Beyond Hartigan Consistency

Merge Distortion Metric for Hierarchical Clustering

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The Ohio State University

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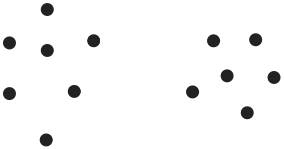
The goal of clustering:

Identify structure in data by grouping it into *clusters*



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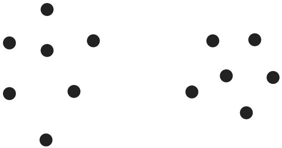
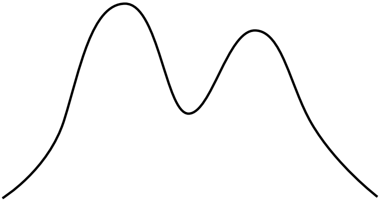


Assumption: data is drawn from some *density*.



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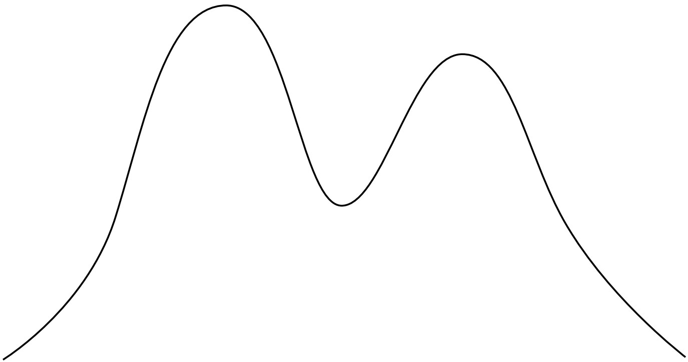
   - Yes. ☺

What *structure* do we wish to recover?

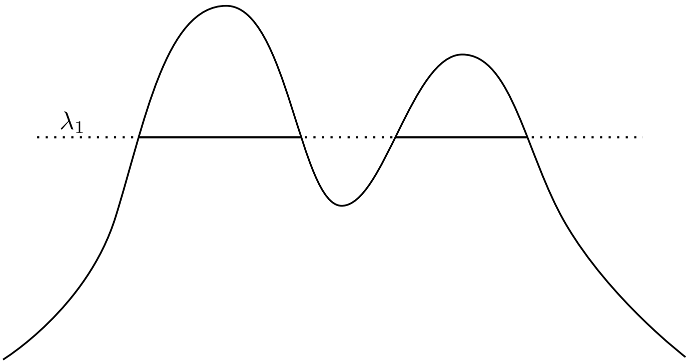
A *cluster* of a density is a *region of high probability.*[1]



[1] Hartigan (1981), Wishart (1969)...

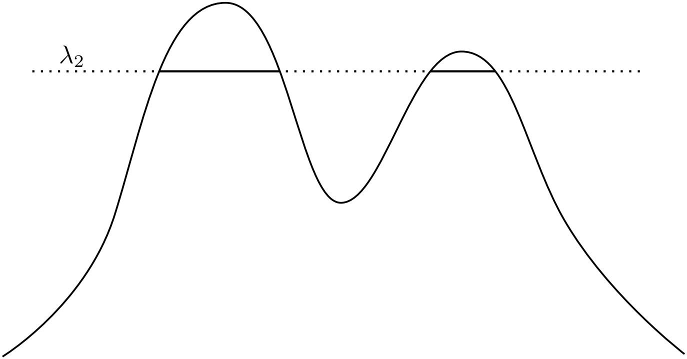
High-density clusters

Connected components of $\{f \geq \lambda_1\}$?



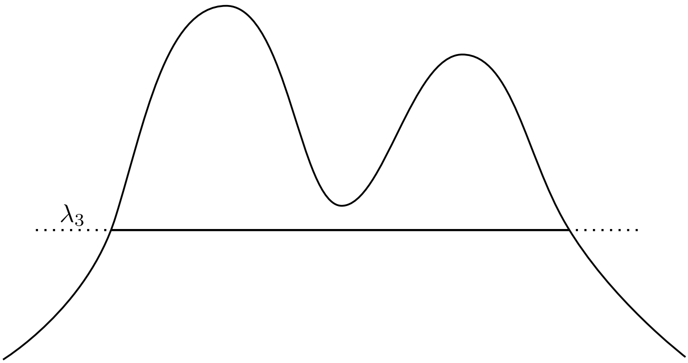
High-density clusters

Connected components of $\{f \geq \lambda_2\}$?



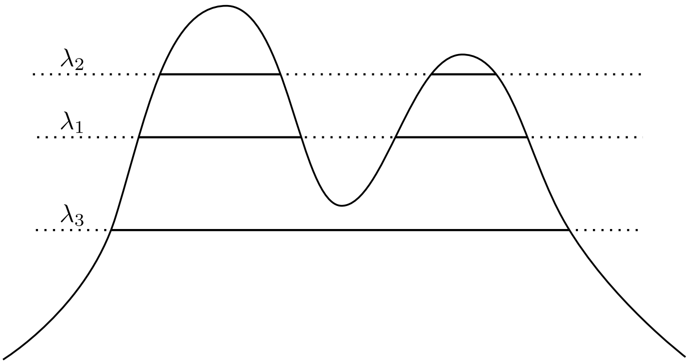
High-density clusters

Connected components of $\{f \geq \lambda_3\}$?



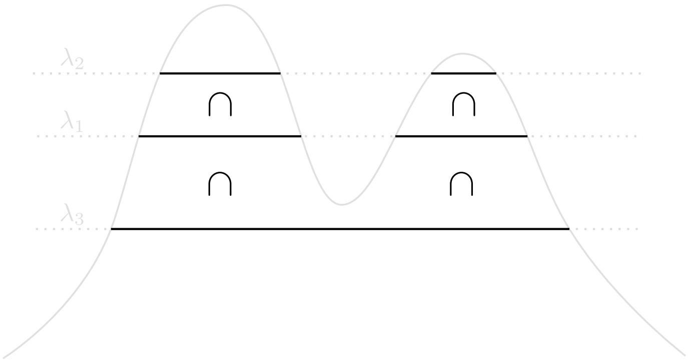
High-density clusters

A *cluster* is a connected component of $\{f \geq \lambda\}$ for any $\lambda > 0$.



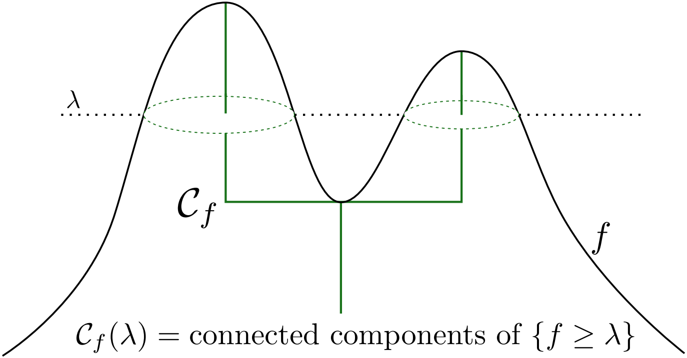
A hierarchy of clusters

Clusters from higher levels nest within clusters from lower levels.



The density cluster tree

This gives rise to a tree structure called the *density cluster tree*.



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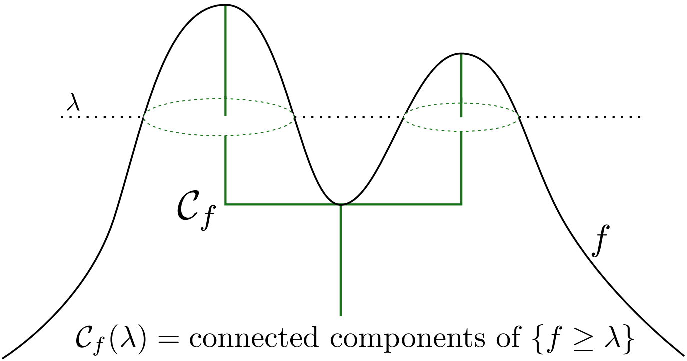
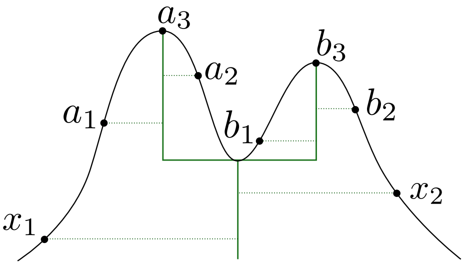
This *density cluster tree* is what we hope to recover from data.

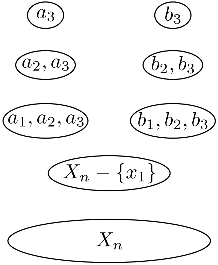


Recovering the *density cluster tree* from data

Draw $X_n \sim f$. Algorithm produces a collection of *empirical clusters*.



$\mathcal{C}_f$



$\hat{\mathcal{C}}_{f,n}$

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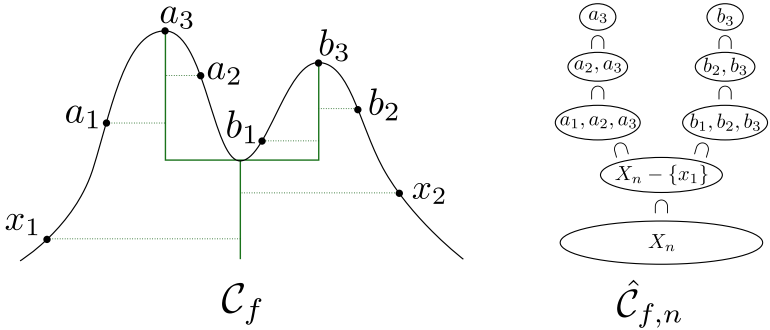
These clusters have hierarchical structure.



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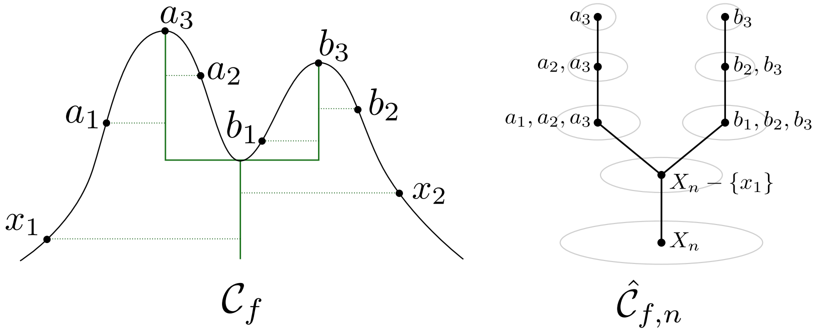
Can represent each cluster as a node in a tree.



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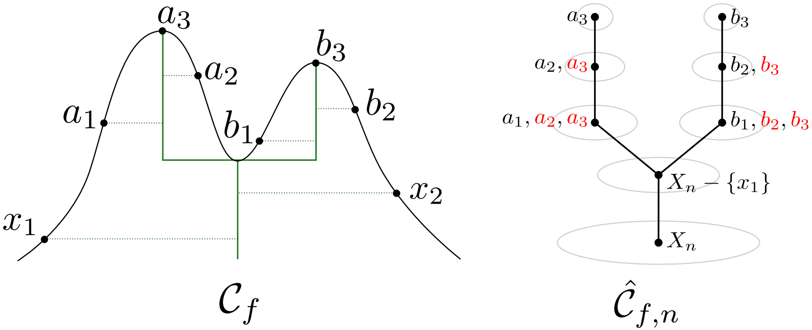

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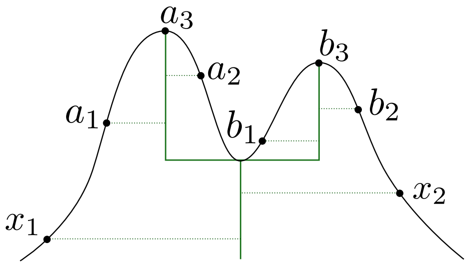

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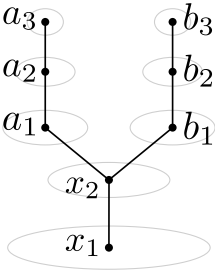

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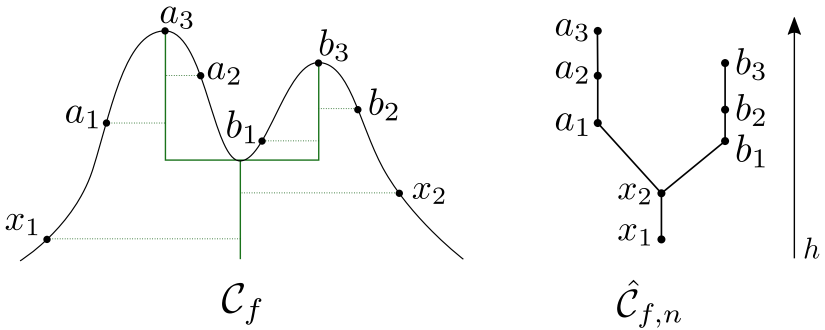
Recovering the *density cluster tree* from data

The *height* of a node is the density of lowest point it contains.



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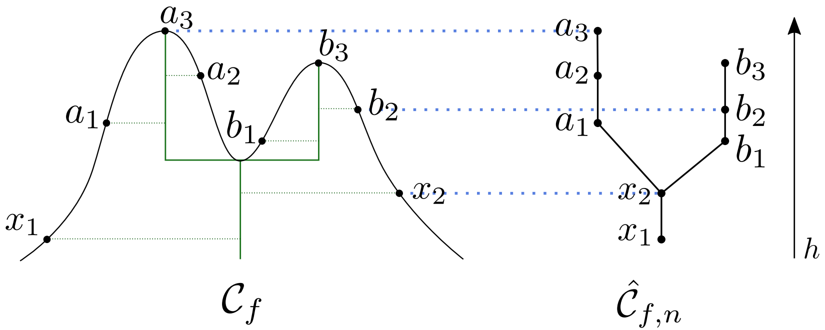
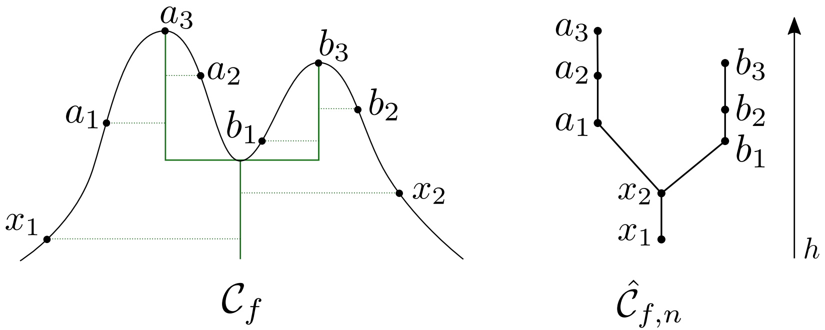


Recovering the *density cluster tree* from data

Goal: As $n \to \infty$, the empirical tree should resemble the true tree.



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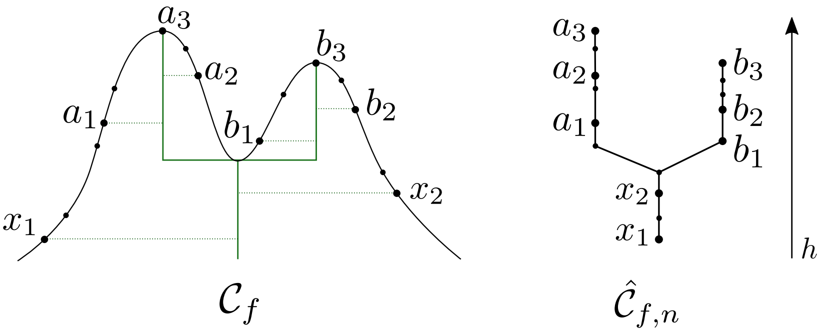

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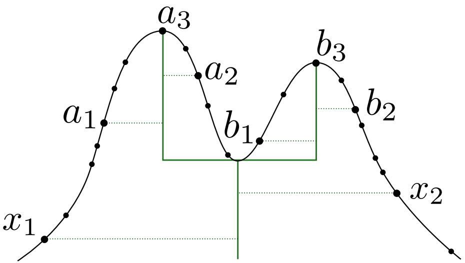

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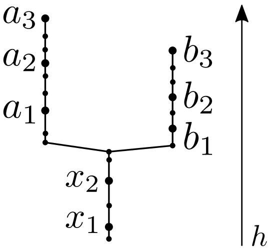

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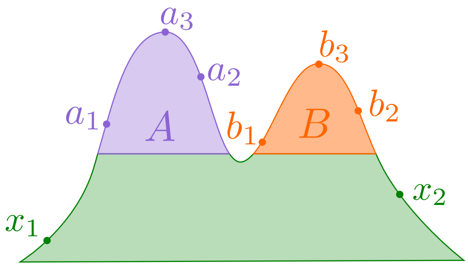
- Informally: Clusters which are disjoint in the true tree should be separated in the empirical tree.

Hartigan Consistency

Let A and B be any disjoint ideal clusters.



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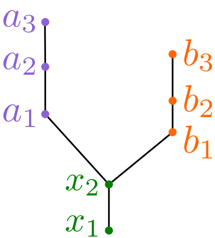

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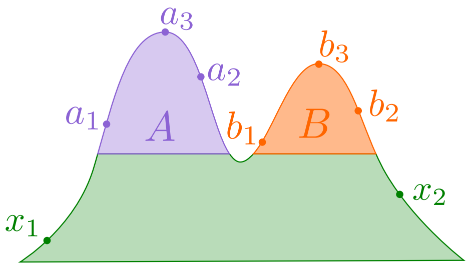
Hartigan Consistency

Find $A_n :=$ the smallest *empirical cluster* containing $A \cap X_n$.



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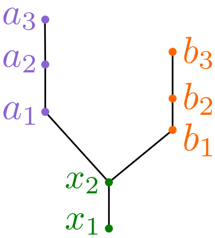

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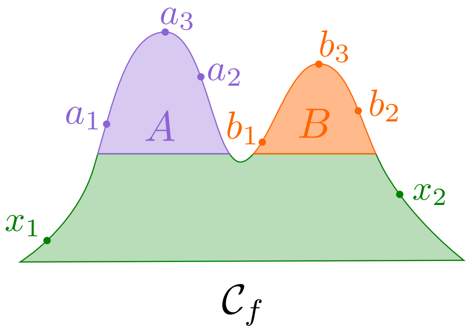

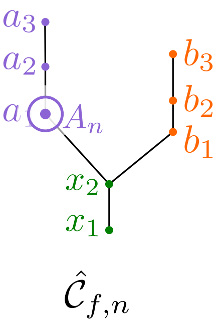

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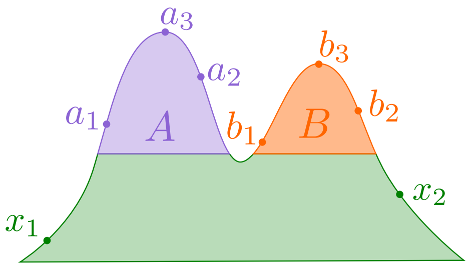

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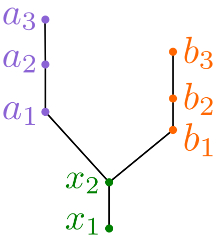

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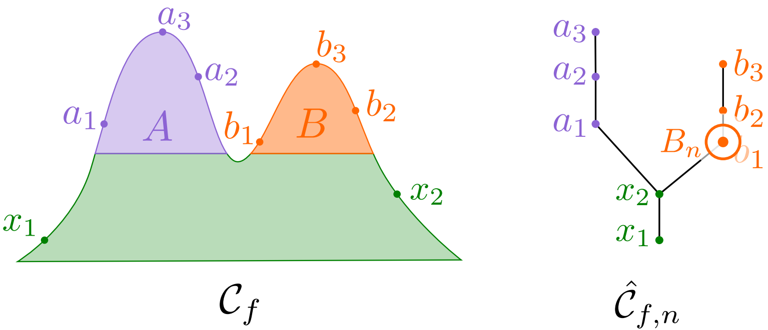

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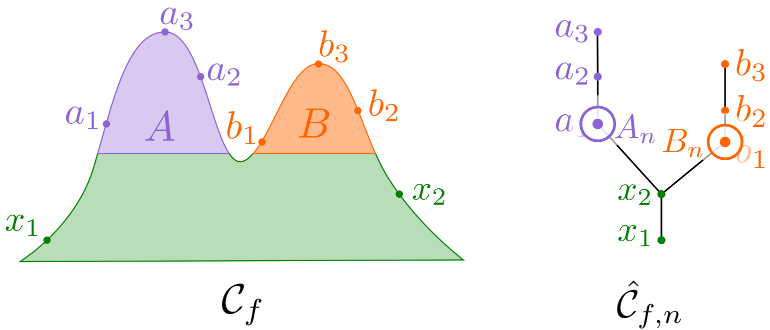
Hartigan consistency: As $n \to \infty$, $\Pr(A_n \text{ is disjoint from } B_n) \to 1$.



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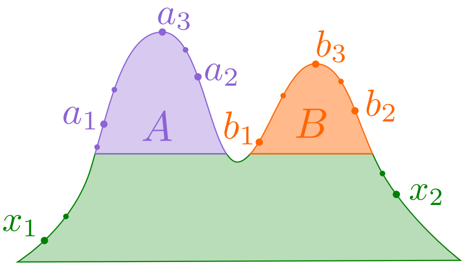

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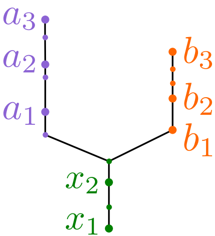

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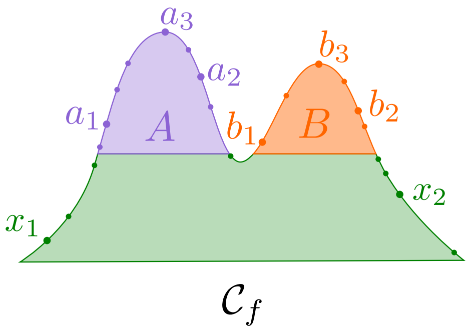

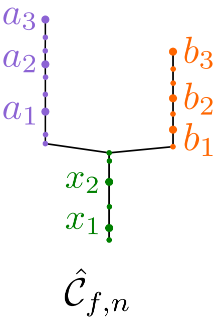

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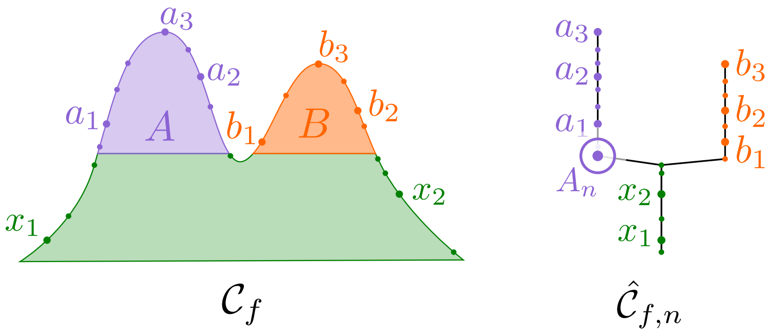

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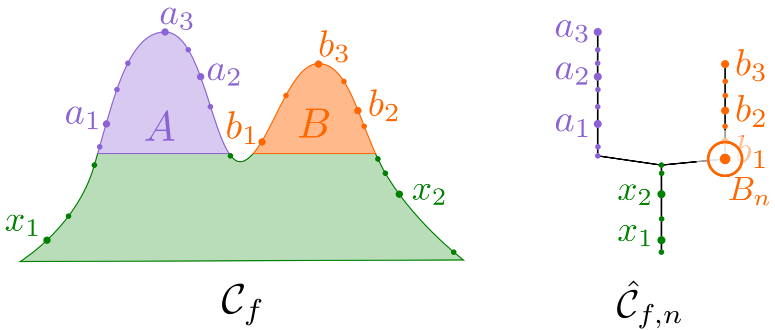

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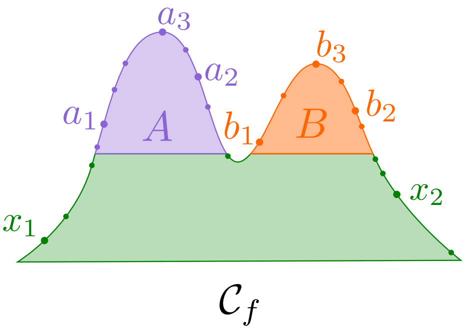

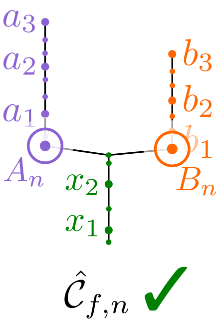

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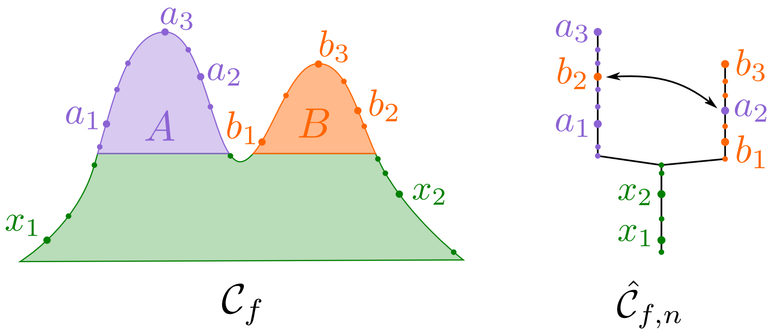

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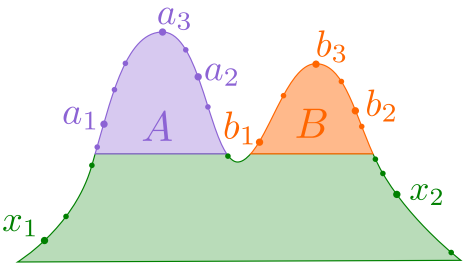

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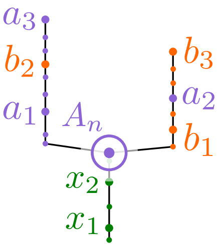

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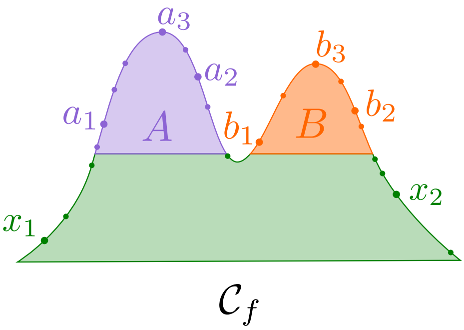

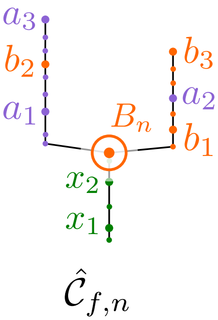

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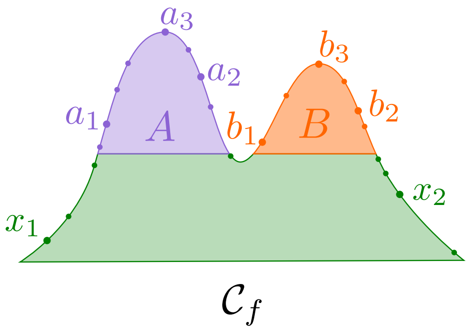

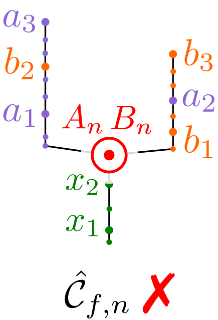

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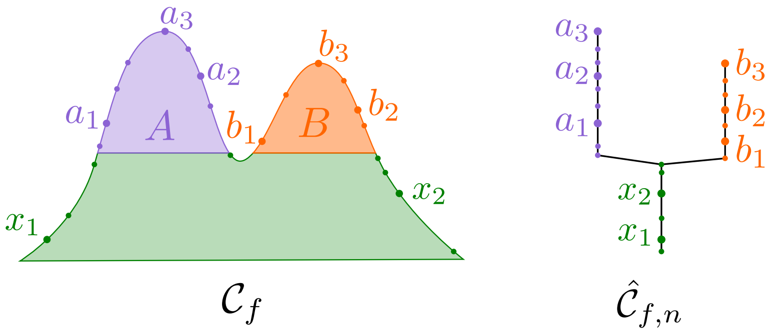
Hartigan lacks a strong notion of *connectedness*.



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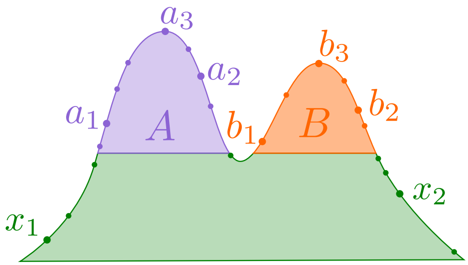
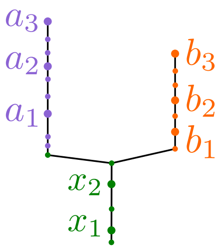


$\mathcal{C}_f$



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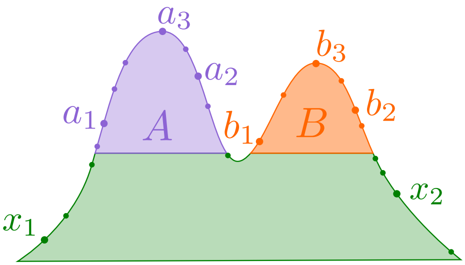

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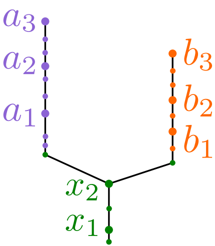

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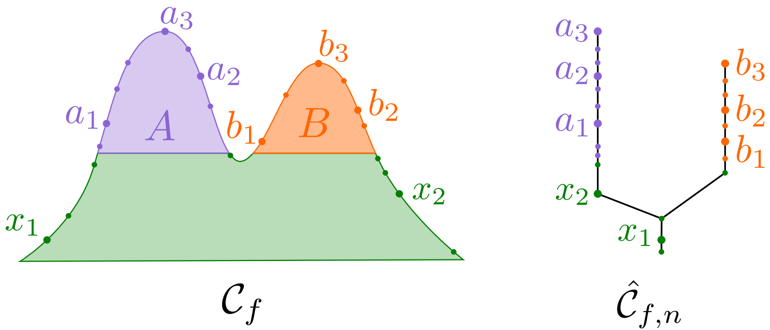

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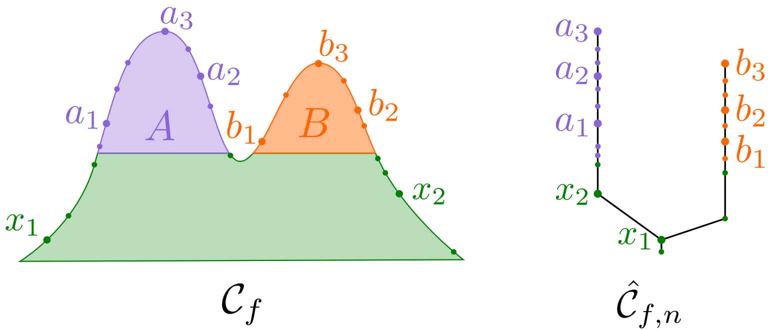

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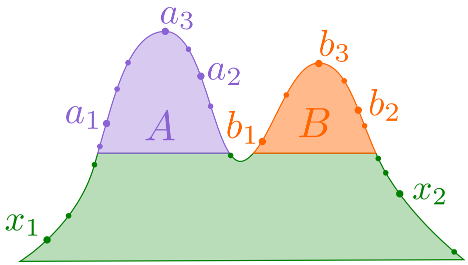

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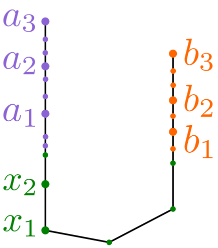

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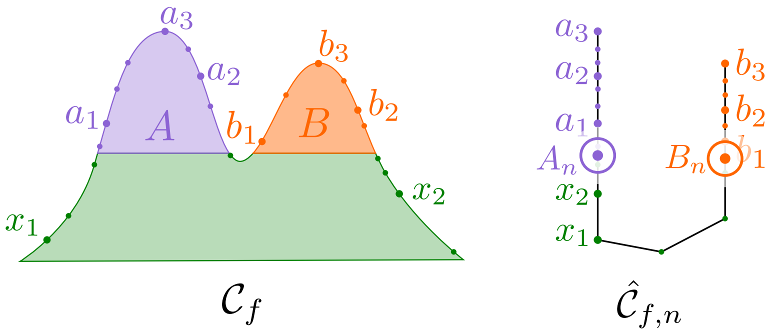

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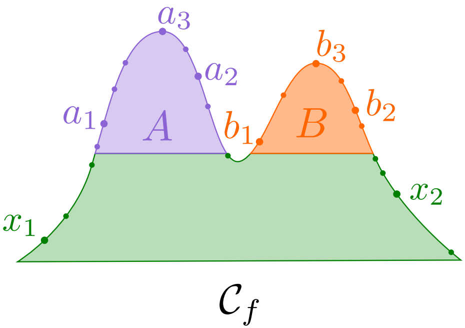

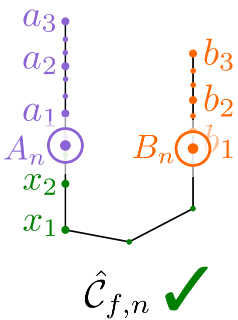

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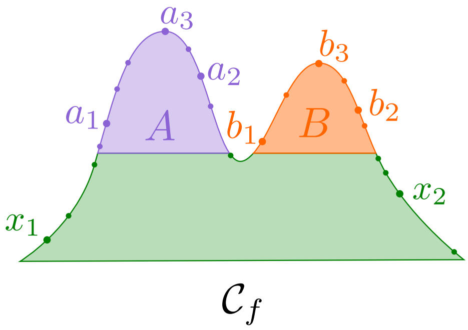
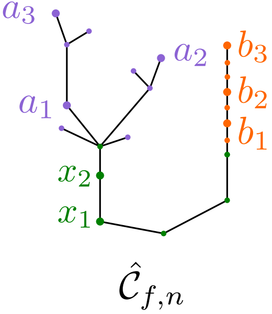
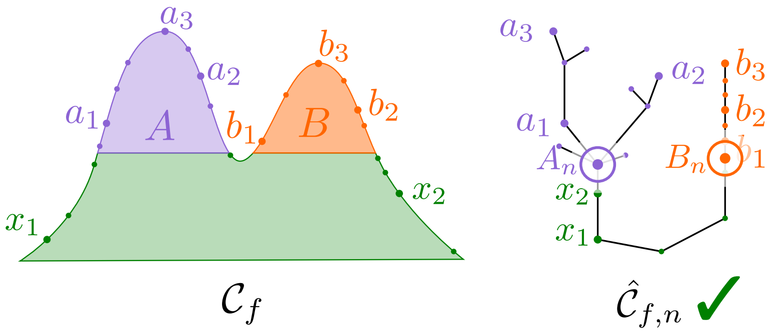
What about this tree?





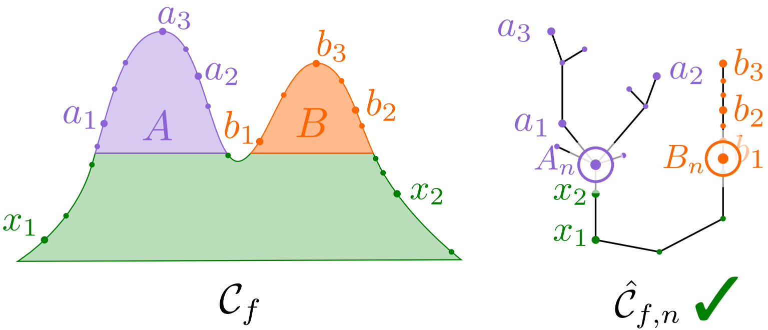
Hartigan consistency is insufficient

What about this tree? Also consistent!



Hartigan consistency is insufficient

A tree can be *Hartigan consistent* yet very different from the true tree.



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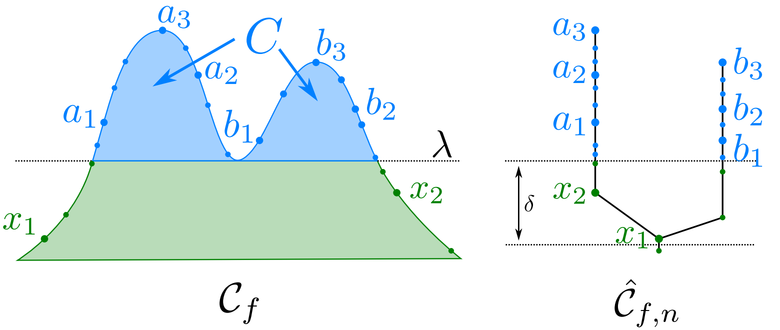
- Together they'll imply *Hartigan consistency*

Minimality

$C \cap X_n$ should be connected at $\lambda - \delta$, with $\delta \to 0$ as $n \to \infty$



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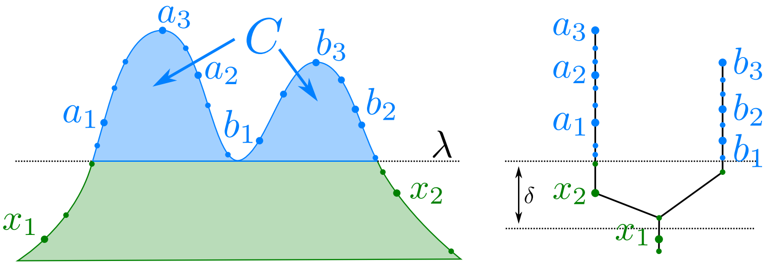

$\mathcal{C}_f$ $\hat{\mathcal{C}}_{f,n}$

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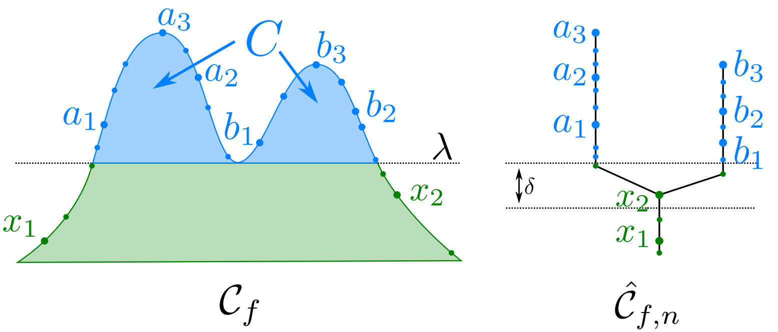

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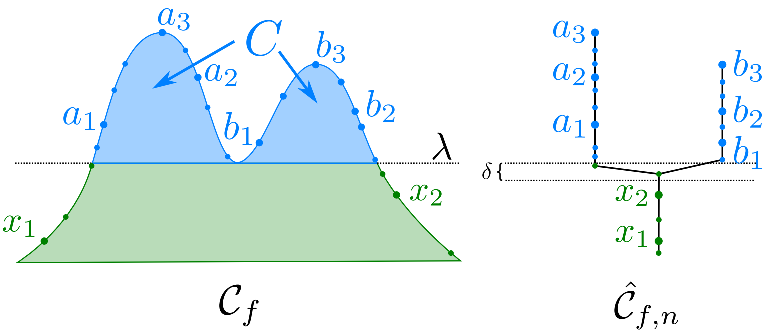
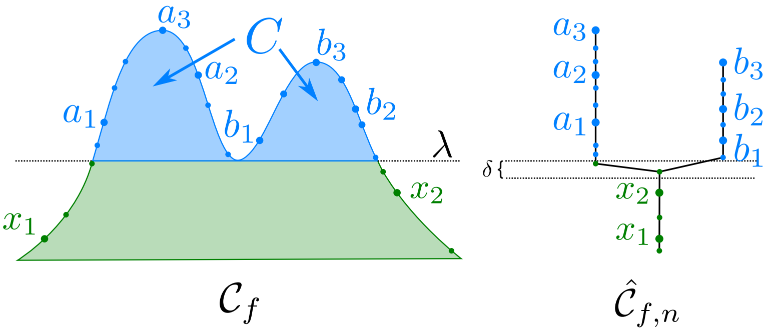


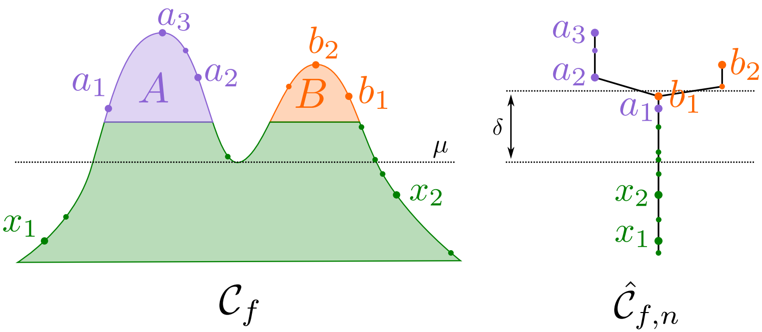
Minimality

$\hat{\mathcal{C}}_{f,n}$ ensures *minimality* if given any cluster C of $\{f \geq \lambda\}$, $C \cap X_n$ is connected at level $\lambda - \delta$ for any $\delta > 0$ as $n \to \infty$.



Separation

$A \cap X_n$ and $B \cap X_n$ should be separated at $\mu + \delta$, with $\delta \to 0$ as $n \to \infty$



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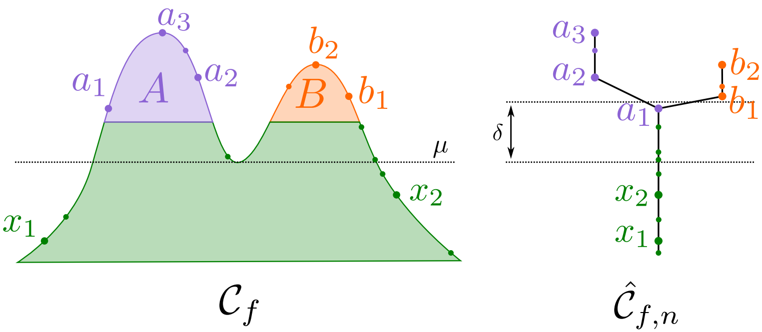

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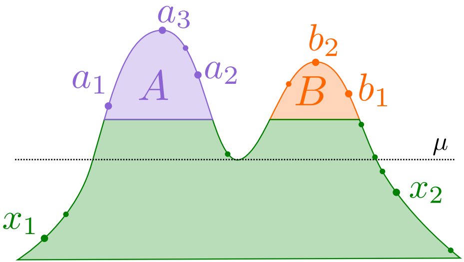
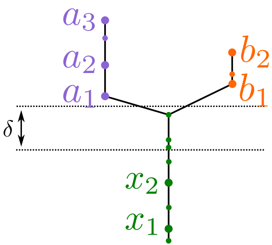


$\mathcal{C}_f$



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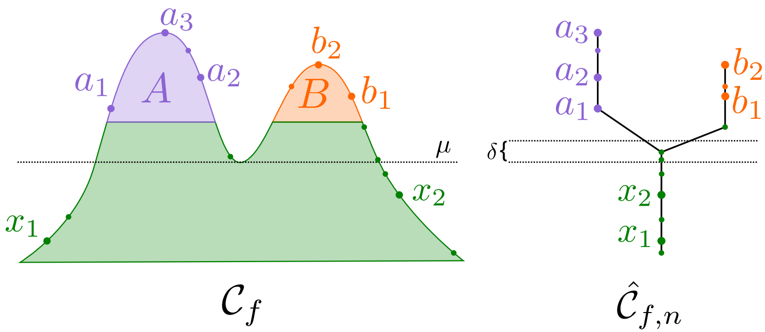

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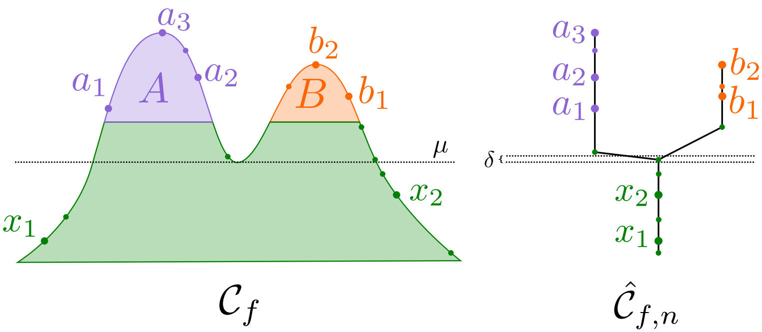

Theorem

If a clustering method ensures minimality *and* separation, *then it is* Hartigan consistent.

$$\textit{Minimality} \text{ and } \textit{Separation} \Longrightarrow \textit{Hartigan Consistency}$$

$$\textit{Hartigan Consistency} \not\Longrightarrow \textit{Minimality} \text{ and } \textit{Separation}$$

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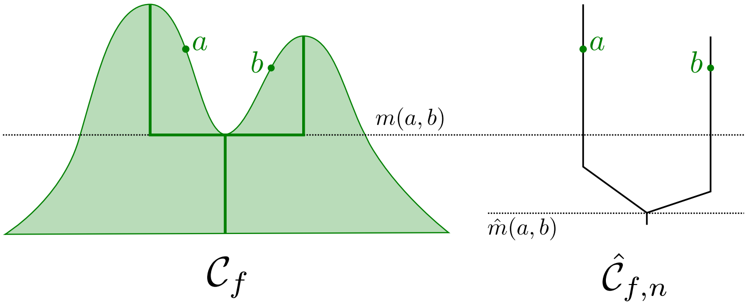

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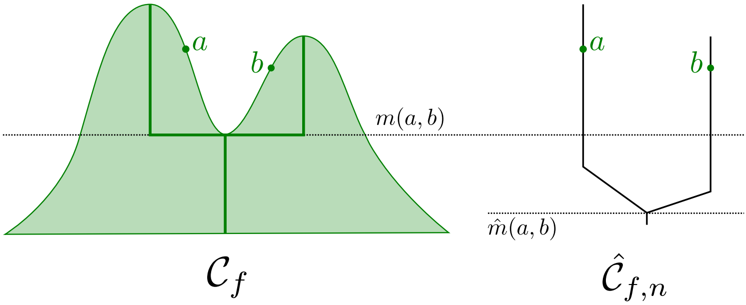

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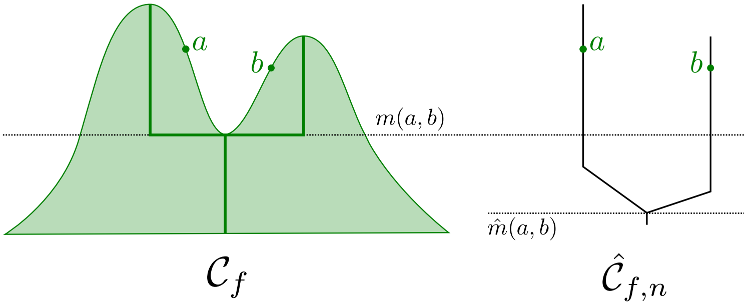

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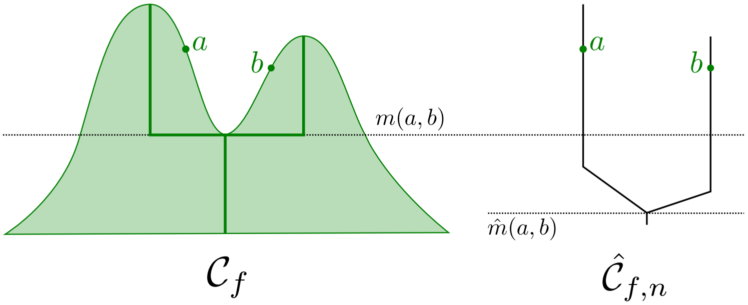

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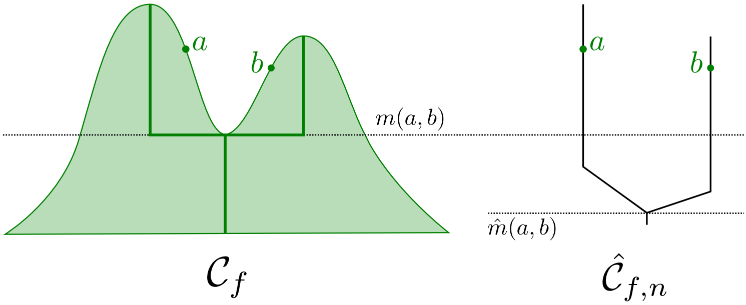

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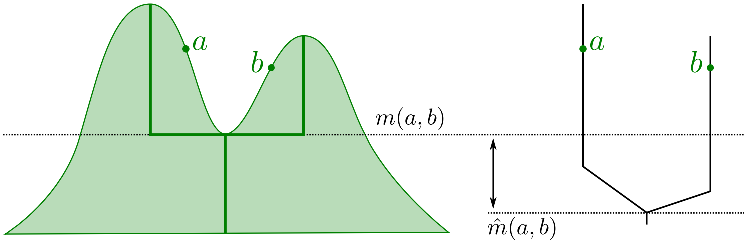

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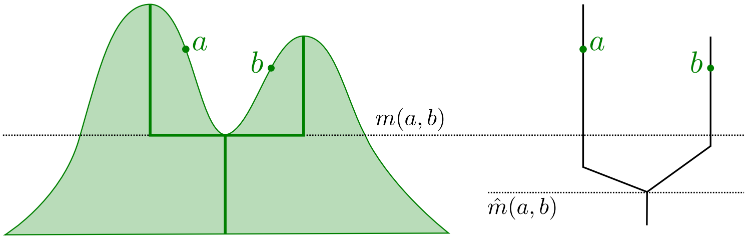

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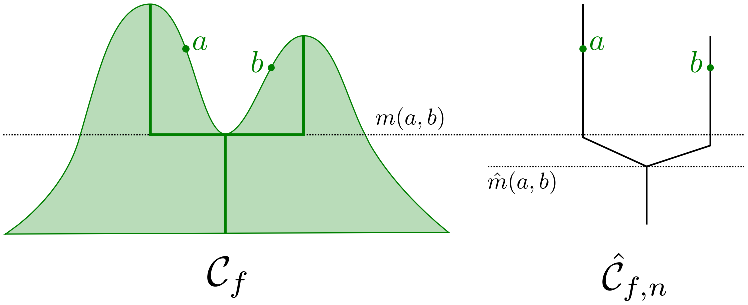

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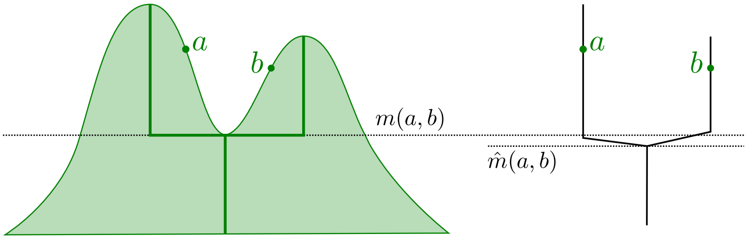

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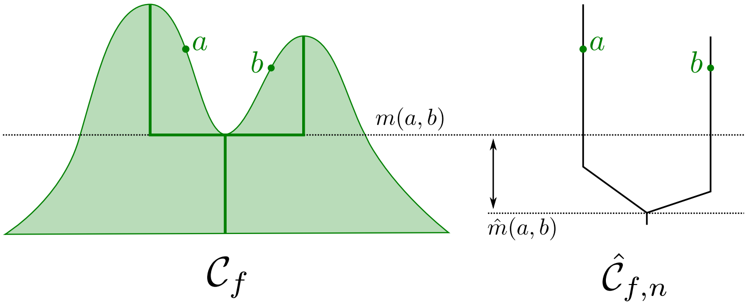

We define the *merge distortion metric* between the density cluster tree and its estimate as:

$$d(\mathcal{C}_f, \hat{\mathcal{C}}_{f,n}) = \max_{x,x' \in X_n} \left| m(x,x') - \hat{m}(x,x') \right| .$$

Theorem

Convergence of $\hat{\mathcal{C}}_{f,n} \to \mathcal{C}_f$

is equivalent to

uniform minimality $+$ *uniform separation*.

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Do algorithms exist which have these properties/converge to the true density cluster tree?

- We analyze two:
- Robust single linkage from (Chaudhuri and Dasgupta, 2010)
- Split tree-based clustering from computational topology

Convergence of robust single linkage

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- Authors proved that it is *Hartigan consistent*
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Theorem

Suppose f is c-Lipschitz, compactly supported, and for any λ, $\{f \geq \lambda\}$ has finitely-many connected components. Then:

- *Robust single linkage converges to the true cluster tree in the merge distortion metric.*

Future work

- What other algorithms converge in the *merge distortion metric*?
- ℓ_2 variant of the metric?
- Fast algorithms for approximating the distance.
- Hierarchical clustering without a density – how do we define distance?

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     - Split-tree-based algorithm.

Thank you!