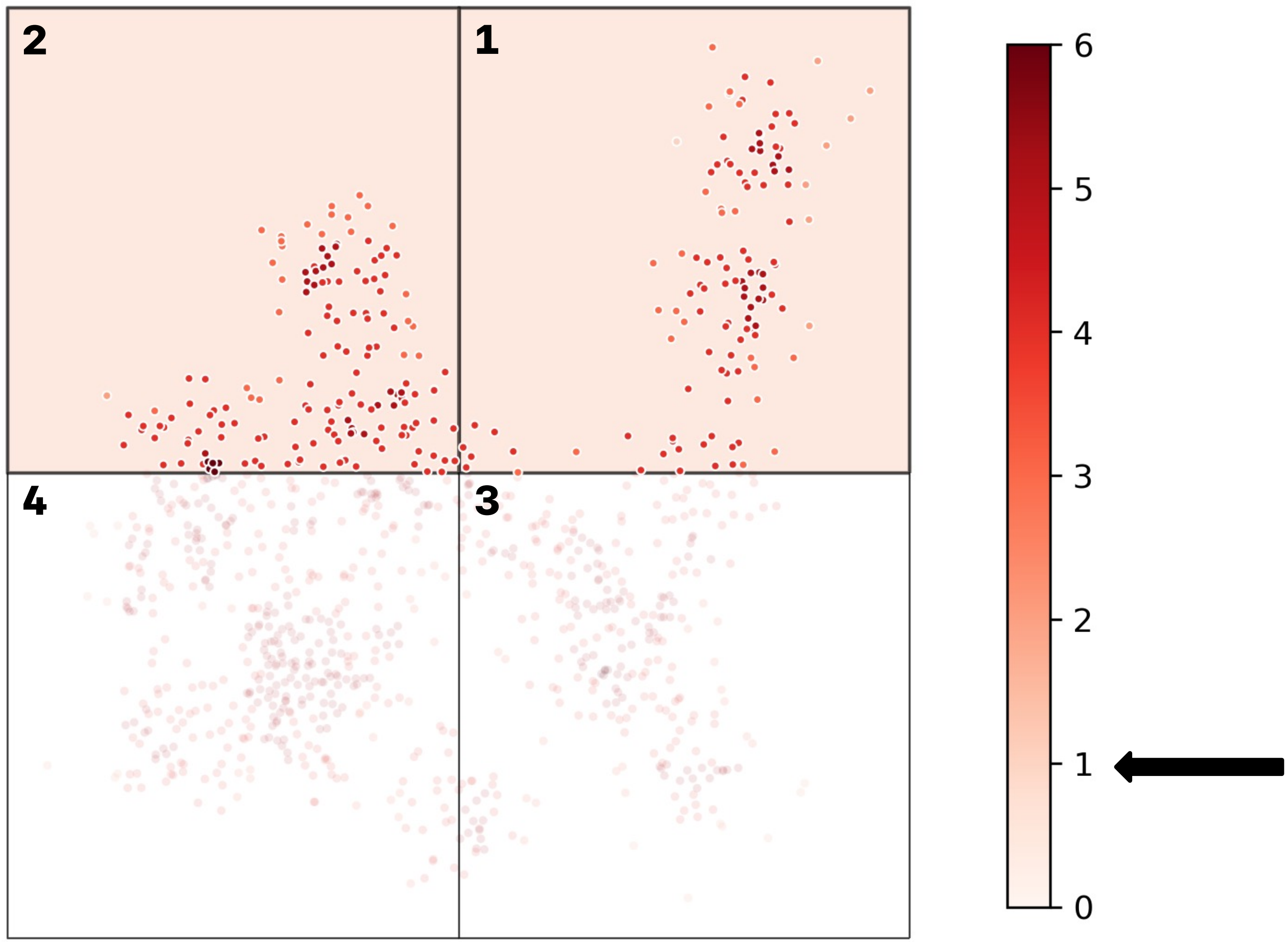
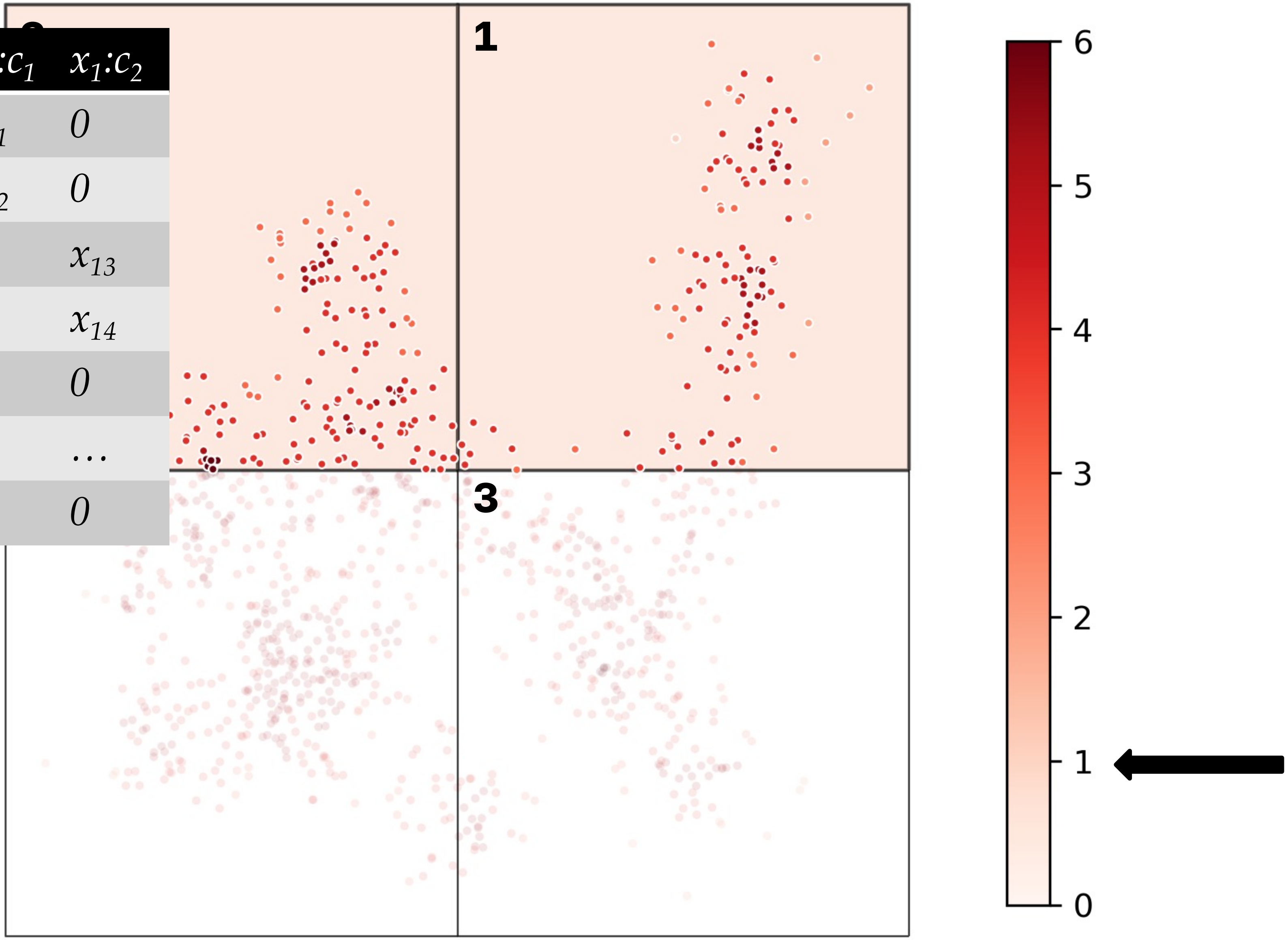


WALK DOWN THE DEPTH LADDER

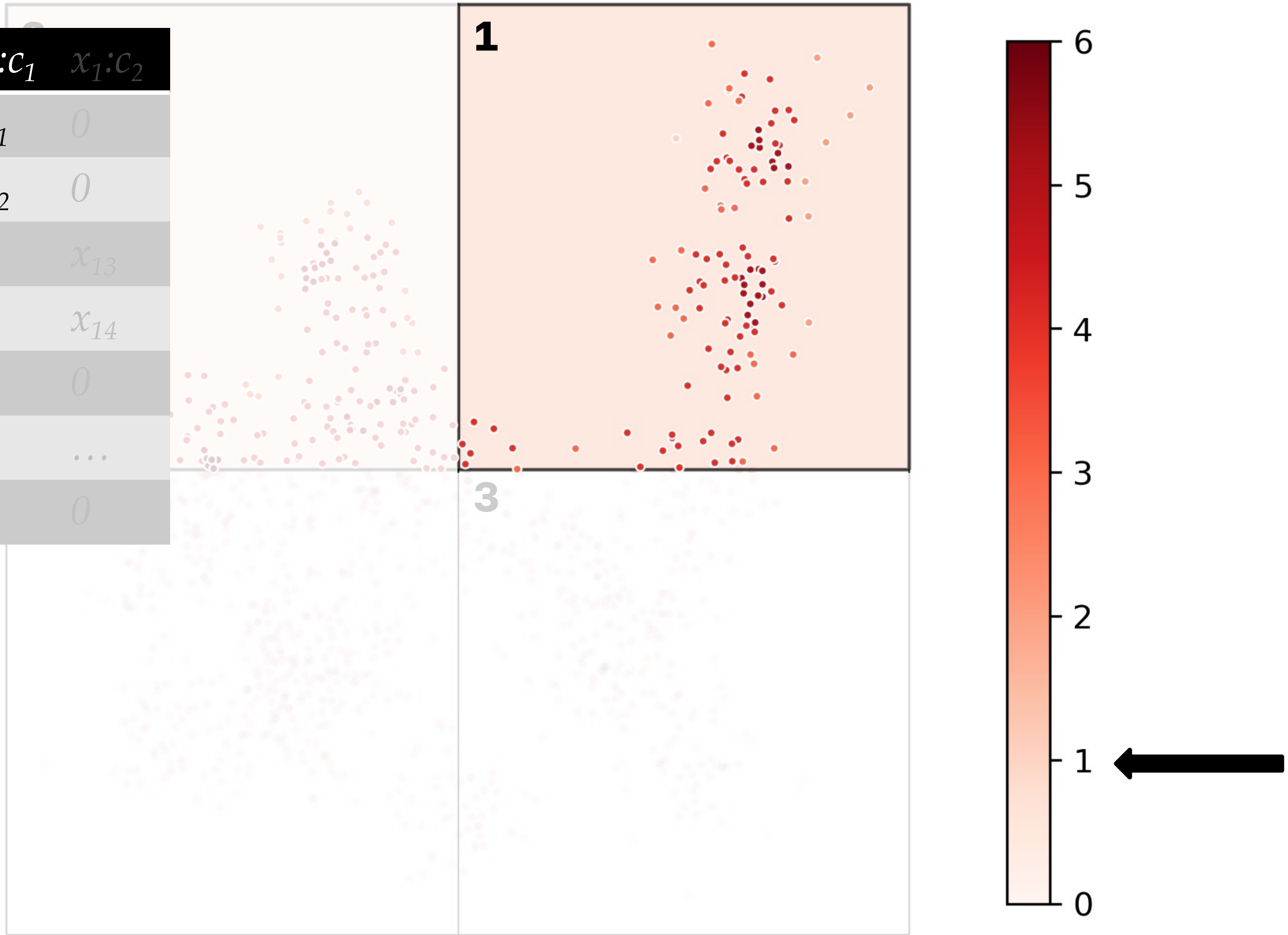
c	c_1	c_2	$x_1{:}c$	$x_1{:}c_1$	$x_1{:}c_2$
0	1	0	0	x_{11}	0
0	1	0	0	x_{12}	0
0	0	1	0	0	x_{13}
0	0	1	0	0	x_{14}
1	0	0	x_{15}	0	0
…	…	…	…	…	…
1	0	0	x_{1n}	0	0



WALK DOWN THE DEPTH LADDER

c	c_1	c_2
0	1	0
0	1	0
0	0	1
0	0	1
1	0	0
…	…	…
1	0	0

$x_1{:}c$	$x_1{:}c_1$	$x_1{:}c_2$
0	x_{11}	0
0	x_{12}	0
0	0	x_{13}
0	0	x_{14}
x_{15}	0	0
…	…	…
x_{1n}	0	0



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c	c_1	c_2
0	1	0
0	1	0
0	0	1
0	0	1
1	0	0
…	…	…
1	0	0

$x_1{:}c$	$x_1{:}c_1$	$x_1{:}c_2$
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0	0	x_{13}
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…	…	…
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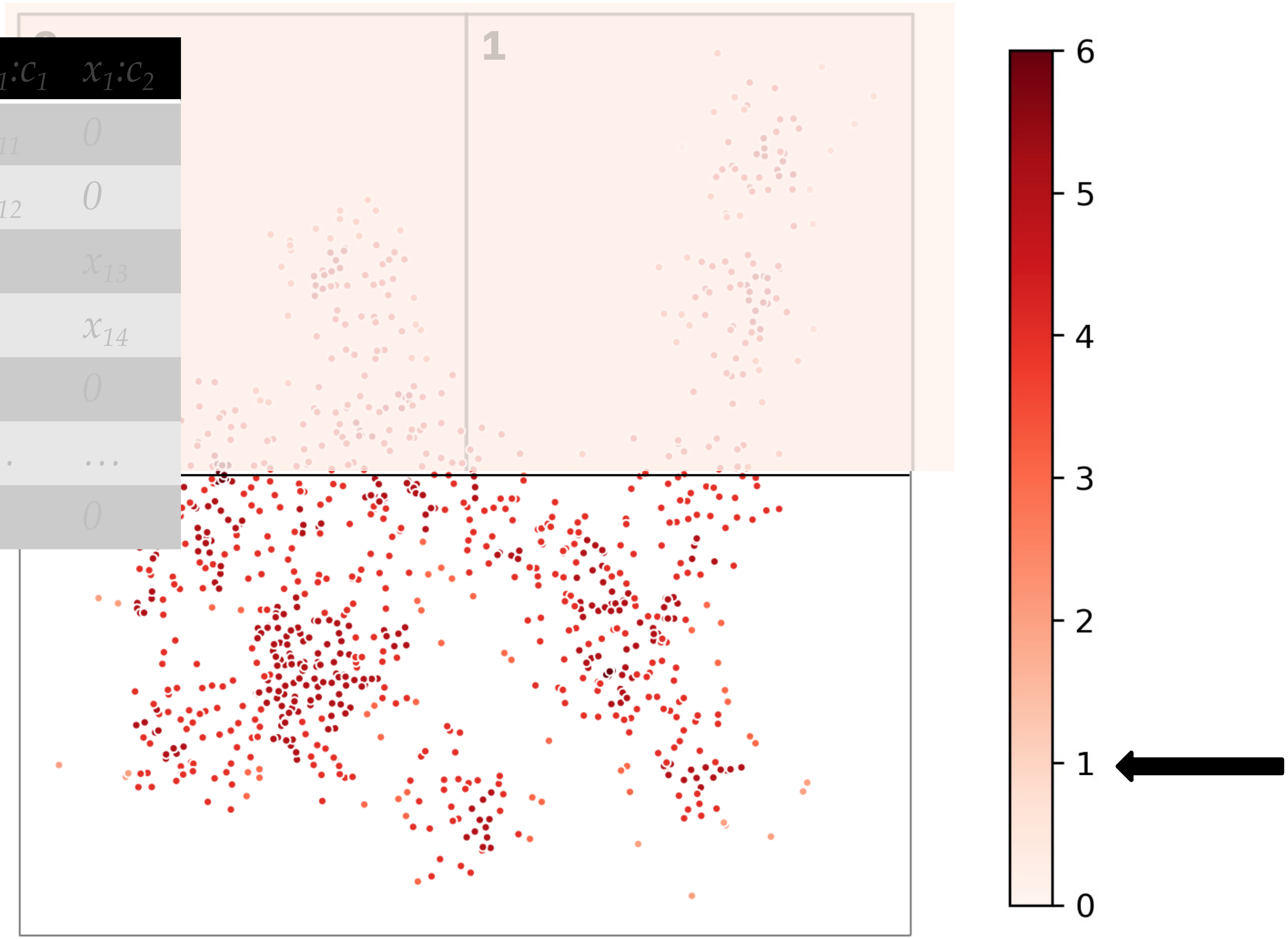

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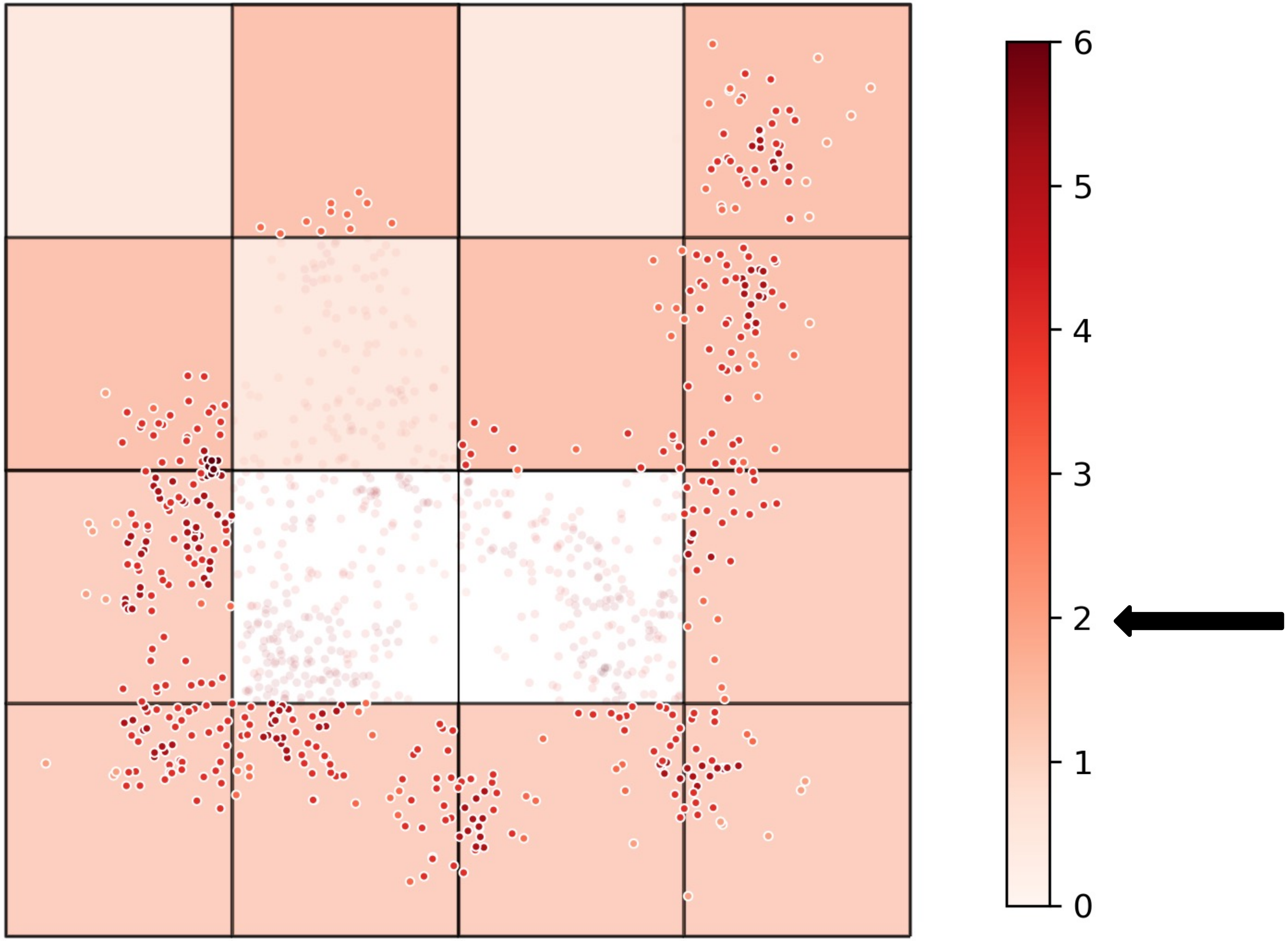

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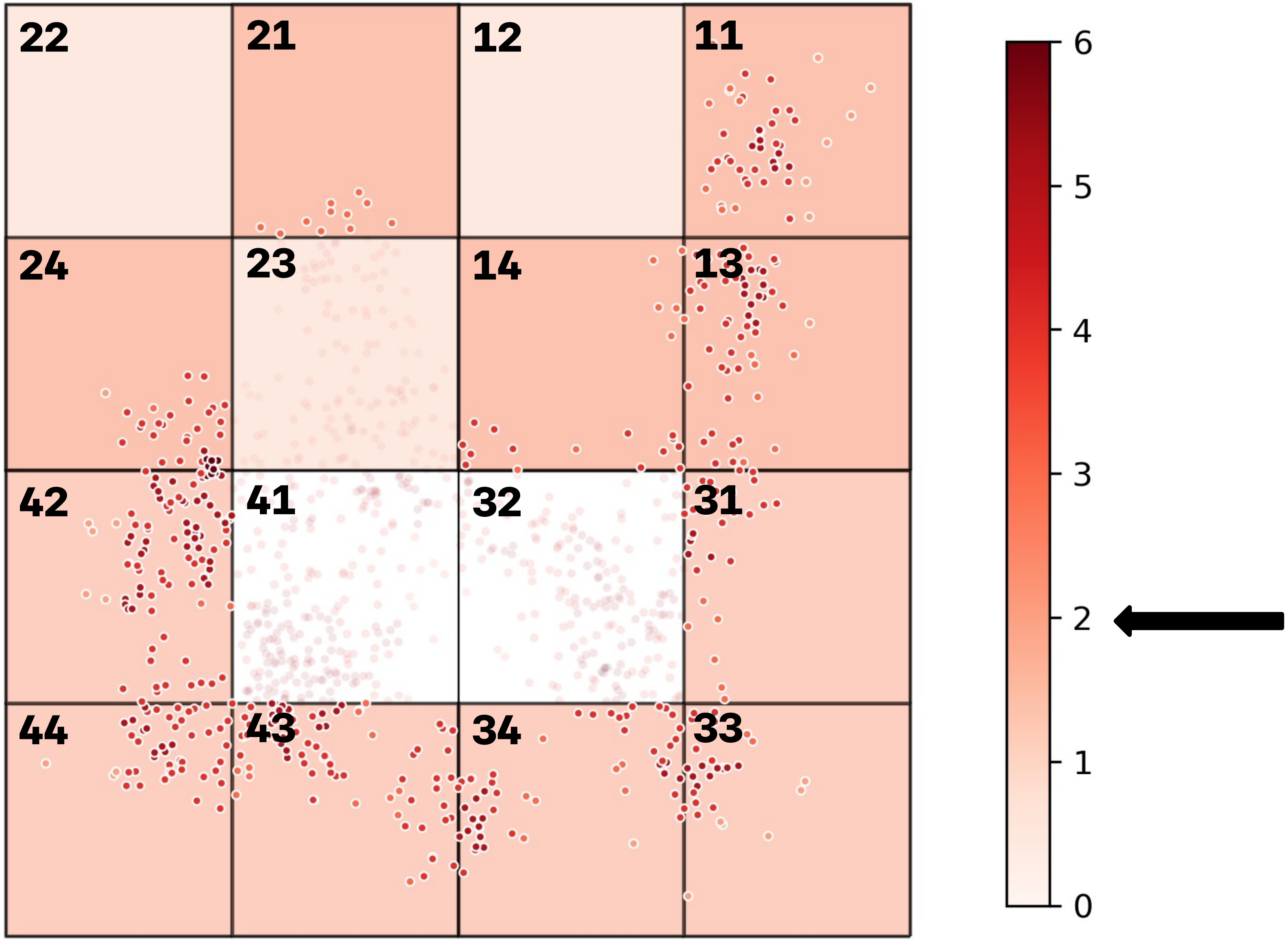

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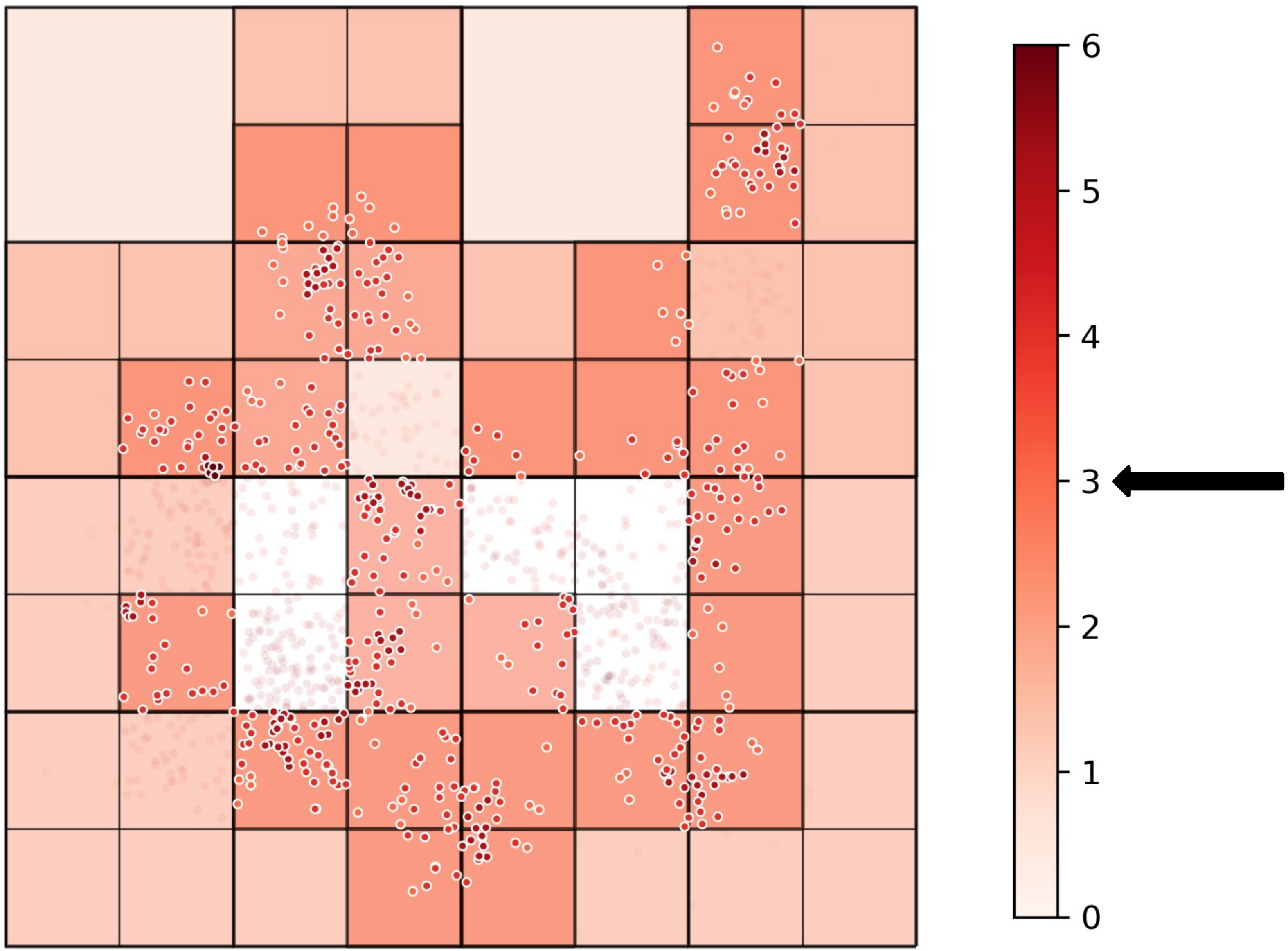

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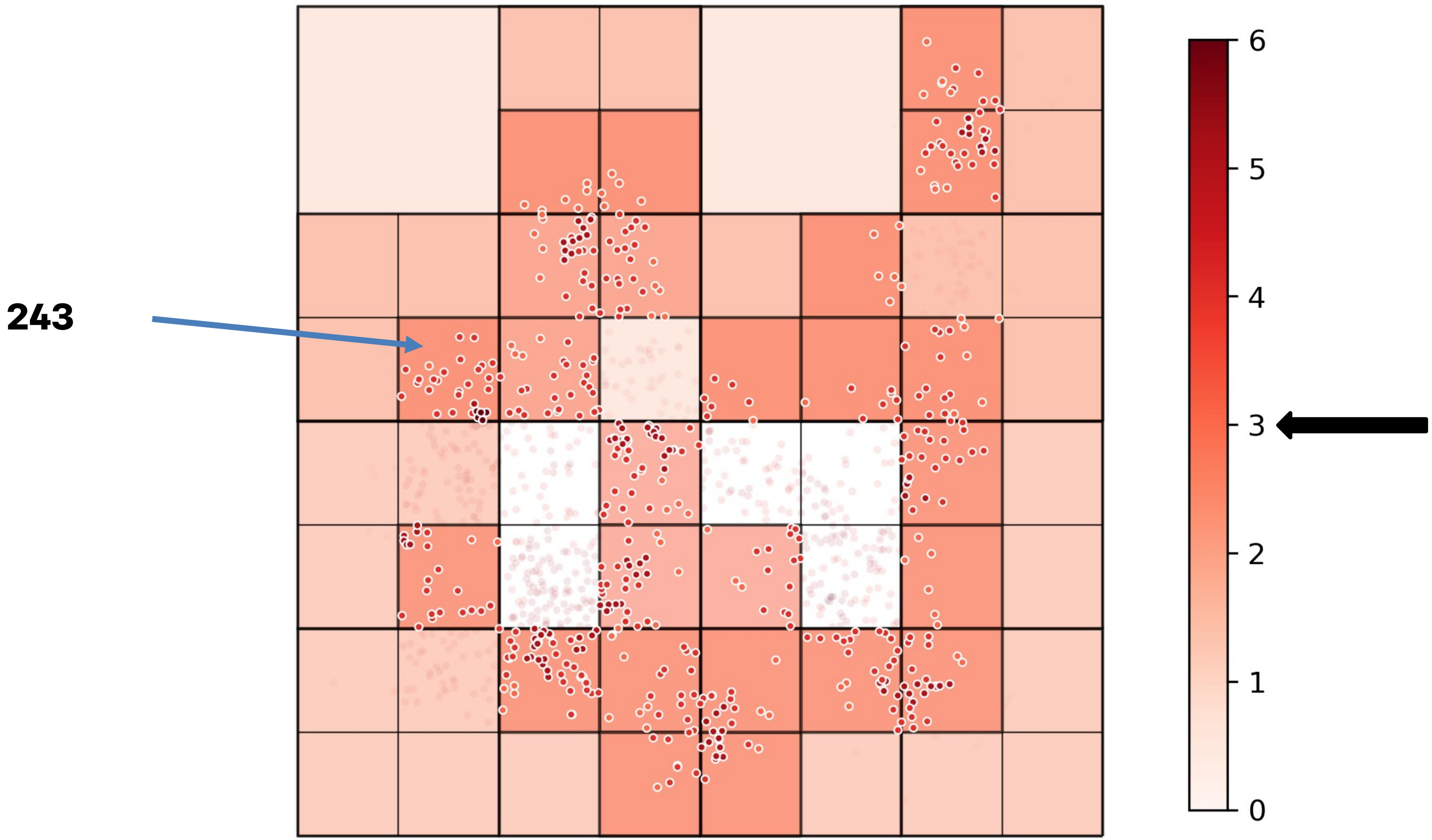
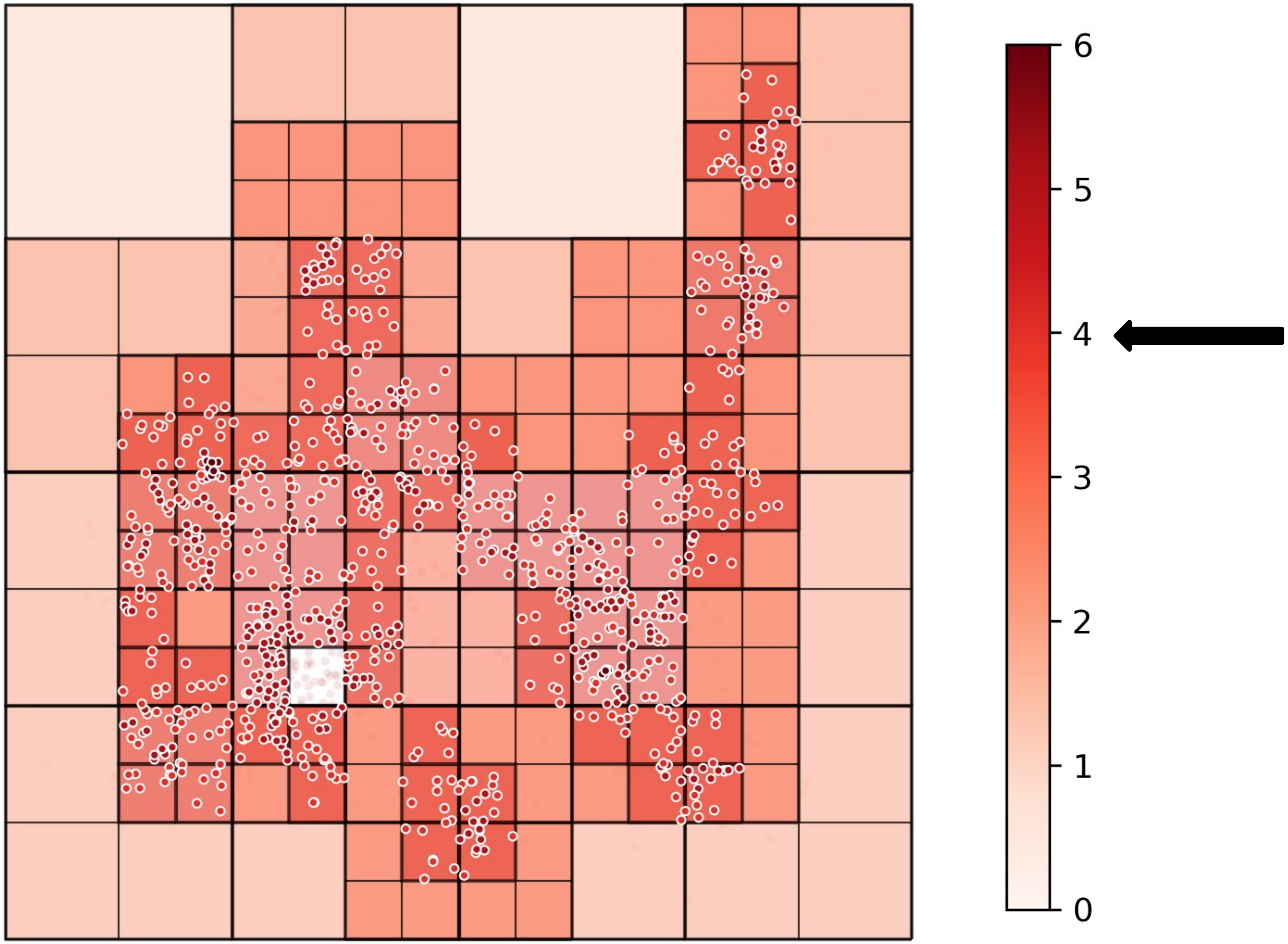
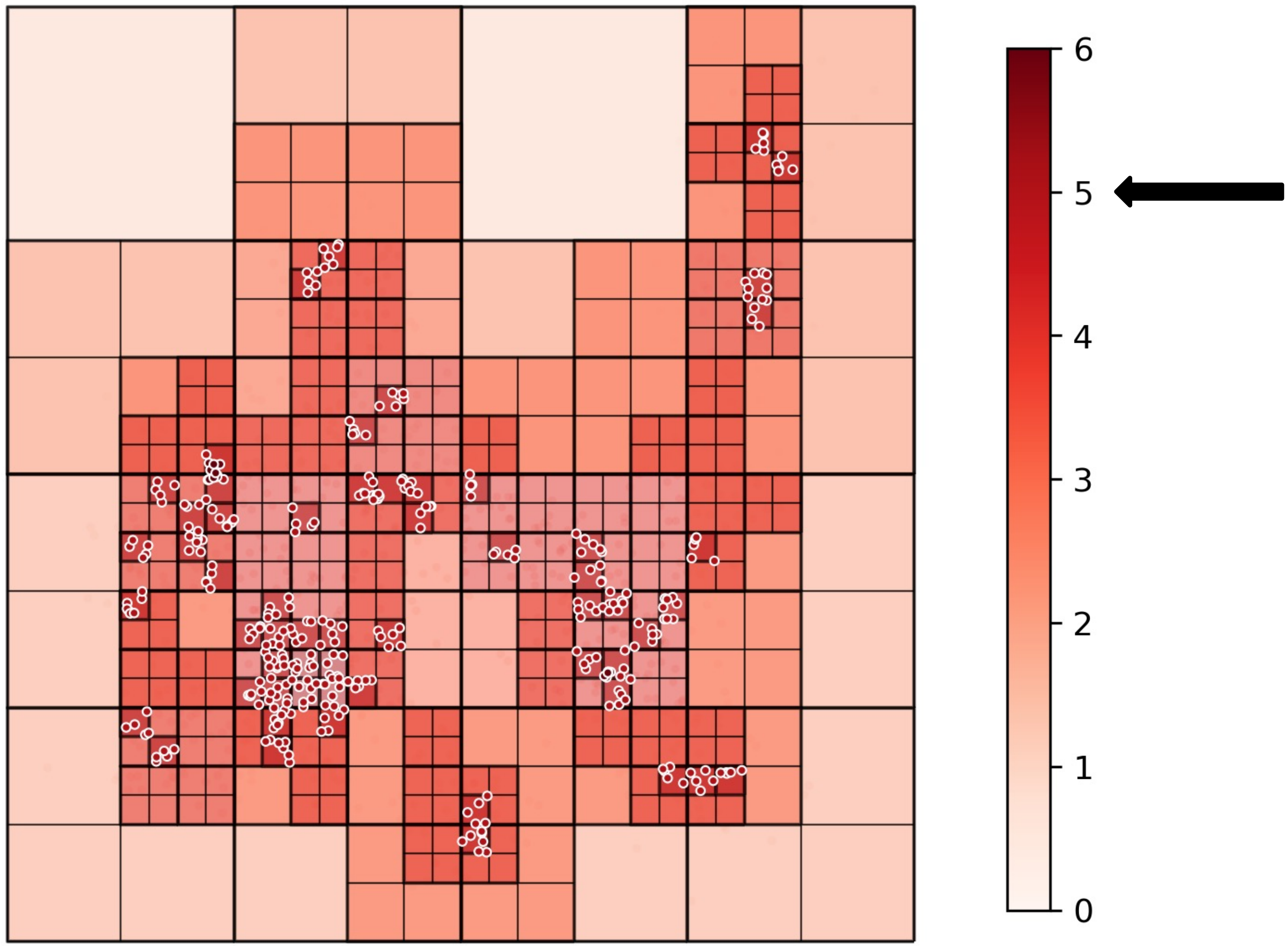


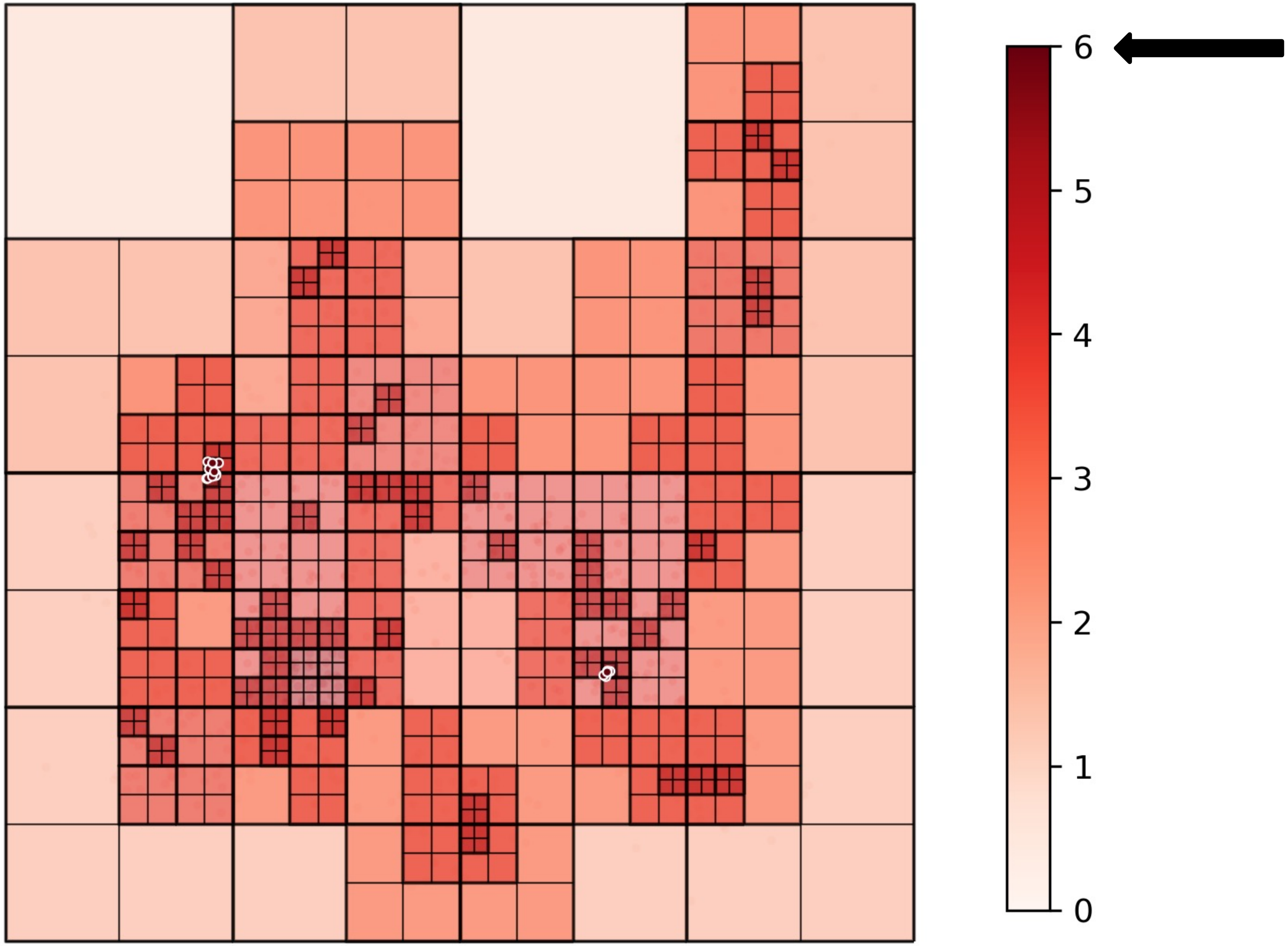
WALK DOWN THE DEPTH LADDER



WALK DOWN THE DEPTH LADDER



WALK DOWN THE DEPTH LADDER



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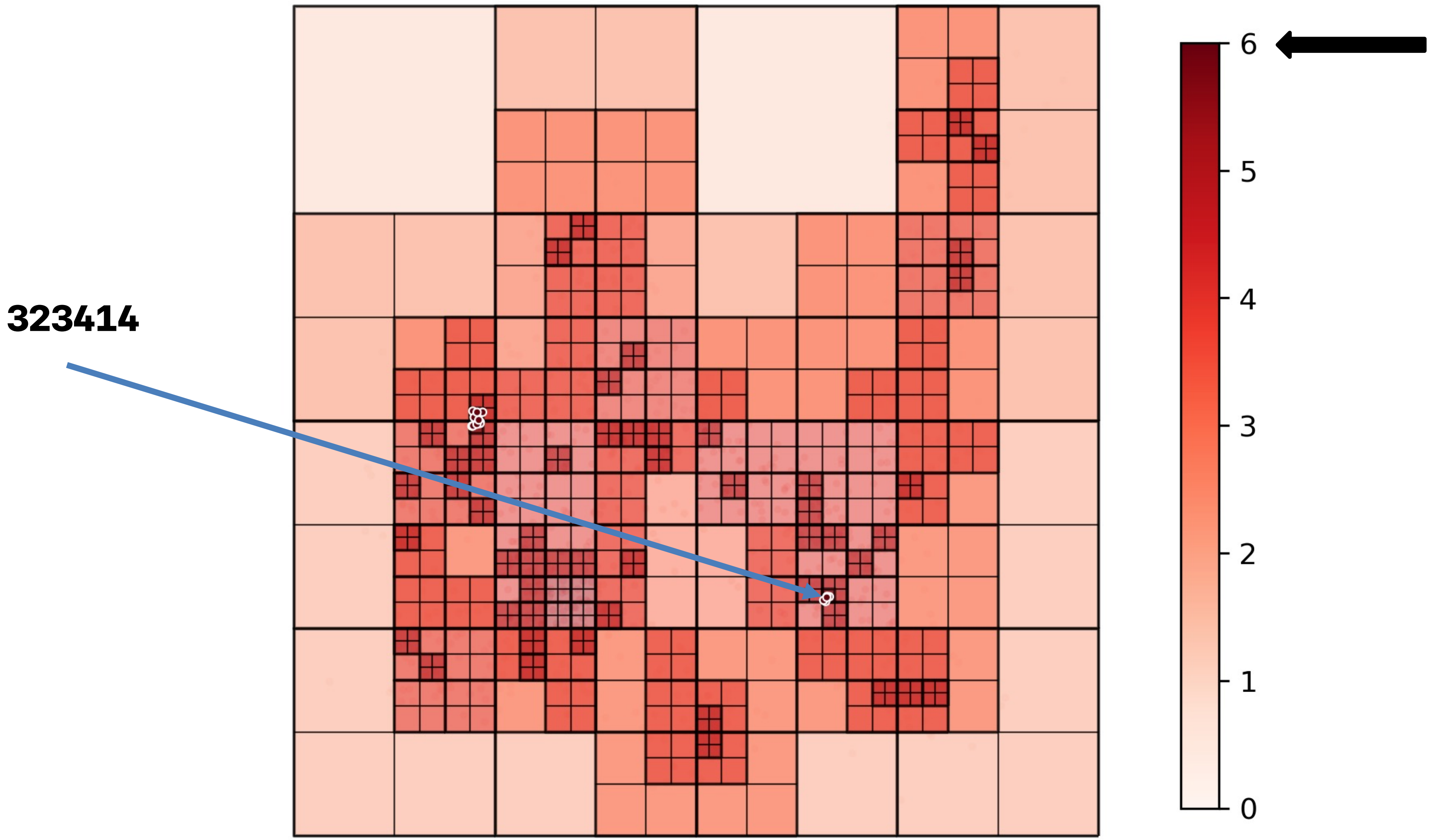

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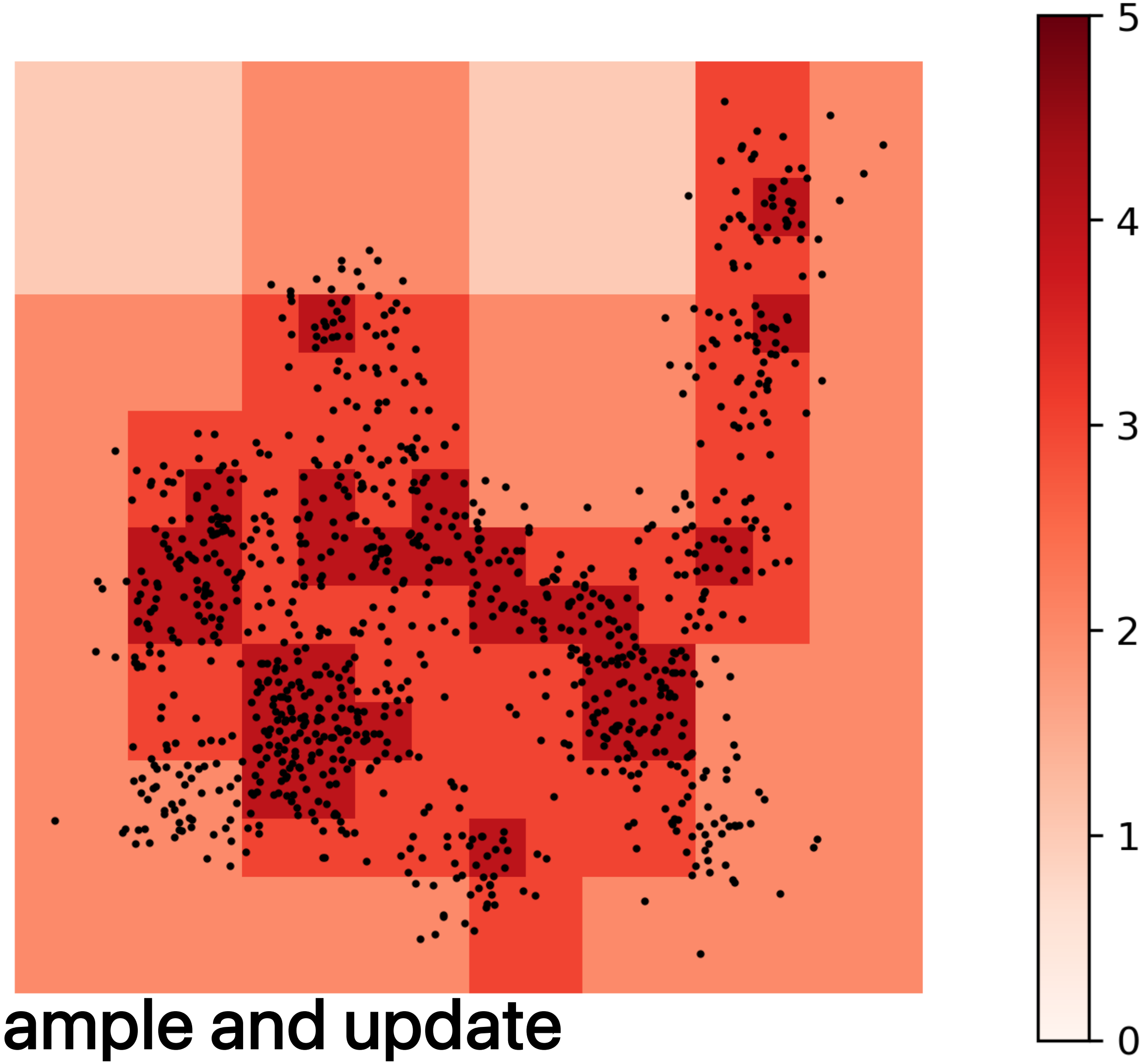
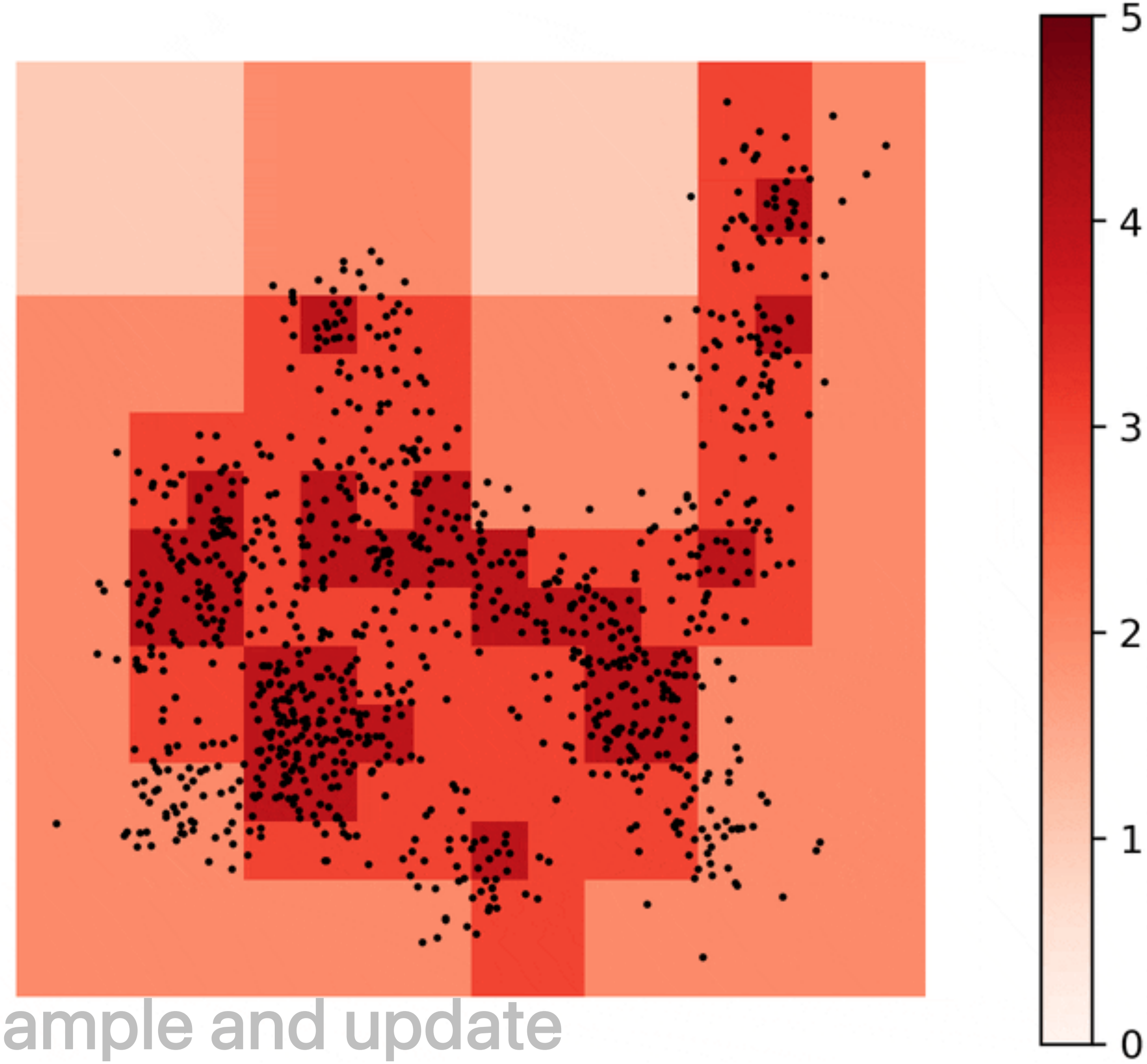


SuperQT

- stable in CV
- totally ordered
- simple out of sample and update

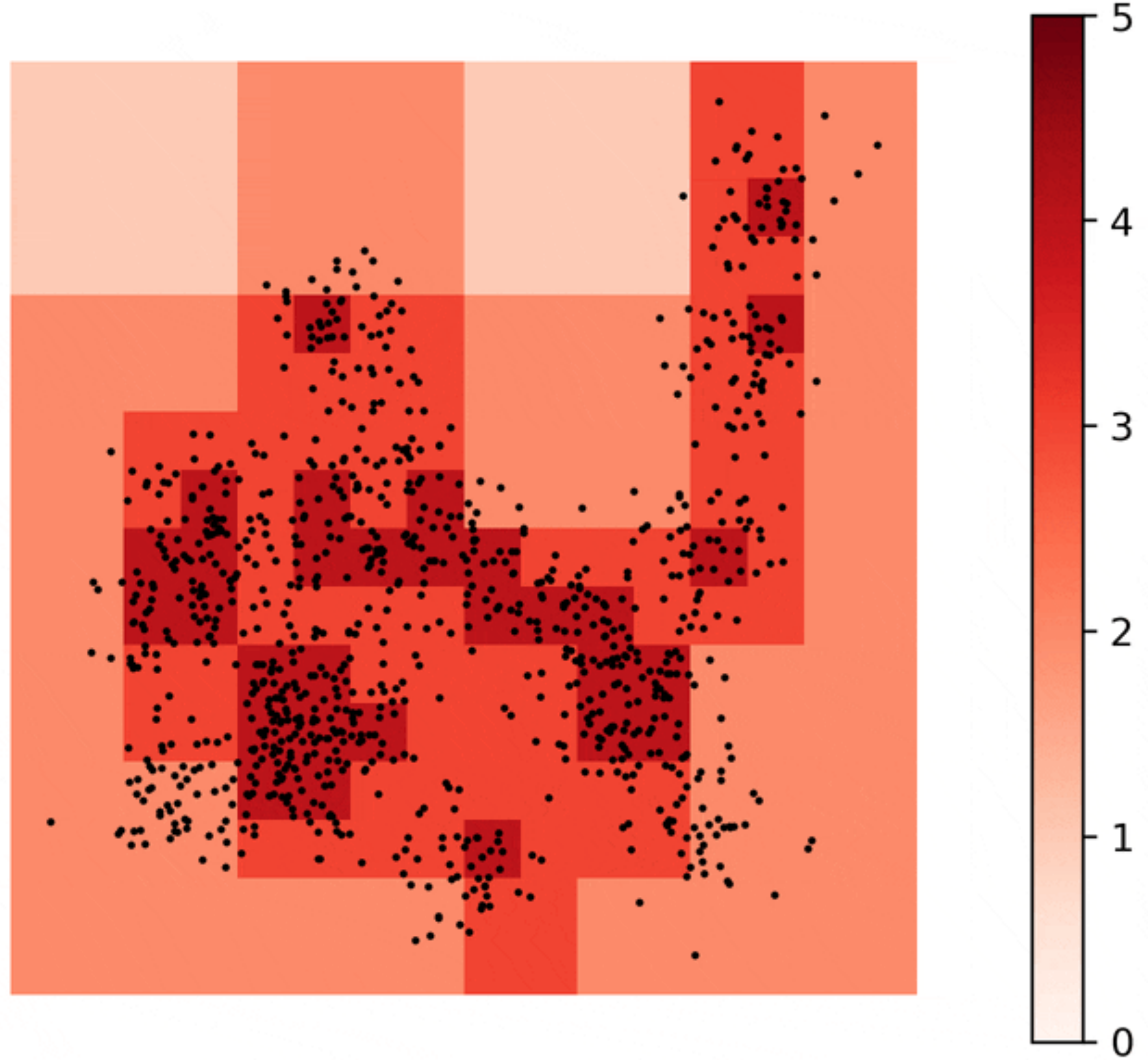
QUADTREES ARE FAIRLY STABLE IN CV



SuperQT
- stable in CV
- totally ordered
- simple out of sample and update

QUADTREES ARE FAIRLY STABLE IN CV

TOTALLY ORDERED
An observation will nest exactly into one cell at any given depth; depth is a function of both fit and density, and big jumps in depth are rare.



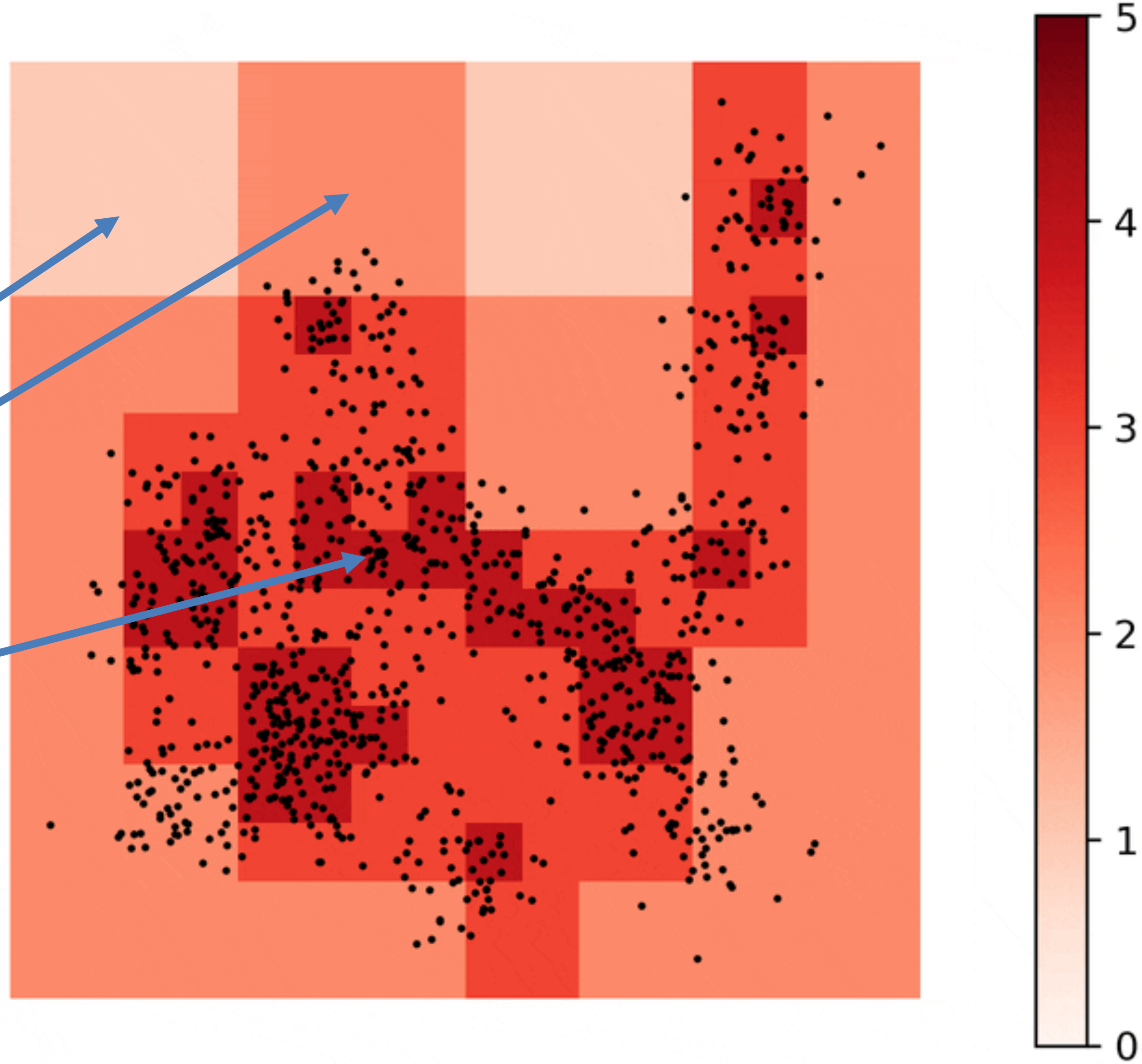
QUADTREES ARE FAIRLY STABLE IN CV

OUT-OF-BAG
For interpolating predictions *within* frame, we always have a model

Always **2**

2 or **21**

4112
or
411

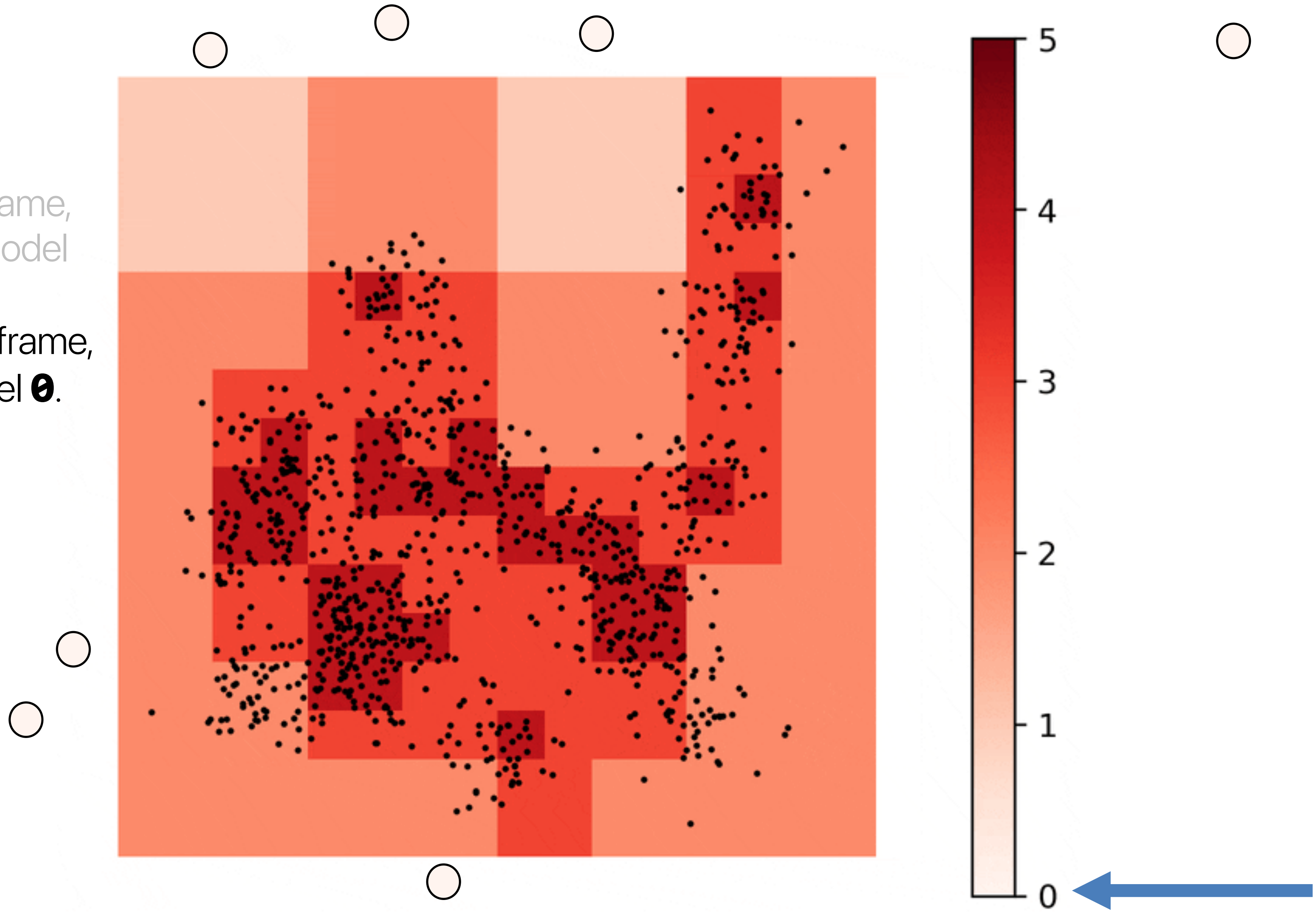


QUADTREES ARE FAIRLY STABLE IN CV

OUT-OF-BAG

For interpolating predictions *within* frame, we always have a model

For *extrapolating* predictions outside frame, we always use model **0**.



QUADTREES ARE FAIRLY STABLE IN CV

OUT-OF-BAG

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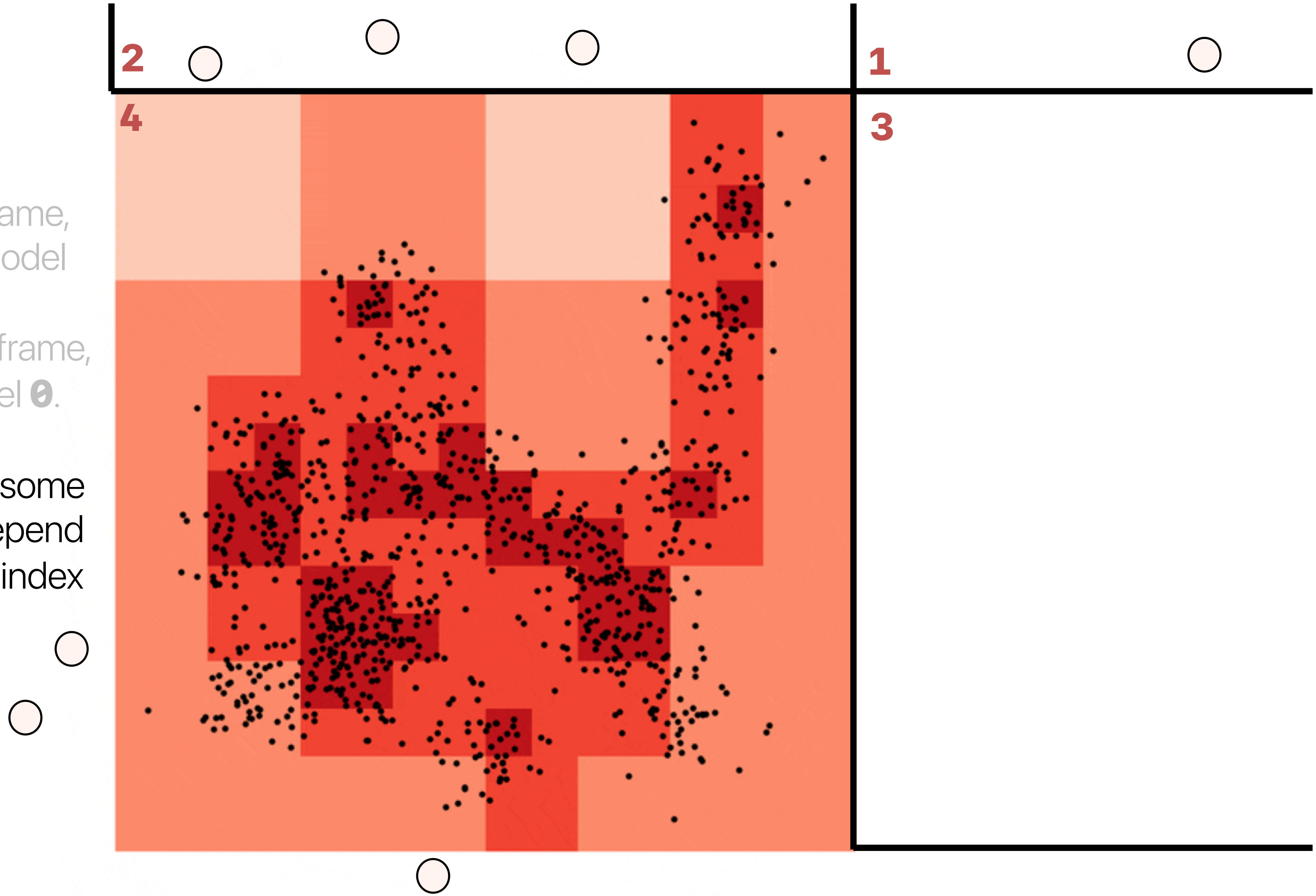
For *extrapolating* predictions outside frame, we always use model **0**.

UPDATING

Treat 0 as a child of some larger frame and prepend all cells with its new index



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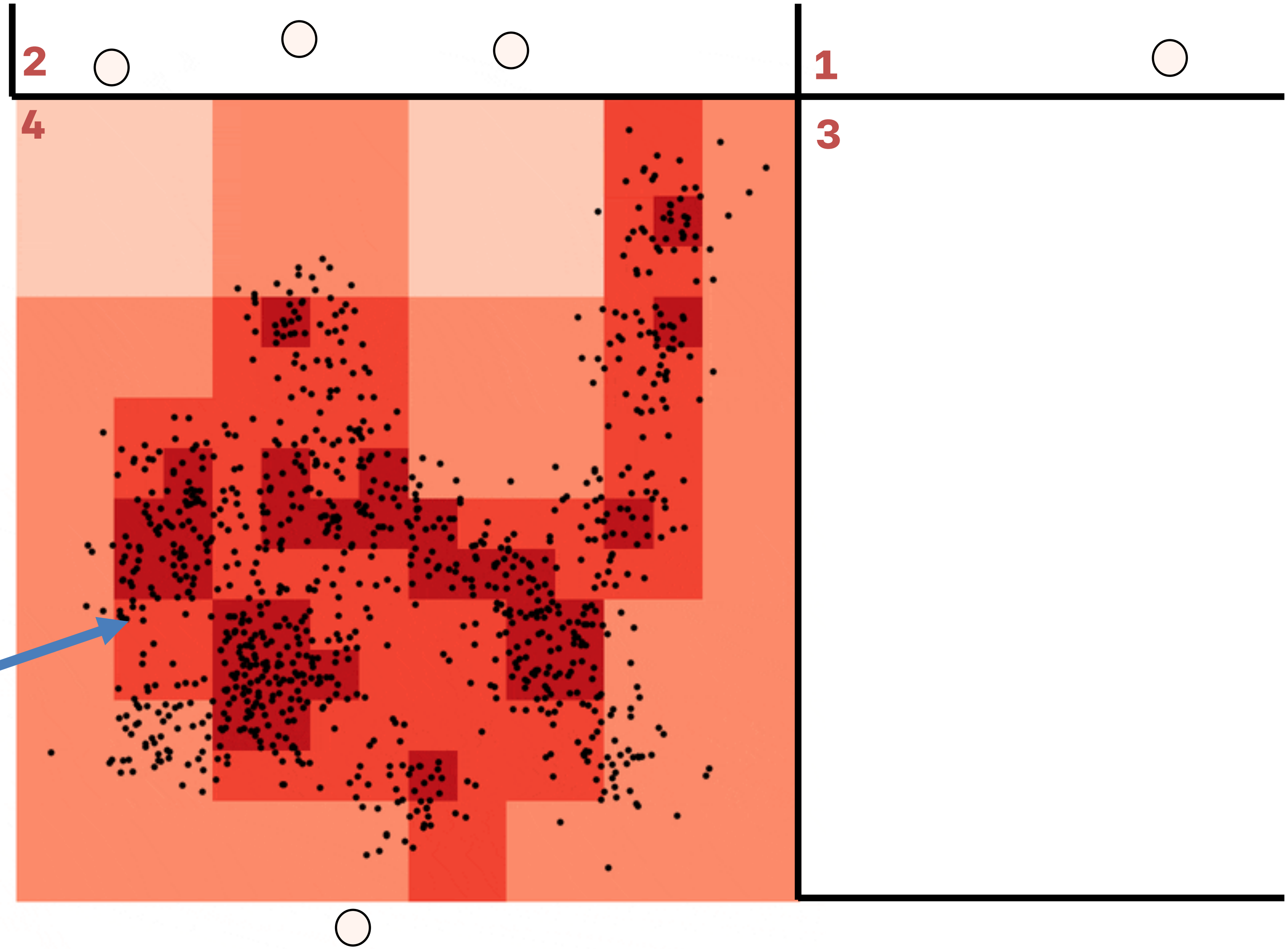

424

updates to

4424

QUADTREES ARE FAIRLY STABLE IN CV

0. INITIALIZE: add root node to queue with label 0 and global model predicting $y \sim X$

1. SPLIT: pop the first node from our queue and split. For each child in that split:

1-1. fit a submodel predicting only child's outcomes using child's data.

1-2. update predictions for the whole map.

1-3. if child model is significantly more skillful than parent **within child (out of sample)**, label samples with child label, return child to queue, & go to 1; otherwise assign all samples to parent's label & drop child.

2. PRUNE: fit a model with all current feature:label interactions (one hot).

2-1. if all terms are helpful, go to 3, otherwise find the depth (d^*) of the least helpful feature:label term

2-2. for each unhelpful term at d^*, merge the feature:child_label term into feature:parent_label, and return to 2.

3. FINALIZE: Fit a final model on final retained feature:label interaction terms

THE SUPERVISED QUADTREE

0. INITIALIZE: add root node to queue with label 0 and global model predicting $y \sim X$
1. SPLIT: pop the first node from our queue and split. For each child in that split:
1-1. fit a submodel predicting only child's outcomes using child's data.
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3. FINALIZE: Fit a final model on final retained feature:label interaction terms

Note that this is *model agnostic*: can use any learner, classification or regression.
- GLMs can split using LRT (χ^2) prune using Wald (t) tests, placing a natural limit on n_{child}
- Always can split using score improvement ($\Delta MSE > \varepsilon$) prune using permutation feature importance ($X_p * I(leaf)$ in best q% of unpruned features)

THE SUPERVISED QUADTREE

0. INITIALIZE: add root node to queue with label 0 and global model predicting $y \sim X$

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2-2. for each unhelpful term at d^*, merge the feature:child_label term into feature:parent_label, and return to 2.

3. FINALIZE: Fit a final model on final retained feature:label interaction terms

Note that this is ***tree agnostic***: can use any spatial tree index

- Pruning is most useful with hierarchical trees, where parent is still "local"
- Overlap (e.g. in RTree) introduces intersection terms (feature:label1:label2).
- Balance is optional, but helpful for submodel efficiency

THE SUPER*TREE

CLUSTERING REGRESSION

jointly solving clustering and regression

GEOGRAPHICAL CLUSTER-REG

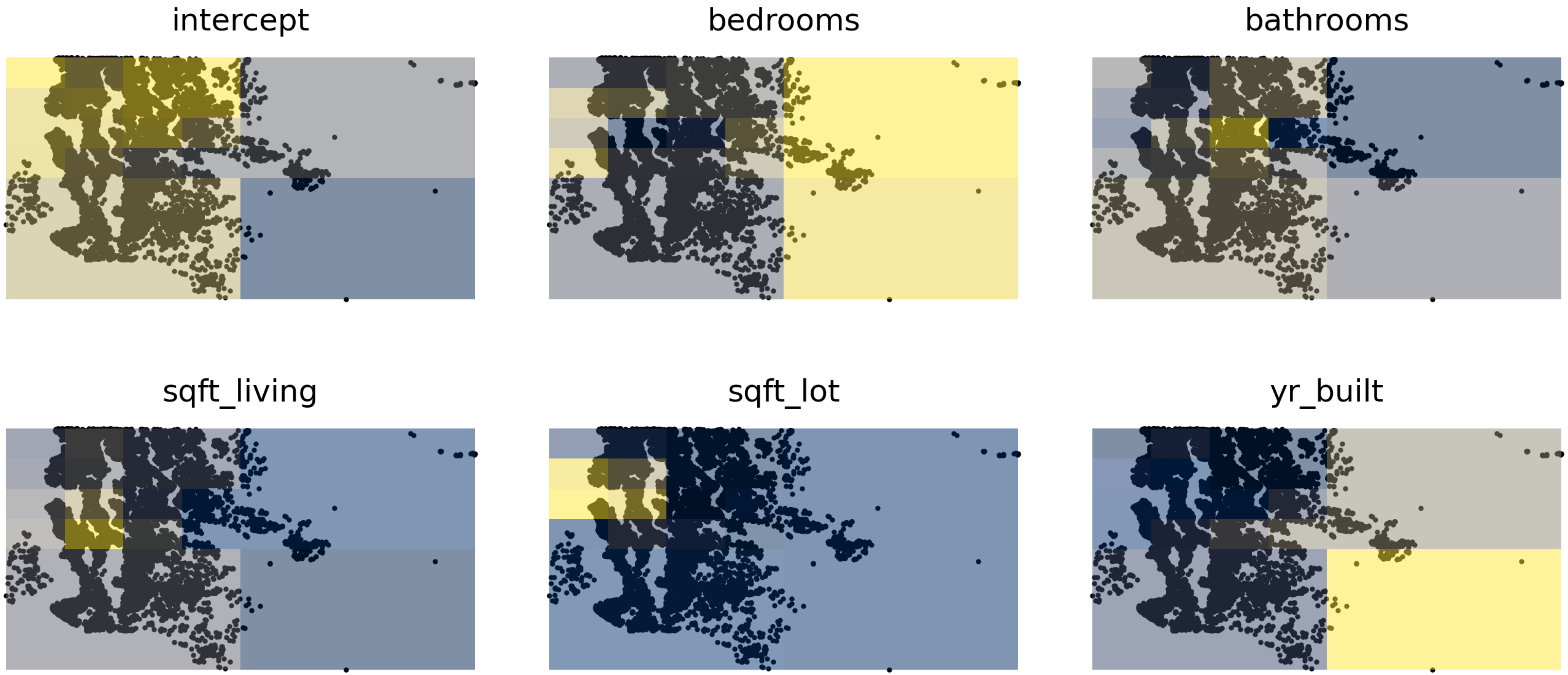
jointly solving clustering and regression

UNDERSTANDING QUADTREES

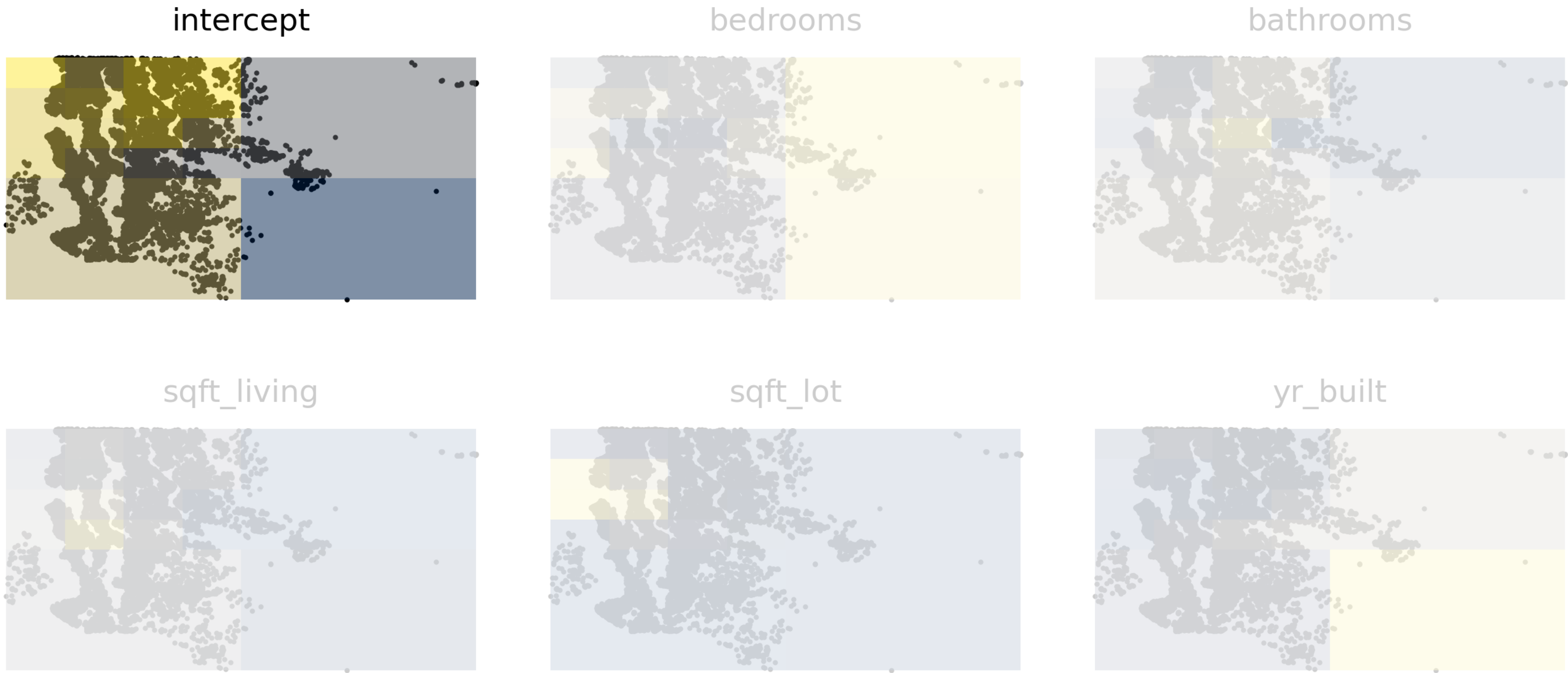
spatial splits for spatial fits

APPLYING QUADTREE REGRESSION

model comparison & basic metrics

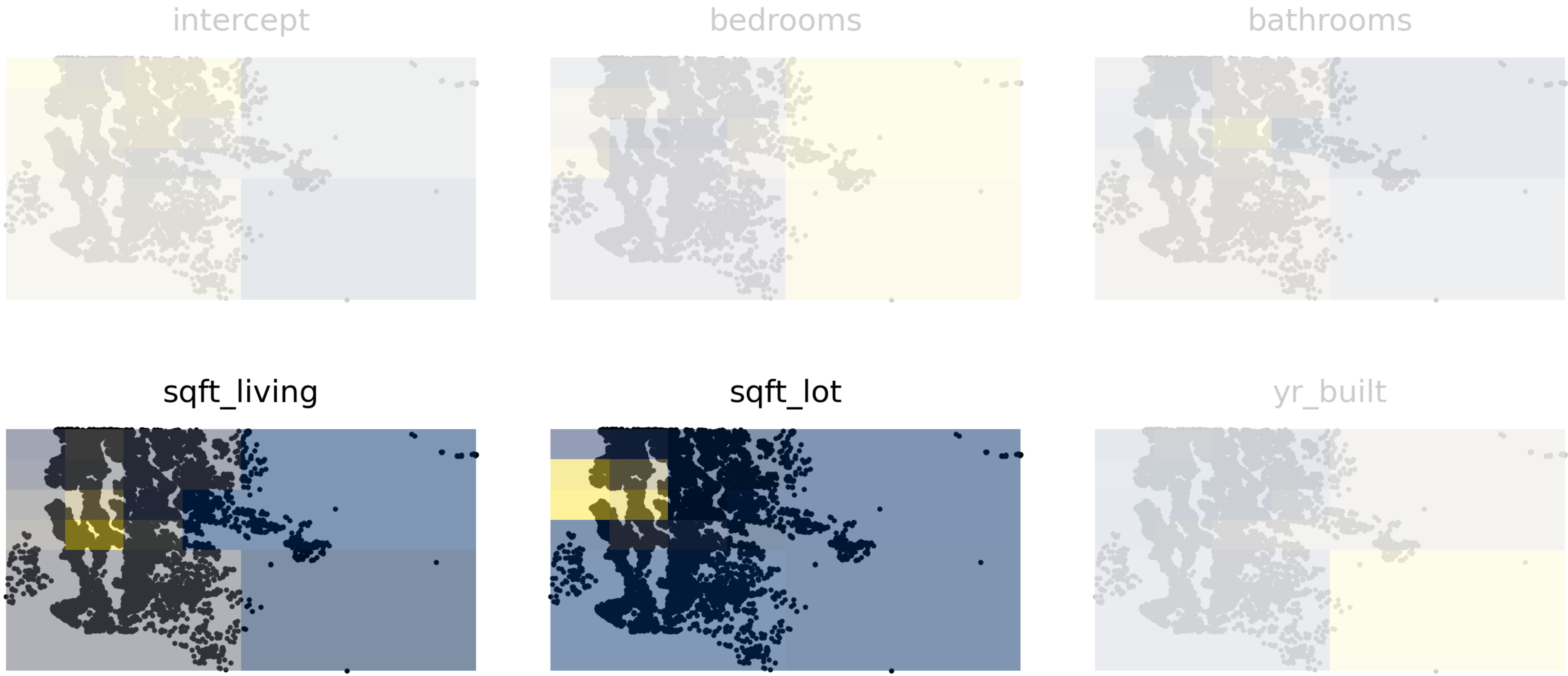


COEFFICIENT SURFACES LOOK LIKE THIS



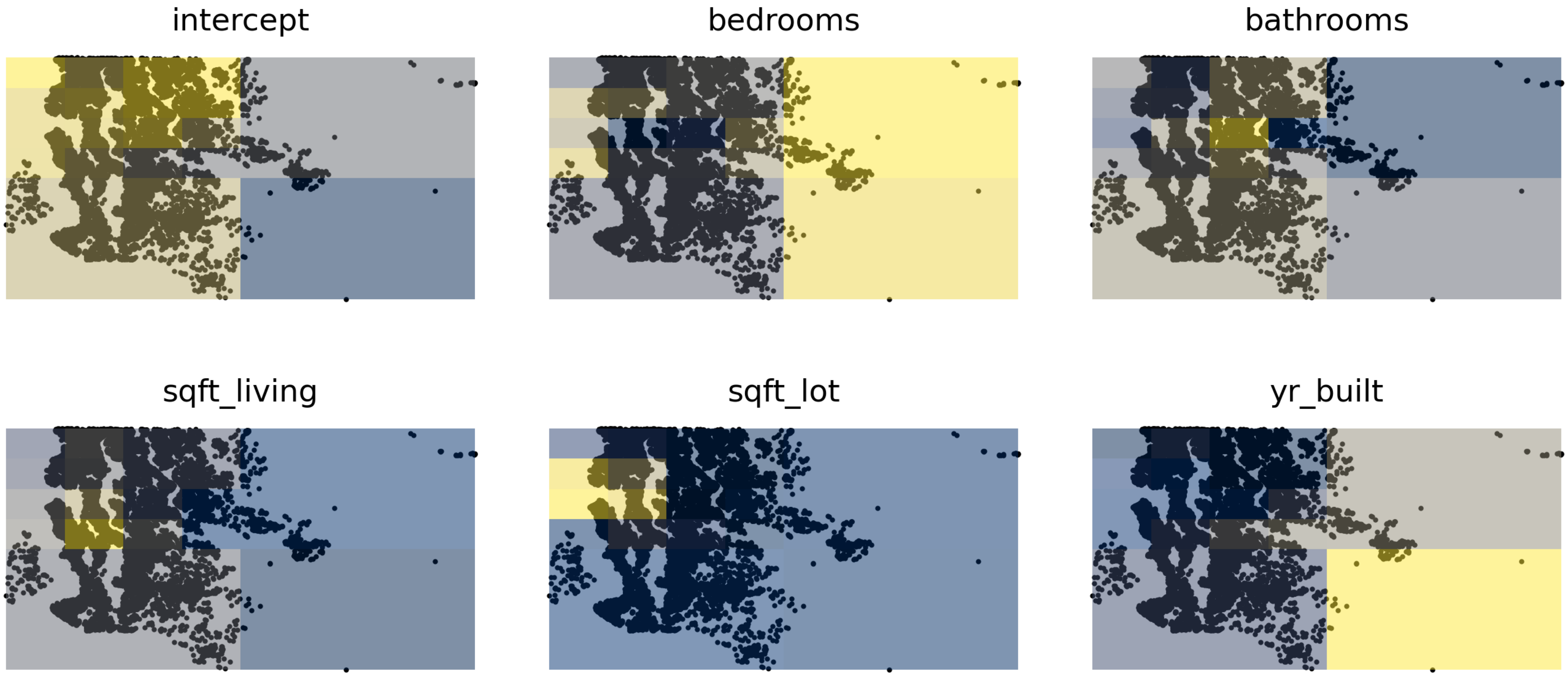
Prices in general are expensive towards the coast, also in the techy areas in the northwest.

COEFFICIENT SURFACES LOOK LIKE THIS



Space is at a premium, with living space slightly more expensive south-center.

COEFFICIENT SURFACES LOOK LIKE THIS



COEFFICIENT SURFACES LOOK LIKE THIS

PLACE	METHOD	MSE	R^2	TIME
Baltimore	OLS	.16	.49	Sub-seconds
n=211	Skater 15 Regimes	.02	.93	Seconds
	MGWR	.01	.95	Seconds
	SuperQT (no prune)	.04 (.02)	.89 (.94)	Seconds
King's Co.	OLS	.13	.53	Seconds
n=31k	Skater 15 Regimes	.05	.811	Hours
	MGWR	DNF	DNF	DNF
	SuperQT (no prune)	.06 (.06)	.78 (.78)	Minutes

COMPARISONS

PLACE	METHOD	MSE	R^2	TIME
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n=211	Skater 15 Regimes	.02	.93	Seconds
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n=31k	Skater 15 Regimes	.05	.811	Hours
	MGWR	DNF	DNF	DNF
	SuperQT (no prune)	.06 (.06)	.78 (.78)	Minutes

Small n: usually need eps+perm (lrt+wald dof issues)

Big n: both lrt+wald and eps+perm are useful

COMPARISONS

PLACE	METHOD	MSE	R^2	TIME
Baltimore	OLS	.16	.49	Sub-seconds
n=211	Skater 15 Regimes	.02	.93	Seconds
	MGWR	.01	.95	Seconds
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COMPETITIVE EVEN AFTER PRUNING

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	MGWR	DNF	DNF	DNF
	SuperQT (no prune)	.06 (.06)	.78 (.78)	Minutes

Pruning is especially powerful in big data:

~90 feature x leaf interactions in Skater & SuperQT

~60 post pruning w/ very small change to fit (for both)

COMPETITIVE EVEN AFTER PRUNING

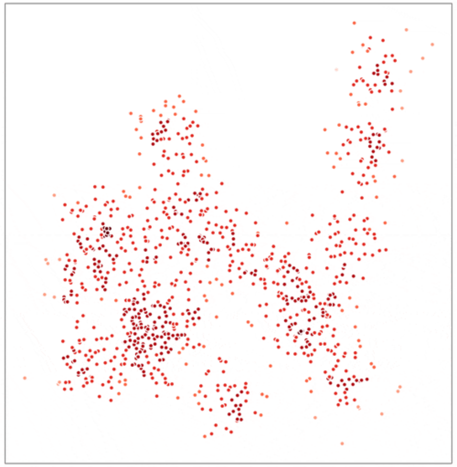
MIT-Licensed

High performance w/ `scipy.sparse`

Available in PySAL by December 2025

SUPER*TREE LEARNERS:

a new metalearner for local data science



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