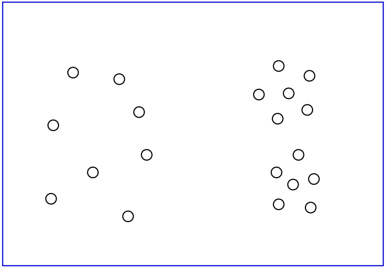
Cluster trees, neighborhood graphs, and continuum percolation

Sanjoy Dasgupta

University of California, San Diego

Part I: Cluster trees

Clustering in $\mathbb{R}^d$



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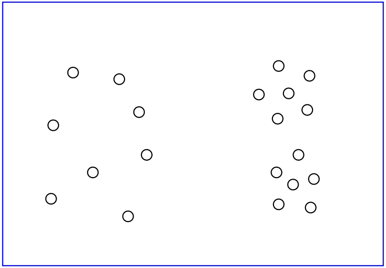

Two common uses of clustering:

- Vector quantization
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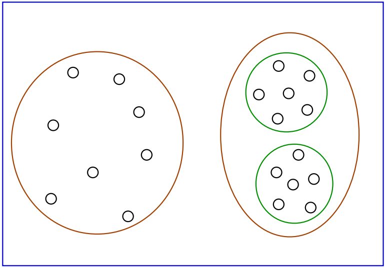

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A hierarchical clustering algorithm

Joseph Kruskal, 1928-2010

The single linkage algorithm:

- Start with each point in its own, singleton, cluster
- Repeat until there is just one cluster:
  - Merge the two clusters with the closest pair of points
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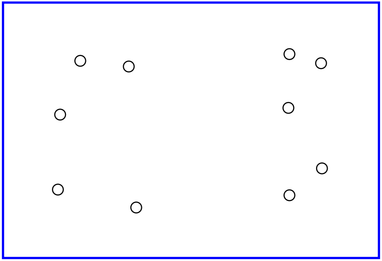

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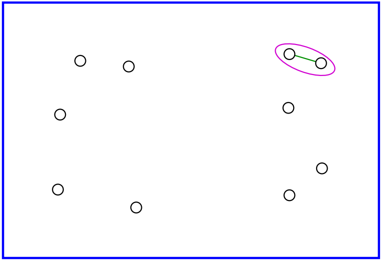

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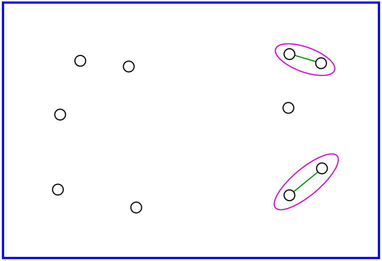

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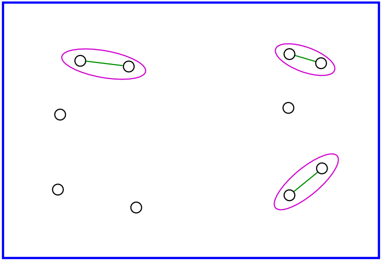

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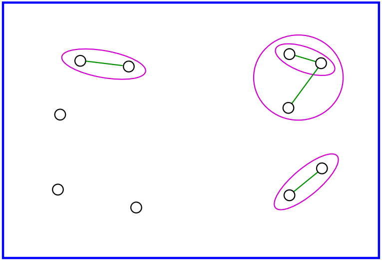

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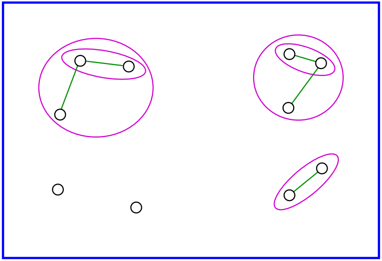

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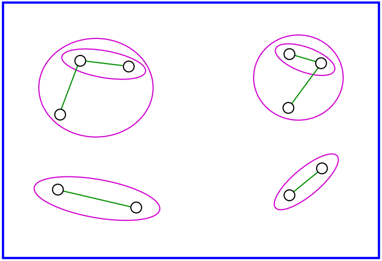

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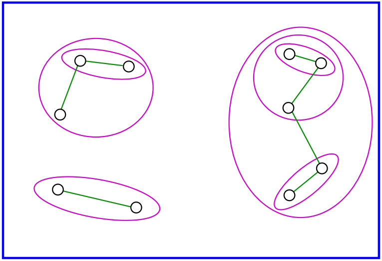

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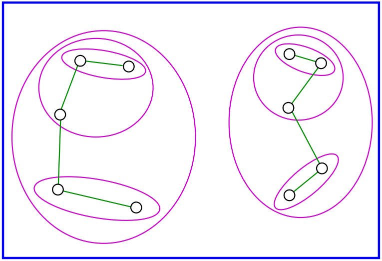

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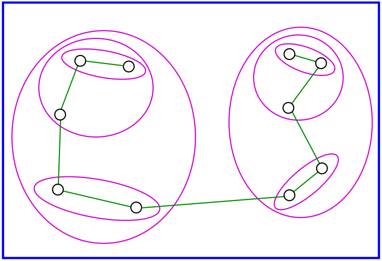

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Statistical theory in clustering

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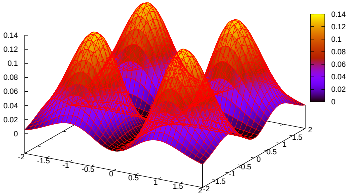

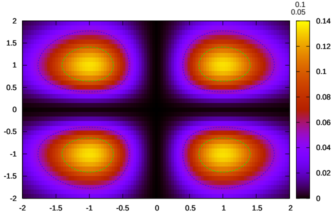

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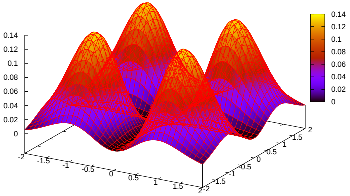
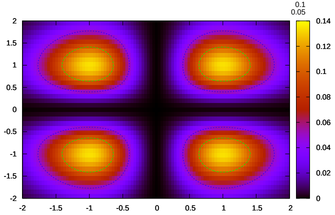
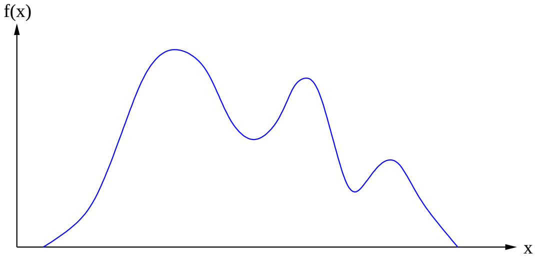




cluster $\equiv$ connected component of $\{x : f(x) \geq \lambda\}$, any $\lambda > 0$

These clusters form an infinite hierarchy, the *cluster tree*.

Converging to the cluster tree



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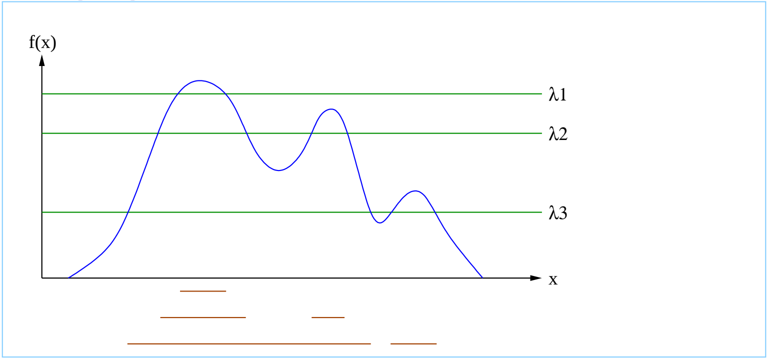

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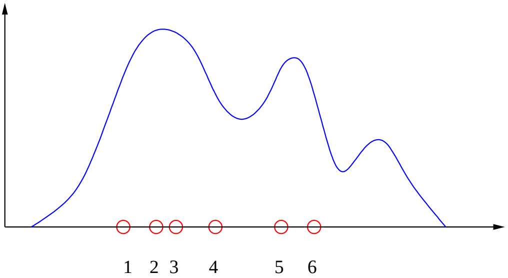

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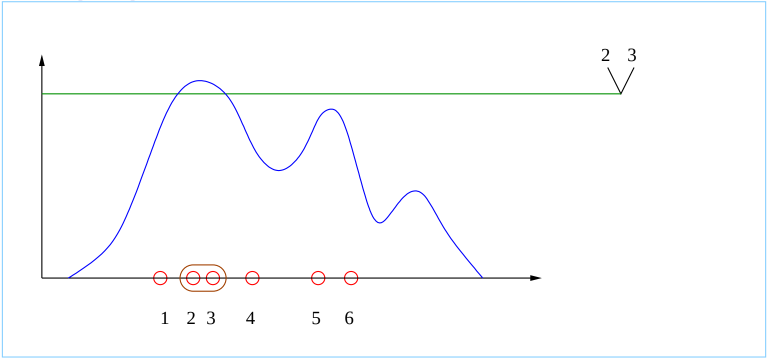

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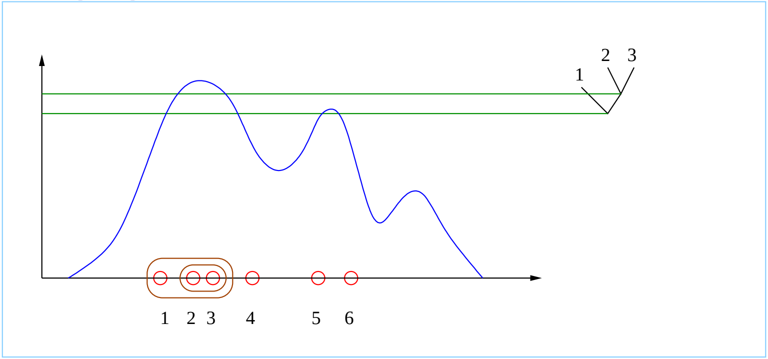

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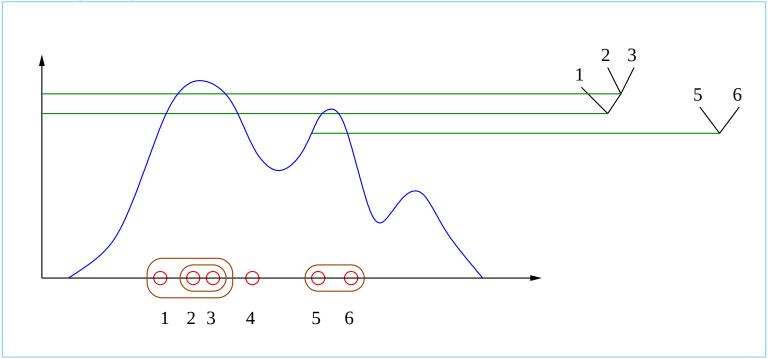

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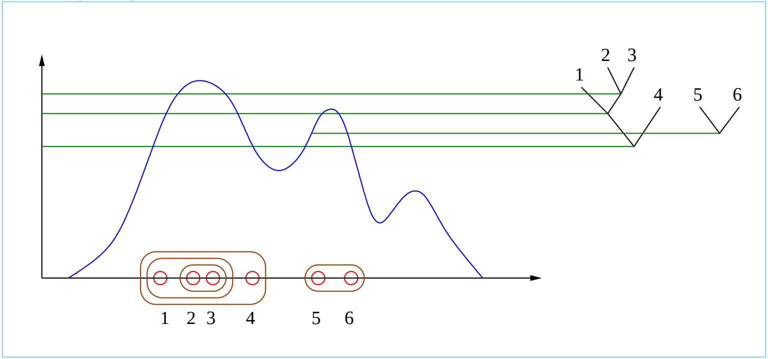

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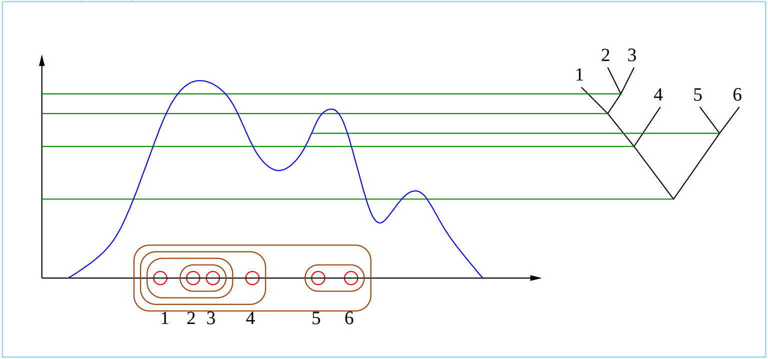

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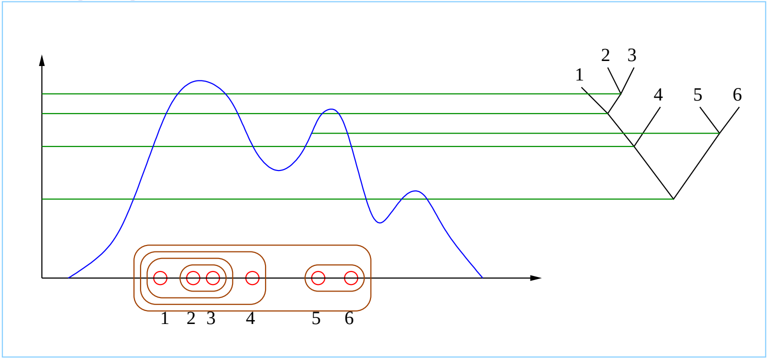

Consistency: Let A, A' be connected components of $\{f \geq \lambda\}$, for any λ. In the tree constructed from n data points X_n, let A_n be the smallest cluster containing $A \cap X_n$; likewise A'_n. Then:

$$\lim_{n \to \infty} \text{Prob}[A_n \text{ is disjoint from } A'_n] = 1$$

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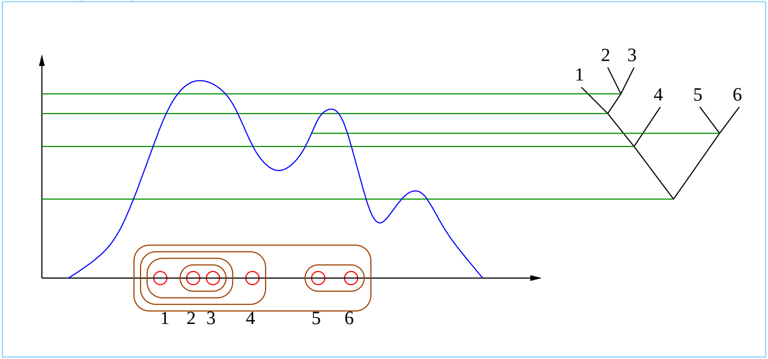

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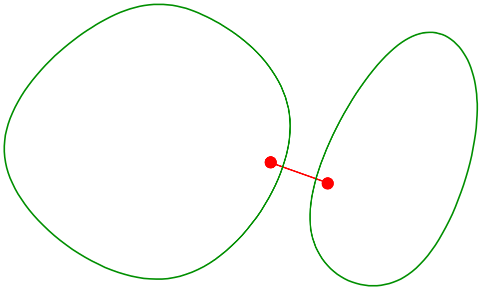
Hartigan 1975: Single linkage is consistent for $d = 1$.

Higher dimension

Hartigan 1982: Single linkage is not consistent for $d > 1$.



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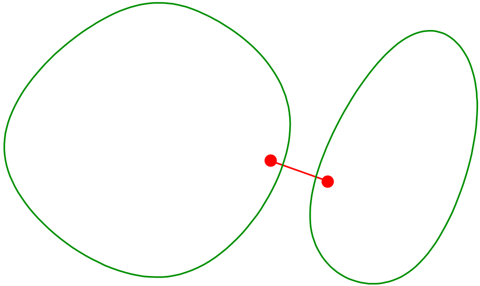


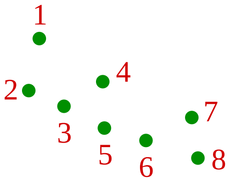
Chaudhuri-D '10: a simple variant of single linkage is consistent in any dimension, with a good finite sample convergence rate.

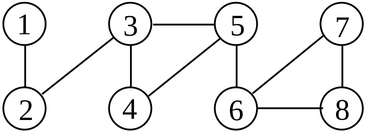
Related work

- Single linkage satisfies a partial consistency property
  Penrose 1995
- Algorithms to capture a user-specified level set $\{x : f(x) \geq \lambda\}$
  Maier-Hein-von Luxburg 2009, Rinaldo-Wasserman 2009,
  Singh-Scott-Nowak 2009
- Other estimators for the cluster tree
  Wishart 1969 (very similar to ours), Wong and Lane 1983,
  Stuetzle and Nugent 2010

Part II: Near neighbor graphs

Capturing a data set's local structure





An undirected graph with

- A node for each data point
- Edges between "neighboring" points

Uses: clustering, semisupervised learning, embeddings, regularization, ...

Two types of neighborhood graph

Connect points at distance $\leq r$

Connect each point to its k nearest neighbors

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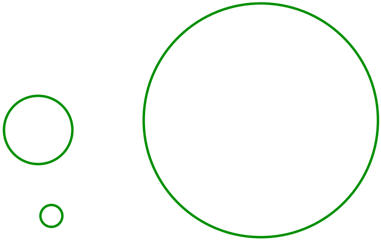
Problem: clusters at different scales



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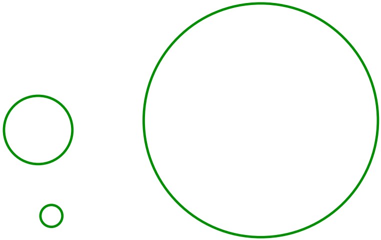

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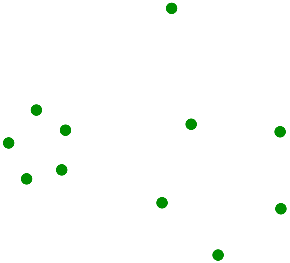
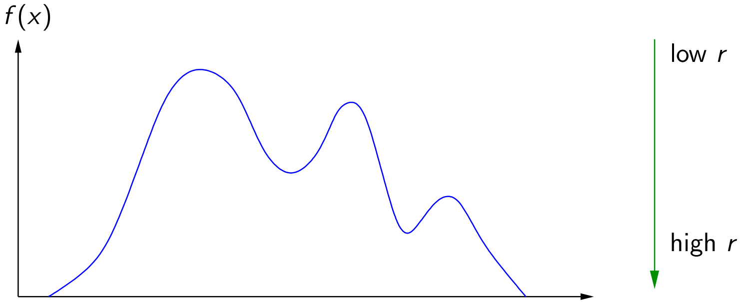
Problem: spurious connections



Single linkage, amended



- For each x_i: set $r(x_i)$ = distance to nearest neighbor
- As r increases from 0 to ∞:
  - Construct graph G_r:
    Nodes $\{x_i : r(x_i) \leq r\}$
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  - Output the connected components of G_r

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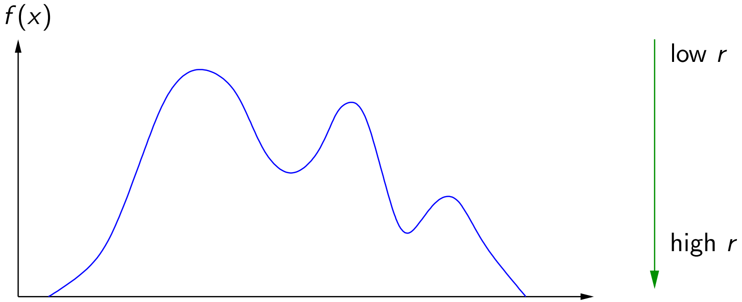

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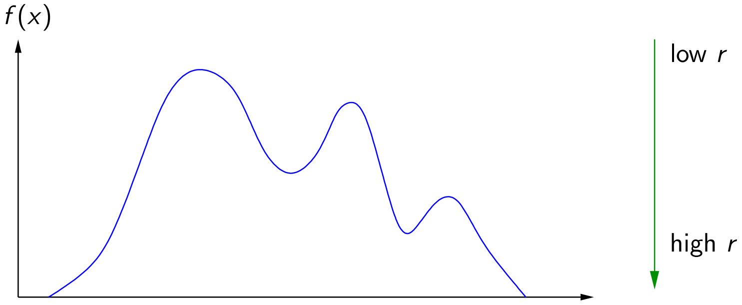

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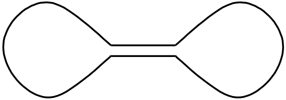
With $\sqrt{2} \leq \alpha \leq 2$ and $k \sim d \log n$, this is consistent for any d!

Which clusters are most salient?

Effect 1: thin bridges



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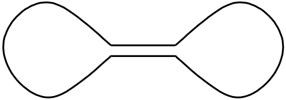

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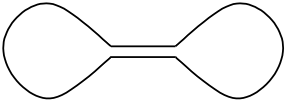

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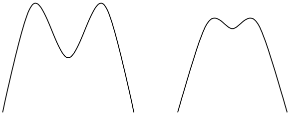

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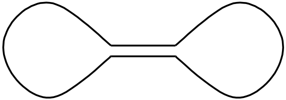

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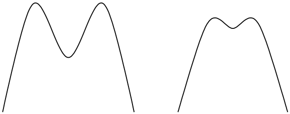

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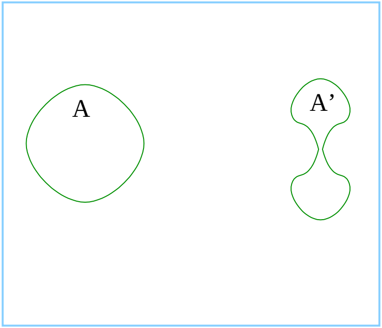
- separated by some set S
- max density in $S_\sigma \leq (1-\epsilon)$(min density in A_σ, A'_σ)



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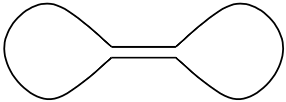

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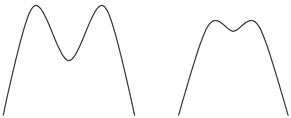

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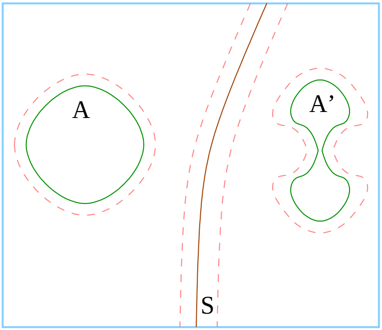

Rate of convergence

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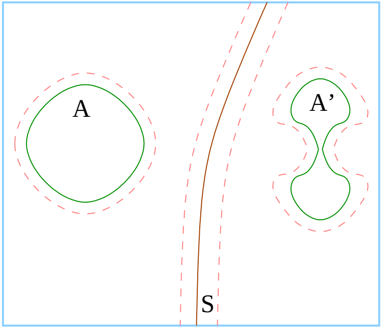

With high probability, for all connected sets A, A':
if A, A' are (σ, ϵ)-separated, and have minimum density λ, then for

$$n \geq \frac{d}{\lambda \epsilon^2 \sigma^d}$$

there will be some intermediate graph G_r such that:

- There is no path between A and A' in G_r
- A and A' are individually connected in G_r

Part III: Continuum percolation

Connectivity in random graphs

Erdos-Renyi random graphs

- n nodes
- Edges placed at random: between each pair of nodes, independently, an edge with probability p

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Random geometric graphs

- n points randomly chosen from an unknown density
- One node per point
- Edges between nodes that are nearby in some sense

Identifying high-density regions

Algorithm:
For each i: $r(x_i)$ = dist to kth nearest neighbor
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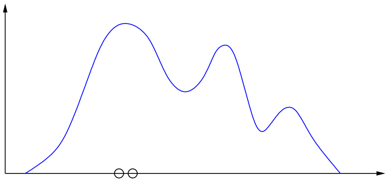
Single linkage has $k = 1$,
hoping: low $r \Leftrightarrow$ high density



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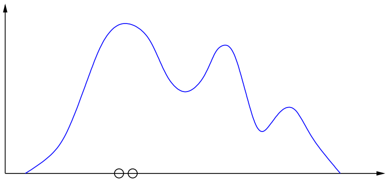
Single linkage has $k = 1$, hoping: low $r \Leftrightarrow$ high density



Vapnik-Chervonenkis bounds:
for *every* ball B in $\mathbb{R}^d$,
$\#$ pts in $B =$
$f(B) \cdot n \pm \sqrt{f(B) \cdot n \cdot d \log n}$.

Identifying high-density regions

Algorithm:
For each i: $r(x_i)$ = dist to kth nearest neighbor
As r increases from 0 to ∞:

- Construct graph G_r:
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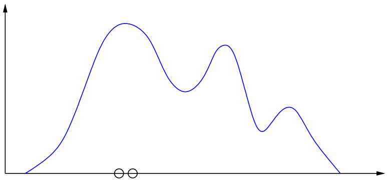

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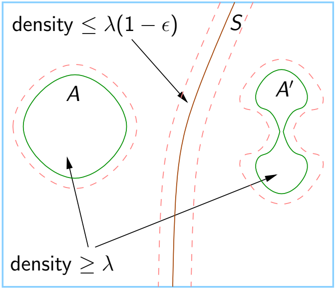
Moral: choose $k \geq d \log n$.

Separation

A, A' are (σ, ϵ)-separated.



(Buffer zone has width σ.)

There is some value r at which:

1. Every point in A, A' has $\geq k$ points within distance r, and is thus a node in G_r
2. Any point in S_σ has $< k$ points within distance r, and thus isn't a node in G_r
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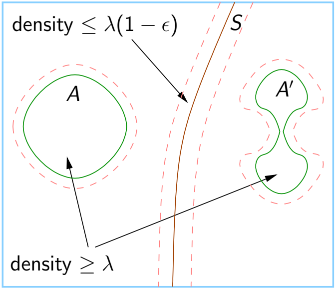

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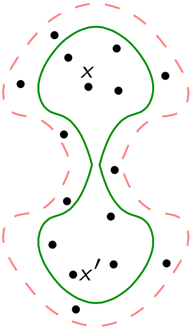
A is disconnected from A' in G_r

Connectedness

At this particular scale r, every point in A and A' (or within distance r of A, A') is active.



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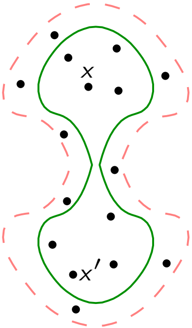

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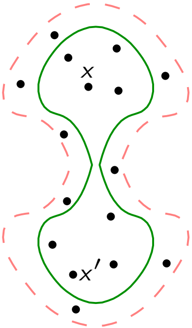

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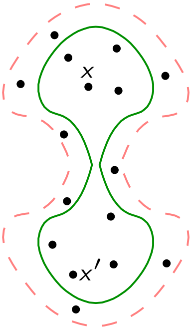

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- $\alpha = 2$: easy to show connectivity
- $\alpha = \sqrt{2}$: our result

Connectedness (cont'd)

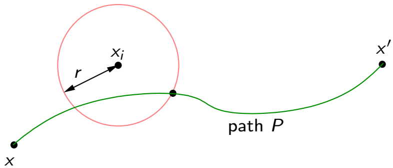
Proof sketch

x, x' are in cluster A, so there is a path P between them.

We'll exhibit data points $x_0 = x, x_1, \ldots, x_\ell = x'$ such that:

- The x_i are within distance r of P (and thus of A, and thus are active in G_r)
- $\|x_i - x_{i+1}\| \leq \alpha r$

So x is connected to x' in G_r.



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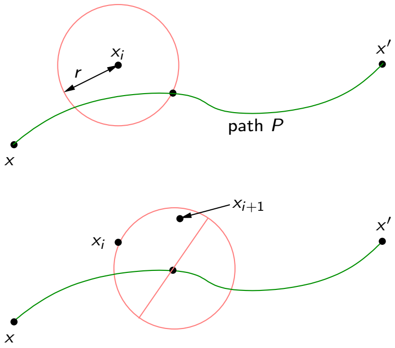

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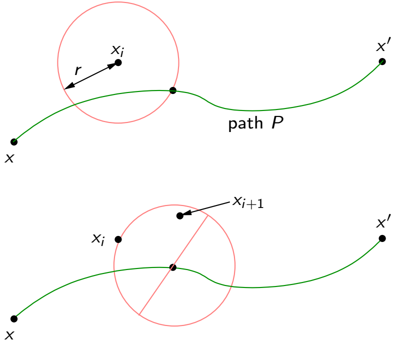

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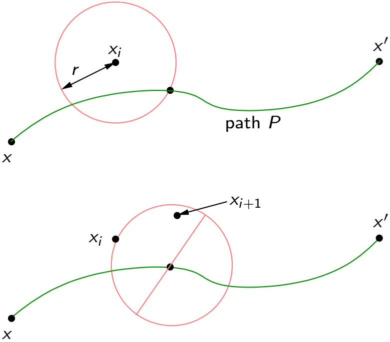
Open problem: will $\alpha = 1$ work?



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Lower bound via Fano's inequality

A game played with a predefined class of distributions $\{\theta_1, \ldots, \theta_\ell\}$.

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Theorem: If Nature chooses I uniformly at random, then the Player must draw at least

$$n \geq \frac{\log \ell}{2\beta}$$

samples in order to guess correctly with probability $\geq 1/2$, where

$$\beta = \frac{1}{\ell^2} \sum_{i,j=1}^{\ell} K(\theta_i, \theta_j).$$

An alternative cluster tree estimator

Original scheme constructs a hierarchy of neighborhood r-graphs:

- For each x_i: set $r_k(x_i)$ = distance to kth nearest neighbor
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Similar rates of convergence for these potentially sparser graphs.

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Open problem: other simple estimators?

Revisiting Hartigan-consistency

Recall Hartigan's notion of consistency:

> *Let A, A' be connected components of $\{f \geq \lambda\}$, for any λ. In the tree constructed from n data points X_n, let A_n be the smallest cluster containing $A \cap X_n$; likewise A'_n. Then:*
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In other words, distinct clusters should (for large enough n) be disjoint in the estimated tree.

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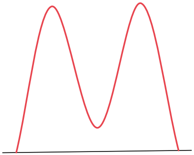
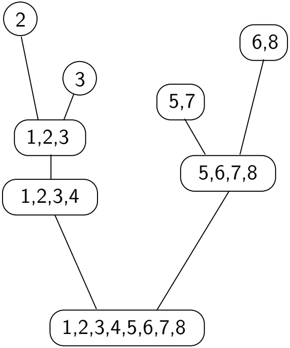
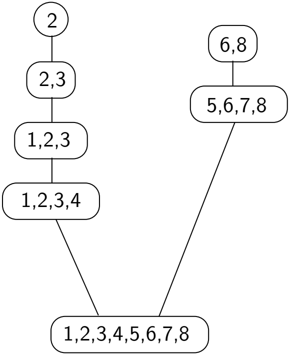
But this doesn't guard against excessive fragmentation within the estimated tree.

Excessive fragmentation: example

Density:







Pruning the cluster tree

- Build the cluster tree as before: at each scale r, there is a neighborhood graph G_r
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Belkin-Eldridge-Wang 2015: A stronger notion of consistency that accounts for fragmentation.

More open problems

1. Other natural notions of cluster for a density f? Are there situations in which a hierarchy is not enough?
2. This notion of cluster is for densities. What about discrete distributions?
3. An $O(n \log n)$ algorithm?

Thanks

Many thanks to my co-authors Kamalika Chaudhuri, Samory Kpotufe, and Ulrike von Luxburg.