# Closing the Computational-Statistical Gap in Best Arm Identification for Combinatorial Semi-bandits

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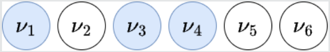
# Computational-Statistical Gap in BAI for Combinatorial Semi-bandits

# Problem: combinatorial BAI with fixed confidence

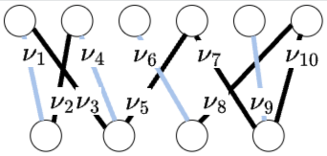
**Input:** $K$ arms $(\nu_k)_{k\in[K]}$ with mean $\boldsymbol{\mu} \in \mathbb{R}^K$ and $\mathcal{X} \subseteq \{0,1\}^K$

**Example: Gaussian reward** $\nu_k = \mathcal{N}(\mu_k, 1), \forall k \in [K]$

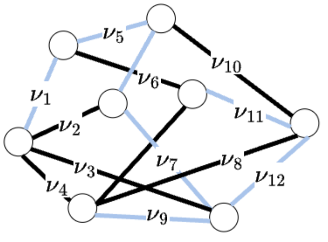
*m*-sets




matchings




spanning trees



# Problem: combinatorial BAI with fixed confidence

**Input:** $K$ arms $(\nu_k)_{k \in [K]}$ with mean $\boldsymbol{\mu} \in \mathbb{R}^K$ and $\mathcal{X} \subseteq \{0,1\}^K$

**Rule:** At each round $t$, the learner

- pulls $\boldsymbol{x}(t) \in \mathcal{X}$ and observes $y_k(t) \sim \nu_k$ iff $x_k(t) = 1$
- decides to stop at round $\tau$ (and outputs $\hat{\boldsymbol{\imath}} \in \mathcal{X}$)

**Goal:** Design a $\delta$-*PAC* algorithm s.t. $\boldsymbol{i}^\star(\boldsymbol{\mu}) \in \operatorname{argmax}_{\boldsymbol{x} \in \mathcal{X}} \langle \boldsymbol{x}, \boldsymbol{\mu} \rangle$ is identified with $\mathbb{P}_{\boldsymbol{\mu}}[\hat{\boldsymbol{\imath}} = \boldsymbol{i}^\star(\boldsymbol{\mu})] \geq 1 - \delta$ and $\mathbb{P}_{\boldsymbol{\mu}}[\tau < \infty] = 1$

(i) *statistically optimal:* information-theoretically *minimal* $\mathbb{E}_{\boldsymbol{\mu}}[\tau]$

(ii) *computationally efficient:* running time *polynomial* in $K$

**Existing $\delta$-PAC algorithms: only (i) or only (ii)**

(Open Question) Possible to design a $\delta$-PAC algorithm achieving both?

# Challenge in solving the lowerbound problem

**Instance-specific sample complexity lower bound [GK16]**

For any $\delta$-PAC algorithm[1], $\mathbb{E}_{\boldsymbol{\mu}}[\tau] \geq T^\star(\boldsymbol{\mu})\mathrm{kl}(\delta, 1-\delta)$, where

$$T^\star(\boldsymbol{\mu})^{-1} = \sup_{\boldsymbol{\omega} \in \Sigma} F_{\boldsymbol{\mu}}(\boldsymbol{\omega}) \text{ with } F_{\boldsymbol{\mu}}(\boldsymbol{\omega}) = \inf_{\boldsymbol{\lambda} \in \mathrm{Alt}(\boldsymbol{\mu})} \sum_{k=1}^{K} \frac{\omega_k(\mu_k - \lambda_k)^2}{2}$$

- $\Sigma = \{\sum_{\boldsymbol{x} \in \mathcal{X}} w_{\boldsymbol{x}} \boldsymbol{x} : \boldsymbol{w} \in \Sigma_{|\mathcal{X}|}\}$: all possible arm allocations
- $\Lambda = \{\boldsymbol{\lambda} \in \mathbb{R}^K : |\boldsymbol{i}^\star(\boldsymbol{\lambda})| = 1\}$: all possible parameters
- $\mathrm{Alt}(\boldsymbol{\mu}) = \{\boldsymbol{\lambda} \in \Lambda : \boldsymbol{i}^\star(\boldsymbol{\lambda}) \neq \boldsymbol{i}^\star(\boldsymbol{\mu})\}$: confusing parameters

[1] Here we assume the arm-$k$ reward distribution is $\nu_k = \mathcal{N}(\mu_k, 1)$

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Each sampling strategy is represented by its arm allocation $\boldsymbol{\omega} \in \Sigma$.

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- $\mathrm{Alt}(\boldsymbol{\mu}) = \{\boldsymbol{\lambda} \in \Lambda : \boldsymbol{i}^\star(\boldsymbol{\lambda}) \neq \boldsymbol{i}^\star(\boldsymbol{\mu})\}$: confusing parameters

The inner optimization measures the distance to the *most confusing parameter* (MCP) with the best action different from $\boldsymbol{i}^\star(\boldsymbol{\mu})$.

$\Rightarrow$ The best sampling strategy has the largest distance to the MCP.

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# Challenge in solving the lowerbound problem

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A standard approach [GK16] achieving asymptotic optimality consists of:

- (Chernoff stopping rule) $\tau = \inf\{t : tF_{\hat{\boldsymbol{\mu}}(t)}(\hat{\boldsymbol{\omega}}(t)) > \ln(\frac{t}{\delta}) + o(1)\}$
- (Optimal allocation) $\boldsymbol{\omega}^\star(\boldsymbol{\mu}) = \mathrm{argmax}_{\boldsymbol{\omega}\in\Sigma} F_{\boldsymbol{\mu}}(\boldsymbol{\omega})$

**Difficulty in determining the most confusing parameter (MCP)**

The domain $\mathrm{Alt}(\boldsymbol{\mu}) = \{\boldsymbol{\lambda} \in \Lambda : \boldsymbol{i}^\star(\boldsymbol{\lambda}) \neq \boldsymbol{i}^\star(\boldsymbol{\mu})\}$ of $F_{\boldsymbol{\mu}}(\boldsymbol{\omega})$

$\Rightarrow$ probably have to solve $\mathcal{O}(2^K)$ many convex programs

[1] Here we assume the arm-$k$ reward distribution is $\nu_k = \mathcal{N}(\mu_k, 1)$

## Computational inefficiency in prior optimal algorithms

- `Track-and-Stop` [GK16] at each round $t$ has to solve

$$\omega^\star(\hat{\mu}(t)) \in \operatorname*{argmax}_{\omega \in \Sigma} F_{\hat{\mu}(t)}(\omega), \quad \text{(computationally expensive)}$$

- `FWS` [WTP21] tracked a vector $\boldsymbol{w}(t)$ and for $\hat{\mu}(t) \in \Lambda$, the gradient $\nabla_\omega f_{\boldsymbol{x}}(\boldsymbol{w}(t), \hat{\mu}(t))$ of each $\boldsymbol{x} \neq \boldsymbol{i}^\star(\hat{\mu}(t))$ has to be computed in order to deal with the *nonsmoothness* of $F_{\hat{\mu}(t)}$
- `CombGame` [JMKK21] proposed a `MCP`-oracle efficient algorithm, but no efficient `MCP` oracle exists prior to our work

**Our Perturbed Frank-Wolfe Sampling (`P-FWS`)**

- `P-FWS` deals with $|\mathcal{X}| \leq 2^K$ actions by *stochastic smoothing*
- All `P-FWS` needs is the linear maximization $\boldsymbol{i}^\star$ oracle

# Our MCP Algorithm: a no-regret algorithm for solving $F_\mu(\omega)$

# A crucial structural observation about $F_\mu(\omega)$

Define $f_{\boldsymbol{x}}(\boldsymbol{\omega}, \boldsymbol{\mu}) = \inf_{\boldsymbol{\lambda} \in \mathbb{R}: \langle \boldsymbol{i}^\star(\boldsymbol{\mu}) - \boldsymbol{x}, \boldsymbol{\lambda} \rangle < 0} \sum_{k=1}^{K} \frac{\omega_k (\mu_k - \lambda_k)^2}{2}$.

**Property of $f_{\boldsymbol{x}}$ and its Lagrangian dual $g_{\omega,\mu}$**

$f_{\boldsymbol{x}}(\boldsymbol{\omega}, \boldsymbol{\mu}) = \max_{\alpha \geq 0} g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}, \alpha)$ (known by [CGL16])

$g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}, \alpha)$ is linear in $\boldsymbol{x}$ and concave in $\alpha$ (our observation)

$$F_{\boldsymbol{\mu}}(\boldsymbol{\omega}) = \min_{\boldsymbol{x} \neq \boldsymbol{i}^\star(\boldsymbol{\mu})} f_{\boldsymbol{x}}(\boldsymbol{\omega}, \boldsymbol{\mu}) = \min_{\boldsymbol{x} \neq \boldsymbol{i}^\star(\boldsymbol{\mu})} \max_{\alpha \geq 0} g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}, \alpha) \tag{1}$$

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**Requirement:** Not only to estimate $F_{\boldsymbol{\mu}}(\boldsymbol{\omega})$ but also the *equilibrium action* $\boldsymbol{x}_e$ s.t. $F_{\boldsymbol{\mu}}(\boldsymbol{\omega}) = \max_{\alpha\geq 0} g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}_e, \alpha)$.

- $\boldsymbol{x}_e$ is needed to solve $\max_{\boldsymbol{\omega}\in\Sigma} F_{\boldsymbol{\mu}}(\boldsymbol{\omega})$ by first-order methods
- existing results [DP19, LNP$^+$21, APFS22, AAS$^+$23] on last-iterate convergence are not applicable

# Our proposed MCP algorithm

**Algorithm 1:** $(\epsilon, \theta)$-$\texttt{MCP}(\boldsymbol{\omega}, \boldsymbol{\mu})$

**for** $n = 1, 2, \cdots$ **do**

(Follow-the-Perturbed-Leader) $\mathcal{Z}_n \sim \exp(1)^K$ and $\eta_n = \frac{c_0}{\sqrt{n}}$

$$\boldsymbol{x}^{(n)} \in \operatorname*{argmin}_{\boldsymbol{x} \neq \boldsymbol{i}^\star(\boldsymbol{\mu})} \left( \sum_{m=1}^{n-1} g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}, \alpha^{(m)}) + \frac{\langle \mathcal{Z}_n, \boldsymbol{x} \rangle}{\eta_n} \right)$$

(Best-Response) $\alpha^{(n)} \in \operatorname*{argmax}_{\alpha \geq 0} g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}^{(n)}, \alpha)$

**if** $\boxed{\sqrt{n} > \frac{c_\theta(1+\epsilon)}{\epsilon \hat{F}}}$, *where* $\begin{cases} \hat{F} = g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}^{(n_\star)}, \alpha^{(n_\star)}) \\ n_\star \in \operatorname{argmin}_{m \leq n} g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}^{(m)}, \alpha^{(m)}) \end{cases}$

**then return** $(\hat{F}, \boldsymbol{x}^{(n_\star)})$;

**end**

# Our proposed MCP algorithm

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(Best-Response) $\alpha^{(n)} \in \operatorname*{argmax}_{\alpha \geq 0} g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}^{(n)}, \alpha)$

**(Computational Cost Per Iteration)**

- $\boldsymbol{x}^{(n)}$ can be computed by at most $D = \max_{\boldsymbol{x} \in \mathcal{X}} \|\boldsymbol{x}\|_0$ calls to $\boldsymbol{i}^\star(\cdot)$
- $\alpha^{(n)}$ is evaluated in $\mathcal{O}(1)$

# Our proposed MCP algorithm

The termination condition is designed based on Lemma 1

**if** $\boxed{\sqrt{n} > \dfrac{c_\theta(1+\epsilon)}{\epsilon \hat{F}}}$, *where* $\begin{cases} \hat{F} = g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}^{(n_\star)}, \alpha^{(n_\star)}) \\ n_\star \in \operatorname{argmin}_{m \le n} g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}^{(m)}, \alpha^{(m)}) \end{cases}$

such that $\mathbb{P}\left[F_{\boldsymbol{\mu}}(\boldsymbol{\omega}) \le \hat{F} \le (1+\epsilon) F_{\boldsymbol{\mu}}(\boldsymbol{\omega})\right] \ge 1 - \theta$ holds.

**(Lemma 1)** If Algorithm 1 runs for $N$ iterations, then

$$\mathbb{P}\left[\underbrace{\frac{1}{N}\sum_{n=1}^{N} g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}^{(n)}, \alpha^{(n)})}_{\ge \min_{n=1}^{N} g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}^{(n)},\alpha^{(n)}) = \hat{F}} - \underbrace{\frac{1}{N}\min_{\boldsymbol{x} \ne \boldsymbol{i}^\star(\boldsymbol{\mu})} \sum_{n=1}^{N} g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}, \alpha^{(n)})}_{\le \frac{1}{N}\sum_{n=1}^{N} g_{\boldsymbol{\omega},\boldsymbol{\mu}}(\boldsymbol{x}_e,\alpha^{(n)}) \le F_{\boldsymbol{\mu}}(\boldsymbol{\omega})} \le \frac{c_\theta}{\sqrt{N}}\right] \ge 1 - \theta.$$

# Our proposed MCP algorithm

**Theorem 1 (MCP)**

Let $(\boldsymbol{\omega}, \boldsymbol{\mu}) \in \Sigma_+ \times \Lambda$. The $(\epsilon, \theta)$-$\mathtt{MCP}(\boldsymbol{\omega}, \boldsymbol{\mu})$ algorithm outputs $(\hat{F}, \hat{\boldsymbol{x}})$:

- $\mathbb{P}\left[F_{\boldsymbol{\mu}}(\boldsymbol{\omega}) \leq \hat{F} \leq (1+\epsilon) F_{\boldsymbol{\mu}}(\boldsymbol{\omega})\right] \geq 1 - \theta$
- the number of calls to $\boldsymbol{i}^\star(\cdot)$: $\mathcal{O}\left(\frac{\|\boldsymbol{\mu}\|_\infty^4 \left\|\boldsymbol{\omega}^{-1}\right\|_\infty^2 K^3 D^5 \ln K \ln \theta^{-1}}{\epsilon^2 F_{\boldsymbol{\mu}}(\boldsymbol{\omega})^2}\right)$

By envelop theorem [WTP21], we obtain an estimation to $\nabla F_{\boldsymbol{\mu}}(\boldsymbol{\omega})$ by

$$\nabla_{\boldsymbol{\omega}} f_{\hat{\boldsymbol{x}}}(\boldsymbol{\omega}, \boldsymbol{\mu}) = \sum_{k=1}^{K} \frac{(\mu_k - \lambda_k^\star)^2}{2},$$

where $\boldsymbol{\lambda}^\star$ is the minimizer to the optimization problem of $f_{\hat{\boldsymbol{x}}}(\boldsymbol{\omega}, \boldsymbol{\mu})$.

# Our P-FWS: the first poly-time statistically optimal algorithm

# Solving $T^\star(\mu)$ with stochastic smoothed objective

- The well-studied stochastic smoothing [FKM05, DBW12] takes the average value in a neighborhood of points:

$$\bar{F}_{\boldsymbol{\mu},\eta} = \mathbb{E}_{\boldsymbol{\mathcal{Z}}\sim \mathsf{Uniform}(B_2)}[F_{\boldsymbol{\mu}}(\boldsymbol{\omega} + \eta \boldsymbol{\mathcal{Z}})]$$

- $F_{\boldsymbol{\mu}}$ is $\ell$-Lipschitz and its smoothed objective satisfies:
  - $\bar{F}_{\boldsymbol{\mu},\eta}$ is $\frac{\ell K}{\eta}$-smooth and $\bar{F}_{\boldsymbol{\mu},\eta}(\boldsymbol{\omega}) \xrightarrow{\eta \downarrow 0} F_{\boldsymbol{\mu}}(\boldsymbol{\omega})$
  - $\nabla \bar{F}_{\boldsymbol{\mu},\eta} = \underset{\boldsymbol{\mathcal{Z}}\sim \mathsf{Uniform}(B_2)}{\mathbb{E}}[\nabla F_{\boldsymbol{\mu}}(\boldsymbol{\omega} + \eta \boldsymbol{\mathcal{Z}})]$

**High-level design of `P-FWS`**

Let $\mathcal{X}_0$ be a set s.t. $\forall k \in [K]$, there exists $\boldsymbol{x} \in \mathcal{X}_0$ s.t. $x_k = 1$.

`P-FWS` alternate between two phases:

$$\begin{cases} \text{pull each } \boldsymbol{x} \in \mathcal{X}_0 \text{ once} & \text{(to avoid high cost and boundary cases)} \\ \text{pull } \boldsymbol{x}(t) \in \operatorname{argmax}_{\boldsymbol{x}\in\mathcal{X}} \left\langle \nabla \bar{F}_{\hat{\boldsymbol{\mu}}(t-1),\eta_t}(\hat{\boldsymbol{\omega}}(t-1)), \boldsymbol{x} \right\rangle & \text{(ideal FW update)} \end{cases}$$

# `P-FWS`: the first poly$(K)$-time optimal algorithm

**Theorem 2 (P-FWS)**

Let $\boldsymbol{\mu} \in \Lambda$ and $\delta \in (0, 1)$. `P-FWS` with proper parameters is $\delta$-PAC and finishes in finite time;

(i) its $\mathbb{P}_{\boldsymbol{\mu}}\left[\limsup_{\delta \to 0} \frac{\tau}{\ln \delta^{-1}} \leq T^\star(\boldsymbol{\mu})\right] = 1$;

(ii) its $\mathbb{E}_{\boldsymbol{\mu}}[\tau]$ being poly$(K)$ in moderate confidence regime;

(iii) the expected number of $\boldsymbol{i}^\star$ upper bounded by poly$(K)$.

# P-FWS: the first poly$(K)$-time optimal algorithm

## Proof Sketch of Theorem 2

Define good events: $\mathcal{E}_t^{(1)}$ when $\hat{\boldsymbol{\mu}}(t)$ is sufficiently close to $\boldsymbol{\mu}$, and $\mathcal{E}_t^{(2)}$ when $\boldsymbol{x}(t)$ is closed to the ideal FW-update.

**(Step 1)** By maximum theorem [FKV14], we derive uniform continuity for $F_{\boldsymbol{\pi}}$ and $\nabla \bar{F}_{\boldsymbol{\pi},\eta}$ in $\boldsymbol{\pi}$
$\Rightarrow$ to simplify the analysis as if $\hat{\boldsymbol{\mu}}(t) = \boldsymbol{\mu}$ for $t \geq M$

**(Step 2)** Under $\mathcal{E}_t^{(1)} \cap \mathcal{E}_t^{(2)}$, we derive a recursive formula for the smoothed FW updates $\Rightarrow$ the FW algorithm converges

**(Step 3)** $\mathbb{E}_{\boldsymbol{\mu}}[\tau] \leq T_0(\delta) + \sum_{t \geq M} \mathbb{P}_{\boldsymbol{\mu}}\left[(\mathcal{E}_t^{(1)} \cap \mathcal{E}_t^{(2)})^c\right]$, where

$$\begin{cases} (\delta\text{-dependent}) \ \frac{T_0(\delta)}{\ln \delta^{-1}} \xrightarrow{\delta \to 0} T^\star(\boldsymbol{\mu}) \\ (\delta\text{-independent}) \ \sum_{t \geq M} \mathbb{P}_{\boldsymbol{\mu}}\left[(\mathcal{E}_t^{(1)} \cap \mathcal{E}_t^{(2)})^c\right] \leq \text{poly}(K) \end{cases}$$

# P-FWS: the first poly$(K)$-time optimal algorithm

**Algorithm 1:** $\texttt{P-FWS}(\{\epsilon_t, \eta_t, n_t, \rho_t, \theta_t\}_t)$

**Initialization:** pull each $\boldsymbol{x} \in \mathcal{X}_0$ four times and update estimates

**for** $t = 4|\mathcal{X}_0| + 1, \cdots$ **do**

  **if** $\sqrt{\frac{t}{|\mathcal{X}_0|}} \in \mathbb{N}$ ***or*** *costly to estimate* $F_{\hat{\boldsymbol{\mu}}(t-1)}(\hat{\boldsymbol{\omega}}(t-1))$ **then**

    pull each $\boldsymbol{x} \in \mathcal{X}_0$ once;

  **else**

    pull $\boldsymbol{x}(t) \in \boldsymbol{i}^\star\left(\nabla \tilde{F}_{\hat{\boldsymbol{\mu}}(t-1),\eta_t,n_t}(\hat{\boldsymbol{\omega}}(t-1))\right)$ and update estimates;

  **if** *not costly to estimate* $F_{\hat{\boldsymbol{\mu}}(t)}(\hat{\boldsymbol{\omega}}(t))$ **then**

    compute $\hat{F}_t$ by $(\epsilon_t, \frac{\delta}{t^2})$-$\texttt{MCP}(\hat{\boldsymbol{\omega}}(t), \hat{\boldsymbol{\mu}}(t))$;

    **return** $\boldsymbol{i}^\star(\hat{\boldsymbol{\mu}}(t))$ **if** $t\hat{F}_t > (1+\epsilon_t)\beta(t, \frac{4|\mathcal{X}_0|-1}{|\mathcal{X}_0|}\delta)$

**end**

$\nabla \tilde{F}_{\hat{\boldsymbol{\mu}}(t-1),\eta_t,n_t}(\hat{\boldsymbol{\omega}}(t-1))$ is a $n_t$-sample estimation to $\nabla \bar{F}_{\hat{\boldsymbol{\mu}}(t-1),\eta_t}(\hat{\boldsymbol{\omega}}(t-1))$

# Preliminary Numerical Results

# Empirical evaluation on $\mathcal{X}$ as the set of spanning trees

All the experiments[2] are performed on a Macbook Air with 16 GB memory.

**Table 1:** Averaged sample complexity at $\delta = 0.1$ over 100 independent runs on a graph with $|\mathcal{X}| = 21\,025$ spanning trees.

| Algorithm | Sample Complexity |
|---|---|
| `P-FWS` (ours) | 1 176 |
| `CombGame` [JMKK21] | 1 277 |

**Table 2:** Averaged sample complexity at $\delta = 0.1$ over 100 independent runs on a graph with $|\mathcal{X}| = 343\,385$ spanning trees.

| Algorithm | Sample Complexity |
|---|---|
| `P-FWS` (ours) | 1 501 |
| `CombGame` [JMKK21] | OOM |

[2] Our code: https://github.com/rctzeng/NeurIPS2023-PerturbedFWS.

# Conclusion and Future Works

# Conclusion and open questions

- Our proposed `P-FWS` is the first algorithm to close the statistical-computational gap for combinatorial BAI by exploring the structural properties of the lowerbound problem.
- It remains largely unexplored whether one can close the computational-statistical gap for other tasks, such as linear BAI or best-policy identification.

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