A New Perspective on Pool-Based Active Classification and False Discovery Control

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Contributions

- Revisiting Classification and TPR maximization subject to FDR-control in a combinatorial setting.
- A common framework for classification and pure exploration for combinatorial bandits
- State of the art action elimination algorithms for both.

Formalities

$[n]$: a finite item space

$y_i \in \{0,1\}$: label for $i \in [n]$

$\mathcal{H}_0 = \{i \in [n] : y_i = 0\}, \mathcal{H}_1 = [n] \setminus \mathcal{H}_1$

Policies:

$\Pi \subset 2^{[n]}$: hypothesis class

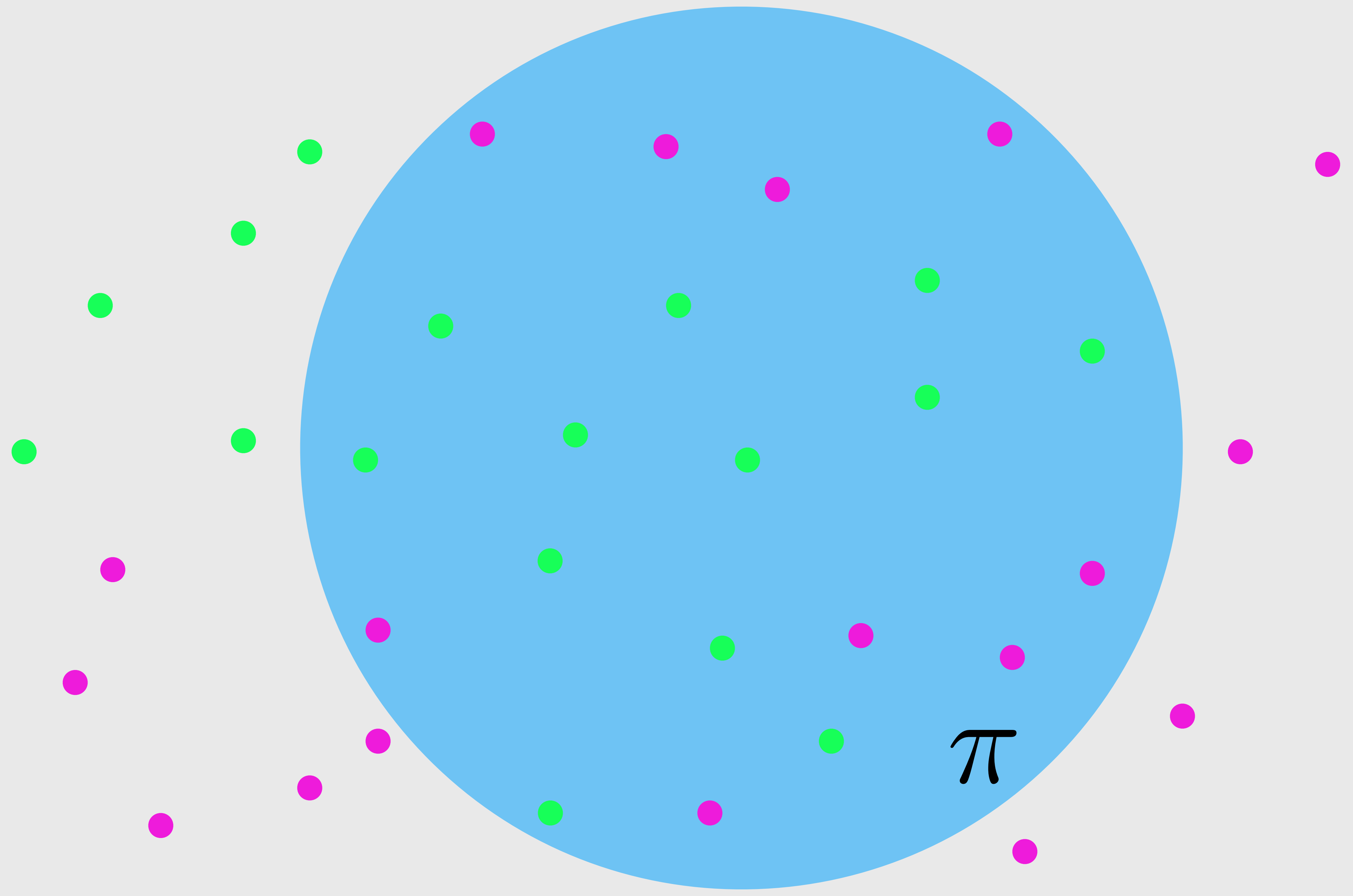
Identify each $\pi \in \Pi$ with a labeler:

$\pi \in \Pi$: $\pi(x) = 1 \iff x \in \pi$

Metrics:

$$R(\pi) := \frac{|\pi \cap \mathcal{H}_0| + |\pi^c \cap \mathcal{H}_1|}{n}$$

$$FDR(\pi) := \frac{|\pi \cap \mathcal{H}_0|}{|\pi|}, \quad TPR(\pi) := \frac{|\pi \cap \mathcal{H}_1|}{|\mathcal{H}_1|}$$



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$$FDR(\pi) := \frac{|\pi \cap \mathcal{H}_0|}{|\pi|}, \quad TPR(\pi) := \frac{|\pi \cap \mathcal{H}_1|}{|\mathcal{H}_1|}$$

Classification Problem:

Identify $\pi^* := \underset{\pi \in \Pi}{\text{argmin}} R(\pi)$

FDR Control Problem:

Identify $\pi^*_\alpha := \underset{\pi \in \Pi, FDR(\pi) \leq \alpha}{\text{argmax}} \; TPR(\pi)$

Revisiting Classification Loss

Re-parametrize: $\mu_x = 2y_x - 1 = \begin{cases} 1 & y_x = 1 \\ -1 & y = 0 \end{cases}$

$$
\begin{aligned}
R(\pi) &= \frac{|\pi \cap \mathcal{H}_0| + |\pi^c \cap \mathcal{H}_1|}{n} \\
&= \frac{1}{n} \sum_{x \in \pi} \mathbf{1}\{y_x = 0\} + \frac{1}{n} \sum_{x \in \pi^c} \mathbf{1}\{y_x = 1\} \\
&= \frac{1}{n} \sum_{x \in \pi} (1 - y_x) + \frac{1}{n} \sum_{x \in \pi^c} y_x \\
&= \frac{|\mathcal{H}_1|}{n} + \sum_{x \in \pi} (1 - 2y_x) \\
&= \frac{|\mathcal{H}_1| + |\pi|}{n} - \frac{1}{n} \sum_{x \in \pi} \mu_x
\end{aligned}
$$

Define:

$$\mu_\pi := \sum_{x \in \pi} \mu_x$$

Key Takeaway:

$$\pi^* = \underset{\pi \in \Pi}{\text{argmin}}\, R(\pi) = \underset{\pi \in \Pi}{\text{argmax}}\, \mu_\pi$$

A combinatorial interpretation of classification!

Detour: Pure Exploration Combinatorial Bandits

Input:

$\nu_i, \mathbb{E}[\nu_i] = \mu_i, i \in [n]$ arm distributions

$\Pi \subset 2^{\mathcal{X}}$ collection of subsets

$\mu_\pi := \sum_{x \in \pi} \mu_x$

Protocol:

In round t choose I_t and receive reward $R_{I_t,t} \sim \nu_{I_t}$

Return:

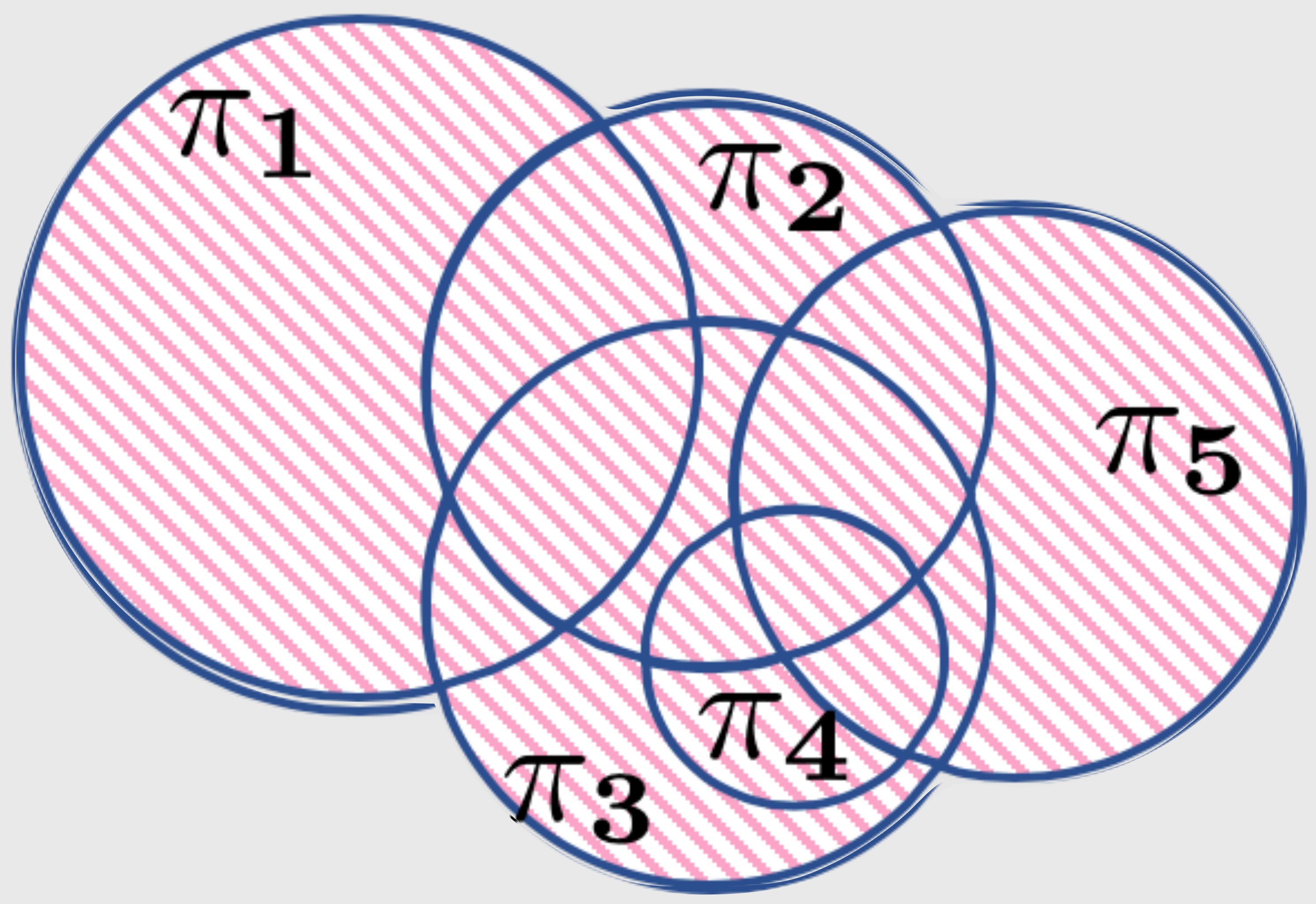
Identify $\pi^* = \operatorname{argmax}_{\pi \in \Pi} \sum_{x \in \pi} \mu_x$

Examples:

- $\Pi = \{\{i\} : i \in [n]\}$. Best-Arm identification.
- $\Pi = \binom{[n]}{k}$. Top-k.
- $\Pi = \{$trees in a weighted graph$\}$. Minimal Spanning Tree
- Classification (stochastic or persistent labels).

Amazingly we can transform classification to a combinatorial bandit problem!

Algorithm: Action Elimination



Action Elimination:

Input: δ, Π

for: $t = 1, 2, \cdots,$

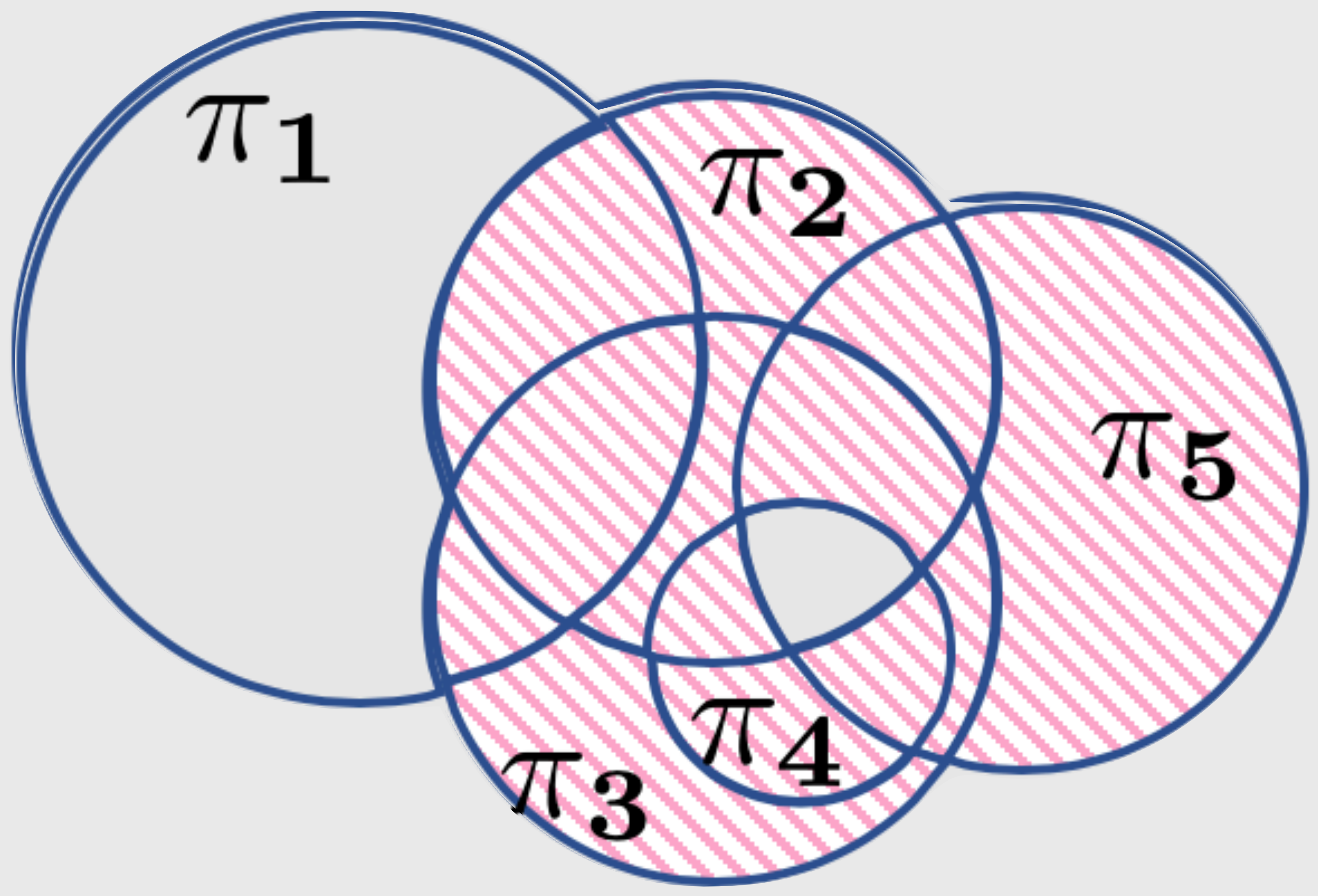
1. **Sample** I_t uniformly at random from $[n]$ (with or without replacement).
2. If $I_s \in \cup_{\pi \in \mathcal{A}} \pi - \cap_{\pi \in \mathcal{A}} \pi$, **observe** μ_{I_t}
3. For each π, π', **update** $\widehat{\mu}(\pi', \pi)$
4. **Eliminate** $\mathcal{A} = \mathcal{A} \setminus \{\pi : \exists \pi', \widehat{\mu}(\pi', \pi) - C(\pi', \pi, t) > 0\}$

Carefully designed to avoid union bounds

Return π^*

Takeaway: **For active classification, we only need to sample points that any labeler is uncertain about.**

Algorithm: Action Elimination



π_5 knocks out π_1

Action Elimination:

Input: δ, Π

for: $t = 1, 2, \cdots,$

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Return π^*

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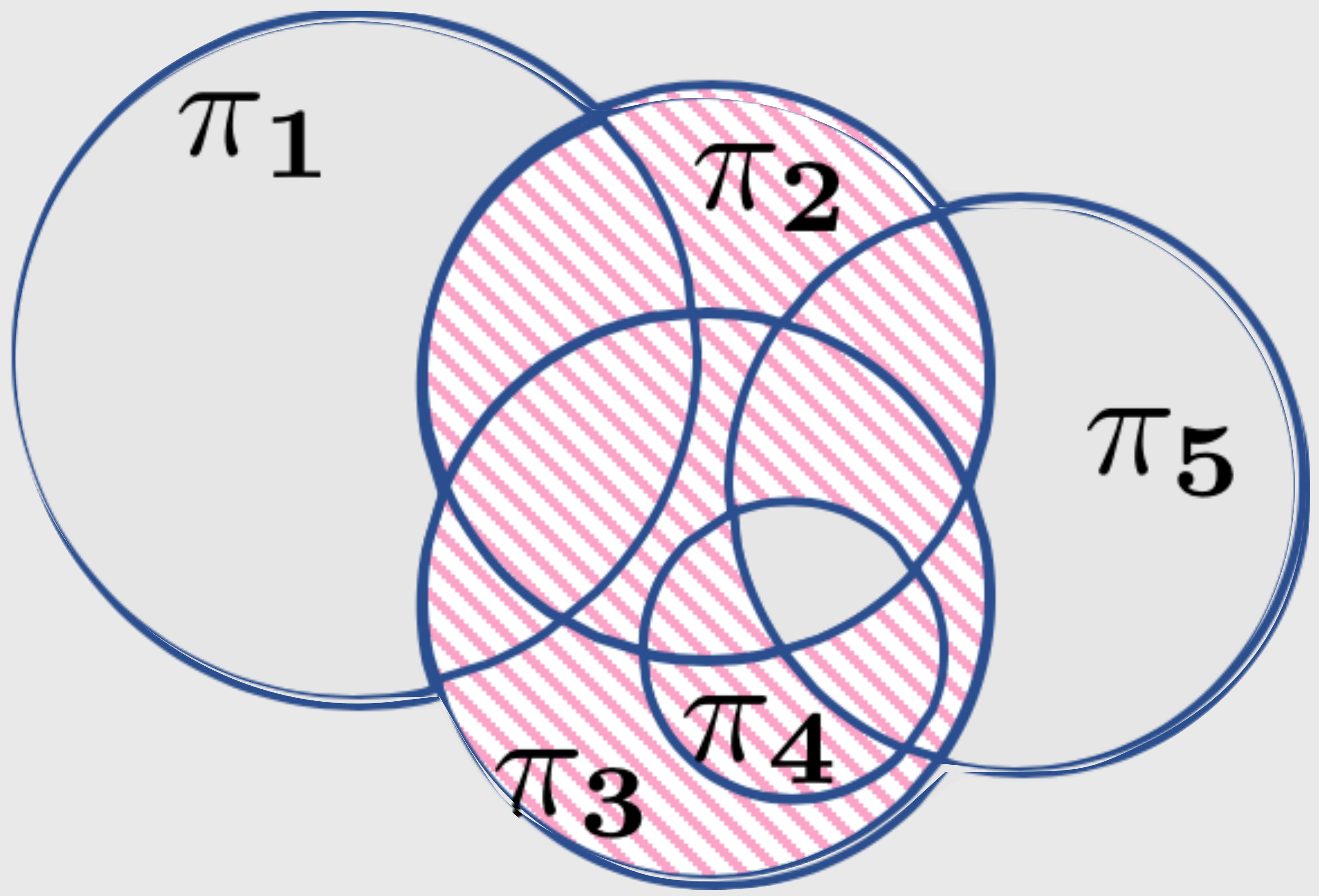

π_2 knocks out π_5

Action Elimination:

Input: δ, Π

for: $t = 1, 2, \cdots,$

1. **Sample** I_t uniformly at random from $[n]$ (with or without replacement).
2. If $I_s \in \cup_{\pi \in \mathcal{A}} \pi - \cap_{\pi \in \mathcal{A}} \pi$, **observe** μ_{I_t}
3. For each π, π', **update** $\widehat{\mu}(\pi', \pi)$
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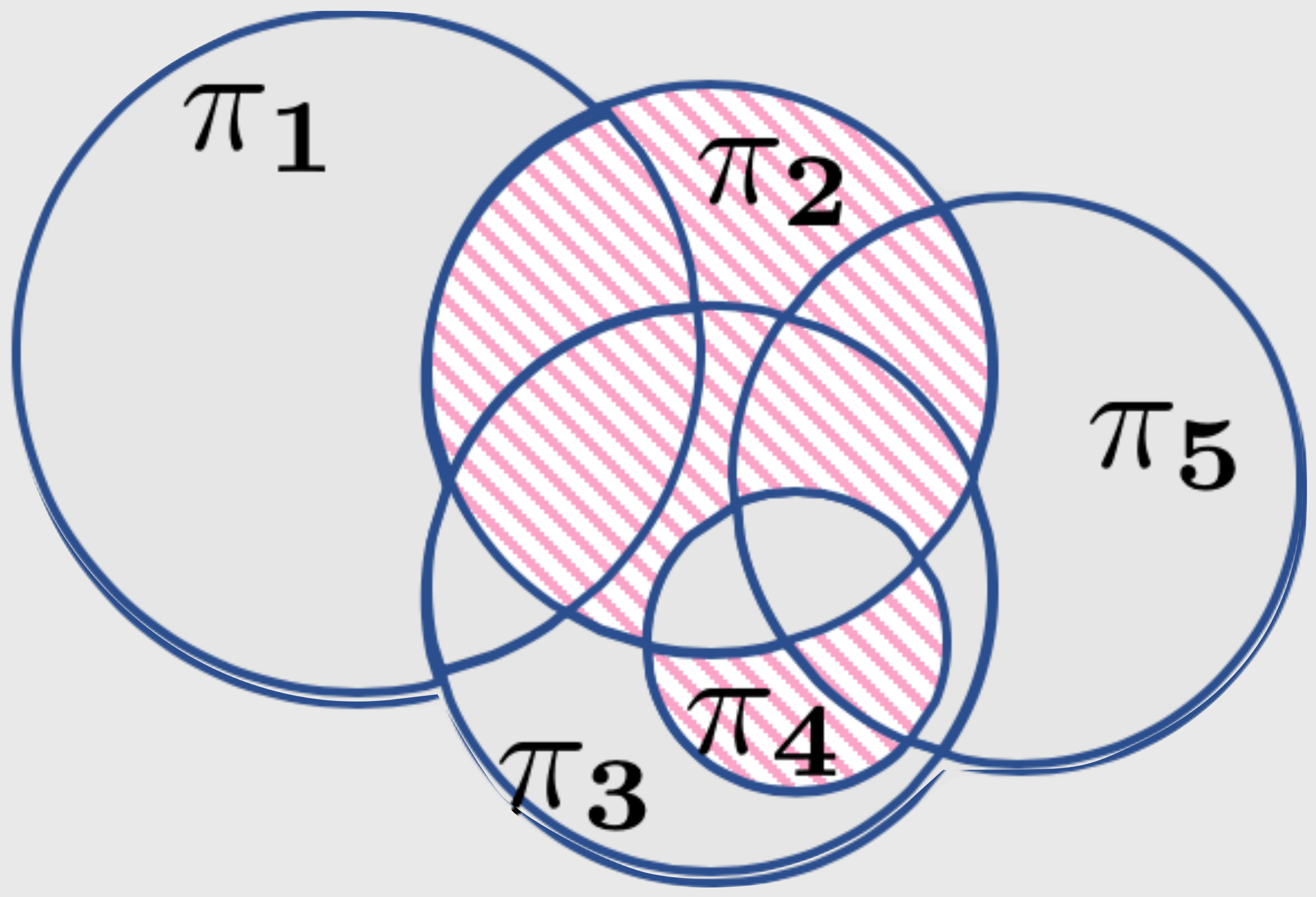
Carefully designed to avoid union bounds

Return π^*

Takeaway: **For active classification, we only need to sample points that any labeler is uncertain about.**

Algorithm: Action Elimination



π_2 knocks out π_3

Action Elimination:

Input: δ, Π

for: $t = 1, 2, \cdots,$

1. **Sample** I_t uniformly at random from $[n]$

(with or without replacement).

2. If $I_s \in \cup_{\pi \in \mathcal{A}} \pi - \cap_{\pi \in \mathcal{A}} \pi$, **observe** μ_{I_t}

3. For each π, π', **update** $\widehat{\mu}(\pi', \pi)$

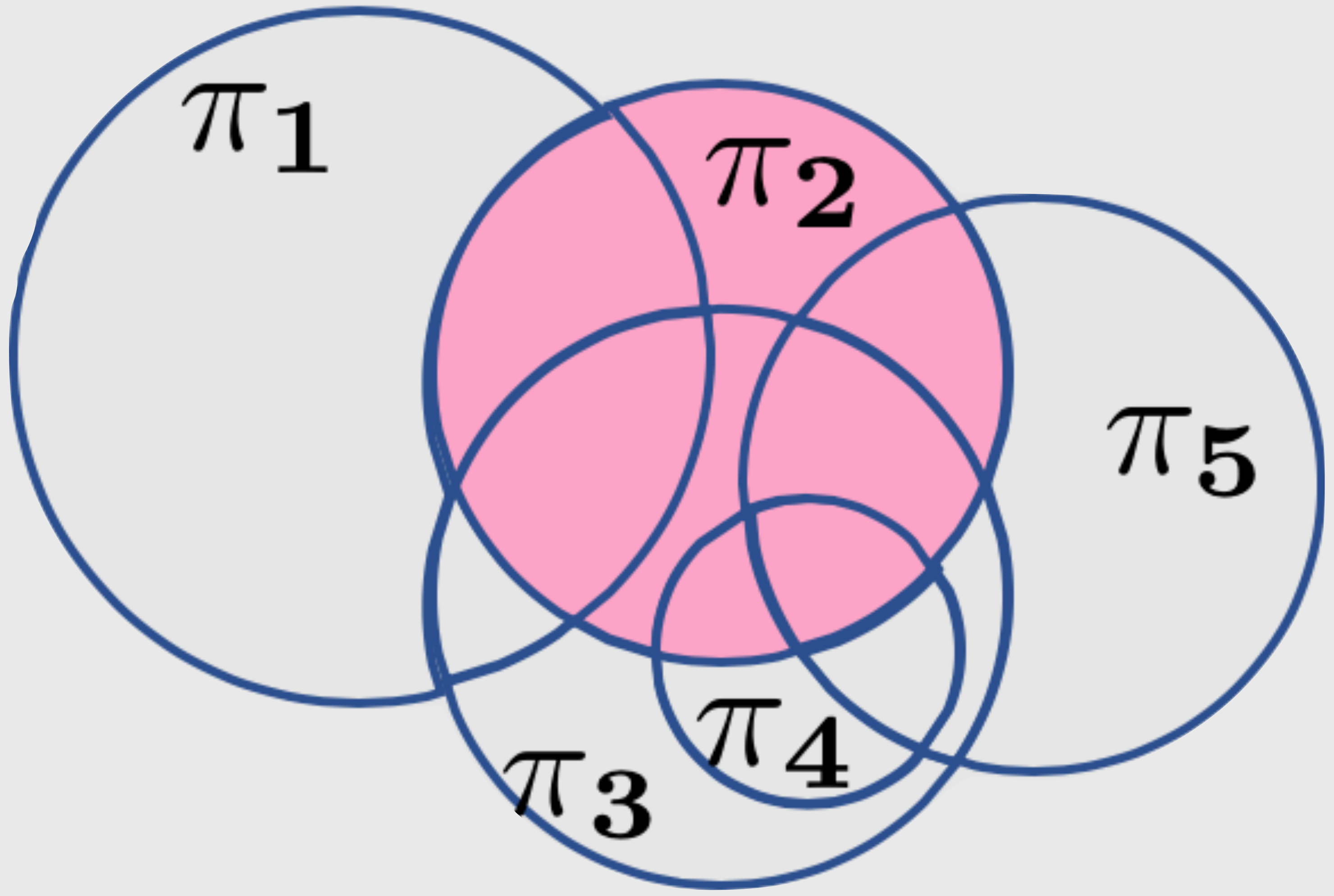
4. **Eliminate** $\mathcal{A} = \mathcal{A} \setminus \{\pi : \exists \pi', \widehat{\mu}(\pi', \pi) - C(\pi', \pi, t) > 0\}$

Carefully designed to avoid union bounds

Return π^*

Takeaway: **For active classification, we only need to sample points that any labeler is uncertain about.**

Algorithm: Action Elimination



π_2 knocks out π_4

Action Elimination:

Input: δ, Π

for: $t = 1, 2, \cdots,$

1. **Sample** I_t uniformly at random from $[n]$ (with or without replacement).
2. If $I_s \in \cup_{\pi \in \mathcal{A}} \pi - \cap_{\pi \in \mathcal{A}} \pi$, **observe** μ_{I_t}
3. For each π, π', **update** $\widehat{\mu}(\pi', \pi)$
4. **Eliminate** $\mathcal{A} = \mathcal{A} \setminus \{\pi : \exists \pi', \widehat{\mu}(\pi', \pi) - C(\pi', \pi, t) > 0\}$

Carefully designed to avoid union bounds

Return π^*

Takeaway: For active classification, we only need to sample points that any labeler is uncertain about.

Guarantees for Action Elimination

Theorem (J., Jamieson 2019) Let $\pi^* = \underset{\pi \in \Pi}{\text{argmin}} R(\pi)$,

$$\tilde{\Delta}_\pi = \frac{|\mu_{\pi^*} - \mu_\pi|}{|\pi^* \Delta \pi|}, \text{ and } B(k, \pi^*) = \{\pi : |\pi \Delta \pi^*| = k\}$$

$$\tau_\pi = \frac{VC(B(|\pi^* \Delta \pi|, \pi^*))}{|\pi^* \Delta \pi|} \frac{\log(n \log(\tilde{\Delta}_\pi^{-2})/\delta)}{\tilde{\Delta}_\pi^2}$$

Then with probability greater than $1-\delta$ the Action Elimination algorithm terminates after a number of samples no more than

$$\sum_{1 \leq i \leq n} \max_{\pi : i \in \pi^* \Delta \pi} \tau_\pi$$

Interpretation: we can stop sampling i after π^* has knocked out any set $i \in \pi^* \Delta \pi$.

Implications: Classification

An active classification complexity that is fundamentally not disagreement coefficient based! Contrasts with the standard DHM algorithm:

- Like DHM we sample in the symmetric difference. Unlike DHM, we can characterize the contribution of each arm.
- For Best-Arm, DHM analysis gives the passive rate $n\Delta_2^2$.
- For 1-d thresholds under Tsybakov noise get the minimax rates (Castro and Nowak 2008):

$$\text{if } \alpha = 0, \log(n)\log(\log(n)/\delta)/h^2 \quad \text{if } \alpha > 0, n^{2\alpha}\log(\log(n)/\delta)/h^2$$

passive rates:

$$n^{2\alpha+1}\log(\log(n)/\delta)/h^2$$

Remarks

- An active classification complexity that is fundamentally not disagreement coefficient based!
- Can quantify the contribution of each arm to the sample complexity
- For 1-d thresholds under Tsybakov noise get the minimax rates (Castro and Nowak 2008):
- An agnostic algorithm that matches the rates of previous binary classification !
- **No need to pull each arm once.**

What about active FDR-control?

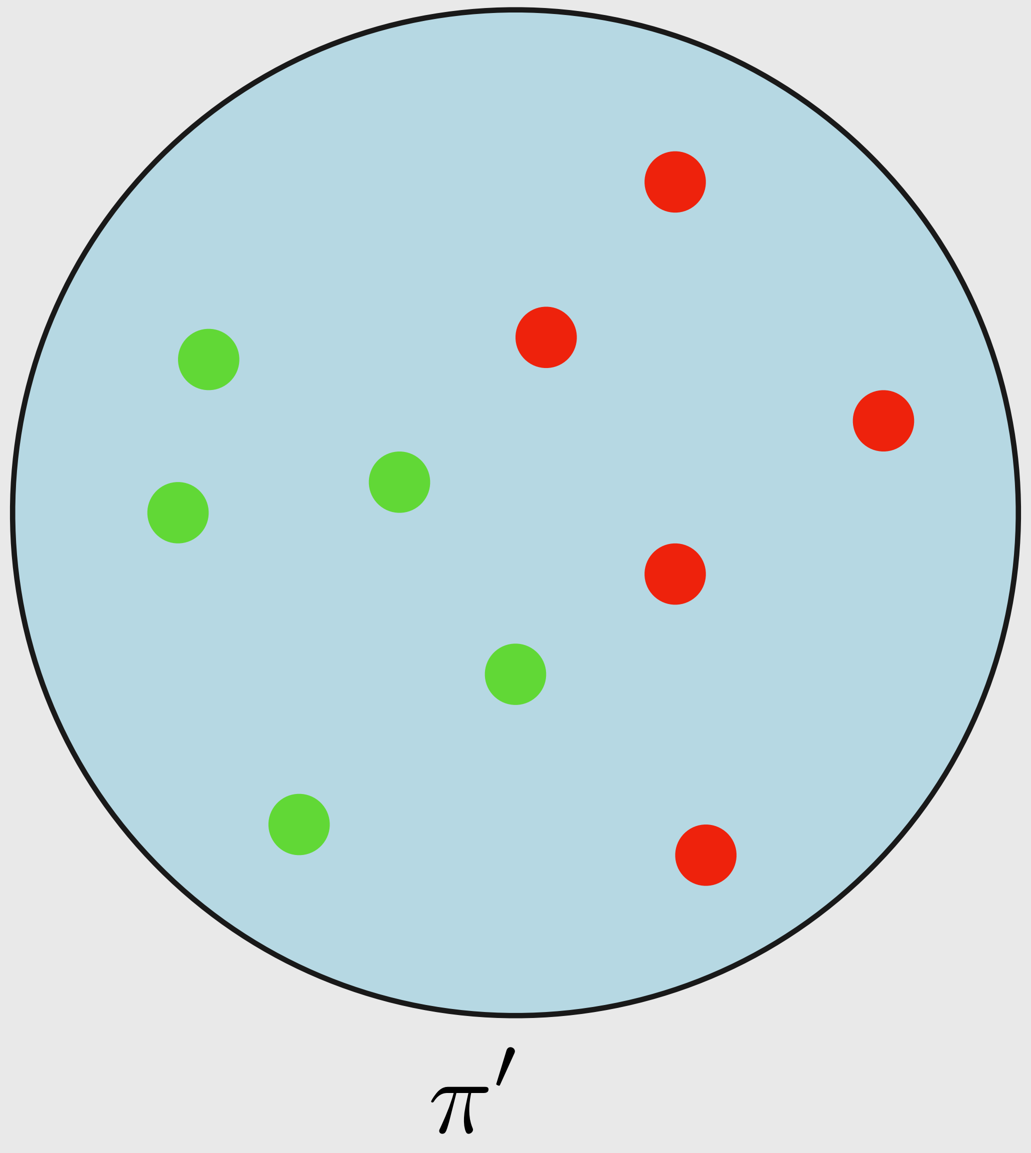
Where to sample: FDR

$$FDR(\pi) = \frac{|\pi \cap \mathcal{H}_0|}{|\pi|} \quad TPR(\pi) = \frac{|\pi \cap \mathcal{H}_1|}{|\mathcal{H}_1|}$$

Find: $\pi^*_\alpha = \underset{FDR(\alpha)\leq\alpha}{\text{argmax}}\ TPR(\alpha)$

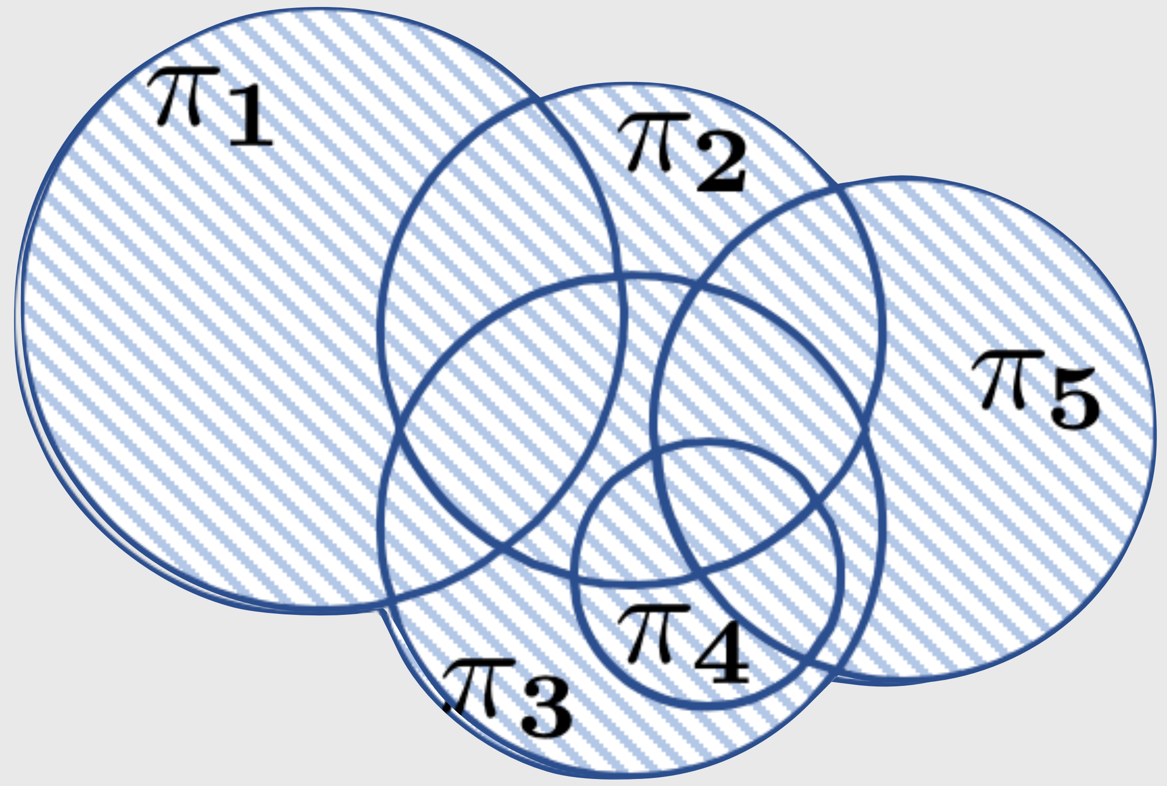
Instead of considering the TPR, can instead consider

$$TP(\pi) = |\pi \cap \mathcal{H}_1| = \sum_{x\in\pi} y_x$$

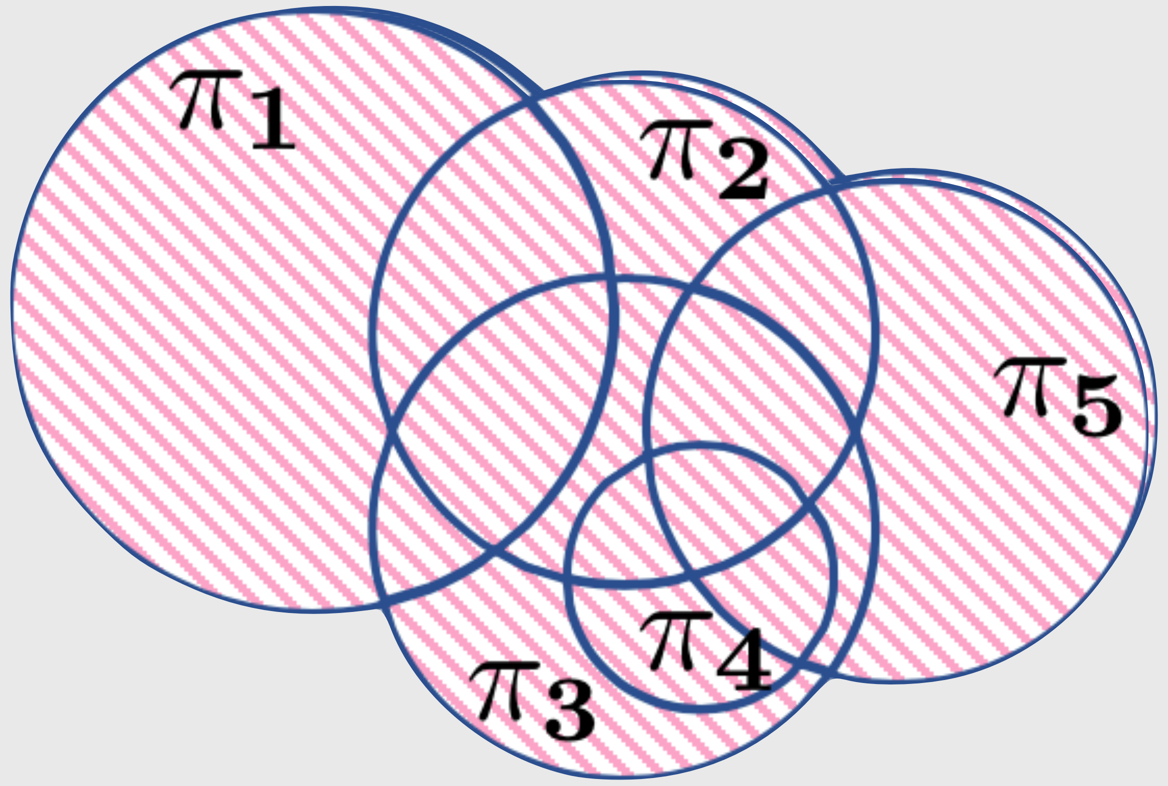


Action-Elimination: FDR

Union



Symmetric Difference



Action Elimination:

Input: δ, Π

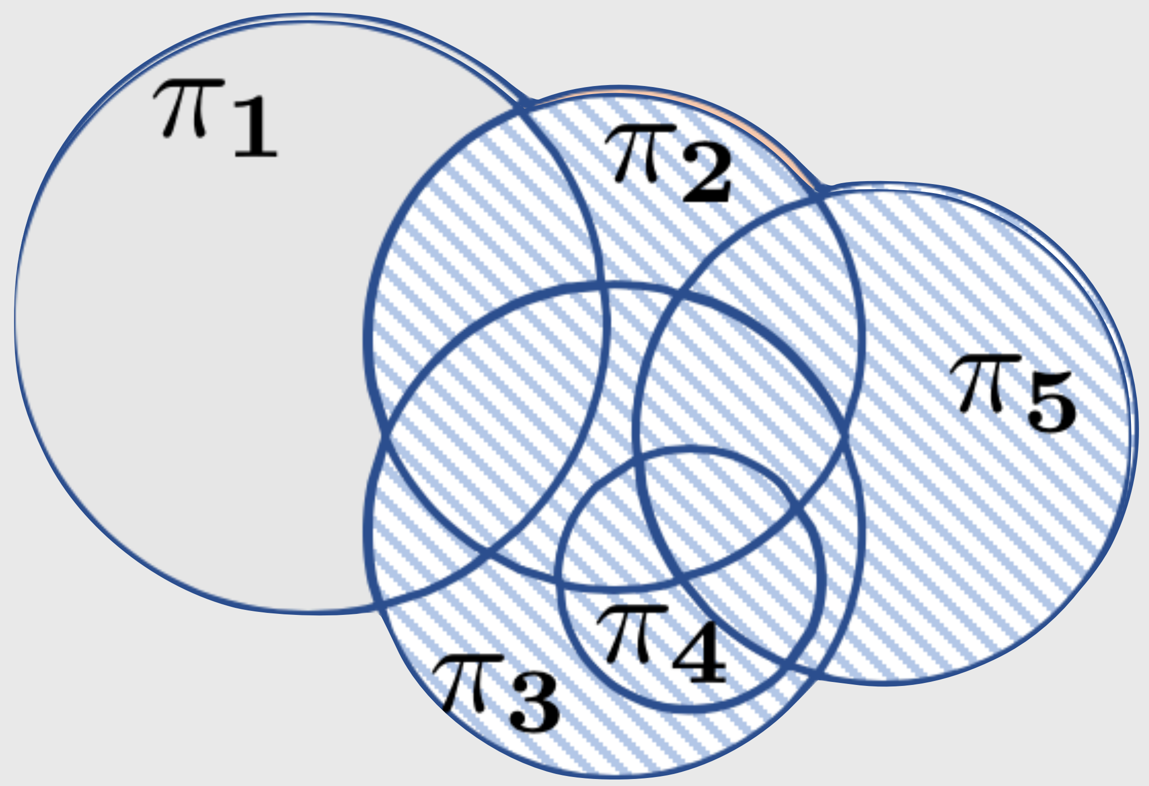
Maintain: $\mathcal{A}$ active sets, $\mathcal{C}$ FDR controlled sets

for: $t = 1, 2, \cdots,$

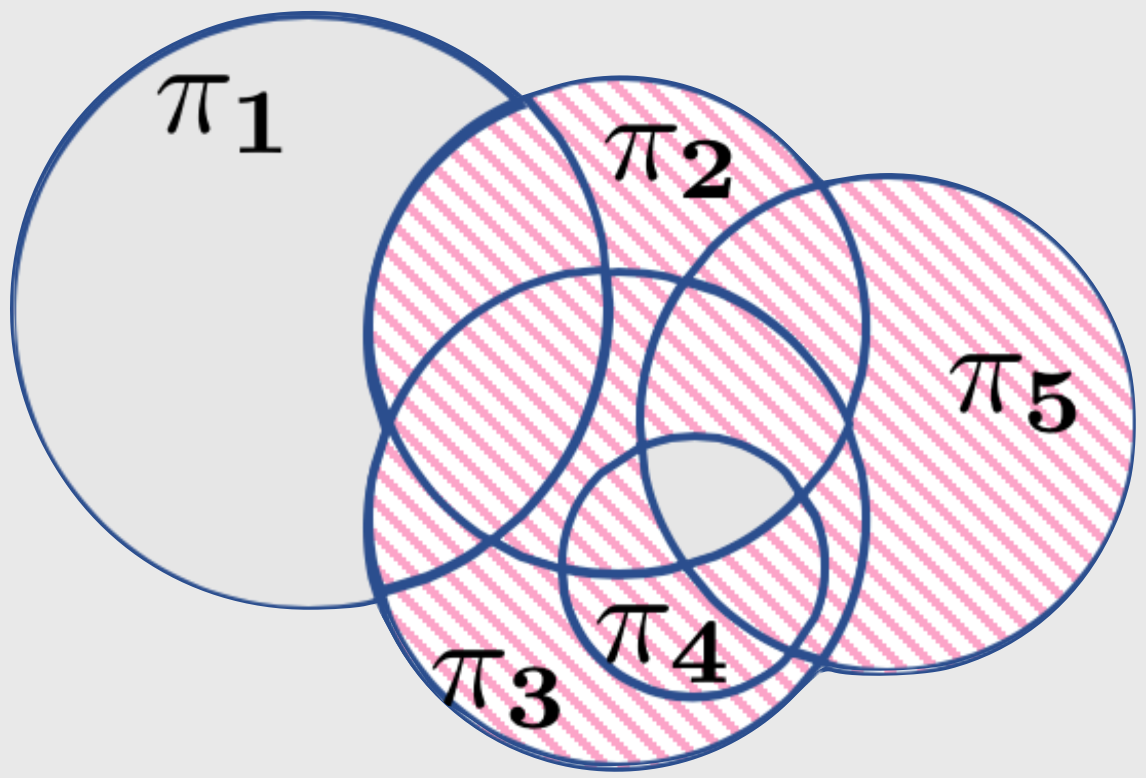
1. **Sample** I_t, J_t uniformly at random from $[n]$ (with or without replacement).
2. If $I_t \in \bigcup_{\pi \in \mathcal{A} \setminus \mathcal{C}} \pi$, observe y_{I_t}
3. If $J_t \in \bigcup_{\pi \in \mathcal{A}} \pi - \bigcap_{\pi \in \mathcal{A}} \pi$, observe y_{I_t}
4. **Update** $\mathcal{C}$ with any new FDR-controlled sets.
5. **Eliminate** $\mathcal{A} = \mathcal{A} \setminus \{\pi : \widehat{FDR}(\pi) + C(\pi, t) < \alpha\}$
6. **Eliminate** $\mathcal{A} = \mathcal{A} \setminus \{\pi : \widehat{TP}(\pi') - \widehat{TP}(\pi) < C(\pi', \pi, t), \pi' \in \mathcal{C}\}$

Action-Elimination: FDR

Union



Symmetric Difference



π_1 not FDRδ-controlled

Action Elimination:

Input: δ, Π

Maintain: $\mathcal{A}$ active sets, $\mathcal{C}$ FDR controlled sets

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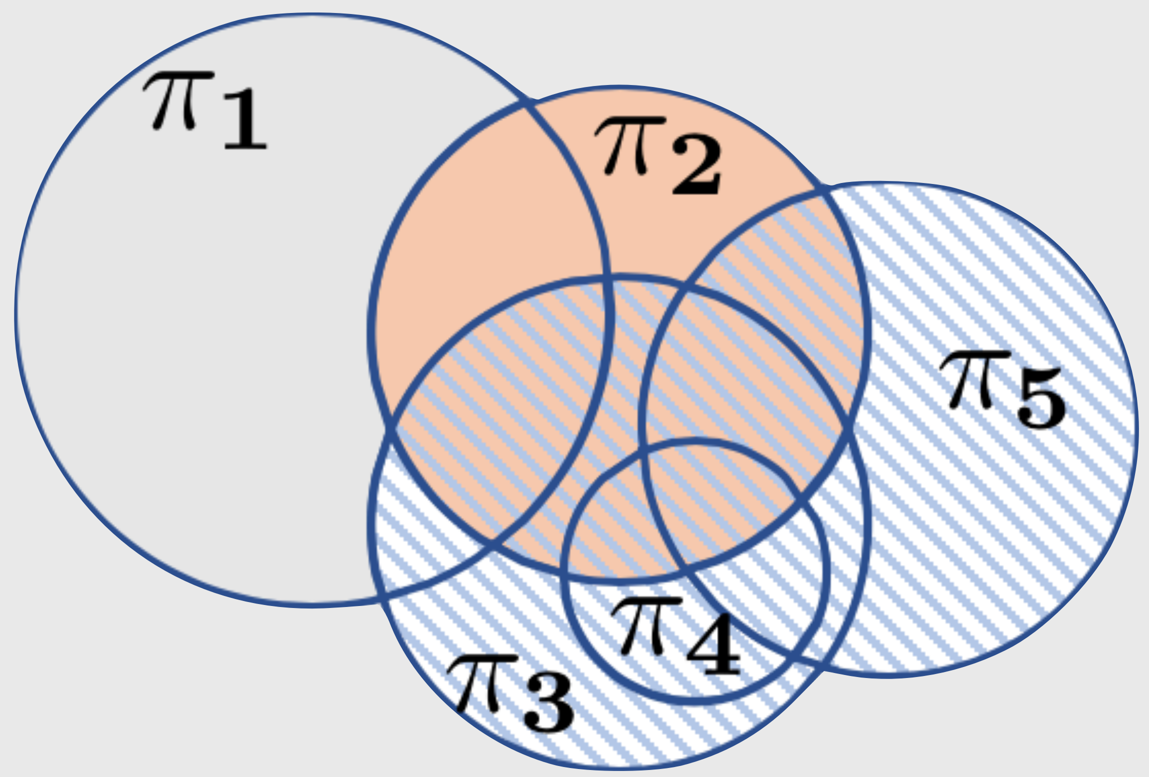
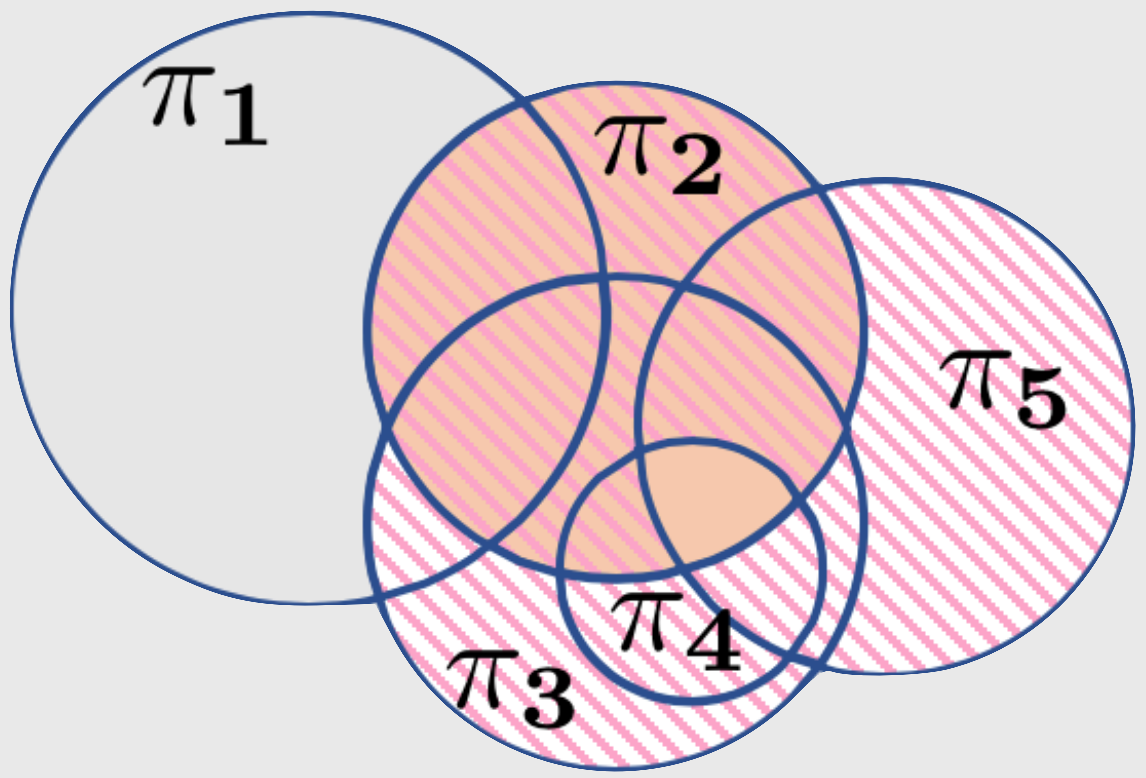
Action-Elimination: FDR

Union



Symmetric Difference



π_2 FDRδ-controlled

Action Elimination:

Input: δ, Π

Maintain: $\mathcal{A}$ active sets, $\mathcal{C}$ FDR controlled sets

for: $t = 1, 2, \cdots,$

1. **Sample** I_t, J_t uniformly at random from $[n]$ (with or without replacement).
2. If $I_t \in \bigcup_{\pi \in \mathcal{A} \setminus \mathcal{C}} \pi$, observe y_{I_t}
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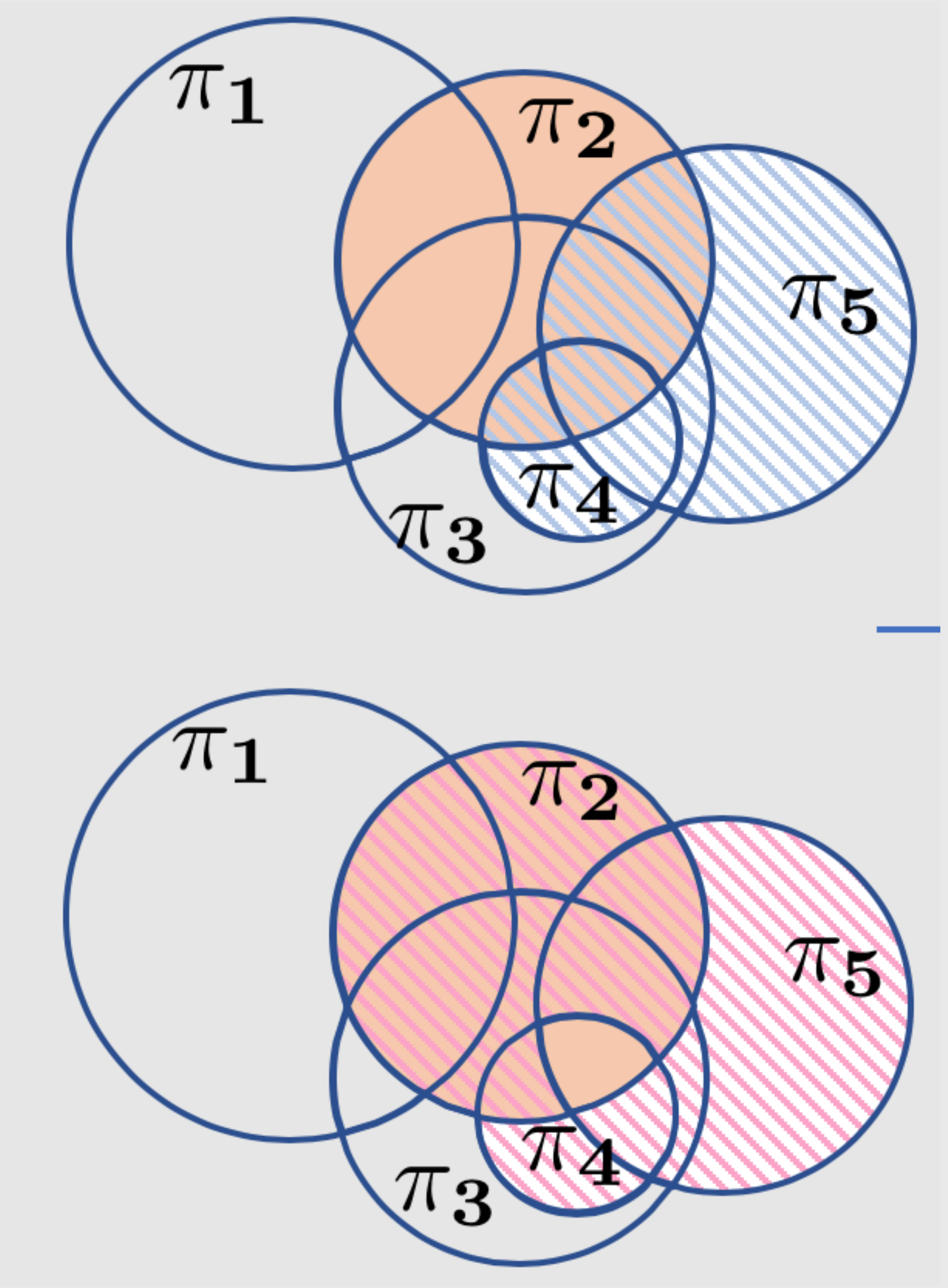
Action-Elimination: FDR

Union

Symmetric Difference



π_2 eliminates π_3

Action Elimination:

Input: δ, Π

Maintain: $\mathcal{A}$ active sets, $\mathcal{C}$ FDR controlled sets

for: $t = 1, 2, \cdots,$

1. **Sample** I_t, J_t uniformly at random from $[n]$ (with or without replacement).
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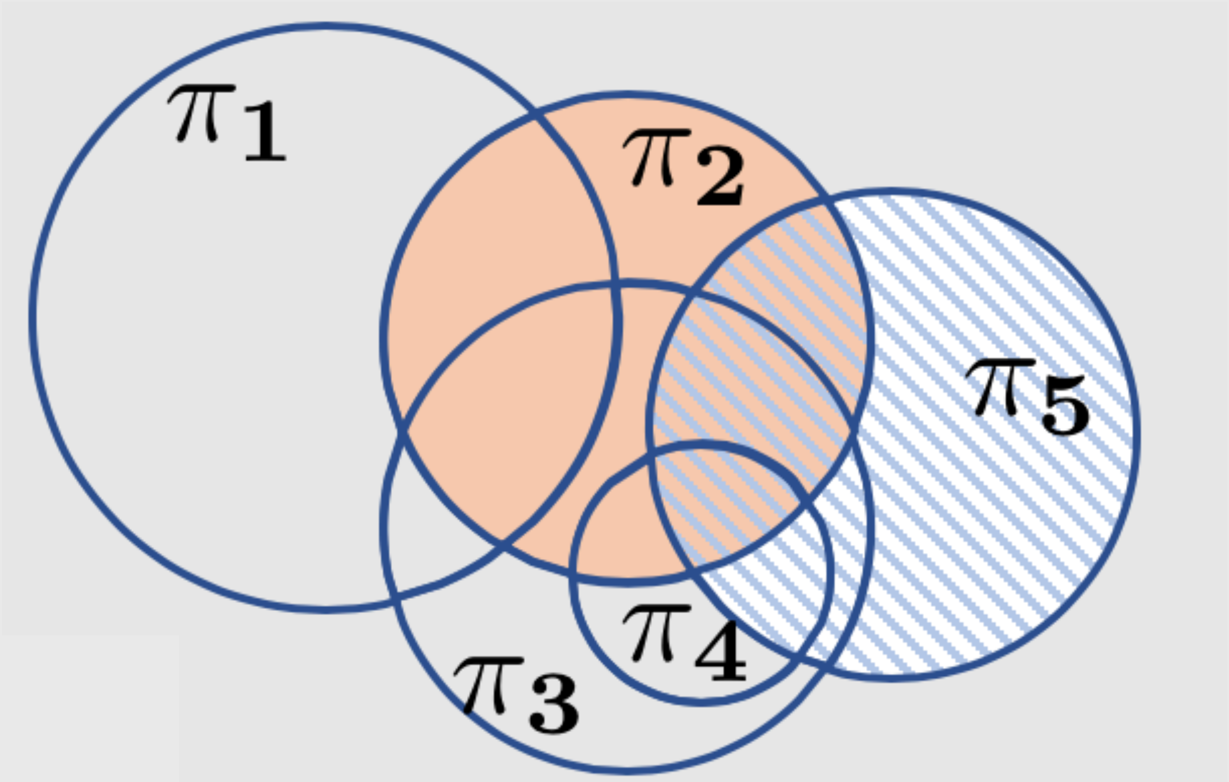
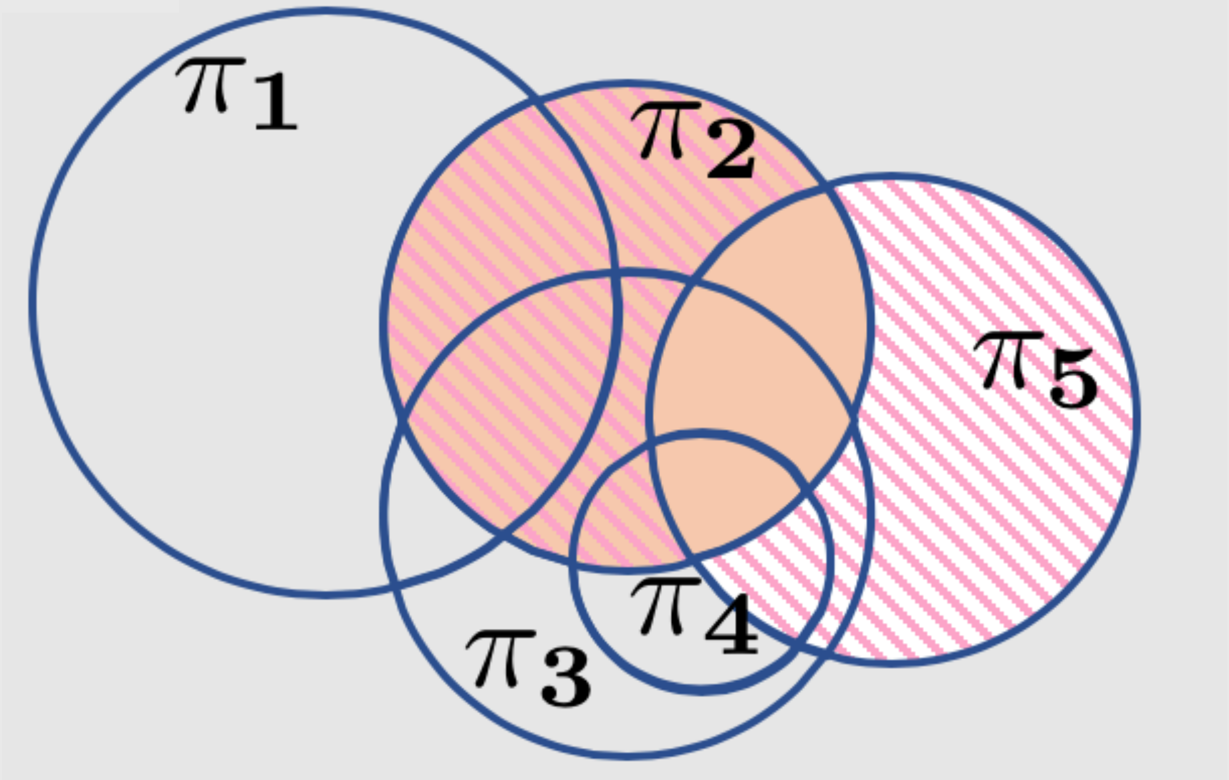
Action-Elimination: FDR

Union

Symmetric Difference





π_2 eliminates π_4 since $\pi_4 \subset \pi_3$

Action Elimination:

Input: δ, Π

Maintain: $\mathcal{A}$ active sets, $\mathcal{C}$ FDR controlled sets

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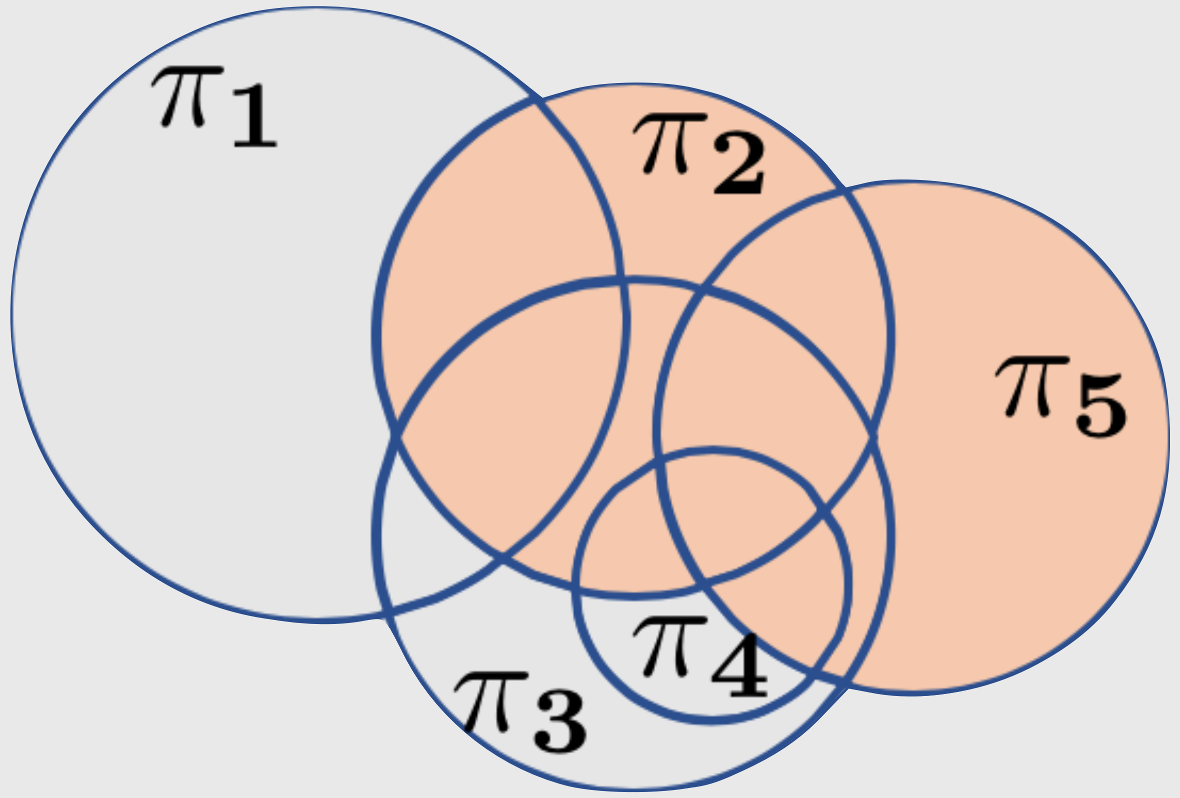
Action-Elimination: FDR

Union



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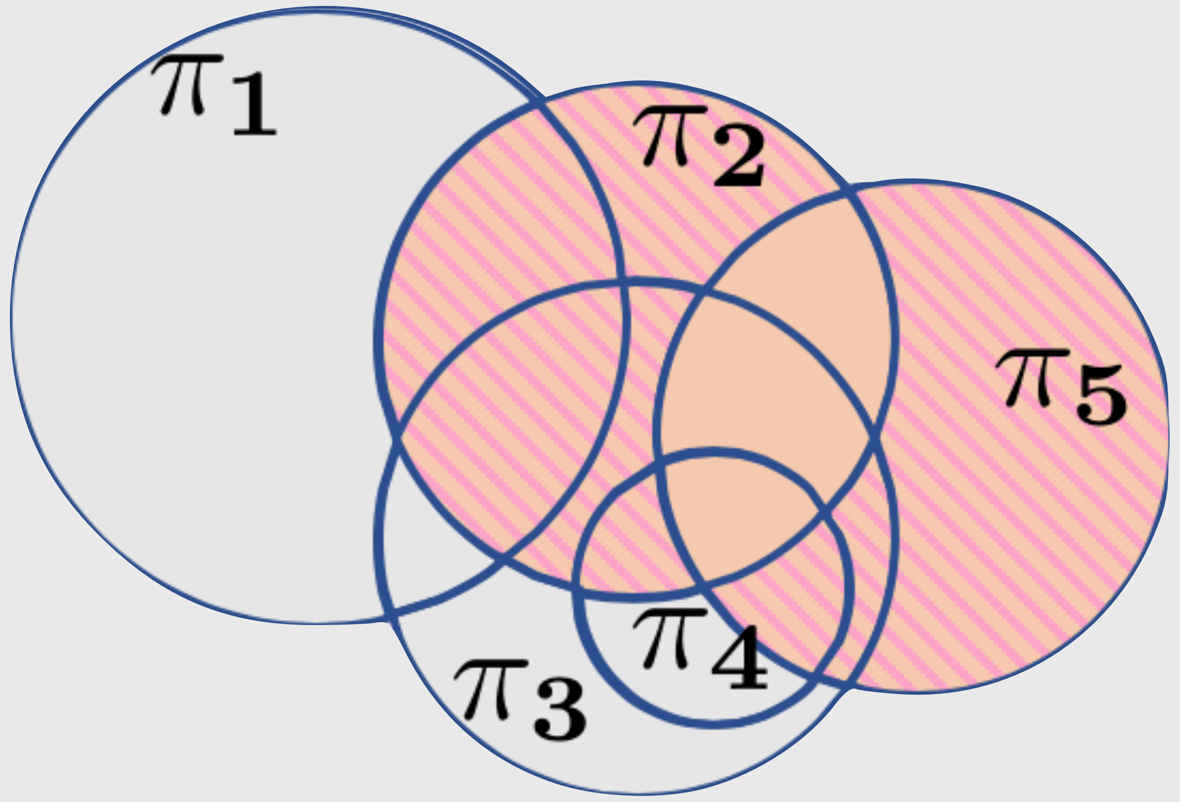

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Guarantees

How long does it take to knock out a set? Define

$$\tilde{\Delta}_\pi = \frac{|TP(\pi^*_\alpha) - TP(\pi)|}{|\pi^*_\alpha \Delta \pi|}, \quad \Delta_{\pi,\alpha} = |FDR(\pi) - \alpha|,$$

and

$$s^{FDR}_\pi = \frac{VC(B(|\pi|)}{|\pi|} \frac{\log(n \log(\tilde{\Delta}^{-2}_{\pi,\alpha})/\delta)}{\tilde{\Delta}^2_{\pi,\alpha}}, s^{TP}_\pi = \frac{VC(B(|\pi^*_\alpha \Delta \pi|, \pi^*_\alpha)}{|\pi^*_\alpha \Delta \pi|} \frac{\log(n \log(\tilde{\Delta}^{-2}_\pi)/\delta)}{\tilde{\Delta}^2_\pi}$$

If π is not FDR-controlled:

$$\min\{s^{FDR}_\pi, \max\{s^{FDR}_{\pi^*}, s^{TPR}_\pi\}\}$$

If π is FDR-controlled:

$$\max\{s^{FDR}_{\pi^*}, s^{TPR}_\pi\}$$

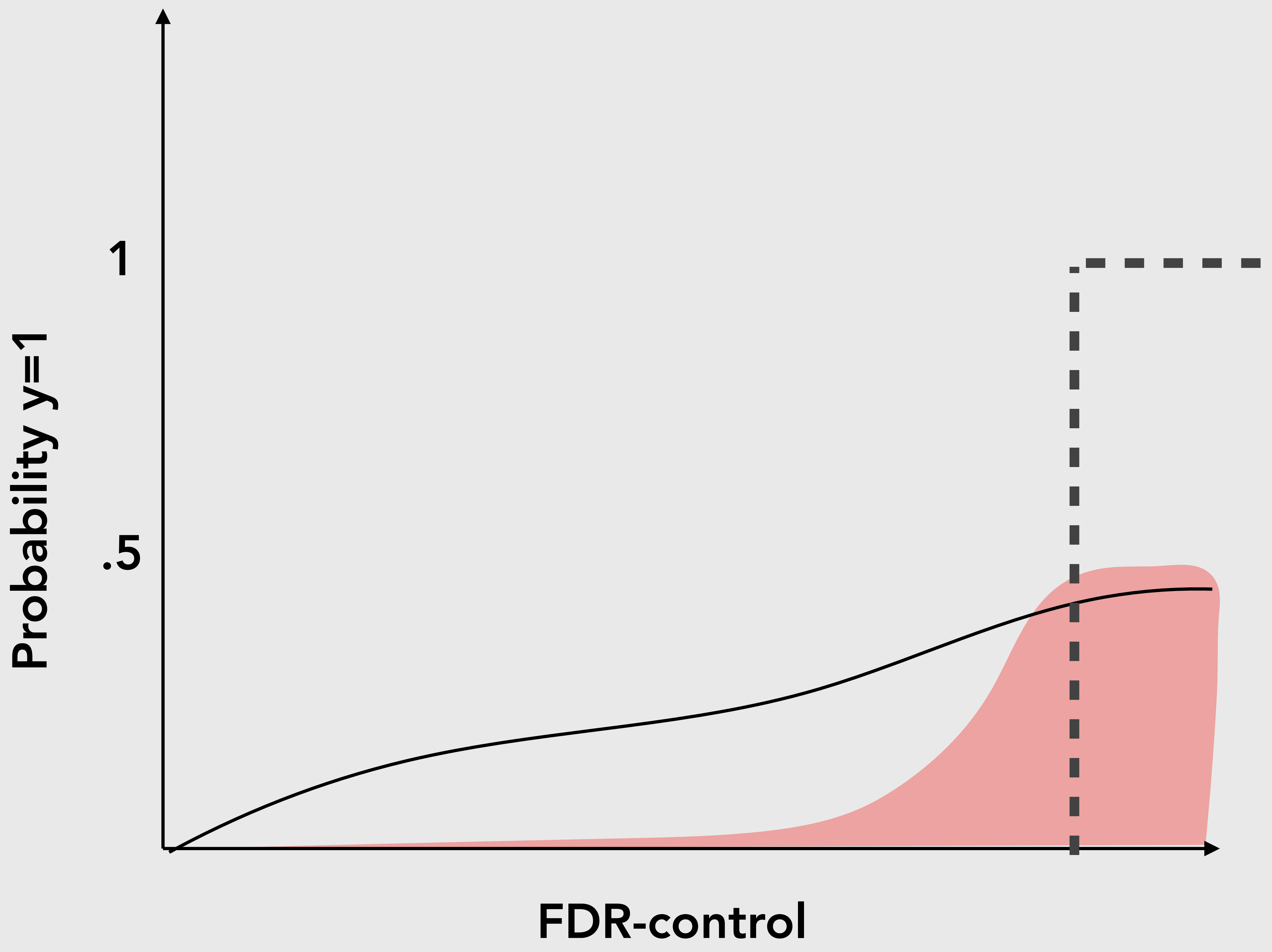
Guarantees

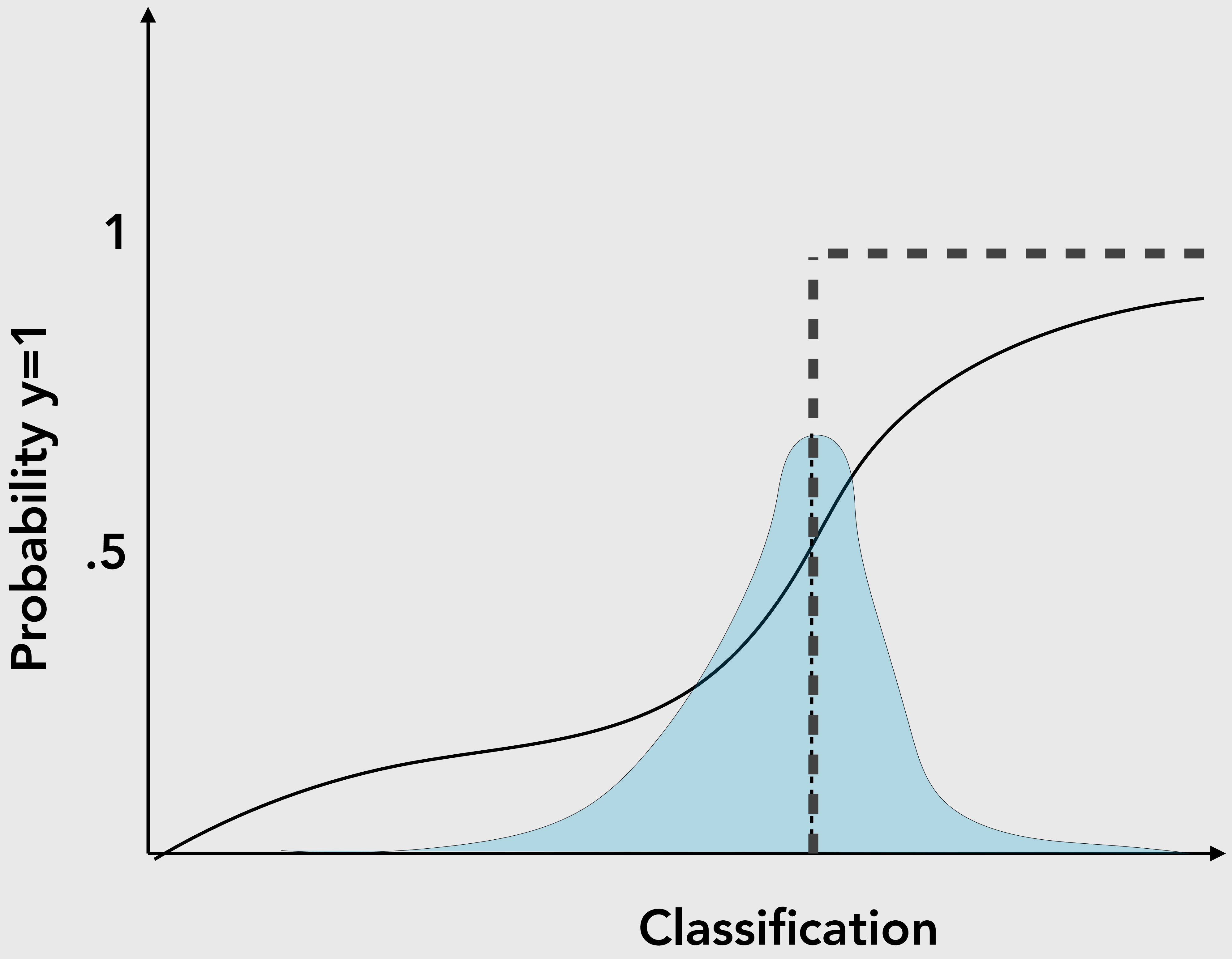
Theorem (J., Jamieson 2019) Let With probability greater than $1-\delta$ the FDR Action Elimination algorithm terminates after a number of samples no more than

$$\sum_{1<i\leq n} \max_{\pi:i\in\pi} \min\{s_{\pi}^{FDR}, \max\{s_{\pi^*}^{FDR}, s_{\pi}^{TPR}\}\} + \max_{\pi:i\in\pi_\alpha^*\Delta\pi} \max\{s_{\pi^*}^{FDR}, s_{\pi}^{TPR}\}$$

The sample complexity is at the time it takes to verify $FDR(\pi^*) \leq \alpha$

Contrasting Sampling Strategies





Moral: If you want FDR-control, it might not make sense to sample using active classification!