

# Handling LP-Rounding for Hierarchical Clustering and Fitting Distances by Ultrametrics

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Joint work with

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Mong-Jen Kao

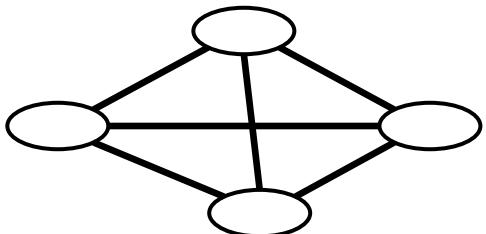
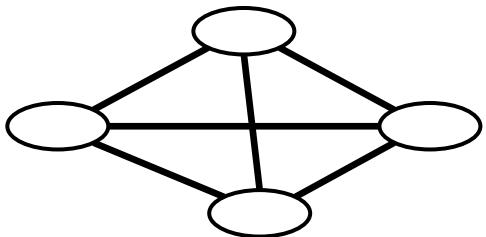
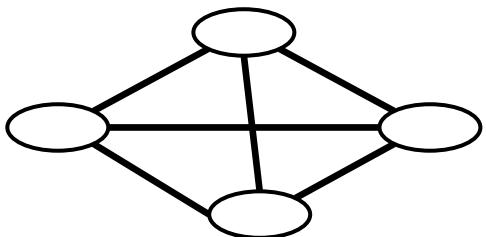
National Yang-Ming Chiao-Tung University, Taiwan

Mu-Ting Lee

National Yang-Ming Chiao-Tung University, Taiwan

# Hierarchical Correlation Clustering (HCC)

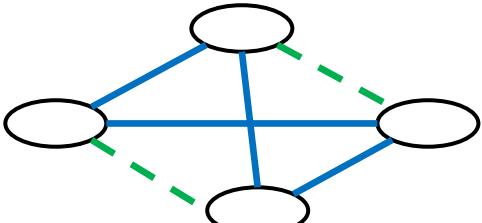
- $\ell$  layers of complete graphs (on the same vertex set)



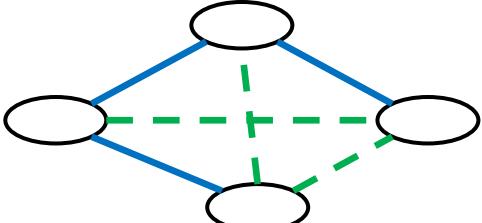
# Hierarchical Correlation Clustering (HCC)

- $\ell$  layers of complete graphs (on the same vertex set)
  - each edge is labeled  or 

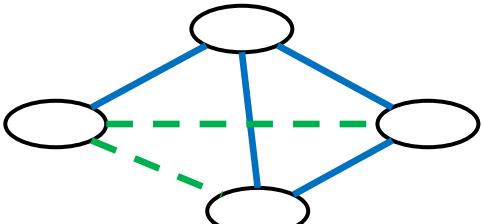
$$\begin{array}{c} \textcolor{blue}{+} \quad \textcolor{green}{\square} \\ E_+^{(3)}, E_-^{(3)} \end{array}$$



$$E_+^{(2)}, E_-^{(2)}$$



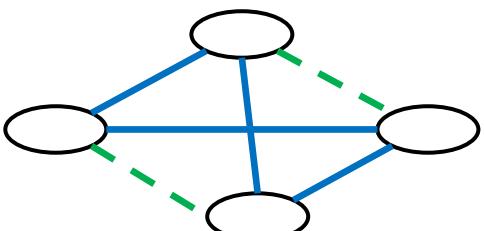
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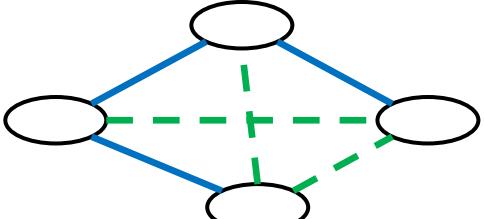
- $\ell$  layers of complete graphs
- $\ell$  weights  $\delta^{(1)}, \dots, \delta^{(\ell)} \geq 0$

$$\begin{array}{c} \textcolor{blue}{+} \\ \textcolor{green}{\exists} \\ E_+^{(3)}, E_-^{(3)} \end{array}$$



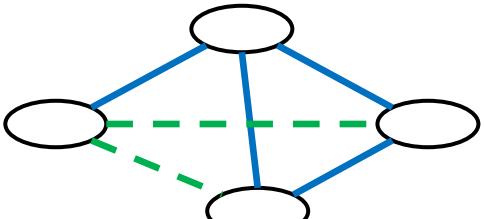
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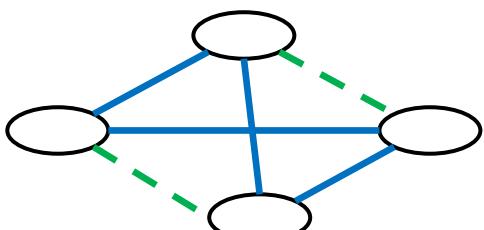


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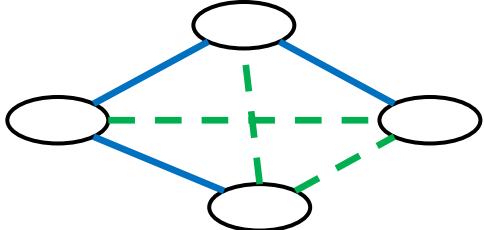
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(partitions)

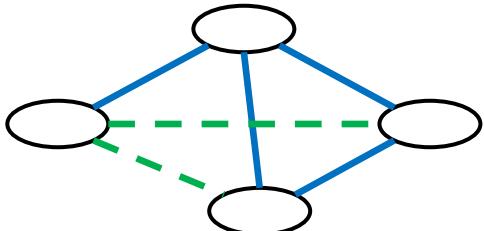
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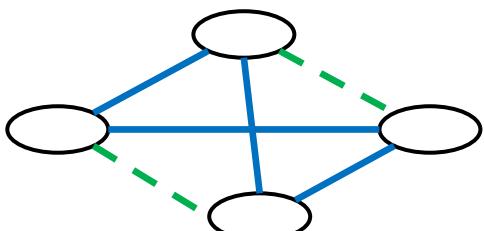


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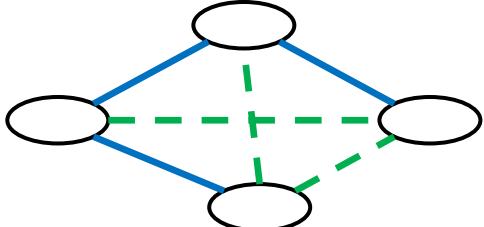
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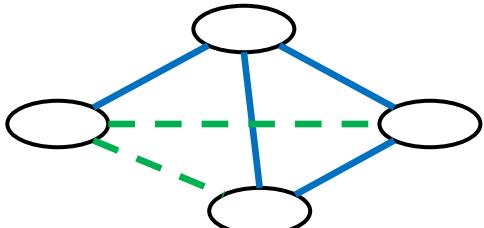
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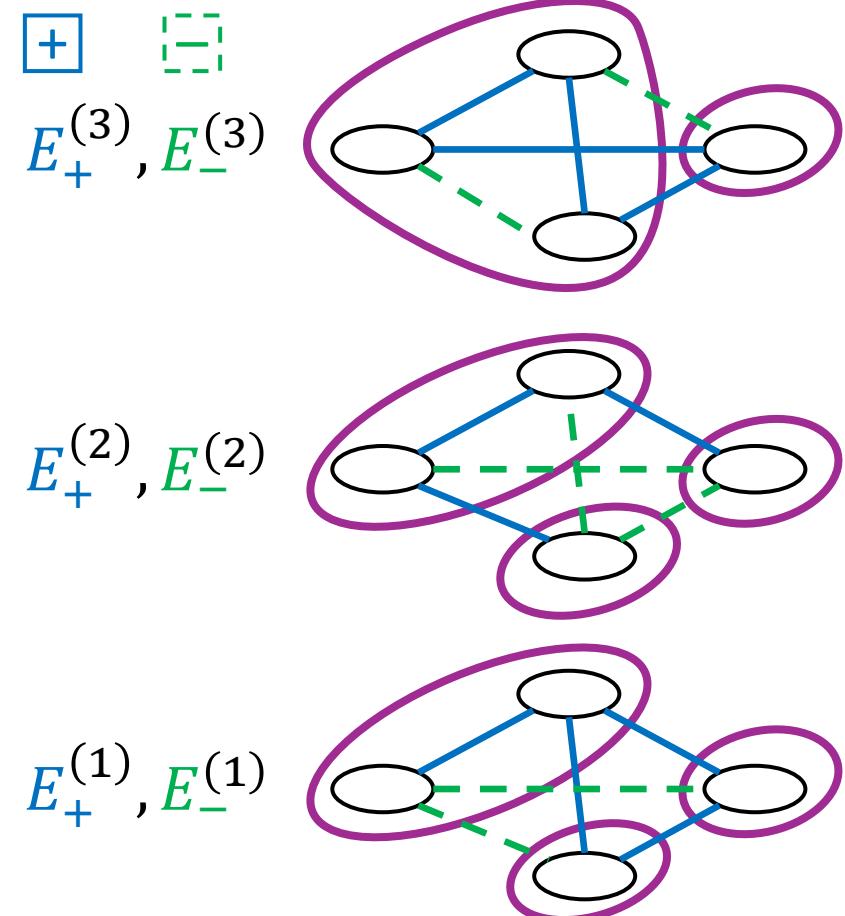
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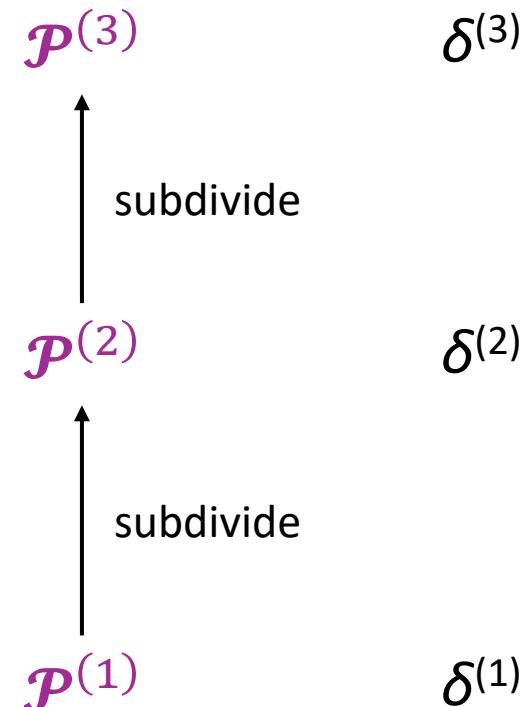
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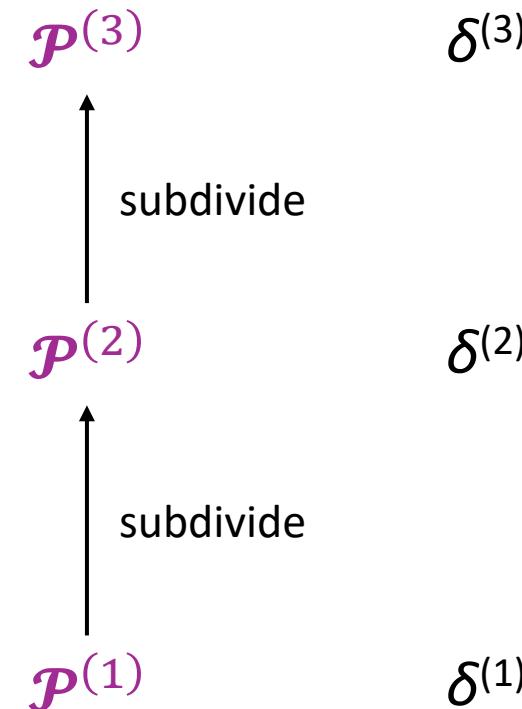
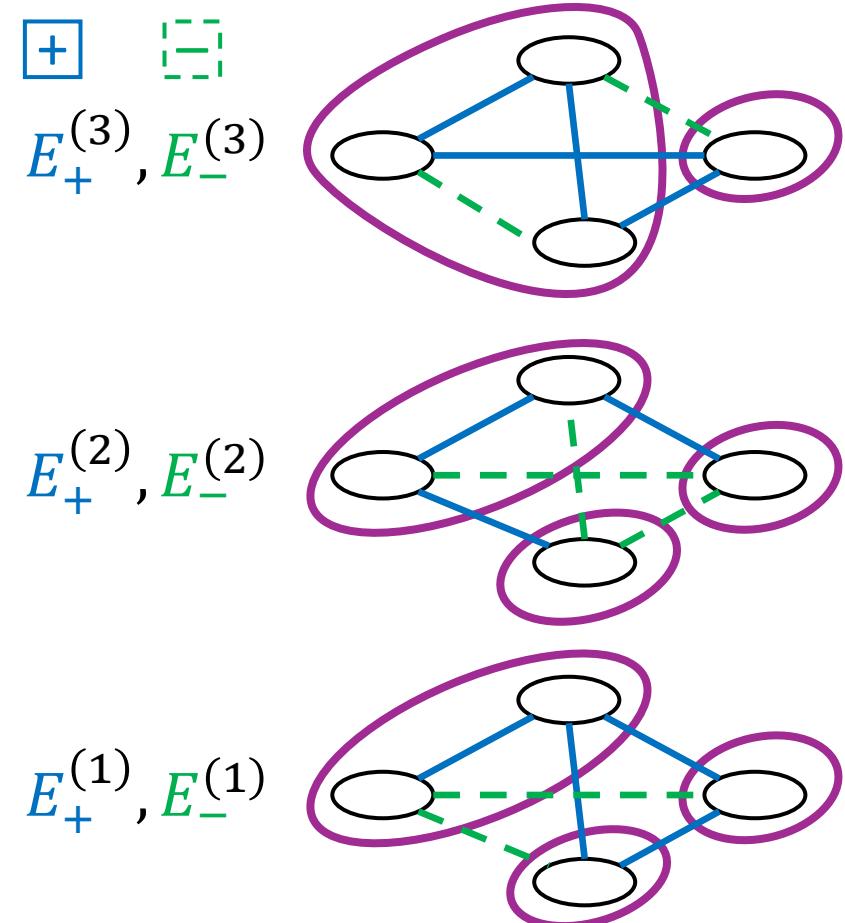


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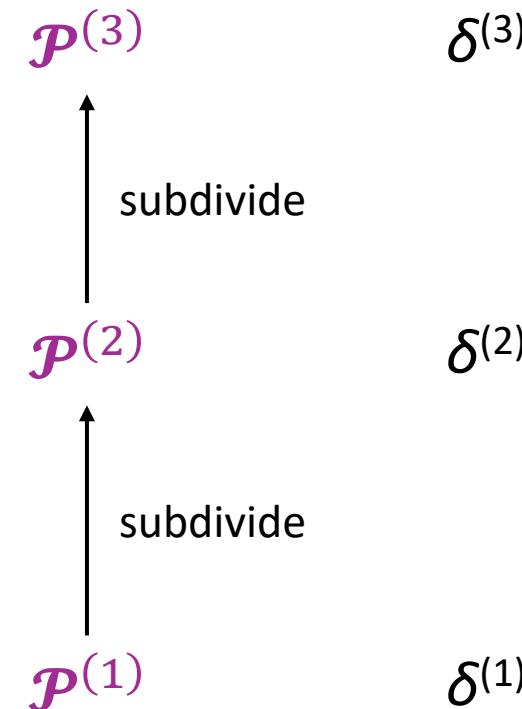
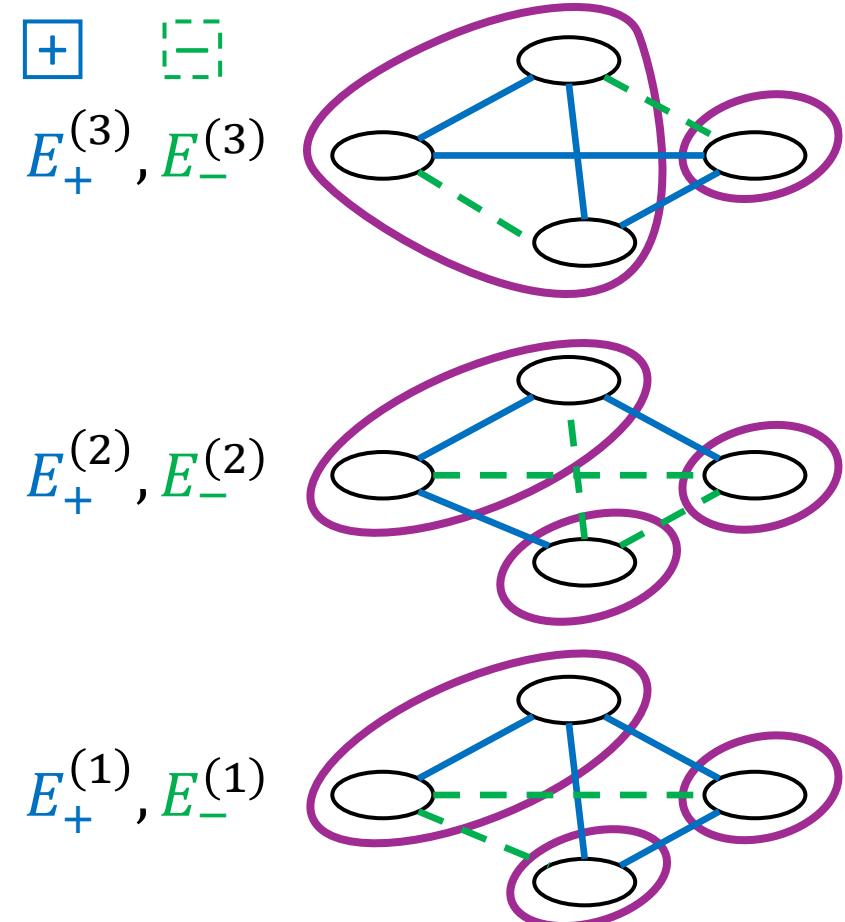
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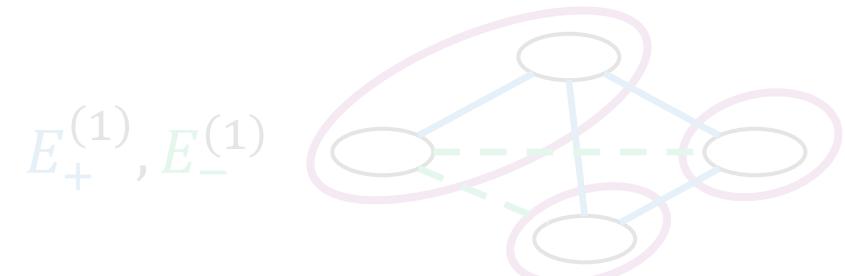
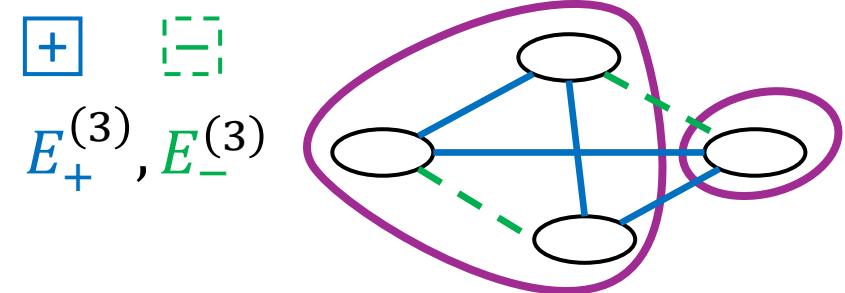
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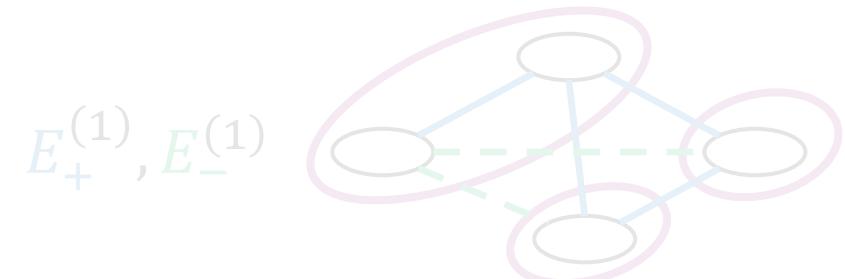
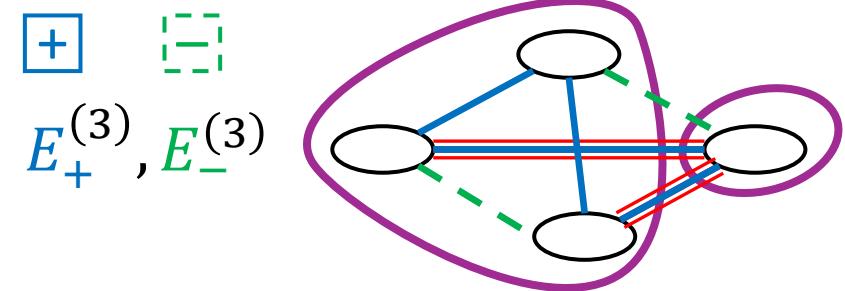


**Definition.** An edge is a *disagreement* if

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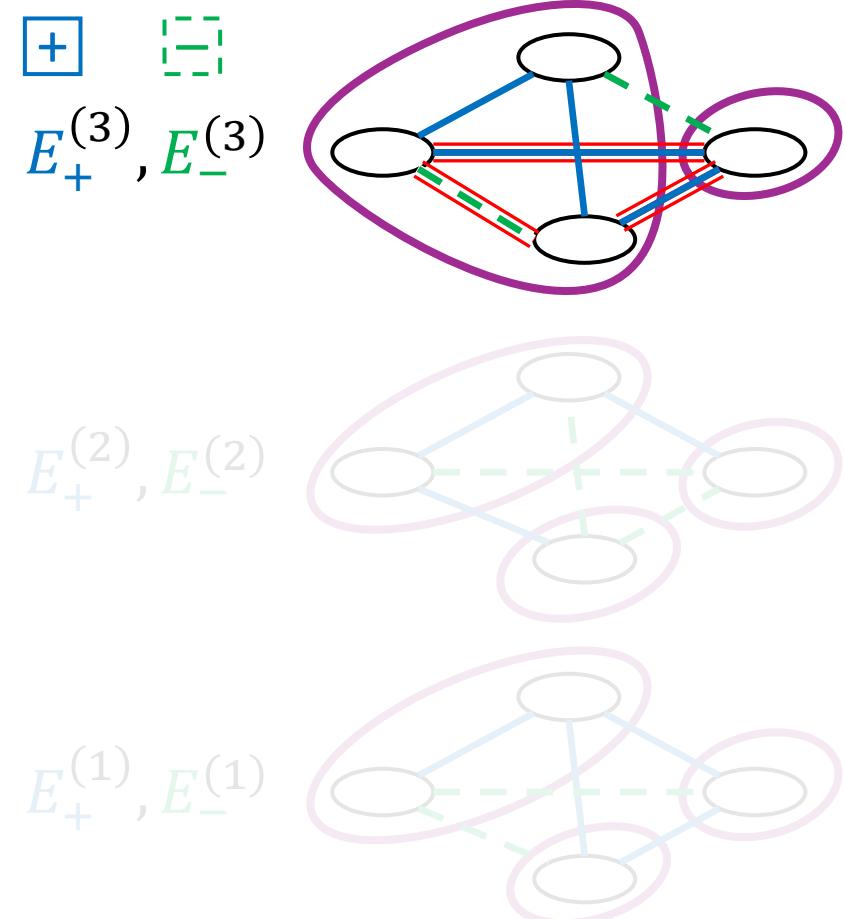


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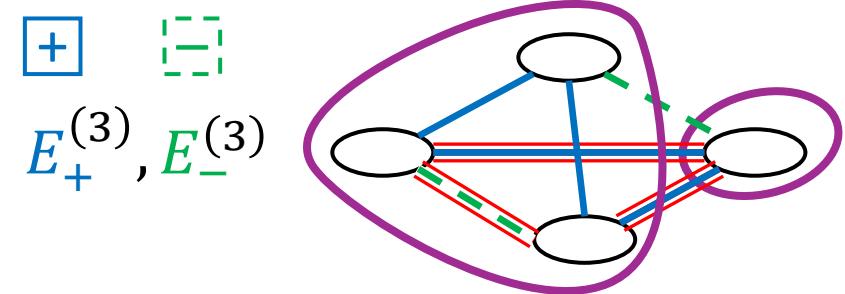


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3 disagreements (at layer 3)

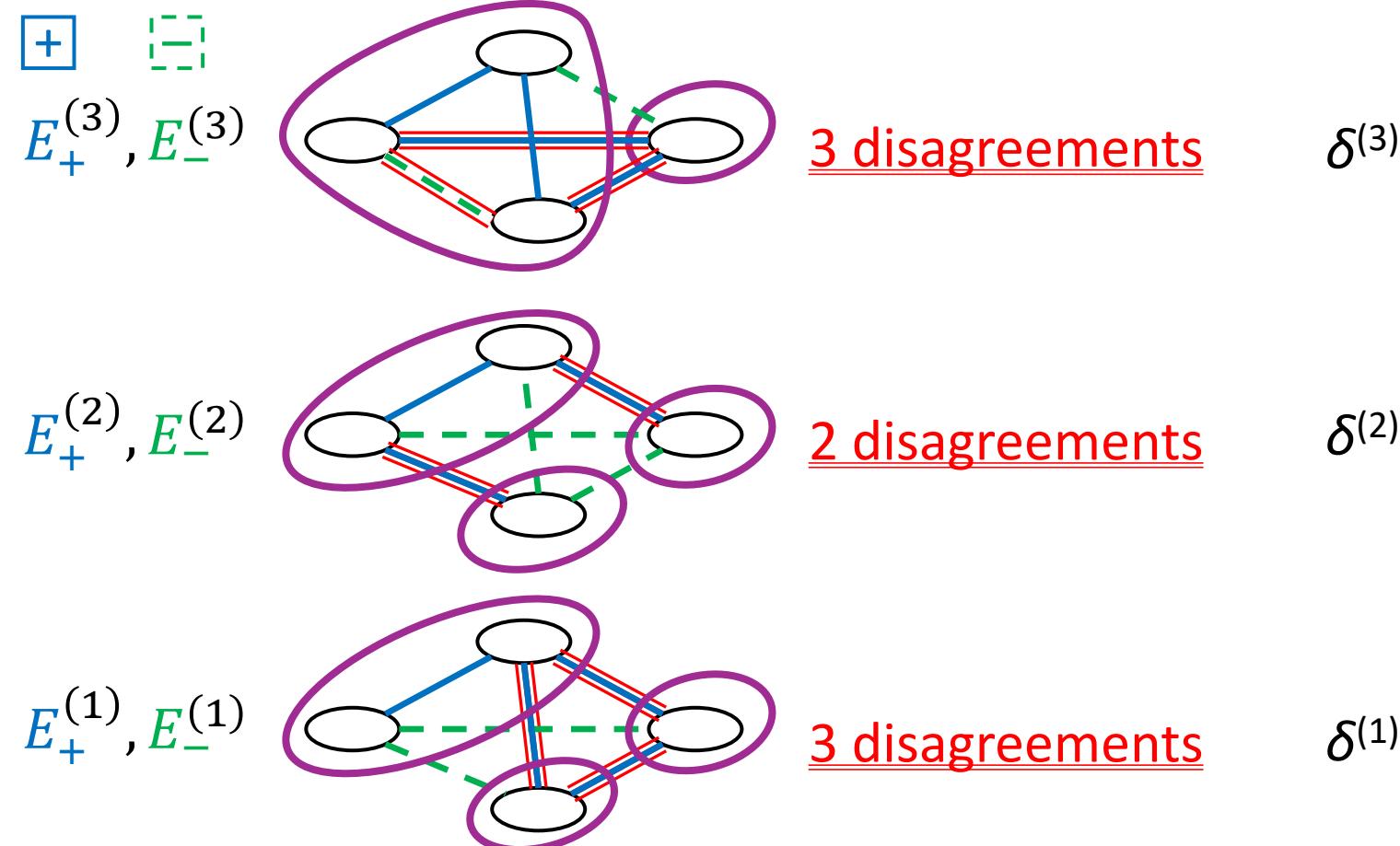
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$\delta^{(3)}$

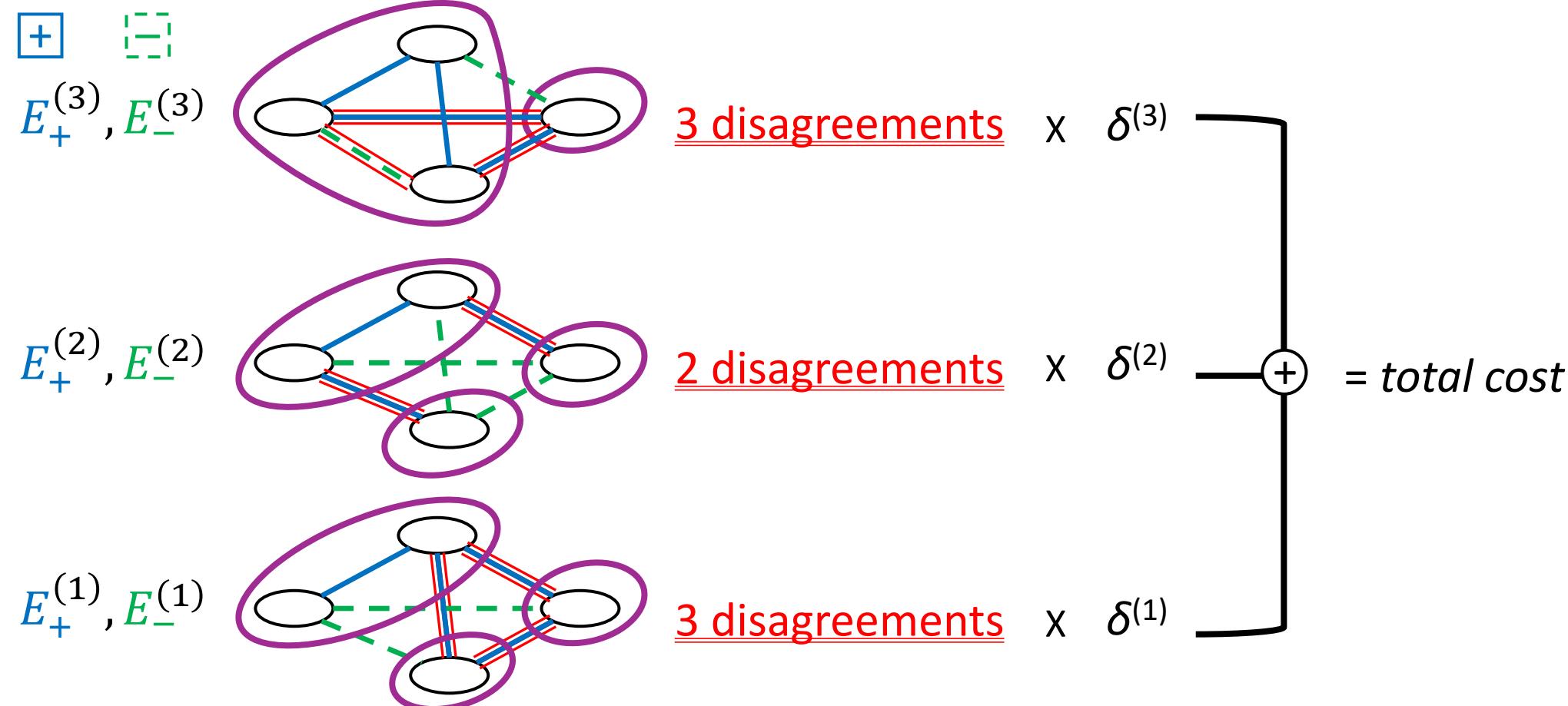
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  - Ailon and Charikar (2005)
  - Cohen-Addad, Das, Kipouridis, Parotsidis, and Thorup (2021)

# Ultrametric Fitting

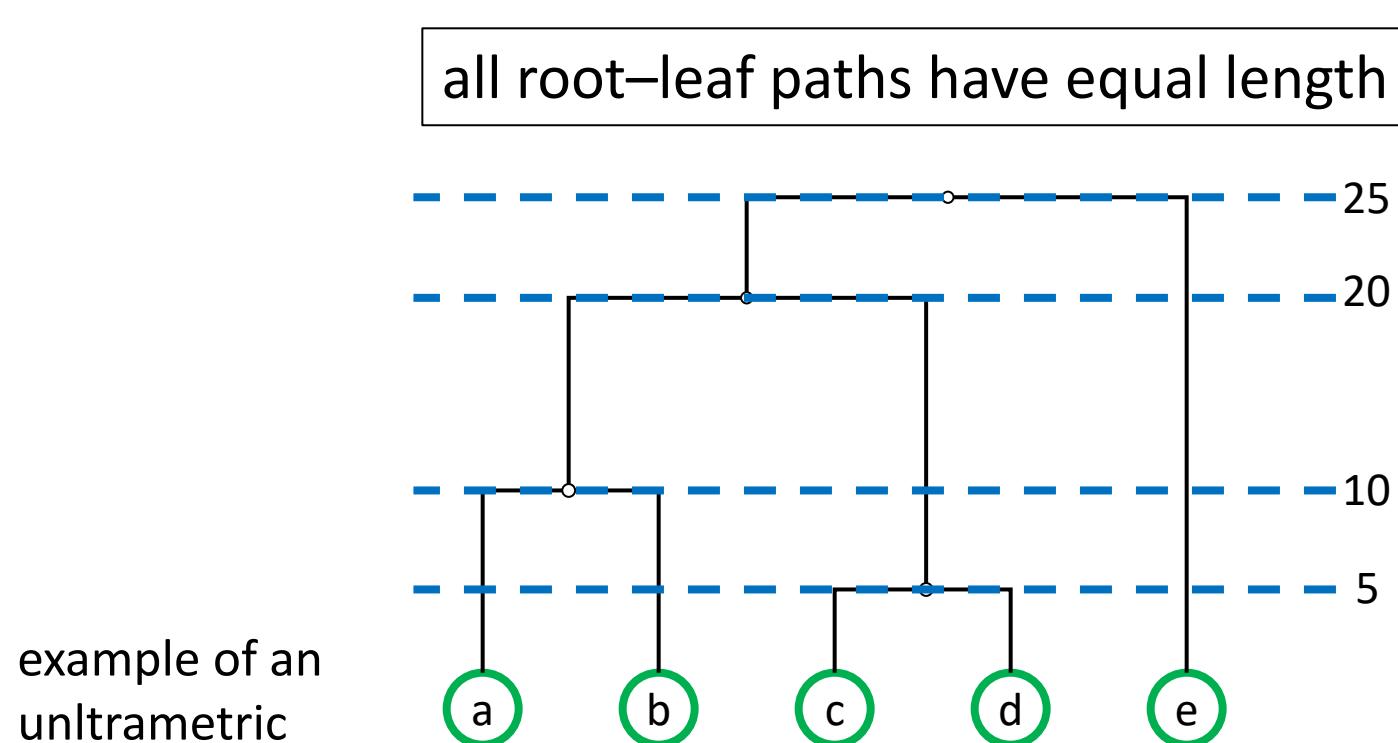
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- Extensively studied since 1960s [Sneath and Sokal, 1962], [Cavalli-Sforza and Edwards, 1967], [Farris, 1972], [Agarwala, Bafna, Farach, Paterson, and Thorup, 1996]
  - Numerical taxonomy, phylogeny reconstruction

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- **$L_1$  Ultrametric Fitting:** best fit  $\equiv$  minimize  $\|D - T\|_1$  —  $\sum_{ij} |D(i,j) - T(i,j)|$
- **$L_0$  Ultrametric Fitting:** best fit  $\equiv$  minimize  $\|D - T\|_0$  —  $\sum_{ij} \mathbb{I}[D(i,j) \neq T(i,j)]$

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(special case of HCC)

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# Previous results on $L_1$ Ultrametric Fitting/HCC

- APX-hard  $k := \#\text{distinct distances in the input distance function } D$
- $\min\{n, O(k \log n)\}$ -approximation for  $L_1$  Ultrametric Fitting
  - Harb, Kannan, and McGregor (APPROX 2005)
- $\min\{k+2, O(\log n \log \log n)\}$ -approximation for  $L_1$  Ultrametric Fitting
  - Ailon and Charikar (FOCS 2005; SIAM J. Comput. 2011)
- first  $O(1)$ -approximation for HCC
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# Our results on HCC

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- **Our result: 25.7846-approximation for HCC**

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- **Our result: (simple) 5-approximation**

# Our Algorithm for HCC

# Standard LP

[Ailon and Charikar, 2005]

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- “Distance” variable  $x_{ij}^{(t)}$  for all  $ij \in E, t \in [\ell]$ 
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- LP relaxation

$$\sum_{ij \in E_+^{(t)}} x_{ij}^{(t)} + \sum_{ij \in E_-^{(t)}} (1 - x_{ij}^{(t)})$$

(fractional) number of disagreements (at layer  $t$ )

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- minimize  $\sum_{t \in [\ell]} \delta^{(t)} \left( \sum_{ij \in E_+^{(t)}} x_{ij}^{(t)} + \sum_{ij \in E_-^{(t)}} (1 - x_{ij}^{(t)}) \right)$

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  - subject to  $x$  satisfies the triangle inequalities for each layer  
 $x$  is monotone w.r.t. layers  
 $x \in [0, 1]$

# Notations

- $\tilde{x}$  : an optimal LP solution
- $\tilde{x}_{ij}^{(t)}$ : the *distance* of  $ij$  at layer  $t$

# Useful Lemma

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- **Lemma.**  $\#(\text{green edges at layer } t \text{ with dist} < 1)$

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“Disregarding edges with distance < 1 in each layer  
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  - Proved using complementary slackness & weak duality

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only incurs an additive factor of 1”

# Algorithm Overview

- Construct a *pre-clustering*  $Q^{(t)}$  for each layer  $t$   
(partition)

$\tilde{x}_e^{(t)}$ : distance of  $e$  (at layer  $t$ )

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(Fix layer  $t$ )

$\mathcal{Q} \leftarrow \{V\}$

while there is  $Q \in \mathcal{Q}$  whose diameter is *large*,

split  $Q$  into two so that #(edges separated & dist < 1) is *small*

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split  $Q$  into two so that #(edges separated & dist < 1) is *small*

- **small-diameter property:** every  $pre-cluster$  has a small diameter
- **few-separated-edges property:** #(edges separated by  $\mathcal{Q}$  & dist < 1) is small

# Algorithm Overview

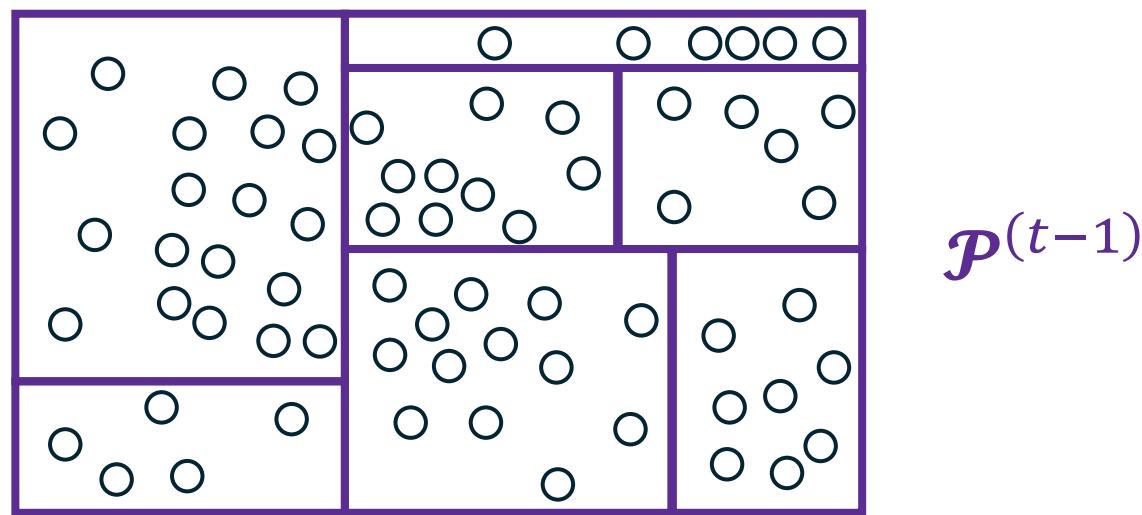
- Construct a *pre-clustering*  $Q^{(t)}$  for each layer  $t$
  - Construct hierarchical clusterings bottom-up:  
(at layer  $t$ ) construct the *clustering*  $\mathcal{P}^{(t)}$  by only merging clusters in  $\mathcal{P}^{(t-1)}$
- ${}^*\mathcal{P}^{(0)} := \{ \{u\}: u \in V \}$

# Algorithm Overview

- Construct a *pre-clustering*  $Q^{(t)}$  for each layer  $t$
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$${}^*\mathcal{P}^{(0)} := \{ \{u\}: u \in V \}$$
  
Hierarchical constraints satisfied!

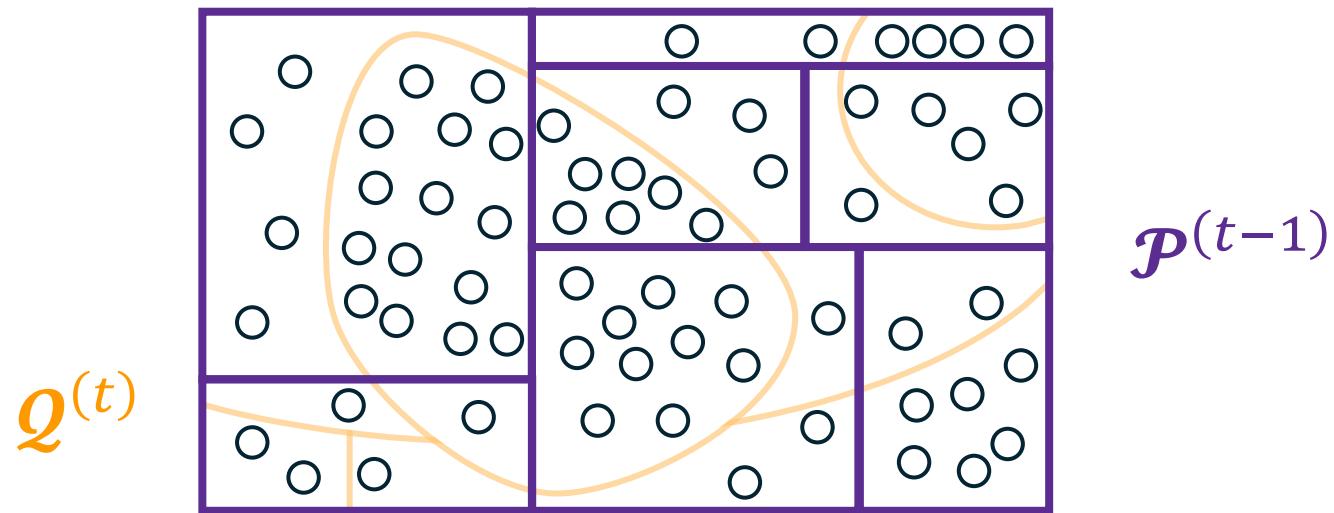
# Algorithm Overview

(Fix layer  $t$ )



# Algorithm Overview

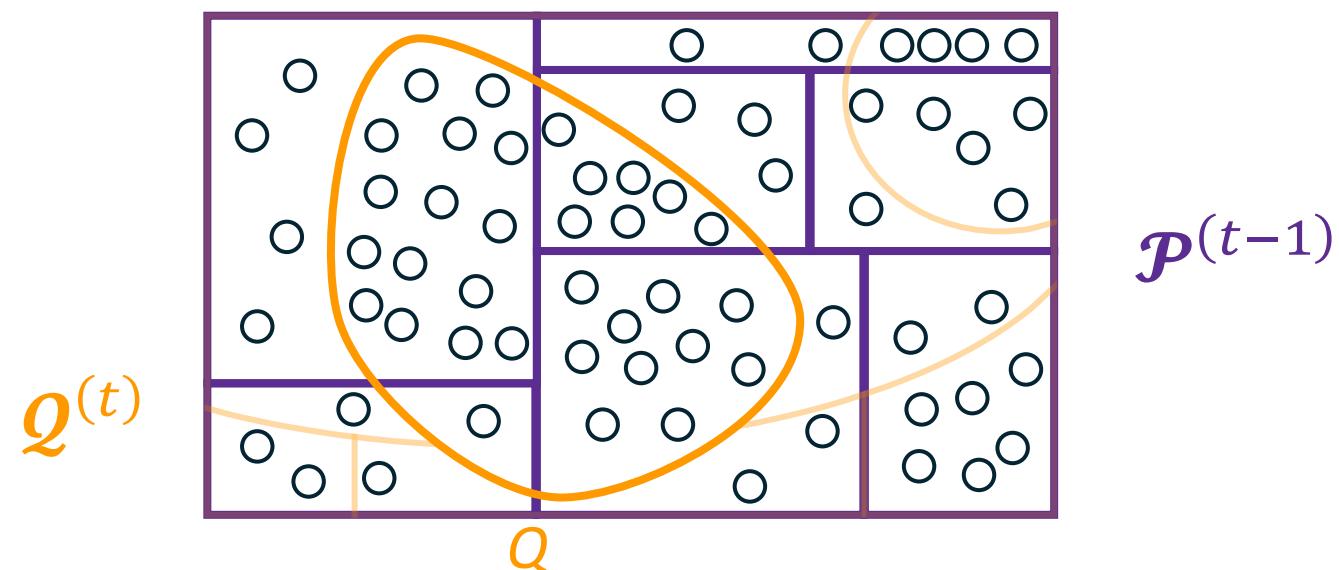
(Fix layer  $t$ )



# Algorithm Overview

(Fix layer  $t$ )

for each pre-cluster  $Q$  at layer  $t$ ,

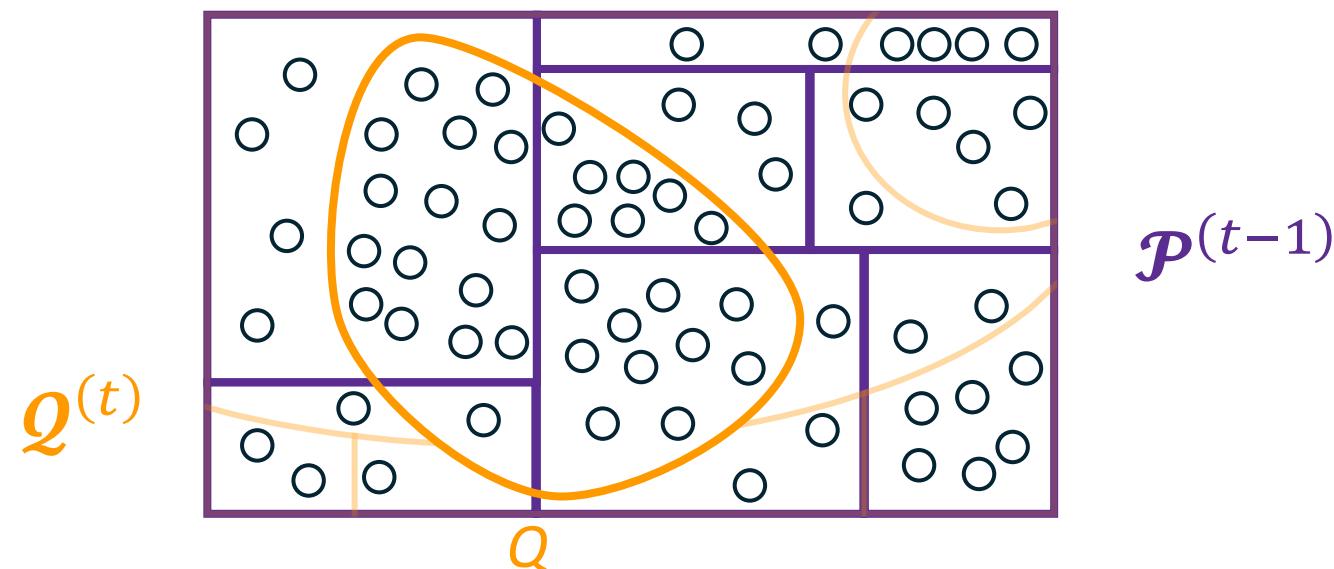


# Algorithm Overview

(Fix layer  $t$ )

for each pre-cluster  $Q$  at layer  $t$ ,

find all  $P' \in \mathcal{P}^{(t-1)}$  that satisfy a *merging condition* with pre-cluster  $Q$



# Algorithm Overview

(Fix layer  $t$ )

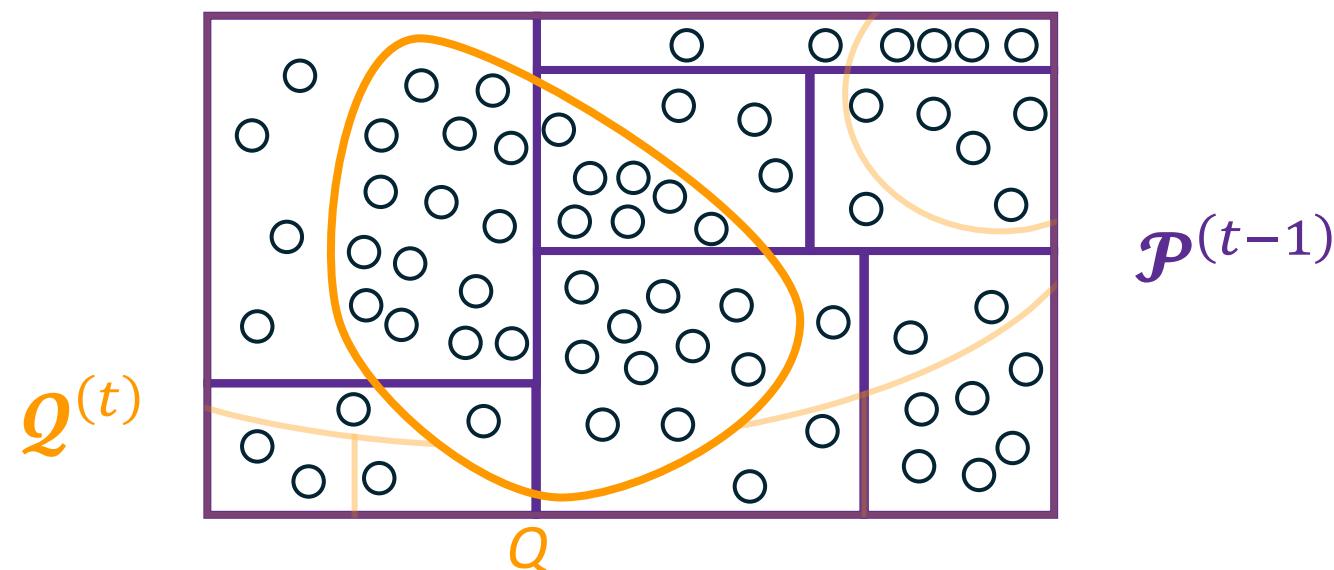
(roughly)

**merging condition:**

most points in  $P'$  are in  $P' \cap Q$

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# Algorithm Overview

(Fix layer  $t$ )

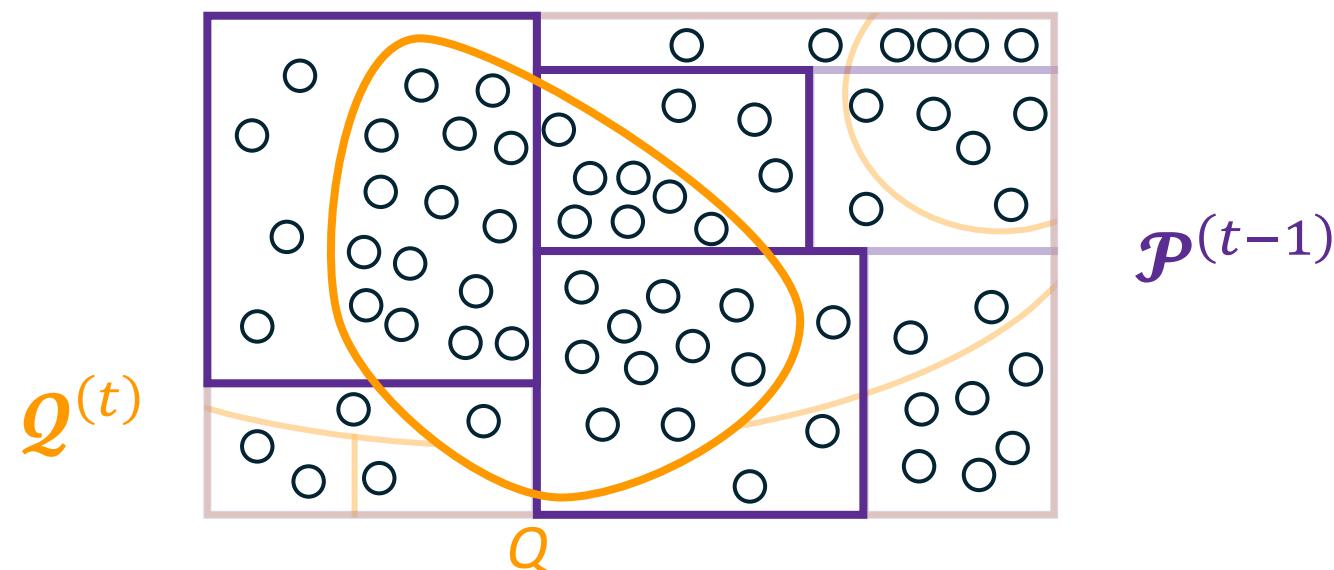
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# Algorithm Overview

(Fix layer  $t$ )

(roughly)

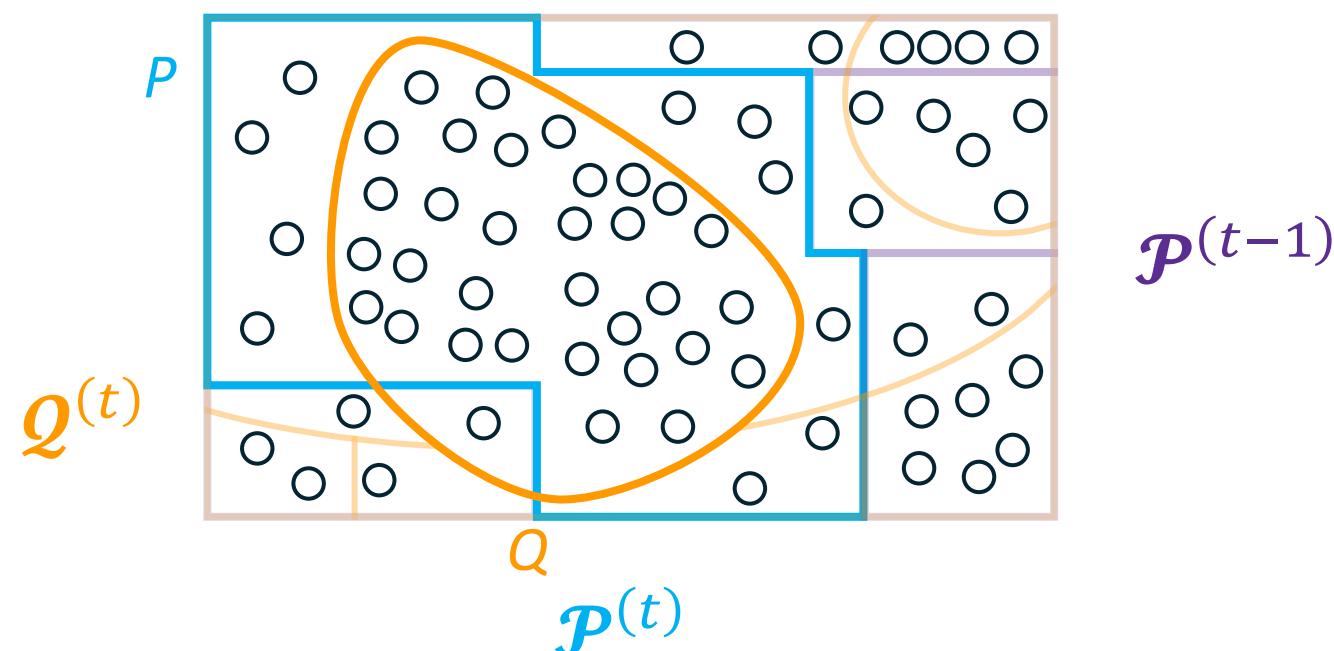
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# Algorithm Overview

(Fix layer  $t$ )

(roughly)

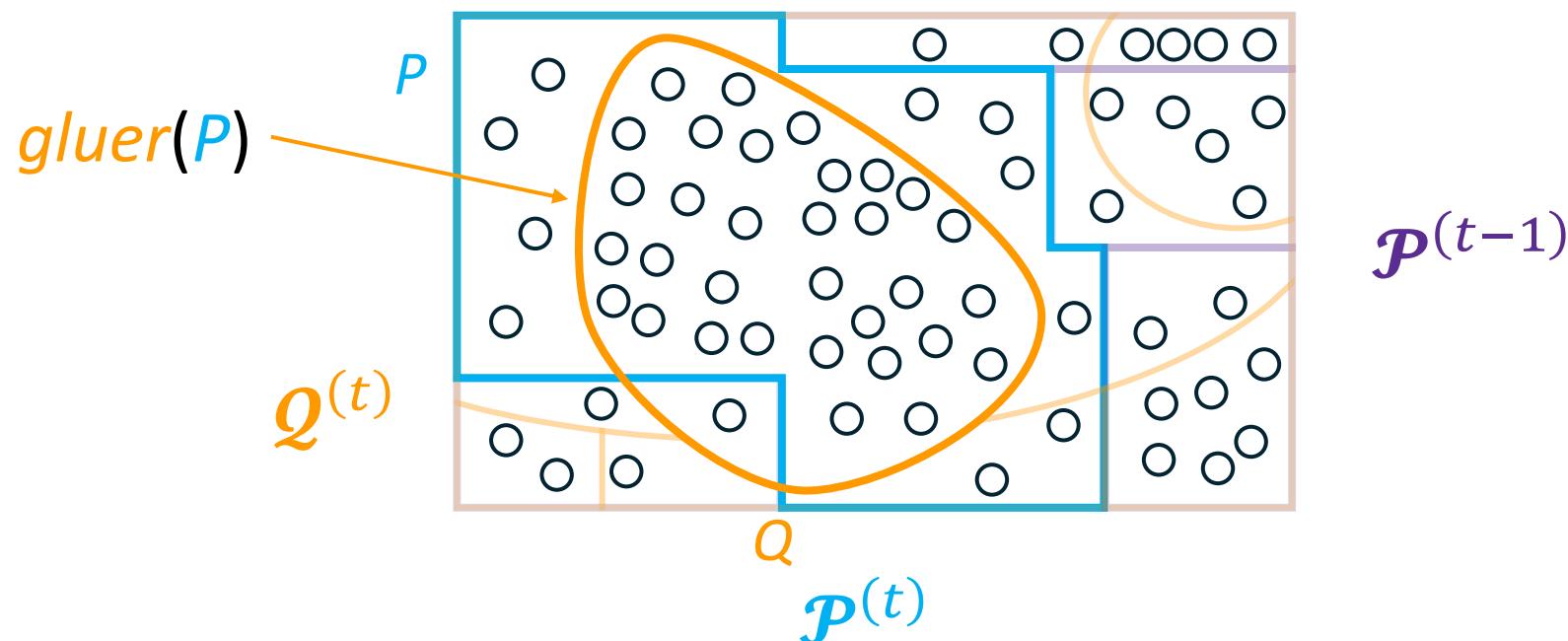
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# Algorithm Overview

(Fix layer  $t$ )

(roughly)

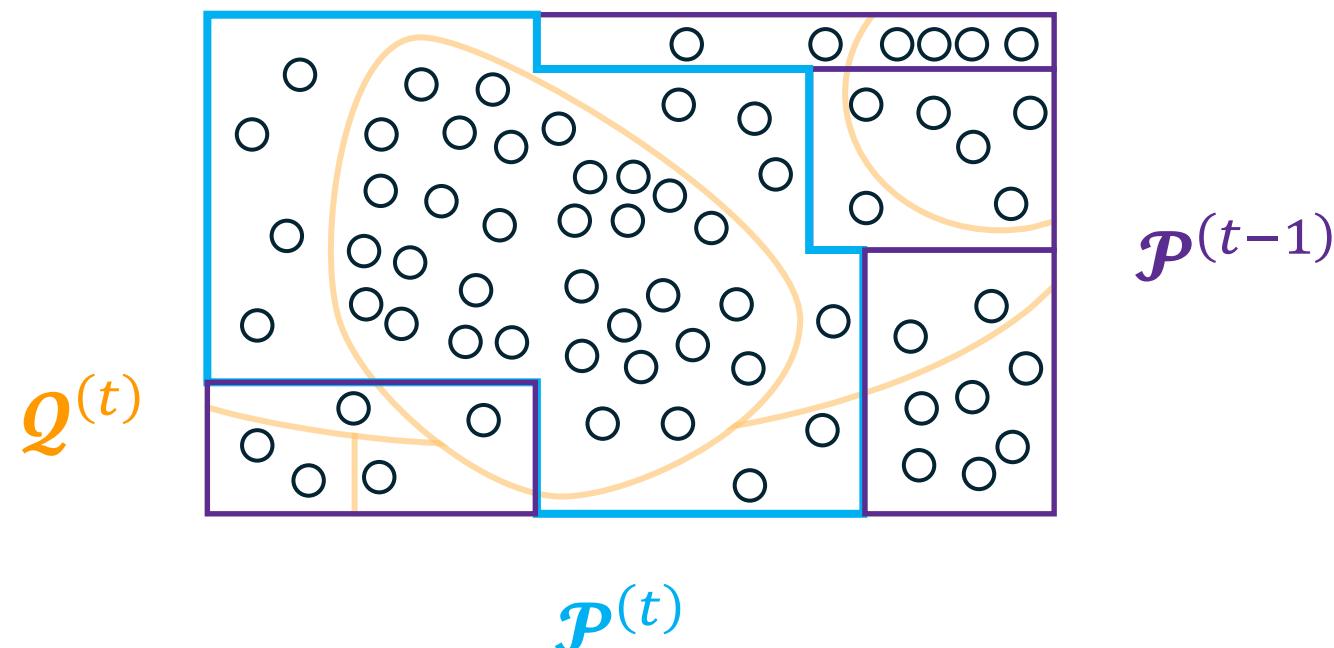
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# Algorithm Overview

(Fix layer  $t$ )

(roughly)

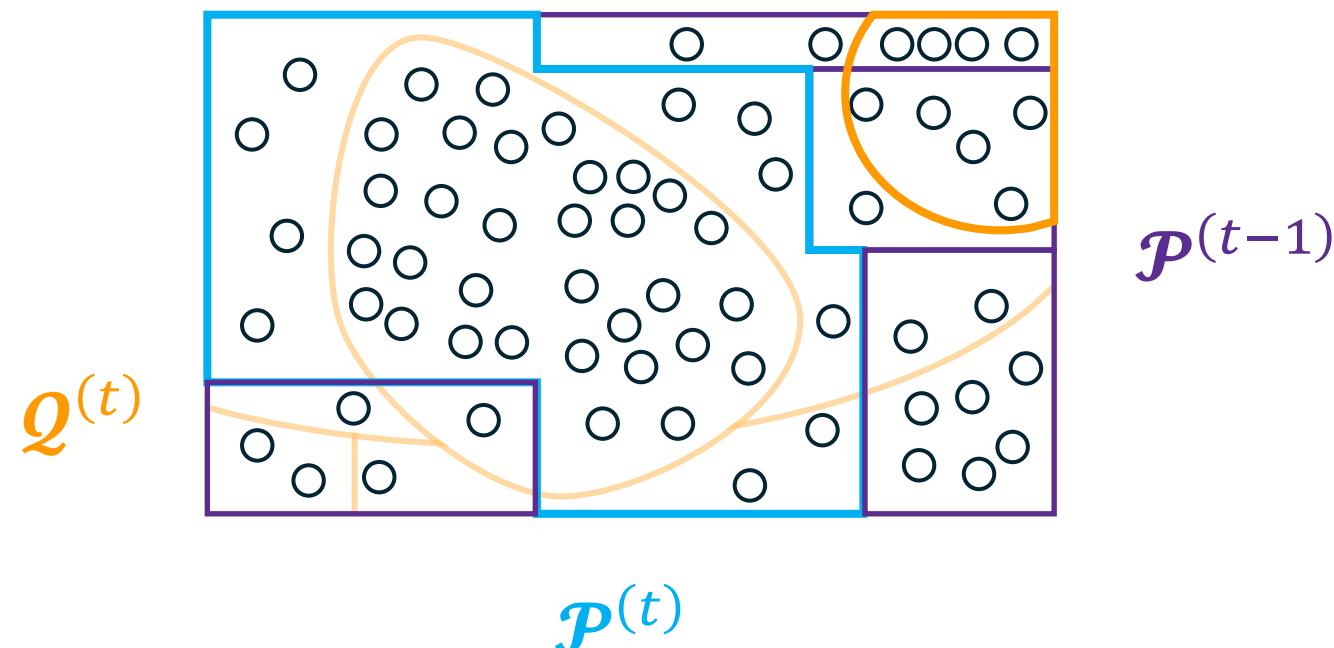
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# Algorithm Overview

(Fix layer  $t$ )

(roughly)

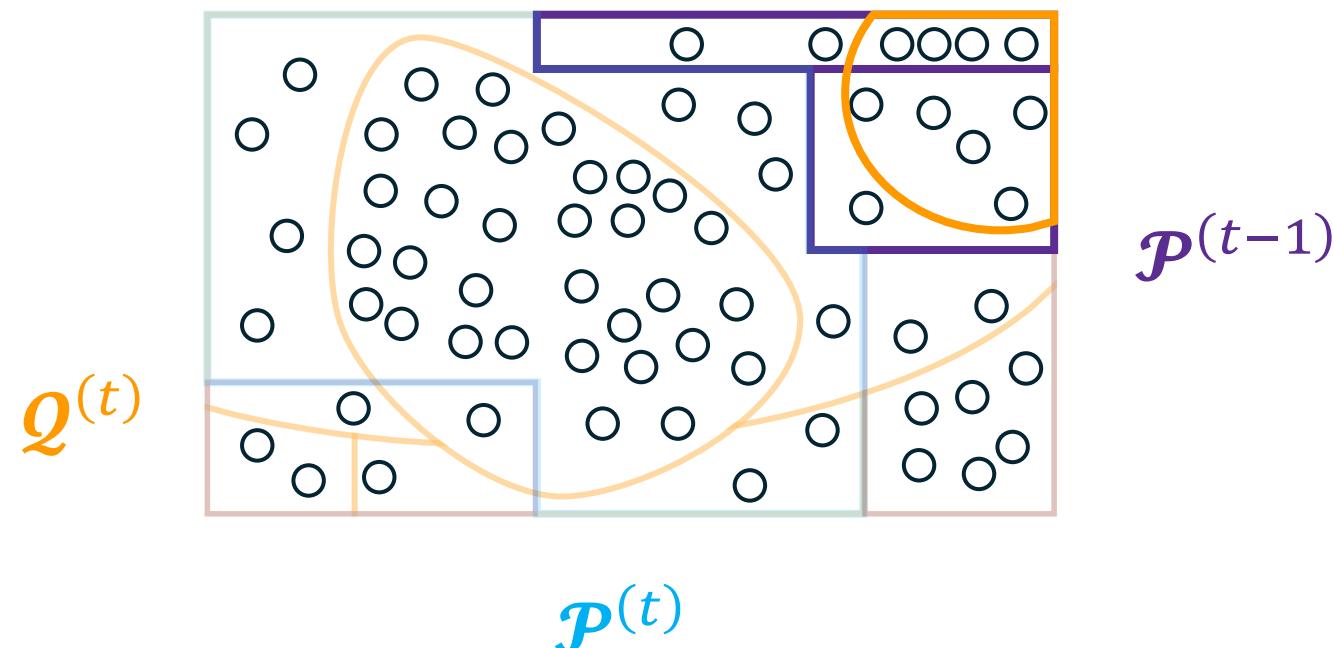
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(Fix layer  $t$ )

(roughly)

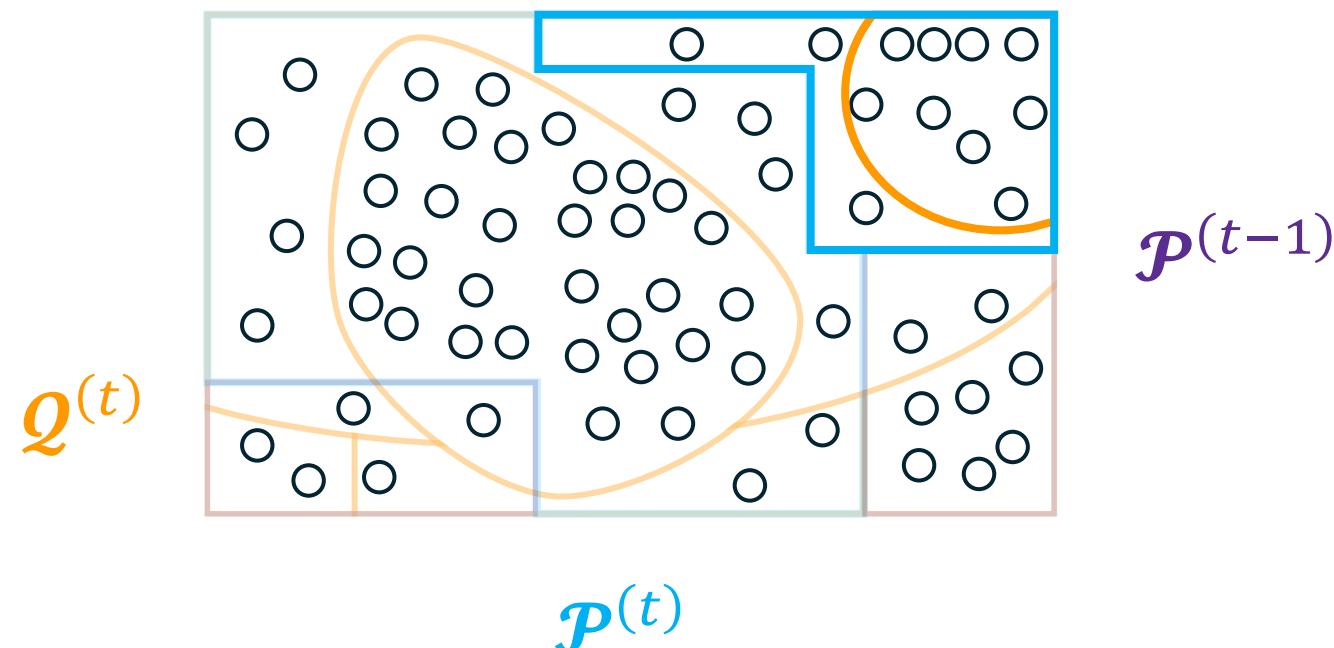
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# Algorithm Overview

(Fix layer  $t$ )

(roughly)

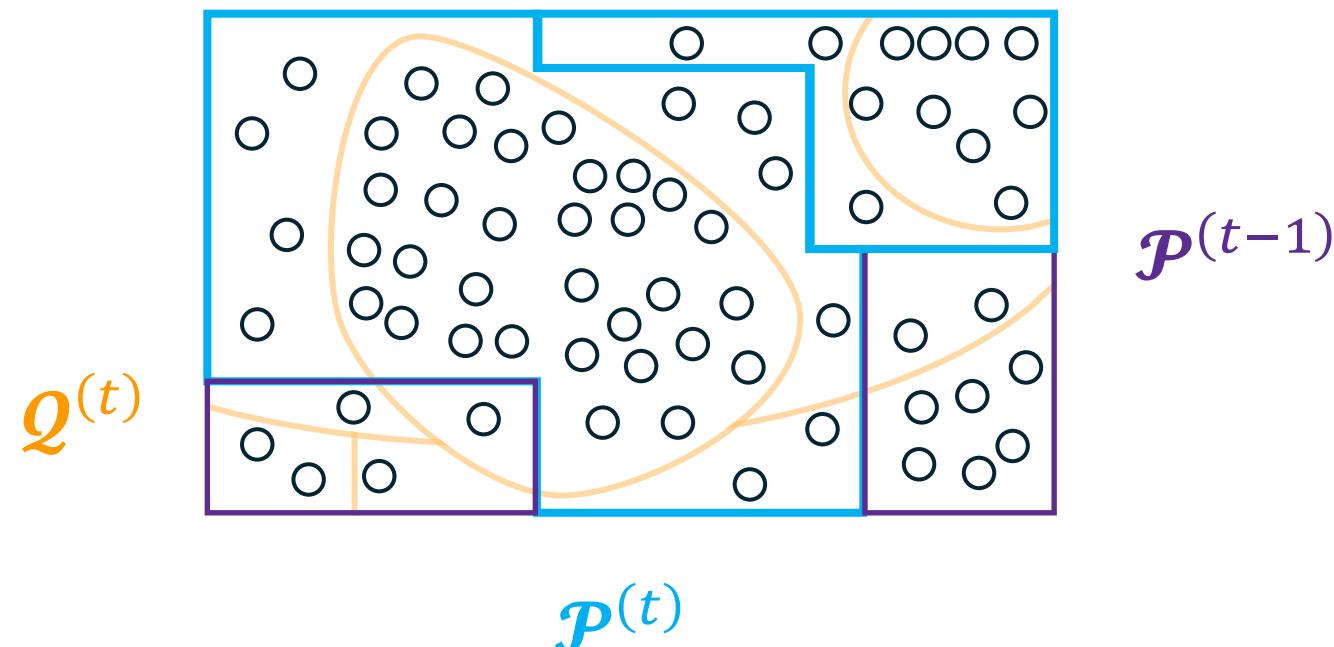
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# Algorithm Overview

(Fix layer  $t$ )

(roughly)

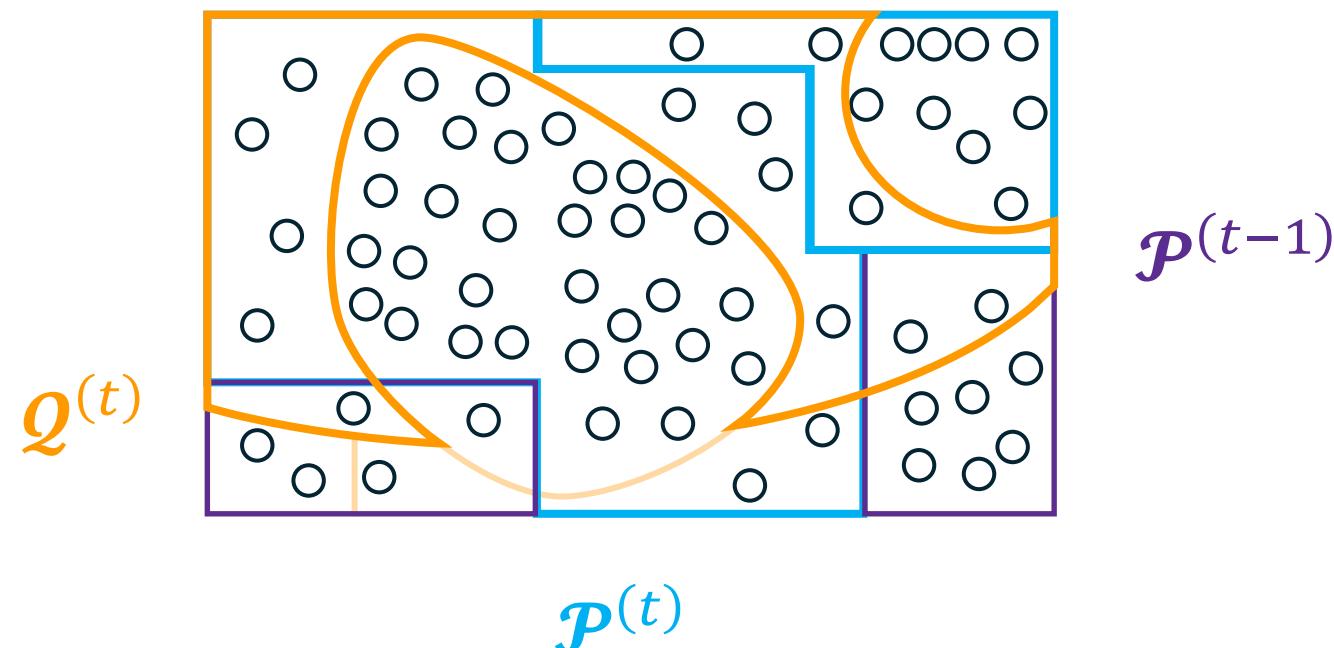
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(Fix layer  $t$ )

(roughly)

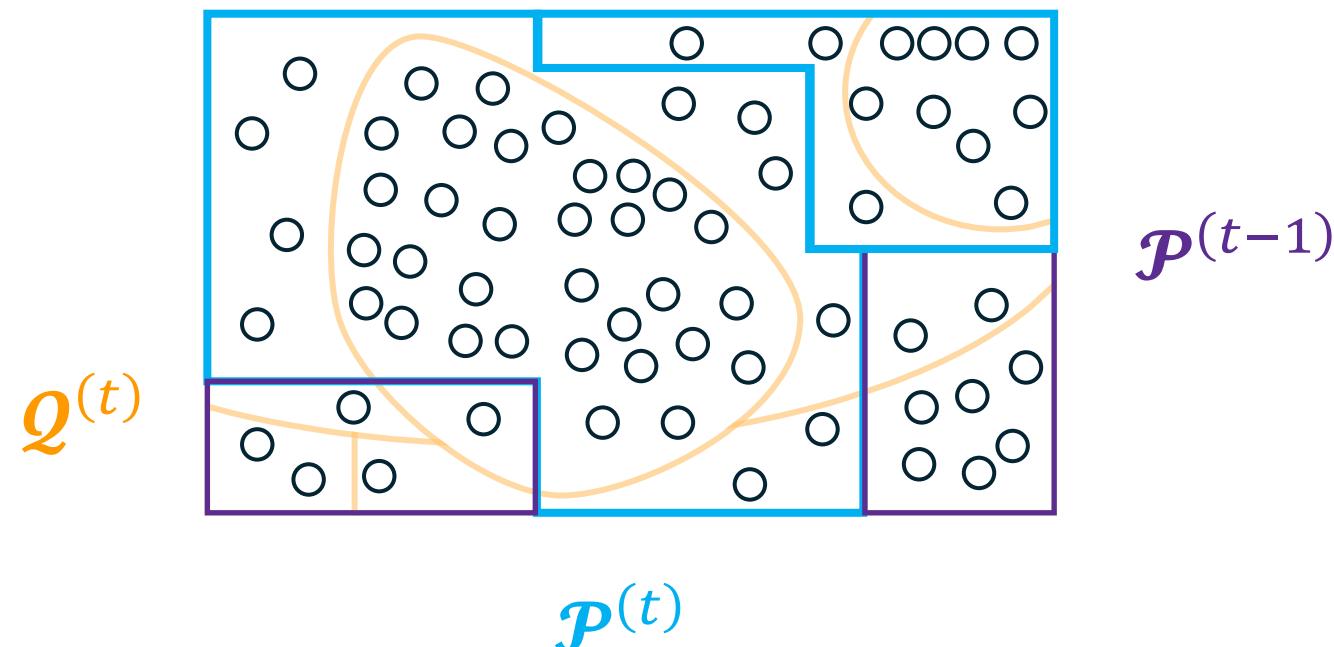
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# Algorithm Overview

(Fix layer  $t$ )

(roughly)

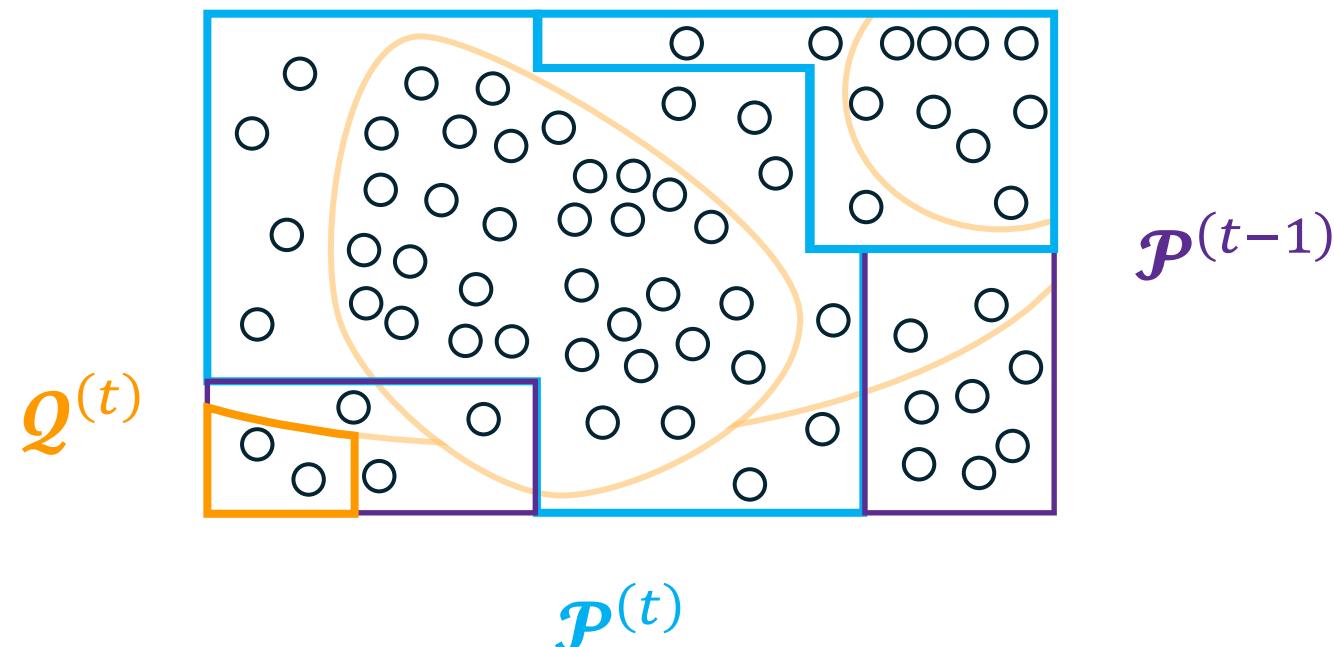
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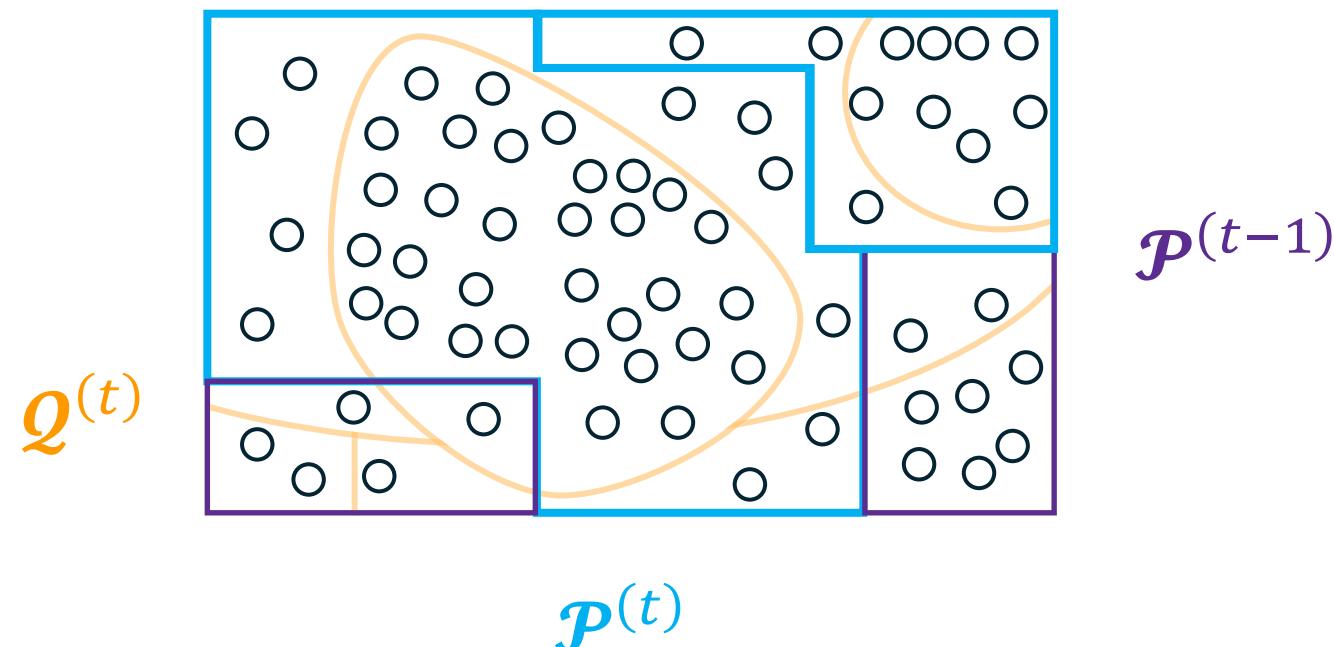
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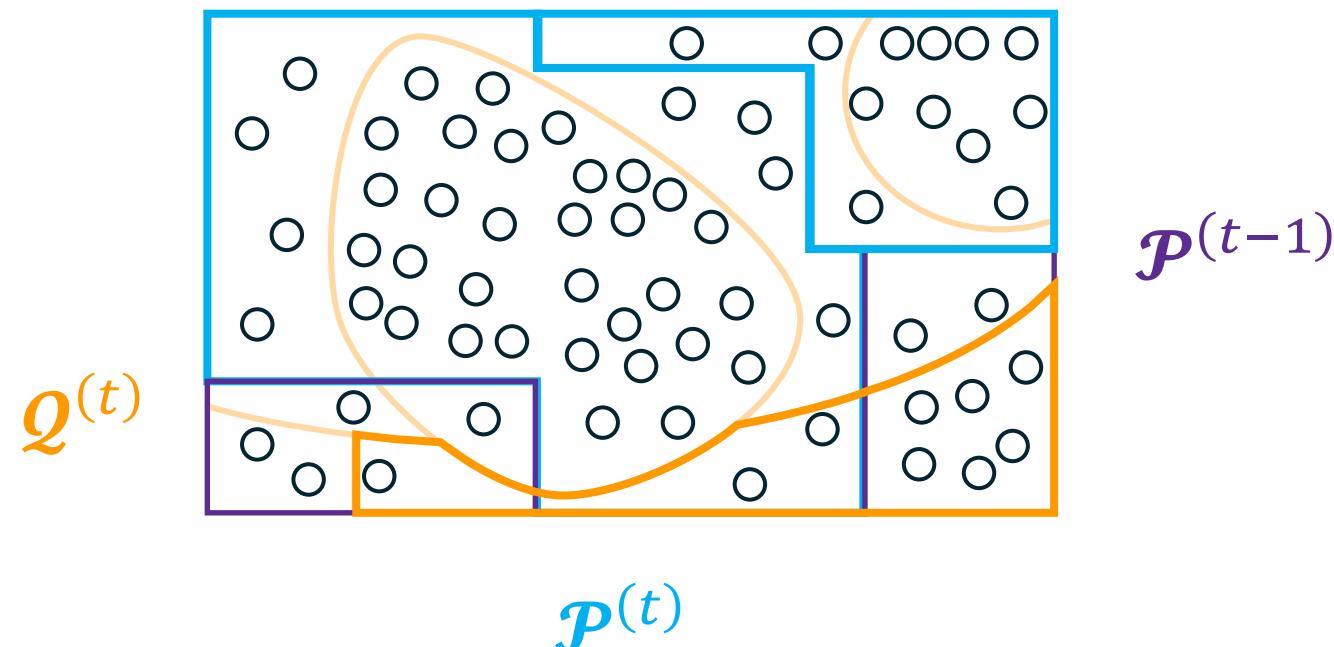
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# Algorithm Overview

(Fix layer  $t$ )

(roughly)

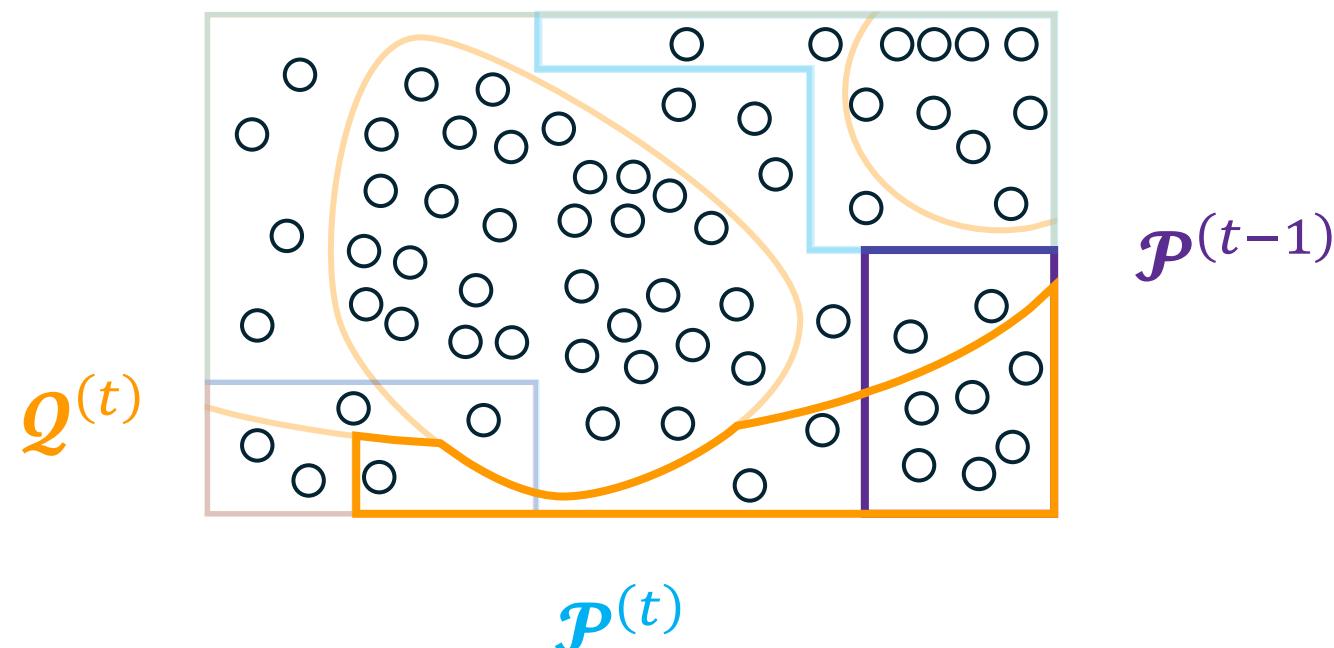
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# Algorithm Overview

(Fix layer  $t$ )

(roughly)

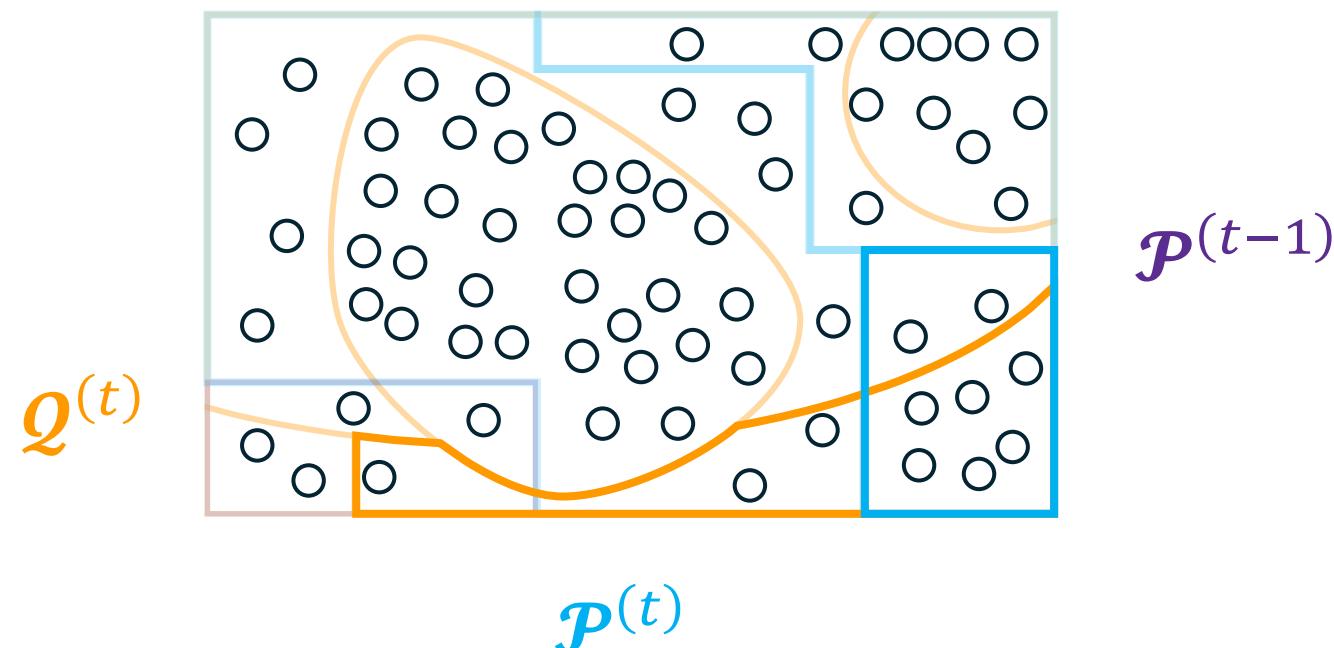
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# Algorithm Overview

(Fix layer  $t$ )

(roughly)

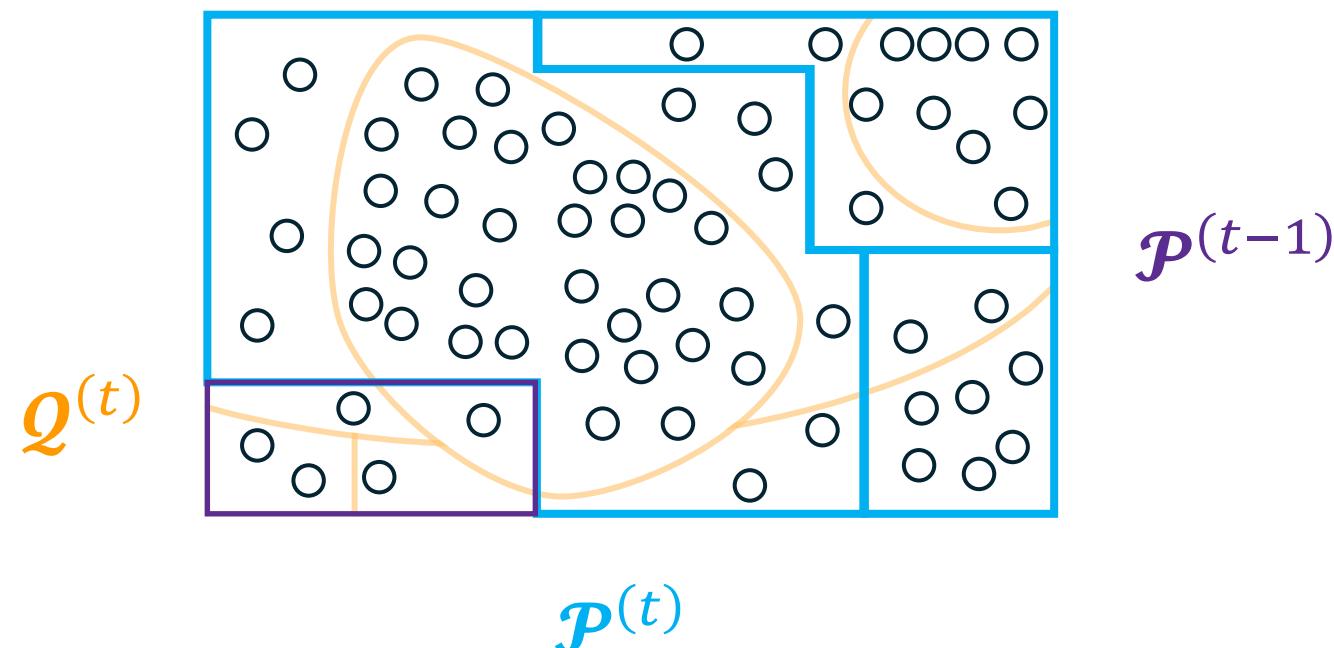
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# Algorithm Overview

(Fix layer  $t$ )

(roughly)

**merging condition:**

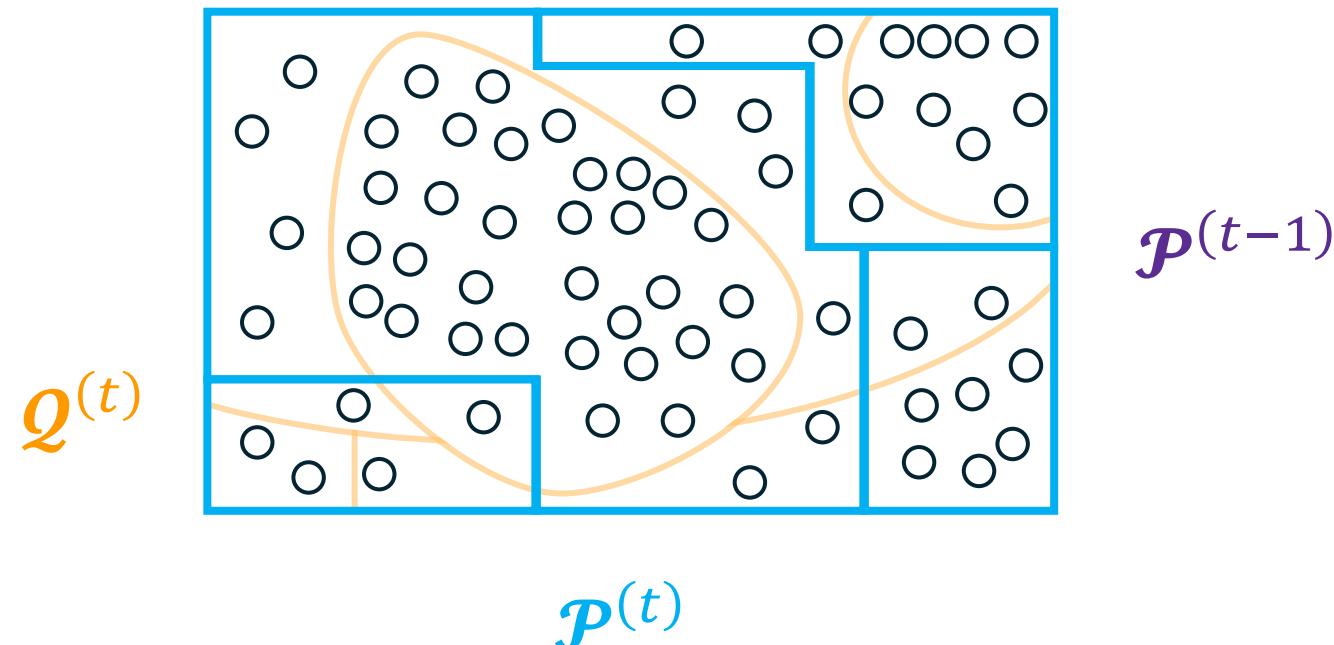
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add all remaining unmerged clusters  $P' \in \mathcal{P}^{(t-1)}$  to  $\mathcal{P}^{(t)}$



# Algorithm Overview

(Fix layer  $t$ )

(roughly)

**merging condition:**

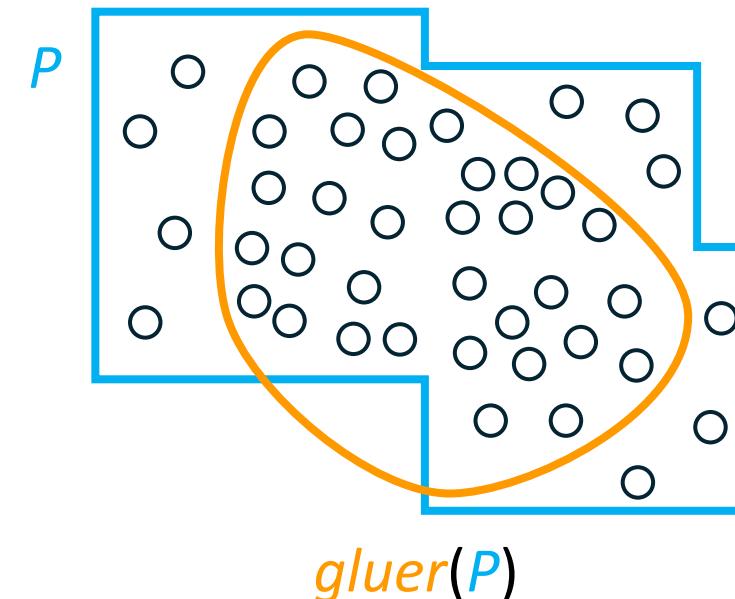
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let  $P$  be the merged cluster; add  $P$  to  $\mathcal{P}^{(t)}$

add all remaining unmerged clusters  $P' \in \mathcal{P}^{(t-1)}$  to  $\mathcal{P}^{(t)}$



- **concentration property:**  
most points in  $P$  are in  $P \cap \text{gluer}(P)$

# Analysis

# Analysis Overview

(Fix layer  $t$ )

- #(disagreements)

$$\leq O(1) \cdot \left( \sum_{ij \in E_+^{(t)}} x_{ij}^{(t)} + \sum_{ij \in E_-^{(t)}} (1 - x_{ij}^{(t)}) \right)$$

LP value at layer  $t$

# Analysis Overview

(Fix layer  $t$ )

- #(disagreements)

$$\leq O(1) \cdot \left( \sum_{ij \in E_+^{(t)}} x_{ij}^{(t)} + \sum_{ij \in E_-^{(t)}} (1 - x_{ij}^{(t)}) \right)$$

LP value at layer  $t$

Objective:  $\sum_{t \in [\ell]} \delta^{(t)} \left( \sum_{ij \in E_+^{(t)}} x_{ij}^{(t)} + \sum_{ij \in E_-^{(t)}} (1 - x_{ij}^{(t)}) \right)$

$\tilde{x}_e^{(t)}$ : distance of  $e$  (at layer  $t$ )

# Analysis Overview

(Fix layer  $t$ )

- #(disagreements) disregarding – edges with  $\text{dist} < 1$ ) **(Useful Lemma)**

$$\leq O(1) \cdot \left( \sum_{ij \in E_+^{(t)}} x_{ij}^{(t)} + \sum_{ij \in E_-^{(t)}} (1 - x_{ij}^{(t)}) \right)$$

$\tilde{x}_e^{(t)}$ : distance of  $e$  (at layer  $t$ )

# Analysis Overview

(Fix layer  $t$ )

- #(disagreements) disregarding – edges with  $\text{dist} < 1$ ) **(Useful Lemma)**

$$\leq O(1) \cdot \#(\text{edges separated by } Q \text{ & } \text{dist} < 1)$$

$$\leq O(1) \cdot \left( \sum_{ij \in E_+^{(t)}} x_{ij}^{(t)} + \sum_{ij \in E_-^{(t)}} (1 - x_{ij}^{(t)}) \right) \quad \text{(few-separated-edges property)}$$

# Analysis Overview

(Fix layer  $t$ )

- #(disagreements disregarding – edges with  $\text{dist} < 1$ )

(Useful Lemma)

Want:

$$\leq O(1) \cdot \#(\text{edges separated by } Q \text{ & } \text{dist} < 1)$$

$$\leq O(1) \cdot \left( \sum_{ij \in E_+^{(t)}} x_{ij}^{(t)} + \sum_{ij \in E_-^{(t)}} (1 - x_{ij}^{(t)}) \right) \quad (\text{few-separated-edges property})$$

$$\tilde{x}_e^{(t)}: \text{distance of } e \text{ (at layer } t\text{)}$$

# Analysis Overview

(Fix layer  $t$ )

- #(disagreements) disregarding – edges with  $\text{dist} < 1$ )

①: #(– edges clustered in  $\mathcal{P}$  &  $\text{dist} = 1$ )

②: #(+ edges separated by  $\mathcal{P}$ )

Want:

$$\boxed{\textcircled{1} + \textcircled{2} \leq O(1) \cdot \#(\text{edges separated by } \mathcal{Q} \text{ & } \text{dist} < 1)}$$

$\tilde{x}_e^{(t)}$ : distance of  $e$  (at layer  $t$ )

# Analysis Overview

(Fix layer  $t$ )

- #(disagreements) disregarding – edges with  $\text{dist} < 1$ )

①: #(– edges clustered in  $\mathcal{P}$  &  $\text{dist} = 1$ )

②: #(+ edges separated by  $\mathcal{P}$ )

①  $\leq O(1) \cdot \#(\text{edges separated by } \mathcal{Q} \text{ & } \text{dist} < 1 \text{ & clustered in } \mathcal{P})$

+ ) ②  $\leq O(1) \cdot \#(\text{edges separated by } \mathcal{Q} \text{ & } \text{dist} < 1 \text{ & separated by } \mathcal{P})$

Want:

① + ②  $\leq O(1) \cdot \#(\text{edges separated by } \mathcal{Q} \text{ & } \text{dist} < 1)$

$\tilde{x}_e^{(t)}$ : distance of  $e$  (at layer  $t$ )

# Analysis Overview

(Fix layer  $t$ )

- #(disagreements) disregarding – edges with  $\text{dist} < 1$ )

- ①: #(- edges clustered in  $\mathcal{P}$  &  $\text{dist} = 1$ )
- ②: #(+ edges separated by  $\mathcal{P}$ )

Our focus: ①  $\leq O(1) \cdot \#(\text{edges separated by } \mathcal{Q} \text{ & } \text{dist} < 1 \text{ & clustered in } \mathcal{P})$

+ ) ②  $\leq O(1) \cdot \#(\text{edges separated by } \mathcal{Q} \text{ & } \text{dist} < 1 \text{ & separated by } \mathcal{P})$

Want:

① + ②  $\leq O(1) \cdot \#(\text{edges separated by } \mathcal{Q} \text{ & } \text{dist} < 1)$

$\tilde{x}_e^{(t)}$ : distance of  $e$  (at layer  $t$ )

# Analysis Overview

 (Fix layer  $t$ )

Our focus: #(- edges clustered in  $\mathcal{P}$  & dist = 1)

$$\leq O(1) \cdot \#(\text{edges clustered in } \mathcal{P} \text{ & separated by } \mathcal{Q} \text{ & dist} < 1)$$

$\tilde{x}_e^{(t)}$ : distance of  $e$  (at layer  $t$ )

# Analysis Overview

(Fix layer  $t$ ,  $P \in \mathcal{P}$ )

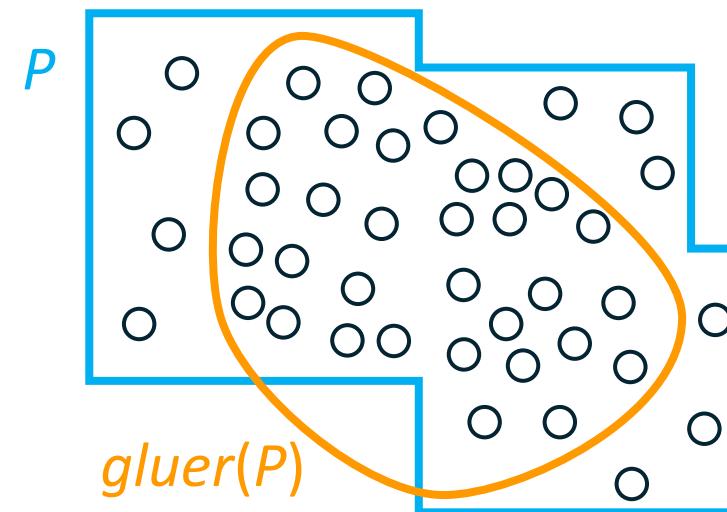
Our focus: #(- edges clustered in  $P$  & dist = 1)

$\leq O(1) \cdot \#(\text{edges clustered in } P \text{ & separated by } Q \text{ & dist} < 1)$

$\tilde{x}_e^{(t)}$ : distance of  $e$  (at layer  $t$ )

# Analysis Overview

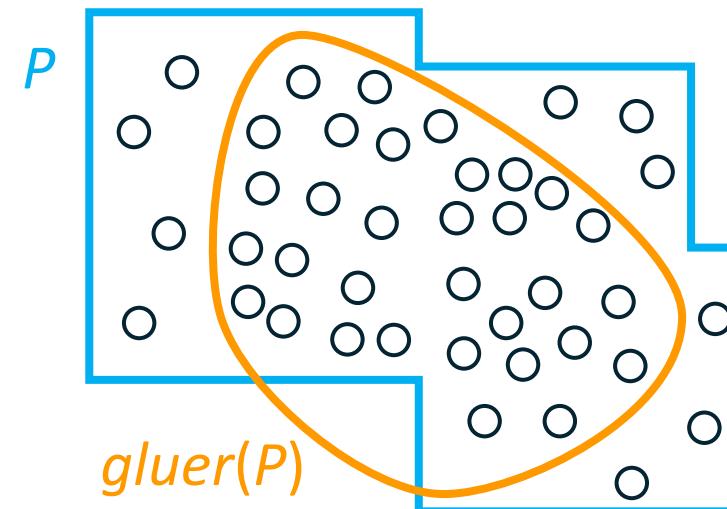
#(- edges clustered in  $P$  & dist = 1)



$$\tilde{x}_e^{(t)}: \text{distance of } e \text{ (at layer } t\text{)}$$

# Analysis Overview

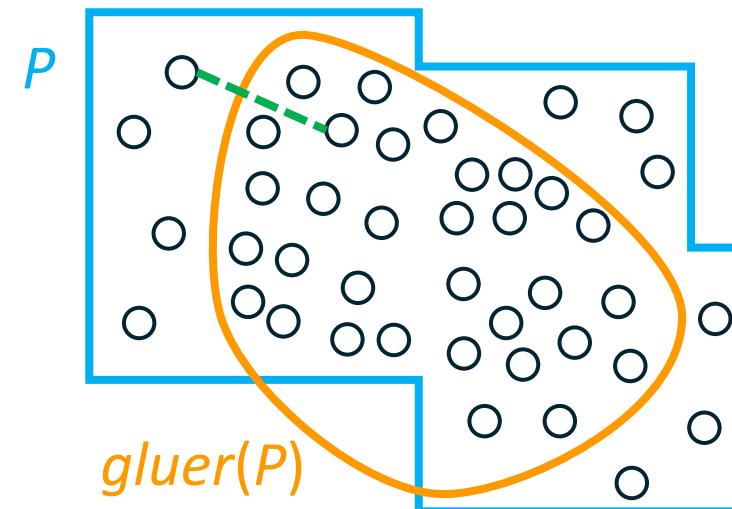
- #(- edges clustered in  $P$ , separated by  $\text{gluer}(P)$  & dist = 1)
- + #(- edges clustered in  $P \setminus \text{gluer}(P)$  & dist = 1)
- #(- edges clustered in  $P \cap \text{gluer}(P)$  & dist = 1)



$\tilde{x}_e^{(t)}$ : distance of  $e$  (at layer  $t$ )

# Analysis Overview

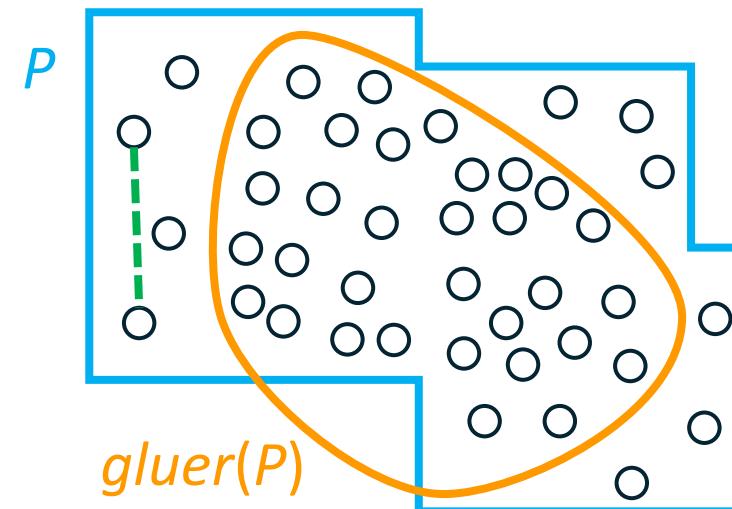
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$$\tilde{x}_e^{(t)}: \text{distance of } e \text{ (at layer } t\text{)}$$

# Analysis Overview

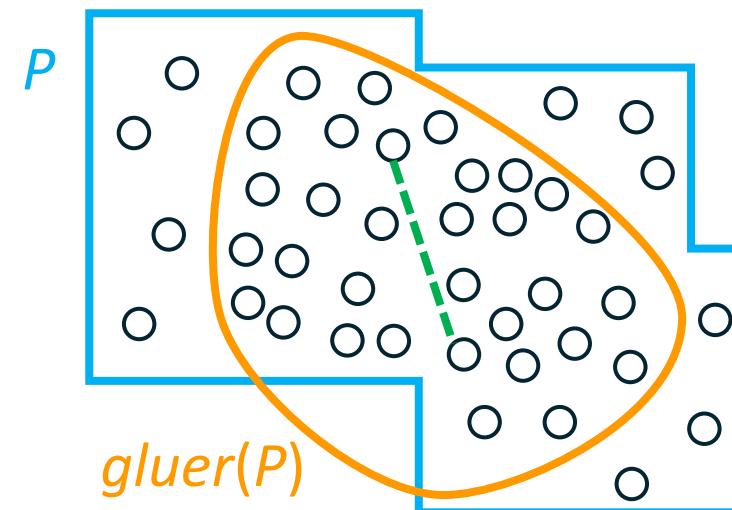
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$\tilde{x}_e^{(t)}$ : distance of  $e$  (at layer  $t$ )

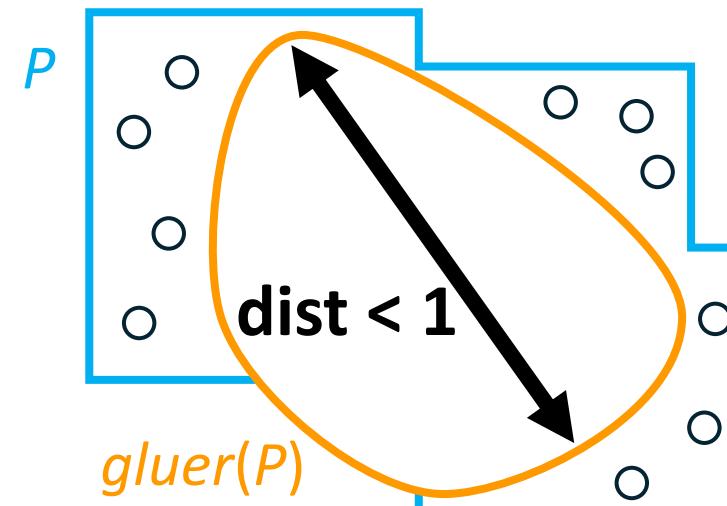
# Analysis Overview

- #(- edges clustered in  $P$ , separated by  $gluer(P)$  & dist = 1)
- + #(- edges clustered in  $P \setminus gluer(P)$  & dist = 1)
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# Analysis Overview

- #(- edges clustered in  $P$ , separated by  $gluer(P)$  &  $dist = 1$ )
- + #(- edges clustered in  $P \setminus gluer(P)$  &  $dist = 1$ )
- #(- edges clustered in  $P \cap gluer(P)$  &  $dist = 1$ ) --- impossible

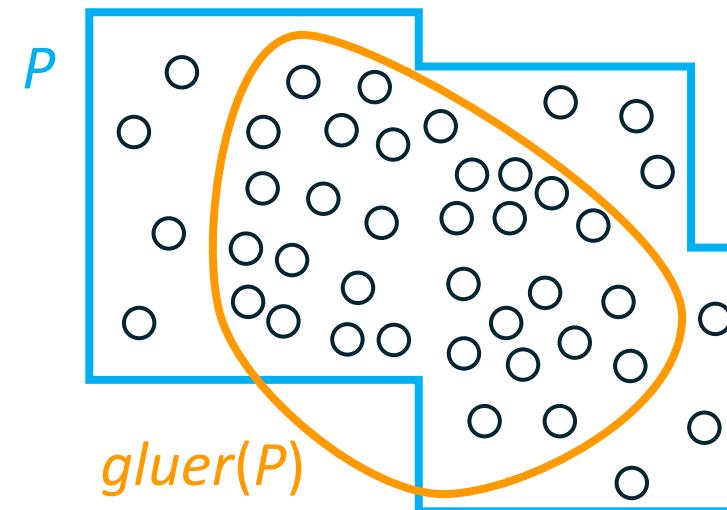


**small-diameter property:**  
every *pre-cluster* has a small diameter

$$\tilde{x}_e^{(t)}: \text{distance of } e \text{ (at layer } t\text{)}$$

# Analysis Overview

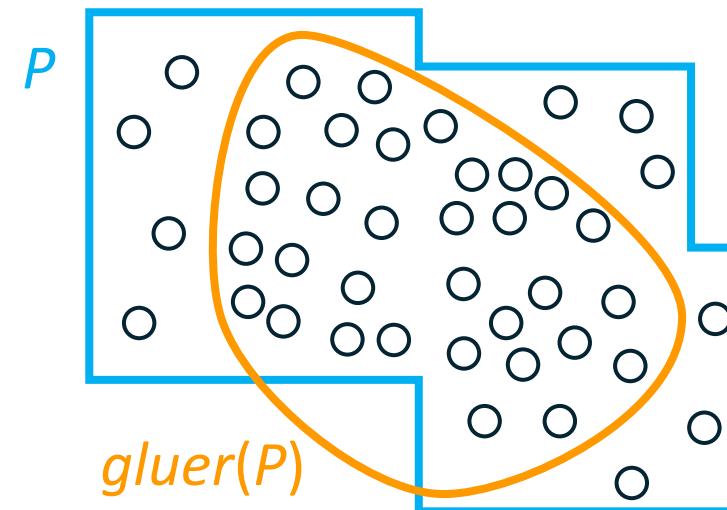
- └ #(- edges clustered in  $P$ , separated by  $gluer(P)$  & dist = 1)
- + #(- edges clustered in  $P \setminus gluer(P)$  & dist = 1)



$$\tilde{x}_e^{(t)}: \text{distance of } e \text{ (at layer } t\text{)}$$

# Analysis Overview

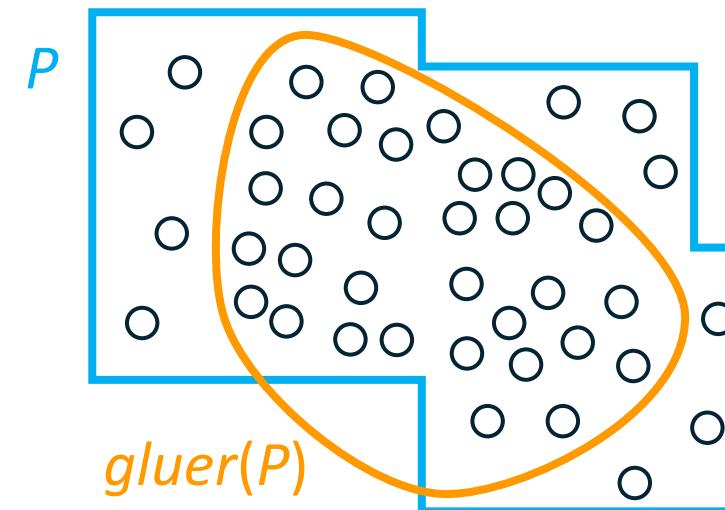
- └ #~~X~~ edges clustered in  $P$ , separated by  $gluer(P)$
- + #~~X~~ edges clustered in  $P \setminus gluer(P)$ 
  - & ~~dist = 1~~
  - & ~~dist > 1~~



$\tilde{x}_e^{(t)}$ : distance of  $e$  (at layer  $t$ )

# Analysis Overview

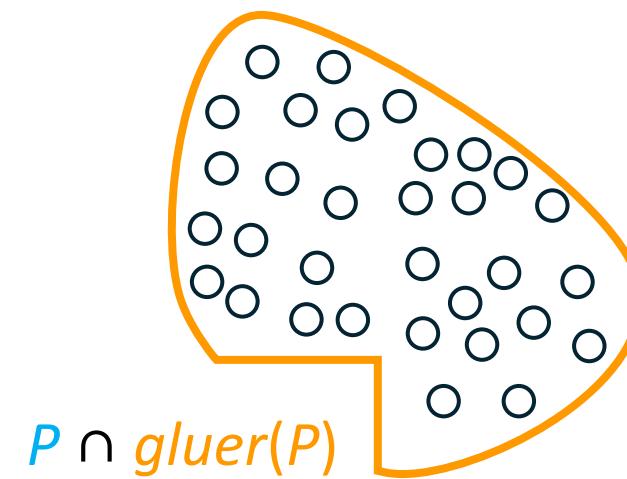
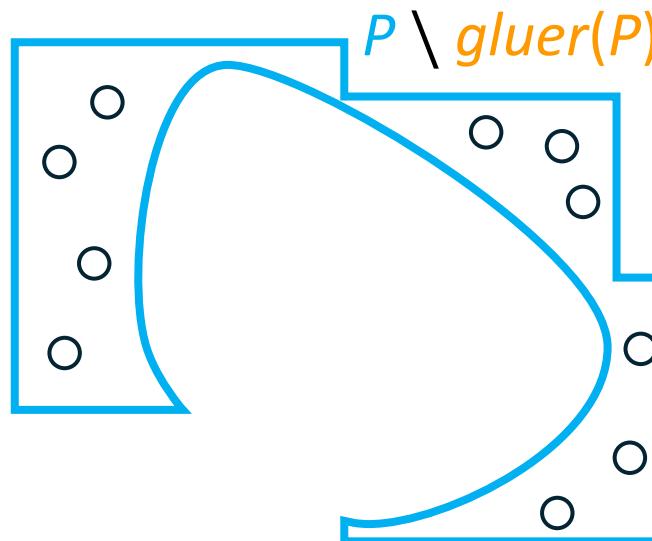
$$\leq \left[ \begin{array}{l} \text{\#(edges clustered in } P, \text{ separated by } \textit{gluer}(P) \text{)} \\ + \text{\#(edges clustered in } P \setminus \textit{gluer}(P) \text{)} \end{array} \right]$$



$\tilde{x}_e^{(t)}$ : distance of  $e$  (at layer  $t$ )

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$$\leq \left[ \begin{array}{l} \#(\text{edges clustered in } P, \text{ separated by } \text{gluer}(P)) \\ + \#(\text{edges clustered in } P \setminus \text{gluer}(P)) \end{array} \right]$$

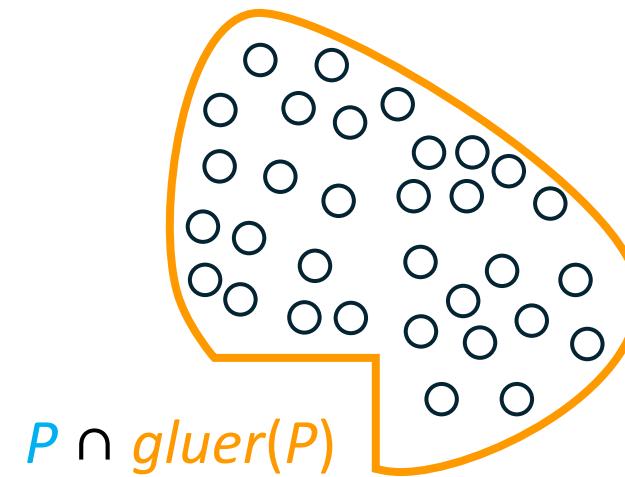
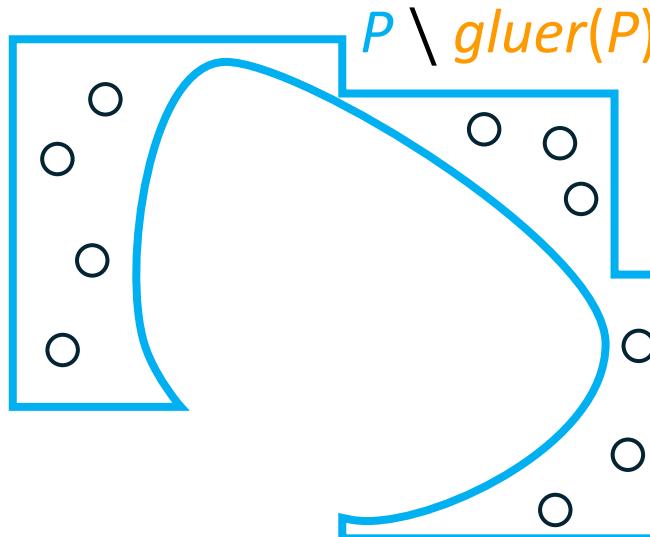


**concentration property:**  
most points in  $P$  are in  $P \cap \text{gluer}(P)$

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- $\leq$   $\left[ \begin{array}{l} \#(\text{edges clustered in } P, \text{ separated by } \text{gluer}(P)) \\ + \#(\text{edges clustered in } P \setminus \text{gluer}(P)) \end{array} \right] \text{ --- negligible}$
- $\approx \#(\text{edges clustered in } P, \text{ separated by } \text{gluer}(P))$

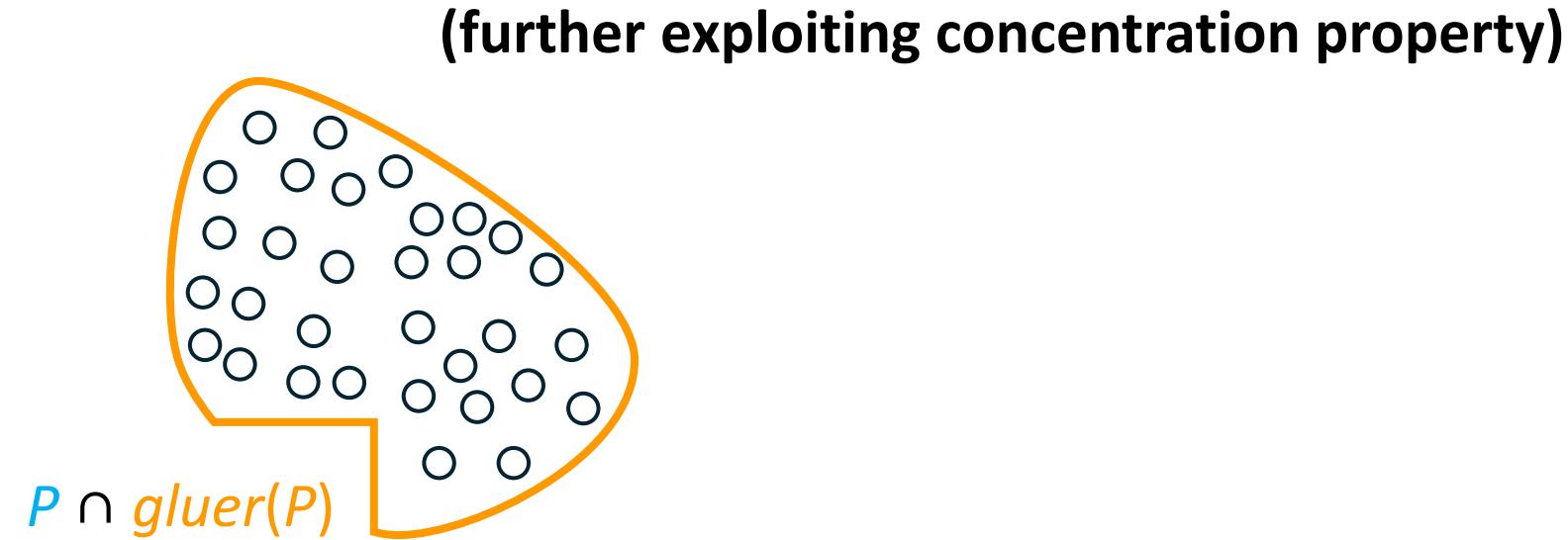
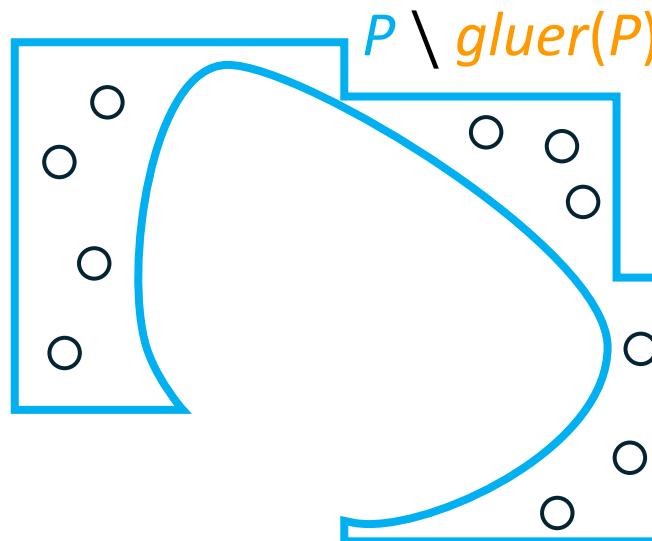


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- $\approx \#(\text{edges clustered in } P, \text{ separated by } \text{gluer}(P))$
- $\approx \#(\text{edges clustered in } P, \text{ separated by } \text{gluer}(P) \text{ & dist} < 1)$



$\tilde{x}_e^{(t)}$ : distance of  $e$  (at layer  $t$ )

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$$\begin{aligned} &\leq \begin{cases} \#(\text{edges clustered in } P, \text{ separated by } \textit{gluer}(P)) \\ + \#(\text{edges clustered in } P \setminus \textit{gluer}(P)) \end{cases} \quad ) \text{ --- negligible} \\ &\approx \#(\text{edges clustered in } P, \text{ separated by } \textit{gluer}(P)) \\ &\approx \#(\text{edges clustered in } P, \text{ separated by } \textit{gluer}(P) \text{ \& dist} < 1) \end{aligned}$$

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$$\therefore \#(-\text{edges clustered in } P \text{ \& dist} = 1)$$

$$\leq O(1) \cdot \#(\text{edges clustered in } P, \text{ separated by } Q \text{ \& dist} < 1)$$

# Conclusion

- **25.7846-approximation for HCC**
- Main ingredients
  - Useful lemma
  - Cut properties (of pre-clusterings)
- 5-approximation for  $L_0$  Ultrametric Fitting
  - with the same ingredients
- Extension to other hierarchical clustering problems?

Thank You