

ACTIVE LEARNING IN REGRESSION OVER FINITE DOMAINS

András Antos

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Based on: [Antos et al., 2010, Carpentier et al., 2011,
Carpentier et al., 2014], PDSS, IDA jegyzet

OUTLINE

1 INTRO: BECSLÉS, DÖNTÉS, FELÜGYELT (PASSZÍV) TANULÁS

- Bayes-döntés
- Bayes-döntés közelítése
- Bayes-becslés
- Regresszióbecslés; négyzetes középhiba minimalizálás

2 INTRODUCTION

3 MODEL, PROTOCOL, LOSSES

4 MAX-LOSS

- Algorithm — GAFS-MAX
- Theory
- Algorithm — GFSP-MAX
- Theory
- Experiments
- Algorithm — UCB-CH-AS-MAX
- Theory

5 CONCLUSIONS

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KÖVETKEZTETÉS

- Megfigyelhető X -ből kell egy (még) nem megfigyelhető Y -ra következtetni
- X, Y val. változók, értékkészletük \mathcal{X} ill. \mathcal{Y} (pl. $\mathbb{R}, \mathbb{R}^d, \{0, 1\}^d, [0, 1]^d$, ezek megszámlálható v. véges része)
- \mathcal{Y} elemei: címkék
- X -ből Y -ra a $g : \mathcal{X} \rightarrow \bar{\mathcal{Y}}$ -vel következtetünk ($\bar{\mathcal{Y}}(\supseteq \mathcal{Y})$ az szóba jövő g -k értékkészletének uniója)
- A $g(X)$ következtetés jóságát méri: $C : \mathcal{Y} \times \bar{\mathcal{Y}} \rightarrow [0, \infty)$ költségfüggvény
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- g jóságát $R(g) \stackrel{\text{def}}{=} \mathbb{E}[C(Y, g(X))]$ *globális kockázat* méri
- g -k, amikre $R(g)$ a legkisebb: *optimális*
- $r(g, x) \stackrel{\text{def}}{=} \mathbb{E}[C(Y, g(X))|X = x]$: *lokális kockázat függvény*
- $\mathbb{E}[r(g, X)] = R(g)$ és

$$r(g, x) = \int_Y C(y, g(x)) dF_{Y|x}(y)$$

ahol $F_{Y|x}$ az Y feltételes, *a posteriori* eloszlásfüggvénye ha $X = x$.

(Általános integrál: diszkrét e.o. \Rightarrow összegzés, absz. folyt. e.o. \Rightarrow Riemann-integrál)

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négyzete, azaz $C_2(y, y') \stackrel{\text{def}}{=} \sum_{s=1}^d |y_s - y'_s|^2 = \|y - y'\|^2$
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 - \Rightarrow pl. $\bar{\mathcal{Y}} = \mathbb{R}$ -re $R(g) = \mathbb{E}[(Y - g(X))^2]$ a *négyzetes körzéphiba* (MSE)

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HIPOTÉZIS, DÖNTÉSFÜGGVÉNY, DÖNTÉSI TARTOMÁNY

Spec. eset: $\mathcal{Y} = \bar{\mathcal{Y}} = \{0, 1\}$, $C(i, j) = C_0(i, j) = \mathbb{I}_{\{i \neq j\}}$

DEFINITIONS

$i = 0,1$ az $\{Y = i\}$: i -dik hipotézis. Y a posteriori eloszlását az $\eta_i(x) \stackrel{\text{def}}{=} \mathbb{P}(Y = i | X = x)$ a posteriori valószínűségek adják.

g = döntésfüggvény. 0 és 1 g -vel való ōsképei \mathcal{X} egy partíciója, ennek $D_i = \{x \in \mathcal{X} : g(x) = i\}$ osztályai a döntési tartományok.

$(D_0, D_1) \Leftrightarrow g$, mert $\mathbb{I}_{\{g(x)=j\}} = \mathbb{I}_{\{x \in D_j\}}$. Igy $r(g, x) =$

$$\mathbb{I}_{\{g(x)=1\}}\eta_0(x) + \mathbb{I}_{\{g(x)=0\}}\eta_1(x) = 1 - \mathbb{I}_{\{x \in D_0\}}\eta_0(x) - \mathbb{I}_{\{x \in D_1\}}\eta_1(x)$$

Olyan g minimalizálja, ami $\forall x$ -et a nagyobb $\eta_j(x)$ -hez tartozó D_j -be sorol

BAYES-DÖNTÉS

- Legyen $\{D_i^*\}$ olyan, hogy $\forall x$

$$x \in D_j^* \Leftrightarrow (\eta_j(x) > \eta_{1-j}(x) \text{ v. } j = 0, \eta_0(x) = \eta_1(x))$$

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g^* (optimális) globális kockázata: *Bayes-kockázat/Bayes-hiba*

$$R(g^*) = \mathbb{E} [\min(\eta_0(X), \eta_1(X))] = \mathbb{E} [\min(\eta_1(X), 1 - \eta_1(X))].$$

OUTLINE

① INTRO: BECSLÉS, DÖNTÉS, FELÜGYELT (PASSZÍV) TANULÁS

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- $\{\eta_i(x)\}$ sokszor ismeretlen.
 - Tfh. η_i -t becsülhető lehet valamely $\tilde{\eta}_i : \mathcal{X} \rightarrow [0, 1]$ -vel.
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- Várakozás: $\tilde{\eta}_i$ -k jó becslések $\Rightarrow \tilde{g}$ hibája $\approx g^*$ hibája (mindig \geq). Kockázatuk különbsége \leq az $\tilde{\eta}_i$ -k becslési hibája:

BAYES-DÖNTÉS KÖZELÍTÉSE 2

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$$r(\tilde{g}, x) - r(g^*, x) \leq \mathbb{I}_{\{\tilde{g}(x) \neq g^*(x)\}} \sum_{i \in \{0,1\}} |\tilde{\eta}_i(x) - \eta_i(x)|$$

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OSZTÁLYOZÁS MINTÁKBÓL

Tf. $\{\eta_i(x)\}$ ismeretlen, de adott n db i.i.d. minta:

$(X_1, Y_1), \dots, (X_n, Y_n) \sim (X, Y)$. Ezek alapján közelítjük g^* -ot. \Rightarrow Osztályozás (v. alakfelismerés, néha (felügyelt) tanulás).

Legyen $|\mathcal{X}| < \infty$, $r_i(x) = \mathbb{P}(X = x, Y = i)$ ($x \in \mathcal{X}, i \in \{0, 1\}$) és $\tilde{r}_{in}(x)$ az $r_i(x)$ becslése az n mintából. Mivel $\eta_i(x) = r_i(x)/\mathbb{P}(X = x)$, legyen $\eta_i(x)$ közelítése

$$\tilde{\eta}_{in}(x) = \frac{\tilde{r}_{in}(x)}{\mathbb{P}(X = x)}, \quad i \in \{0, 1\}$$

és \tilde{g}_n egy hozzájuk rendelt döntésfüggvény. ($\mathbb{P}(X = x)$ -k ismeretlenek $\Rightarrow \tilde{\eta}_{in}(x)$ -k nem meghatározhatók, de \tilde{g}_n -hez nem is kell, mert $\tilde{g}_n(x) = \operatorname{argmax}_i \tilde{\eta}_{in}(x) = \operatorname{argmax}_i \tilde{r}_{in}(x)$.)

$$R(\tilde{g}_n) - R(g^*) \leq \mathbb{E} \left[\sum_{i \in \{0, 1\}} |\tilde{\eta}_{in}(X) - \eta_i(X)| \right] = \sum_{x \in \mathcal{X}} \sum_{i \in \{0, 1\}} |\tilde{r}_{in}(x) - r_i(x)|.$$

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- Legyen $\tilde{r}_{in}(x) = \frac{1}{n} \sum_{t=1}^n \mathbb{I}_{\{X_t=x, Y_t=i\}}$ rel. gyakoriság.
- Nagy számok erős tv.-e: $n \rightarrow \infty \Rightarrow \forall x \in \mathcal{X}, i \in \{0, 1\}$,
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- \Rightarrow Jobb oldal 0-hoz tart m.m. és $R(\tilde{g}_n) - R(g^*) \geq 0 \Rightarrow$ az is $\rightarrow 0$.
- Így $R(g^*)$ -ot „majdnem biztosan” tetszőlegesen megközelítő hibájú $\{\tilde{g}_n\}$ sorozatot kaptunk
- $|\mathcal{X}| < \infty$ esetén az eljárás erősen konzisztens.

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Ha n összemérhető az (X, Y) pár effektív értékkészletével, akkor bár az egyes tagok kicsik, az összeg már nem lesz az, így $R(\tilde{g}_n)$ megbízhatatlanná válik.

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BAYES-BECSLÉS

Spec. eset: $\mathcal{Y}, \bar{\mathcal{Y}} \subseteq \mathbb{R}$, többnyire végtelen, folytonos, C az Y és $g(X)$ valamely távolságát méri a; hibázás nagysága is számít.
Ekkor g becslésfüggvény.

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Bayes-becslésnek nevezzük az optimális g^* becslésfüggvényeket, azaz amikre $R(g^*) = \min_g R(g)$.

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- Legyen $Y \in \mathbb{R}$ véges szórású és $C(y, y') = C_2(y, y') = (y - y')^2$.
- \Rightarrow keressük g^* -t, amire $R(g^*) = \mathbb{E} [(g^*(X) - Y)^2]$ min.
- Tétel \Rightarrow ha $r(g^*, x) = \min_{y \in \bar{\mathcal{Y}}} \mathbb{E} [(Y - y)^2 | X = x]$ m.m. $x \in \mathcal{X}$ -re, akkor g^* Bayes-becslés.

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THEOREM (STEINER)

$C = C_2$ esetén $\forall g$ -re $r(g, x) = r(\mu, x) + (\mu(x) - g(x))^2$
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Regressziós függvény: $\mu(x) = \mathbb{E}[Y|X = x]$; minden x -re Y feltételes várhatóértékét adja ha $X = x$.

THEOREM (STEINER)

$C = C_2$ esetén $\forall g$ -re $r(g, x) = r(\mu, x) + (\mu(x) - g(x))^2$
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REGRESSZIÓBECSLÉS; MSE MINIMALIZÁLÁS

- Legyen $Y \in \mathbb{R}$ véges szórású és $C(y, y') = C_2(y, y') = (y - y')^2$.
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5 CONCLUSIONS

ACTIVE LEARNING

● Regression:

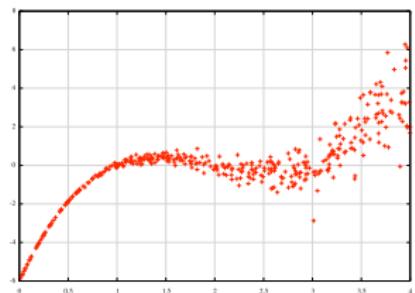
- Goal: Learn f
- Data: $(X_1, Y_1), \dots, (X_n, Y_n)$, where

$$Y_t = f(X_t) + Z_t,$$

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$$\mathbb{E}[Z_t | X_t] = 0,$$

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- Assumption: X_{t+1} can be selected based on

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“Active learning” — more efficient than passive learning for some problem classes

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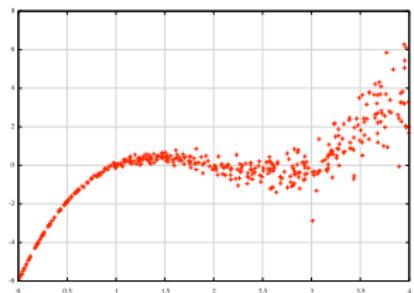
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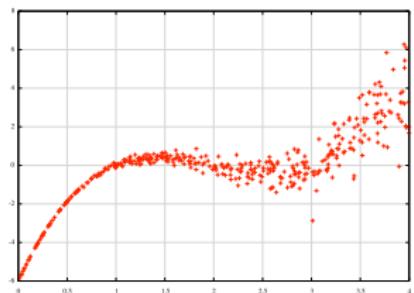
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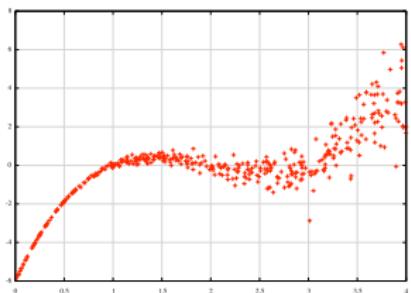
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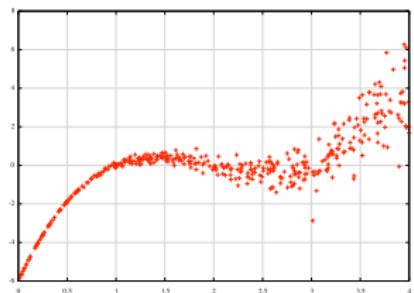
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OPTIMAL EXPERIMENT DESIGN/PLANNING/ALLOCATION

- E.g. [Fedorov, 1972]: mostly homoscedastic Gaussian noise: $\text{Var}[Y|X = x] = \text{Var}[Z|X = x] \equiv \sigma^2 = \text{const}$
- E.g.: Generalized linear model: $\mu, \phi(X) \in \mathbb{R}^d$ basis func.

$$Y = f(X) + Z = \mu^T \phi(X) + Z$$

X has finite domain $\mathcal{X} = \{x_1, \dots, x_K\}$, w.l.o.g. $x_k = k$. Now $\phi = [\phi(1) \cdots \phi(K)] \sim d \times k$ matrix \Rightarrow optimization problem: given \mathcal{X} , how many times should we choose k to minimize some loss

- $K > d$: hard and interesting
- Spec. case: $K = d$, $\{\phi(1), \dots, \phi(K)\} \subseteq \mathbb{R}^K$ is a basis in \mathbb{R}^K
- Further simplification: $\phi(k) = e_k$, $\phi = I$, i.e., $f(x_k) = \mu_k$,

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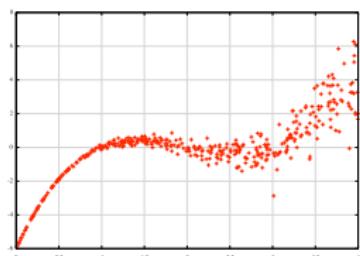
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HETEROSCEDASTICITY

What if Z is heteroscedastic (non-Gaussian), i.e.,

$$\text{Var}[Z|X = x] = \sigma^2(x),$$

and $\sigma^2(x)$ is unknown?



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MODEL & PROTOCOL OF LEARNING

- Given $(\mathcal{D}_k)_{1 \leq k \leq K}$ distributions with means $(\mu_k)_{1 \leq k \leq K}$ supported in $[0, 1]$.

PROTOCOL OF LEARNING

- Request sample from option/arm $X_t \in \{1, \dots, K\}$

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Loss of $\hat{\mu}_{kn}$ after seeing n samples: $L_{kn} = \mathbb{E} [(\hat{\mu}_{kn} - \mu_k)^2]$. If k is chosen \sim some a given p_1, \dots, p_K , $p_k \geq 0$, ($\sum_k p_k = 1$),

$$L_n^{(p)} = \sum_k p_k L_{kn}.$$

EXAMPLES

• Treatment efficiency testing

• Hypothesis testing

• Model selection (AIC, BIC, etc.)

• Feature selection

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ADAPTIVE STRATIFIED SAMPLING

- **Problem:** Estimate $\mu = \mathbb{E}[Y]$.

- **Assumptions:** We are given

- strata S_1, S_2, \dots, S_n , $n > 0$ with weights $w_k = \mathbb{P}(S_k) > 0$.

- $\mu_k = \mathbb{E}[Y|S_k]$ for all k .

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- **Goal:** Sample $Y|S_k$ and construct $\hat{\mu}_{kn}$ s.t. the loss of $\hat{\mu}_n = \sum_k w_k \hat{\mu}_{kn}$, $L_n = \mathbb{E}[(\hat{\mu}_n - \mu)^2] \rightarrow \min!$

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EXAMPLES

Running polls adaptively

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Unknown $p \rightarrow$ pessimistic (worst-case) approach. Loss after seeing n samples:

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- $\forall k$ learner sequentially decides the frequency of $\{X_t = k\}$
- $T_{kn} \stackrel{\text{def}}{=} \sum_{t=1}^n \mathbb{I}_{\{X_t=k\}} \geq 0$: number of samples allocated to arm k till time n

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OUTLINE

1 INTRO: BECSLÉS, DÖNTÉS, FELÜGYELT (PASSZÍV) TANULÁS

- Bayes-döntés
- Bayes-döntés közelítése
- Bayes-becslés
- Régesszióbecslés; négyzetes középhiba minimalizálás

2 INTRODUCTION

3 MODEL, PROTOCOL, LOSSES

4 MAX-LOSS

- Algorithm — GAFS-MAX
- Theory
- Algorithm — GFSP-MAX
- Theory
- Experiments
- Algorithm — UCB-CH-AS-MAX
- Theory

5 CONCLUSIONS

OPTIMAL ALLOCATION (MAX-LOSS)

- Assume $\sigma_k^2 = \text{Var}[Y_{kt}] = \text{Var}[Y|X=k]$ are known (and > 0 now). Choose $\{T_{kn}\}_k$ in advance (not data-dependent).
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- Goal: Minimize $L_n = \max_k L_{kn}$!
- Solution: Optimal choice must make all L_{kn} the same:

$$T_{kn}^* = n \frac{\sigma_k^2}{\Sigma^2} \stackrel{\text{def}}{=} n\lambda_k \quad (\text{mod rounding}),$$

where $\Sigma^2 = \sum_k \sigma_k^2$, λ_k is *optimal allocation ratio* for arm k .

- \Rightarrow To get $\{T_{kn}^*\}_k$ only $\{\sigma_k\}_k$ is needed
- (How to extend this if $\exists \sigma_k = 0$?) W.l.o.g. assume $\Sigma^2 > 0$.

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- Reminds to *multi-armed bandit problems*
[Auer et al., 2002]. *Exploration-exploitation trade-off!* (But different performance criterion.)
- How to explore?

• Greedy, softmax, Thompson sampling

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• *Bayesian Bandit* (Beta-Binomial)

• *Softmax*

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- Sample arm $X_{t+1} \in \operatorname{argmax}_k \frac{\hat{\sigma}_{kt}^2}{T_{kt}}$! (based on earlier samples)

- Is this a good idea?
- Reminds to *multi-armed bandit problems*
[Auer et al., 2002]. *Exploration-exploitation trade-off!* (But different performance criterion.)
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 - Upper confidence bounds
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EXPLORE OR EXPLOIT?

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- Algorithm — GAFS-MAX
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⑤ CONCLUSIONS

ALGORITHM GAFS-MAX

Greedy Allocation with Forced Selection \Rightarrow GAFS

Algorithm GAFS-MAX(α)

- ➊ First K trials: choose each arm once, initialize $\forall k : T_{kK} = 1, \hat{\sigma}_{kK} = 0$
- ➋ At time $t = K + 1, \dots, n$ do:
- ➌ $U_{t-1} \in \operatorname{argmin}_{1 \leq k \leq K} T_{k,t-1}$
- ➍ Let

$$X_t = \begin{cases} U_{t-1}, & \text{if } T_{U_{t-1}, t-1} < \alpha\sqrt{t-1} + 1 \\ \in \operatorname{argmax}_{1 \leq k \leq K} \frac{\hat{\sigma}_{k,t-1}^2}{T_{k,t-1}}, & \text{otherwise} \end{cases}$$

- ➎ Choose option X_t , $T_{kt} := T_{k,t-1} + \mathbb{I}_{\{X_t=k\}}$
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UPPER BOUND GAFS-MAX

THEOREM

Let $\lambda_{\min} = \min_{k: \lambda_k > 0} \lambda_k$. Then there is $C = \text{poly}(1/\lambda_{\min})$, s.t. for any n

$$R_n(\mathcal{A}_{\text{GAFS-MAX}}) \leq Cn^{-3/2}\sqrt{\ln n}.$$

PROOF – PREPARATIONS

OBSERVATIONS

With high probability:

- **Claim 1:** If $T_{kn} \geq f(n)$ then

$$\hat{\lambda}_{kn} - \lambda_k = O\left(\sqrt{\frac{\ln n}{f(n)}}\right)$$

- **Claim 2:** If $\hat{\lambda}_{kn} - \lambda_k = O(\sqrt{\ln n/f(n)})$ then

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- Forcing $\Rightarrow T_{kn} \geq \sqrt{n}$
- Use Claim 1 & 2 with $f(n) = \sqrt{n} \Rightarrow$

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- $\Rightarrow T_{kn} \geq \frac{\lambda_k}{2}n$ if n is large enough
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- Wald's second identity $\Rightarrow L_{kn} - L_n^* = O(n^{-3/2} \sqrt{\ln n}).$



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Greedy Forced Selection with Phases \Rightarrow GFSP

Phase m : times $\{t_m - K + 1, \dots, t_m\} \cup \{t_m + 1, \dots, t_m + m\}$

Algorithm GFSP-MAX

- 1 First $2K$ trials: choose each arm twice, initialize $\forall k : T_{k,2K} = 2, \hat{\sigma}_{k,2K}^2$
- 2 In phase m , $t_m \stackrel{\text{def}}{=} m(2K + m - 1)/2 + 2K$ and do:
 - 3 At times $t_m - K + 1, \dots, t_m$: choose each arm once
 - 4 $\hat{\Sigma}^2 \stackrel{\text{def}}{=} \sum_k \hat{\sigma}_{k,t_m-K}^2, \hat{\lambda}_{m,k} \stackrel{\text{def}}{=} \hat{\sigma}_{k,t_m-K}^2 / \hat{\Sigma}^2$
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 - 6 $T_{k,t_m+m} := T_{k,t_m-1+m-1} + m\hat{\lambda}_{k,m} + 1$
 - 7 Observe $Y_{t_m-K+1}, \dots, Y_{t_m+m}$
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 - ➍ $\hat{\Sigma}^2 \stackrel{\text{def}}{=} \sum_k \hat{\sigma}_{k,t_m-K}^2, \hat{\lambda}_{m,k} \stackrel{\text{def}}{=} \hat{\sigma}_{k,t_m-K}^2 / \hat{\Sigma}^2$
 - ➎ At times $t_m + 1, \dots, t_m + m$: choose arm k $m\hat{\lambda}_{k,m}$ times (+rounding!)
 - ➏ $T_{k,t_m+m} := T_{k,t_m-1+m-1} + m\hat{\lambda}_{k,m} + 1$
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ALGORITHM GFSP-MAX

Greedy Forced Selection with Phases \Rightarrow GFSP

Phase m : times $\{t_m - K + 1, \dots, t_m\} \cup \{t_m + 1, \dots, t_m + m\}$

Algorithm GFSP-MAX

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ANALYSYS GFSP-MAX

- Observe: After phase m :
 - each arm is chosen $\geq m + 2$ times,
 - number of all trials: $2K + Km + (1 + 2 + \dots + m) \approx m^2/2$.
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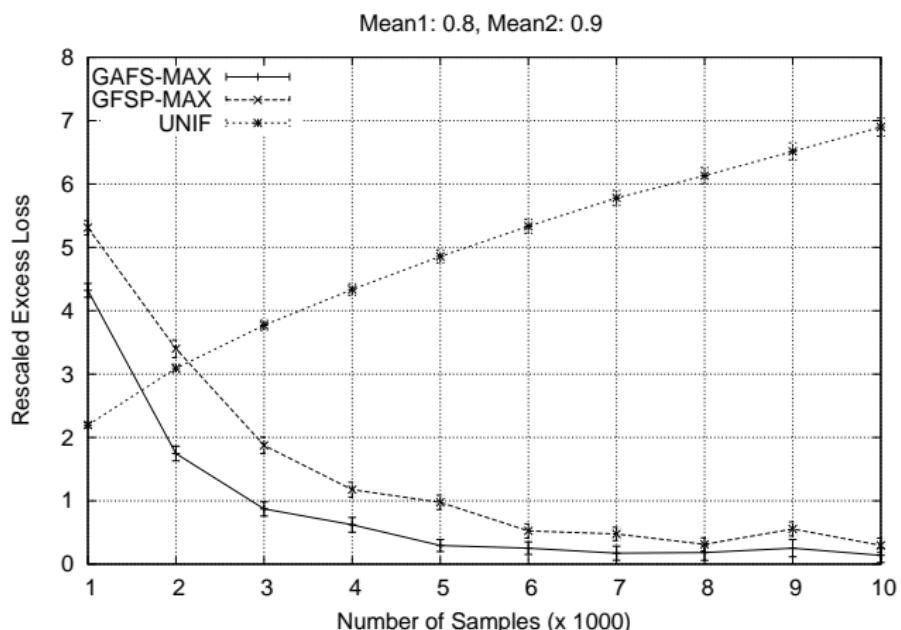
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BERNOULLI OPTIONS, $K = 2$ 

The rescaled excess loss, $n^{3/2} R_n$, against n

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UPPER BOUND UCB-CH-AS-MAX

THEOREM

Let $\lambda_{\min} = \min_{k: \lambda_k > 0} \lambda_k$. Then there is $C = \text{poly}(1/\lambda_{\min}, 1/\Sigma)$, s.t. for any n , if it is known in advance, and UCB-CH-AS-MAX runs with $\delta = n^{-5/2}$, then

$$R_n(\mathcal{A}_{\text{UCB-CH-AS-MAX}}) \leq Cn^{-3/2}\sqrt{\ln n}.$$

PROOF (SKETCH)

For $\delta > 0$, let $\xi = \xi_{K,n}(\delta)$ be event

$$\bigcap_{\substack{1 \leq k \leq K \\ 1 \leq t \leq n}} \left\{ \left| \frac{1}{t} \sum_{i=1}^t Y_{ki}^2 - \left(\frac{1}{t} \sum_{i=1}^t Y_{ki} \right)^2 - \sigma_k^2 \right| \leq 3 \sqrt{\frac{\ln(1/\delta)}{2t}} \right\}.$$

- Hoeffding: $\mathbb{P}(\xi) \geq 1 - 4Kn\delta$.
- There is $C = \text{poly}(1/\lambda_{\min}, 1/\Sigma)$, s.t. if UCB-CH-AS-MAX runs with δ , then $\forall n$ on ξ , $\forall k$: $|T_{k,n} - T_{k,n}^*| \leq C\sqrt{n \ln(1/\delta)}$.

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With high probability: $|T_{k,n} - T_{k,n}^*| = O(\sqrt{n \ln(1/\delta)})$.

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OPEN QUESTIONS

- Lower bounds: are results sharp?
- Extensions:

• What happens if we consider more complex models?
• What happens if we consider more complex losses?
• What happens if we consider more complex environments?

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Unbounded (sub-Gaussian) distributions — done

General distributions — done

Non-convex optimization — done

Sampling — done

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