On the Complexity of Best Arm Identification with Fixed Confidence

Discrete Optimization with Noise

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The Problem

Best-Arm Identification with Fixed Confidence

K options = probability distributions $\boldsymbol{\nu} = (\nu_a)_{1 \le a \le K}$

$\nu_a \in \mathcal{F}$ exponential family parameterized by its expectation μ_a

ν_1

ν_2

ν_3

ν_4

ν_5

At round t, you may:

- choose an option $A_t = \phi_t(A_1, X_1, \dots, A_{t-1}, X_{t-1}) \in \{1, \dots, K\}$
- observe a new independent sample $X_t \sim \nu_{A_t}$

so as to identify the best arm $a^* = \operatorname{argmax}_a \mu_a$ and $\mu^* = \max_a \mu_a$
as fast as possible: stopping time τ .

Fixed-budget setting	Fixed-confidence setting
given $\tau = T$	minimize $\mathbb{E}[\tau]$
minimize $\mathbb{P}(\hat{a}_\tau \neq a^*)$	under constraint $\mathbb{P}(\hat{a}_\tau \neq a^*) \le \delta$

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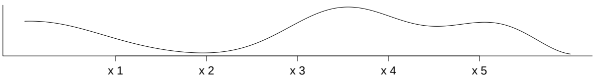

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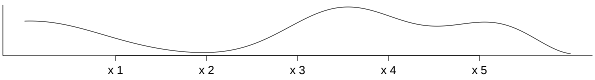

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Fixed-budget setting	Fixed-confidence setting
given $\tau = T$ minimize $\mathbb{P}(\hat{a}_\tau \neq a^*)$	minimize $\mathbb{E}[\tau_\delta]$ under constraint $\mathbb{P}(\hat{a}_\tau \neq a^*) \leq \delta$

Intuition

Most simple setting: for all $a \in \{1, \dots, K\}$,

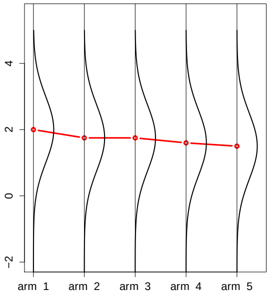
$$\nu_a = \mathcal{N}(\mu_a, 1)$$

For example: $\mu = [2, 1.75, 1.75, 1.6, 1.5]$.

At time t:

➜ you have sampled n_a times the option a

➜ your empirical average is $\bar{X}_{a,n_a}$.



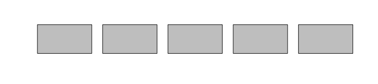
$\longrightarrow$ if you stop at time t, your probability of prefering arm $a \geq 2$ to arm $a^* = 1$ is:

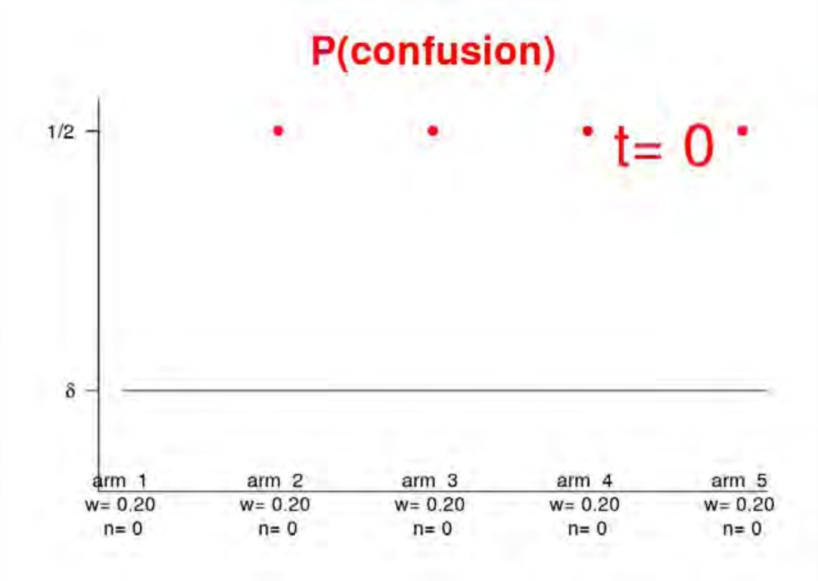
$$\mathbb{P}\left(\bar{X}_{a,n_a} > \bar{X}_{1,n_1}\right) = \mathbb{P}\left(\frac{\bar{X}_{a,n_a} - \mu_a - (\bar{X}_{1,n_1} - \mu_1)}{\sqrt{1/n_1 + 1/n_a}} > \frac{\mu_1 - \mu_a}{\sqrt{1/n_1 + 1/n_a}}\right)$$

$$= \bar{\Phi}\left(\frac{\mu_1 - \mu_a}{\sqrt{1/n_1 + 1/n_a}}\right)$$

where $\bar{\Phi}(u) = \int_u^\infty \frac{e^{-u^2/2}}{\sqrt{2\pi}} du$

Uniform Sampling





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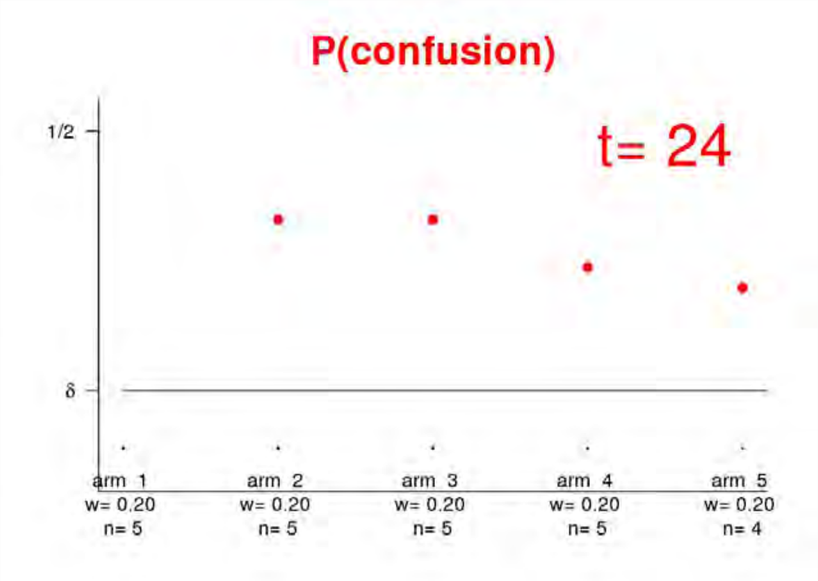

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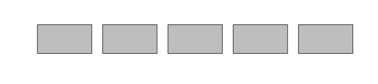

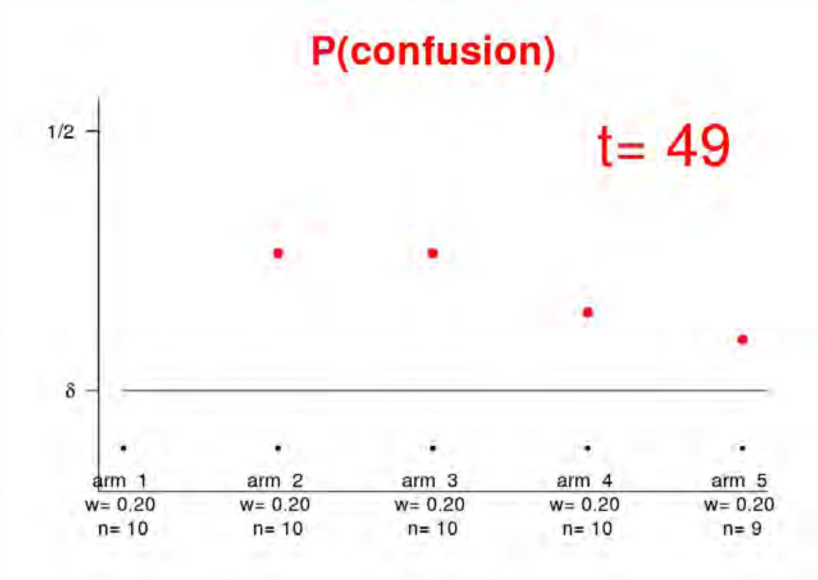

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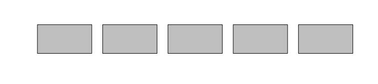

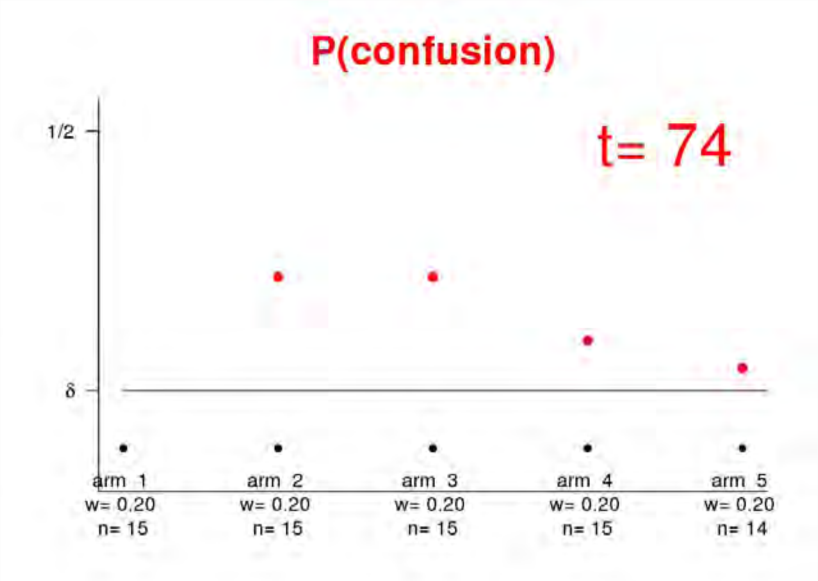

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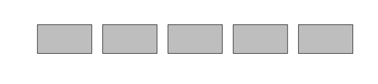
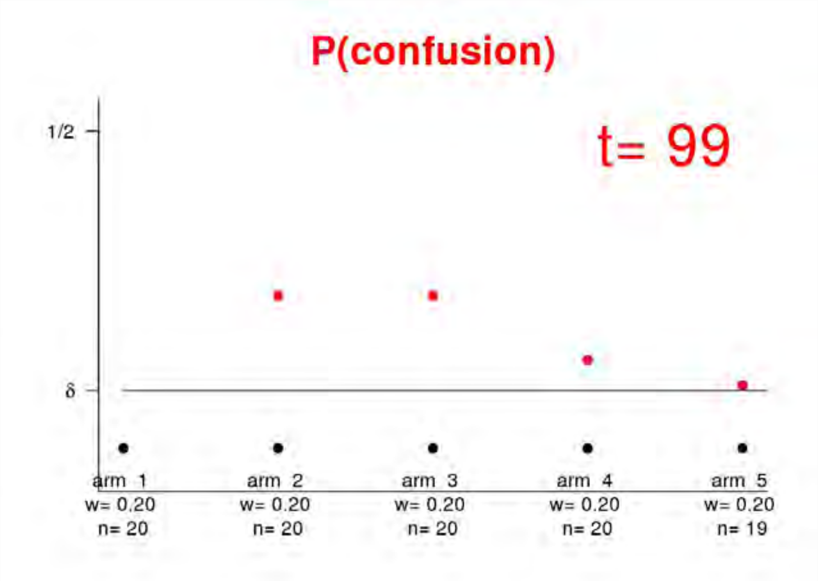

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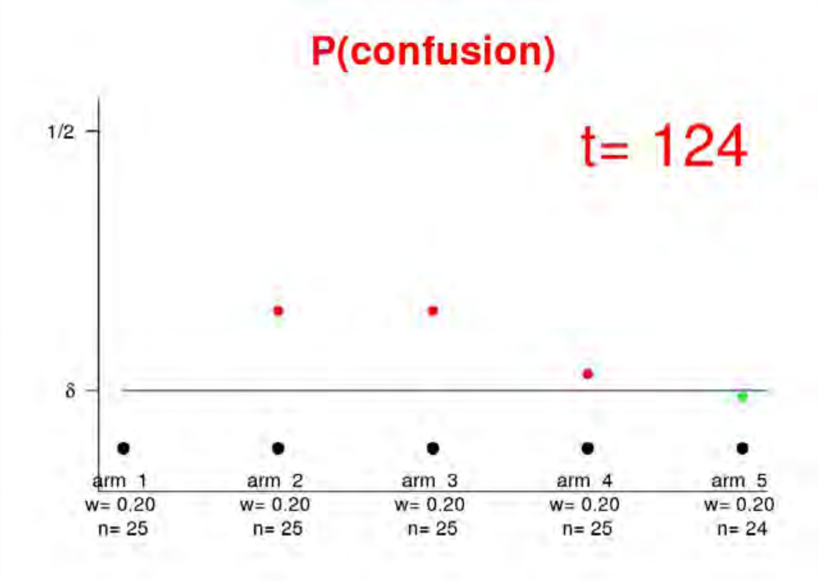

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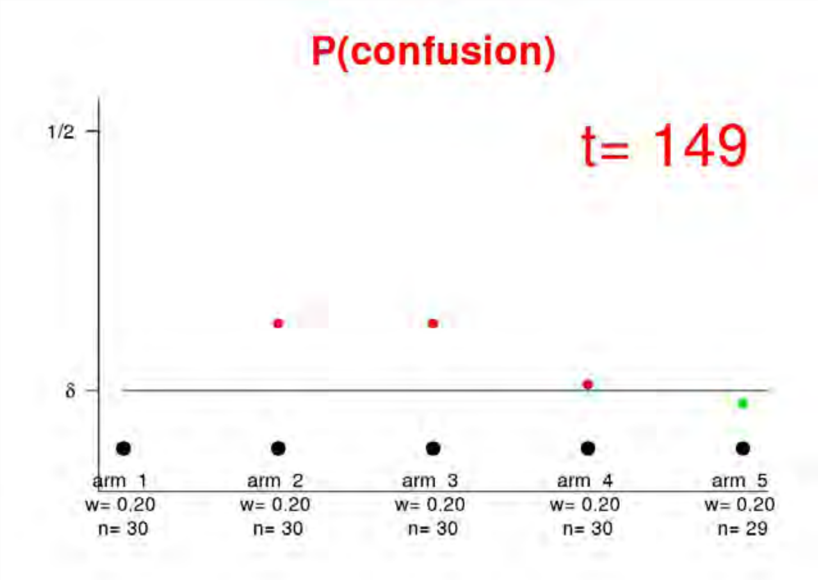

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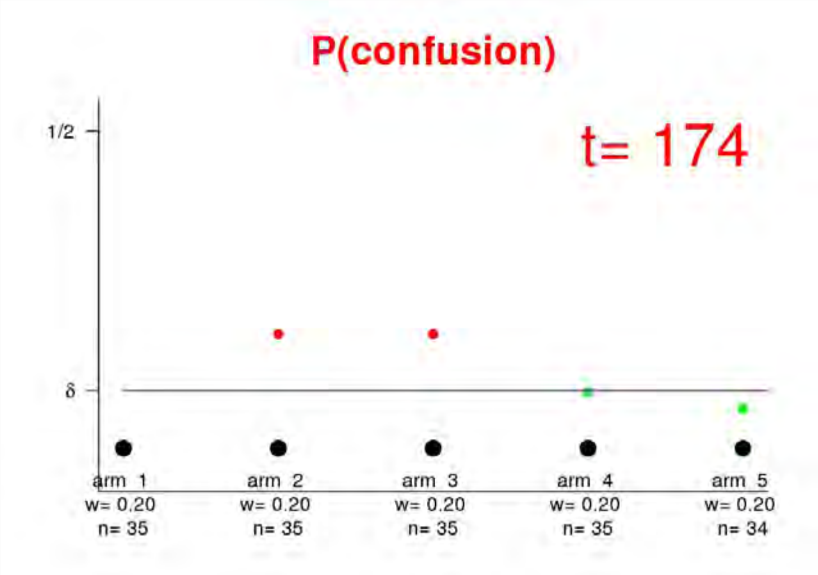

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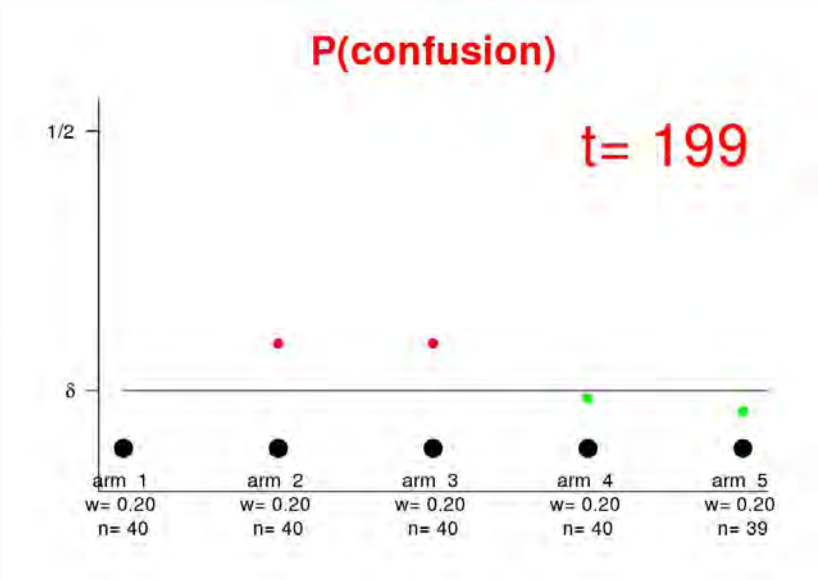

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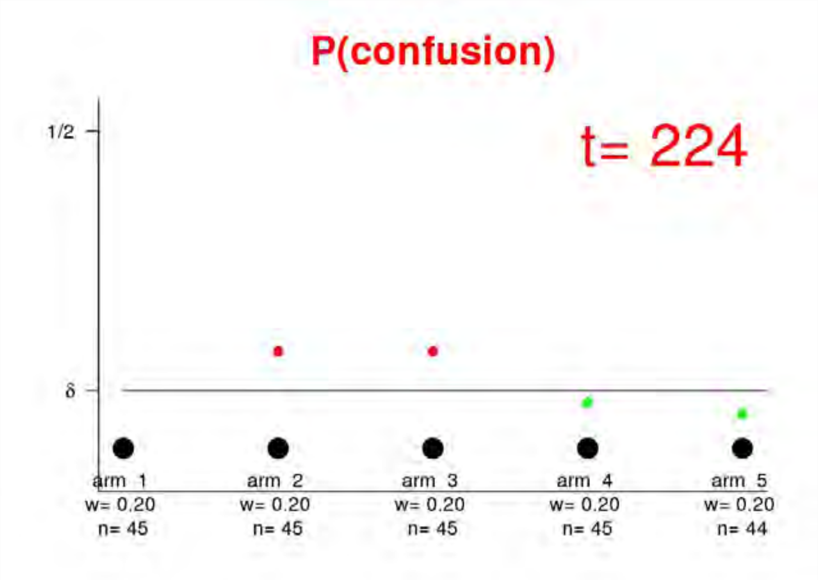

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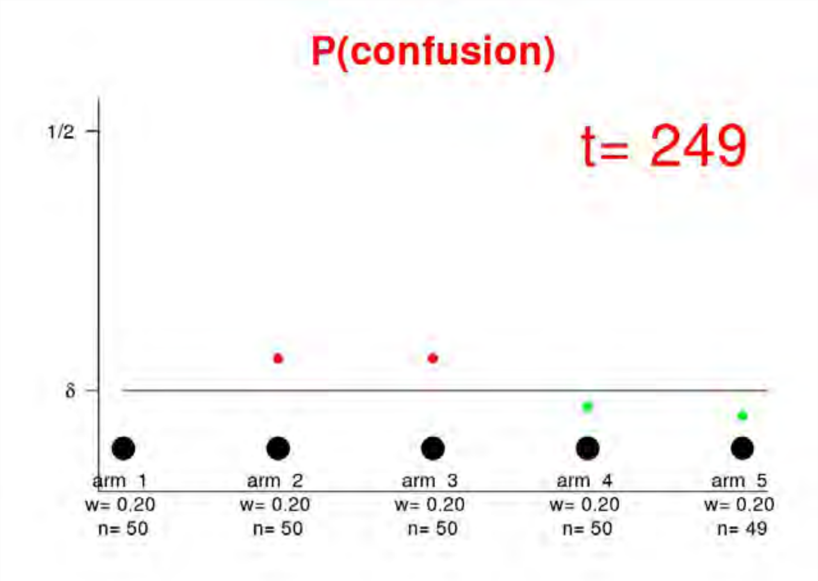

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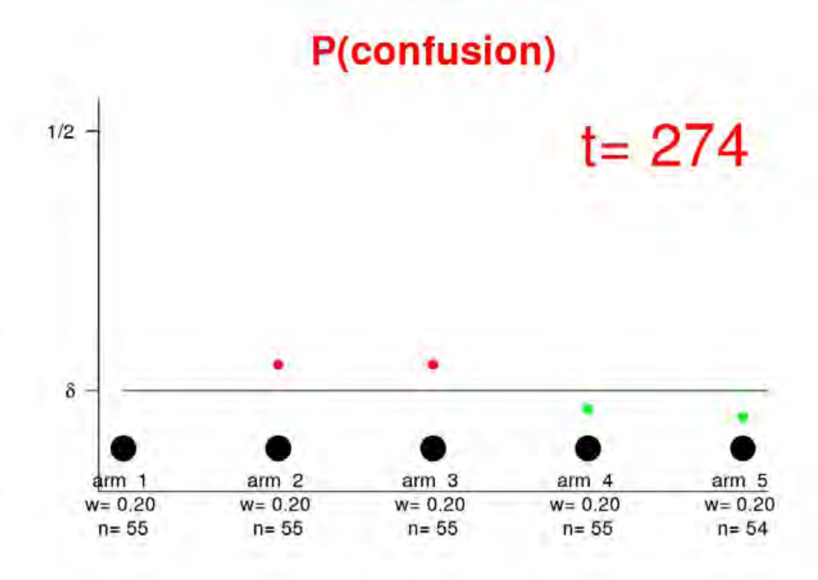

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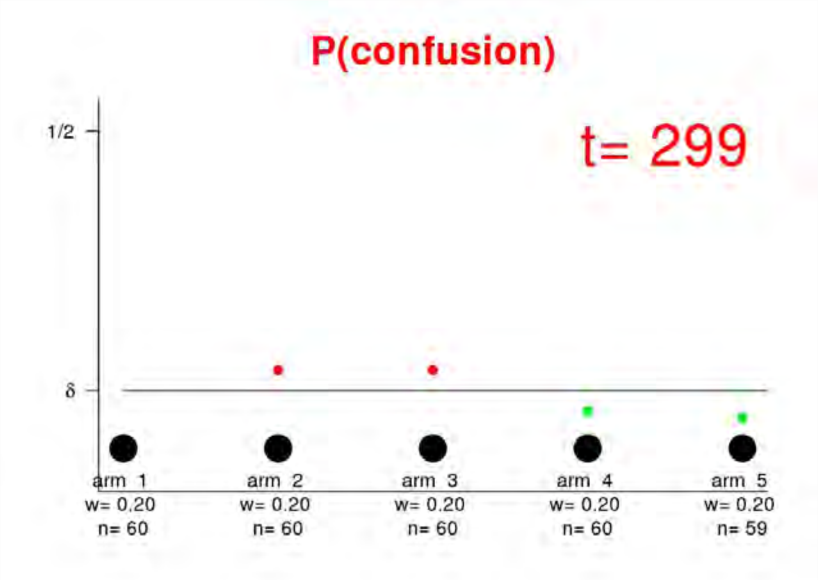

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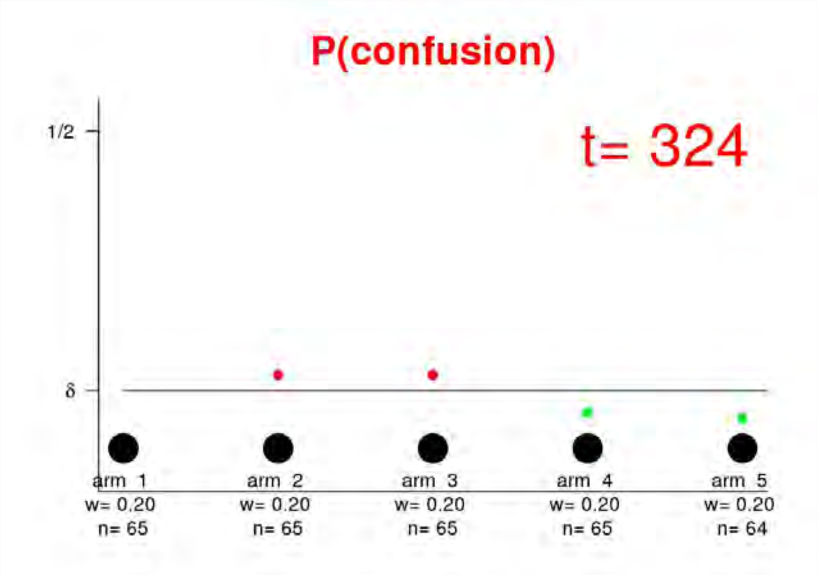

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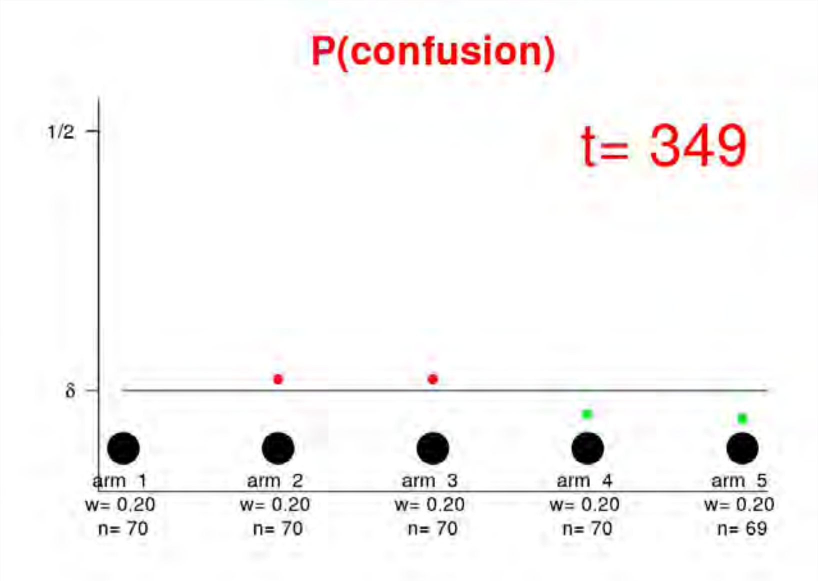

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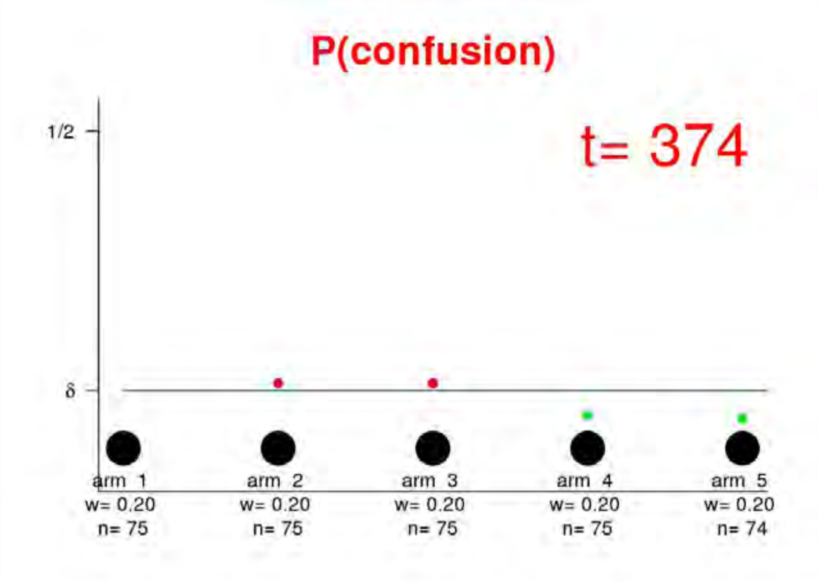

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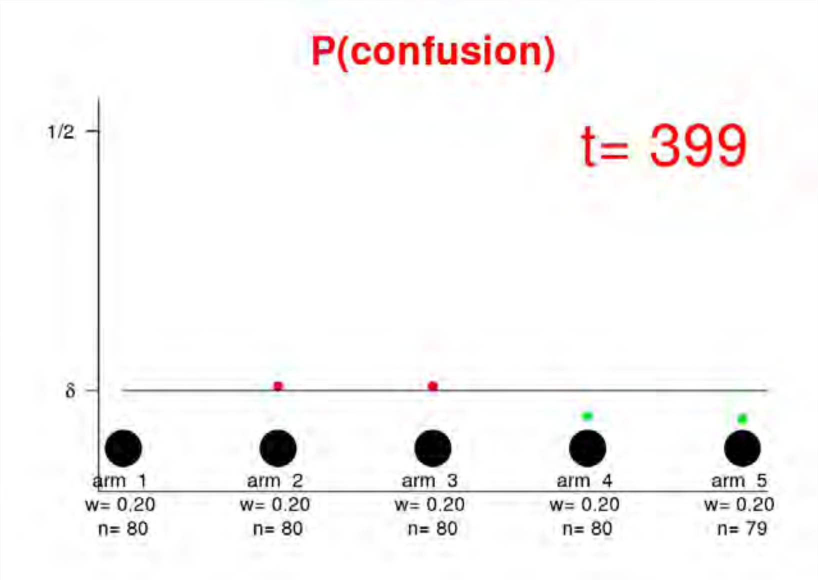

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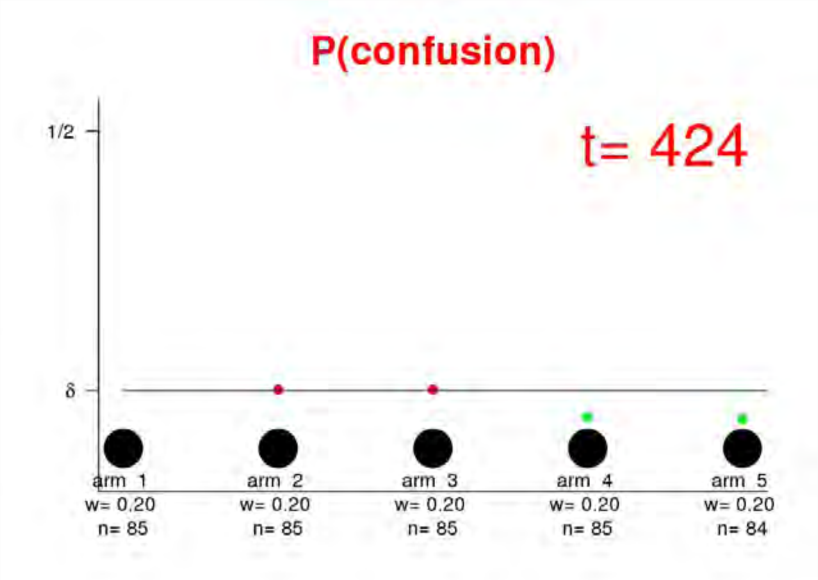

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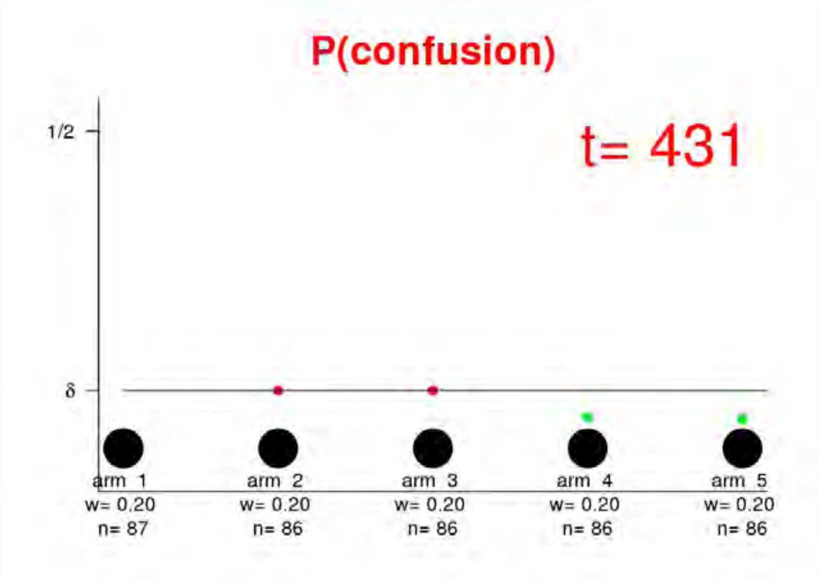

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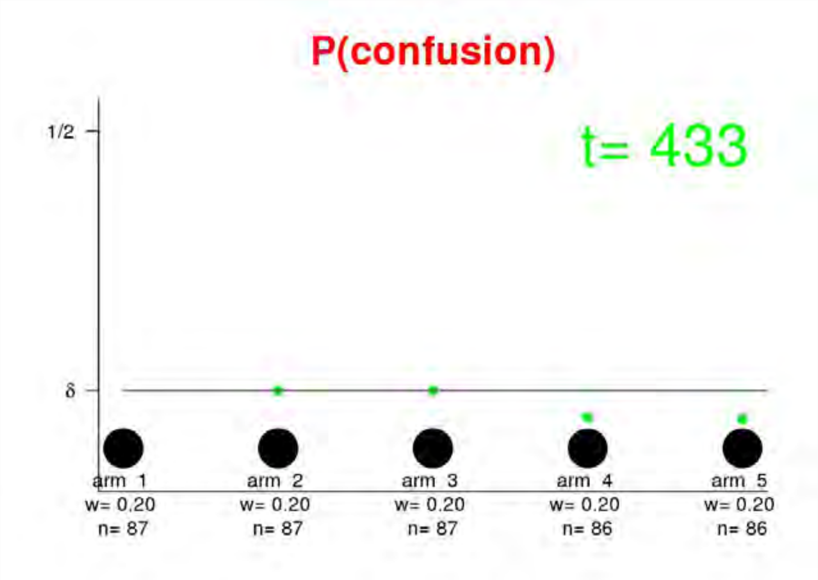
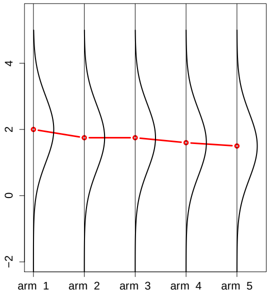


Intuition: Equalizing the Probabilities of Confusion

Most simple setting: for all $a \in \{1, \ldots, K\}$,

$$\nu_a = \mathcal{N}(\mu_a, 1)$$

For example: $\mu = [2, 1.75, 1.75, 1.6, 1.5]$.



Active Learning

➜ **You allocate a relative budget w_a to option a, with $w_1 + \cdots + w_K = 1$.**

At time t:

➜ you have sampled $\mathbf{n_a} \approx \mathbf{w_a t}$ times the option a

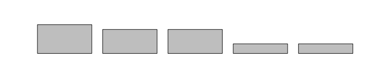
➜ your empirical average is $\bar{X}_{a,n_a}$.

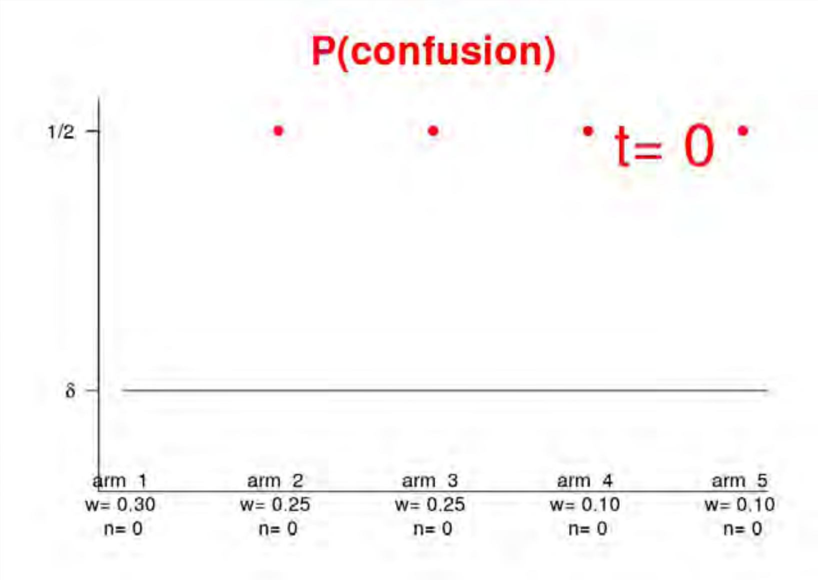
$\longrightarrow$ if you stop at time t, your probability of prefering arm $a \geq 2$ to arm $a^* = 1$ is:

$$\mathbb{P}\left(\bar{X}_{a,n_a} > \bar{X}_{1,n_1}\right) = \mathbb{P}\left(\frac{\bar{X}_{a,n_a} - \mu_a - (\bar{X}_{1,n_1} - \mu_1)}{\sqrt{1/n_1 + 1/n_a}} > \frac{\mu_1 - \mu_a}{\sqrt{1/n_1 + 1/n_a}}\right)$$

$$= \bar{\Phi}\left(\frac{\mu_1 - \mu_a}{\sqrt{1/n_1 + 1/n_a}}\right)$$

Improving: trial 1





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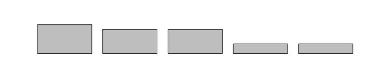

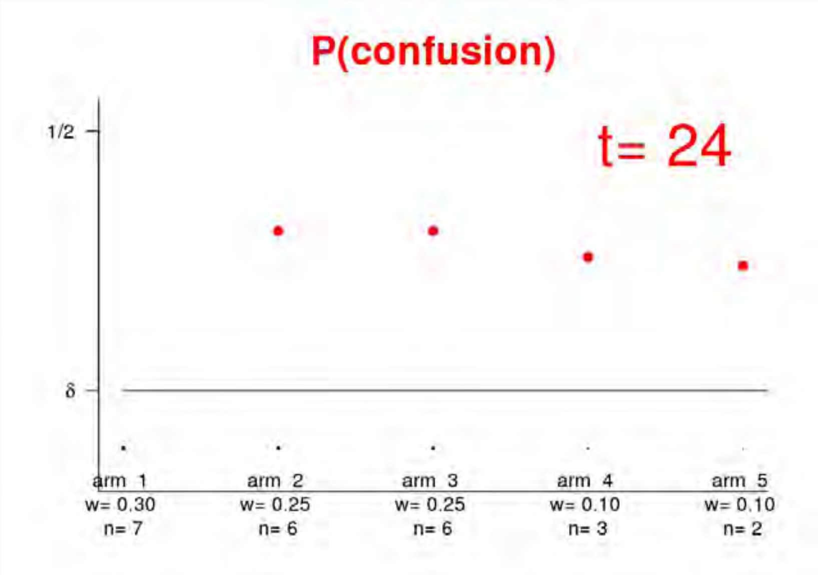

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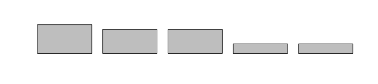

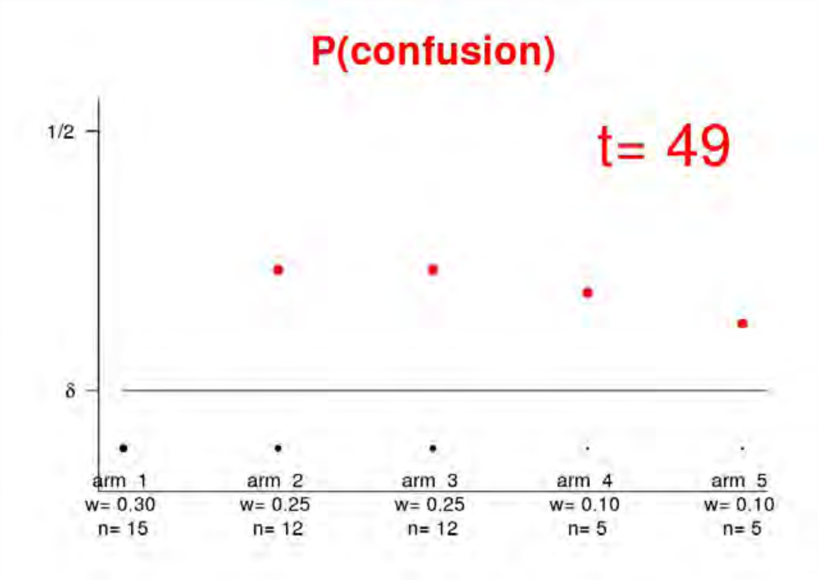

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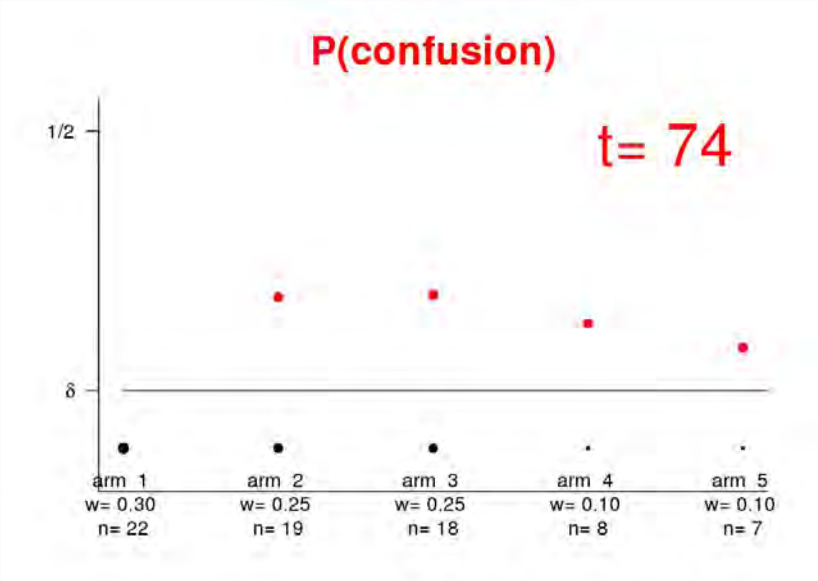

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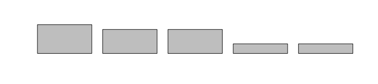

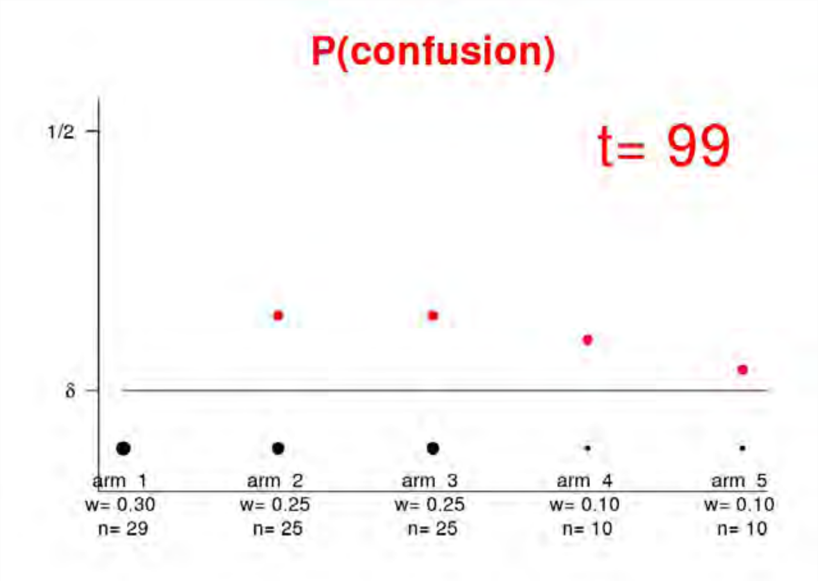

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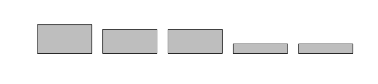

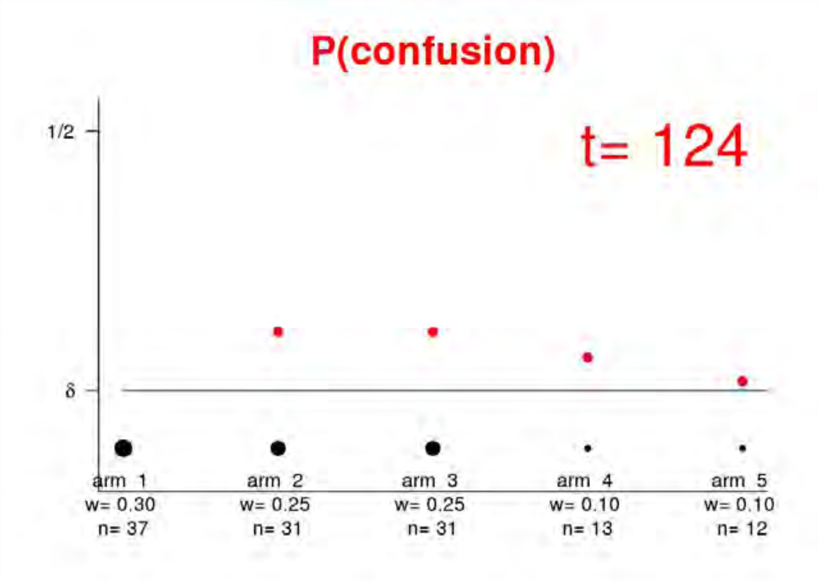

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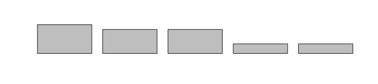

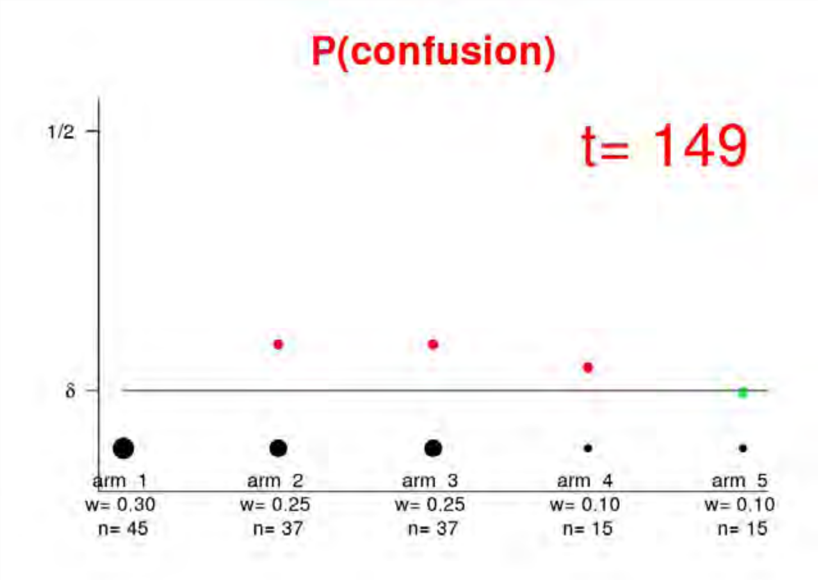

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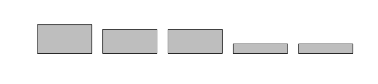

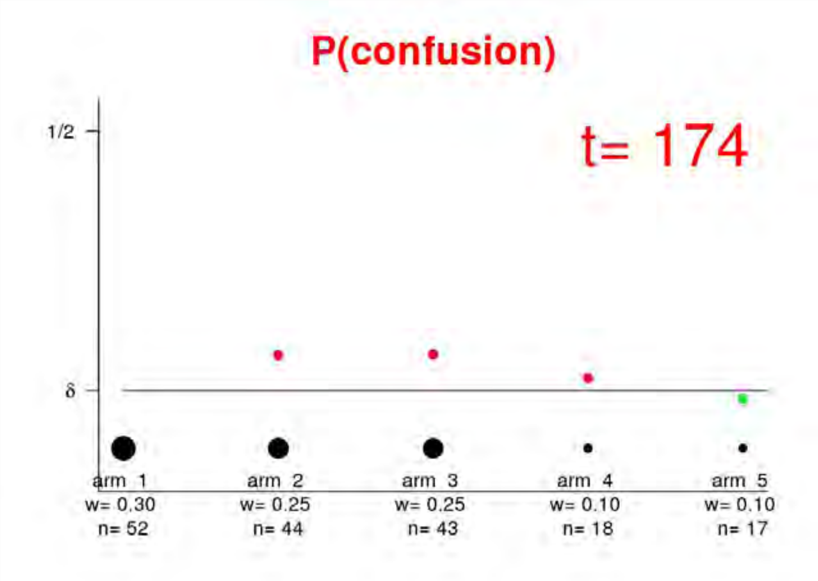

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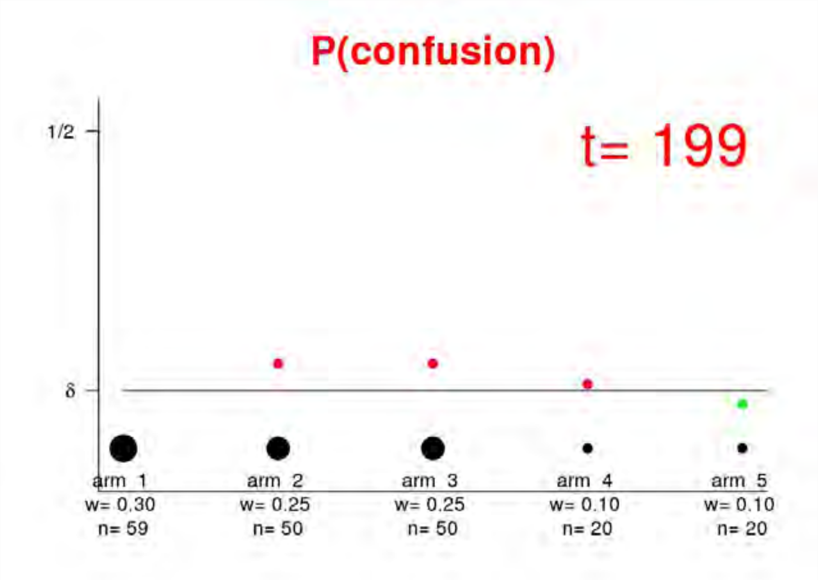

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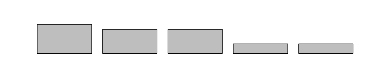

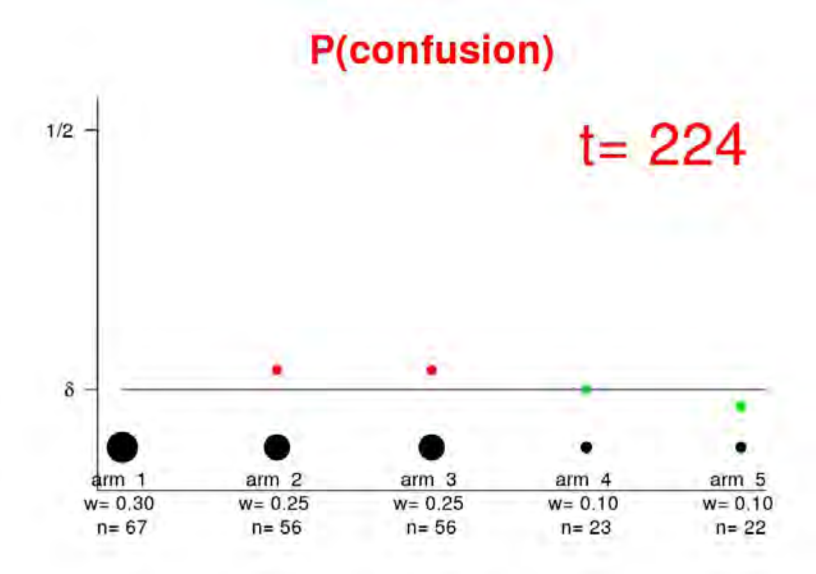

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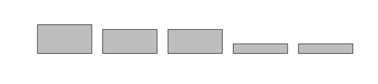

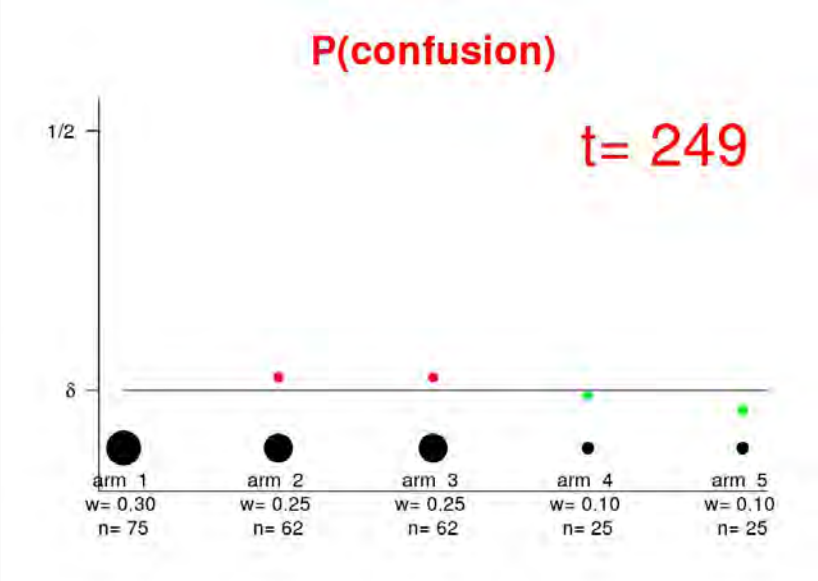

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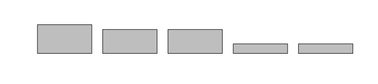

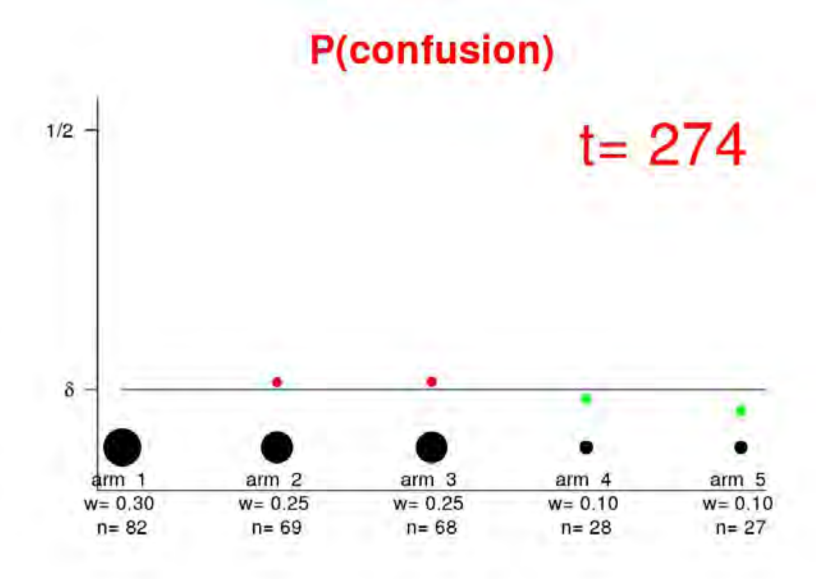

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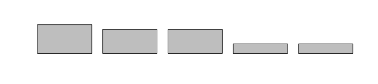

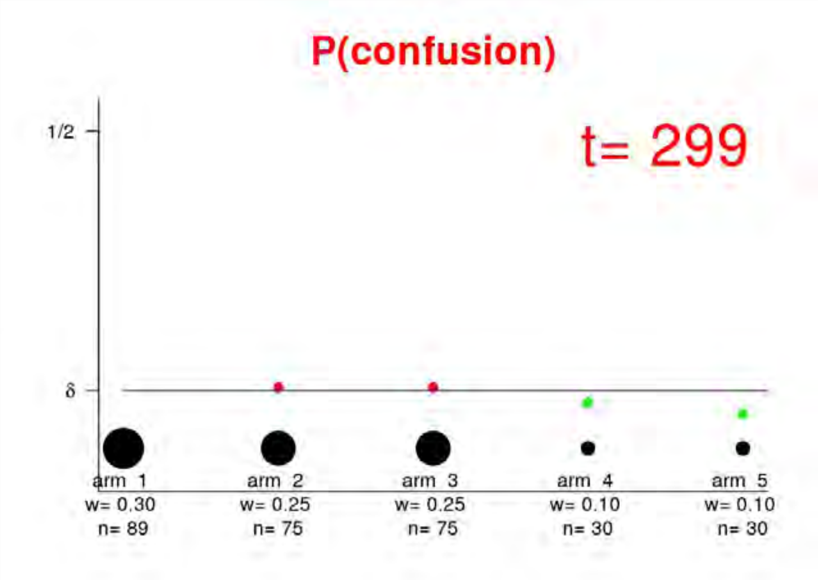

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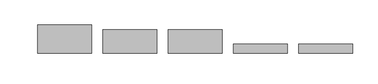

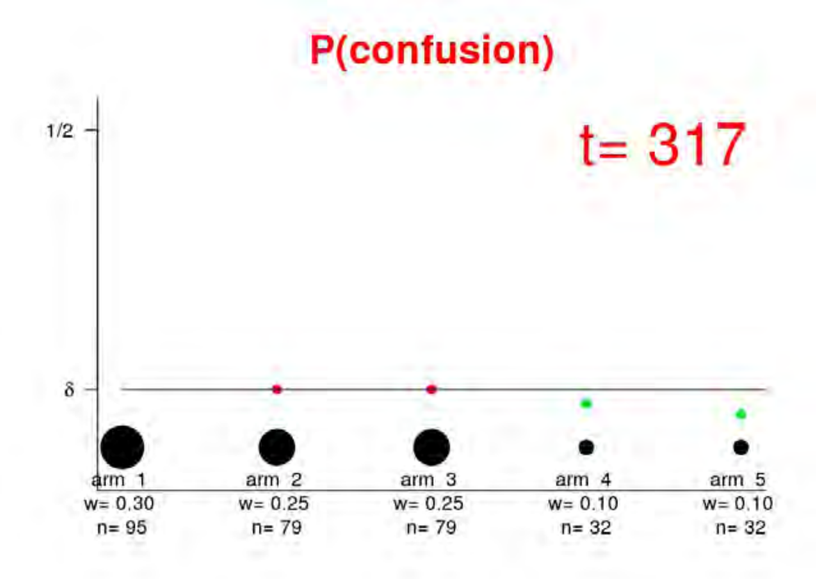

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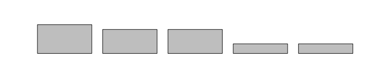
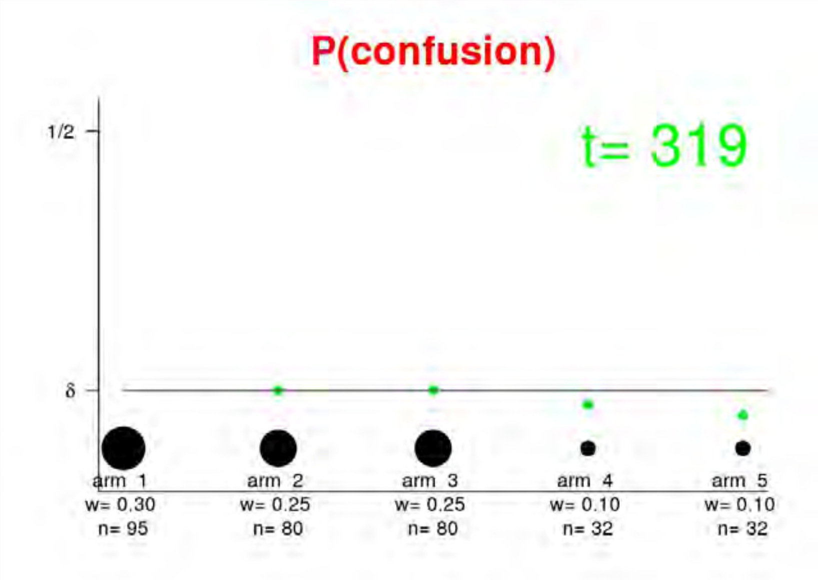
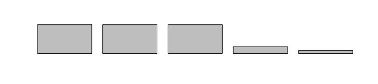
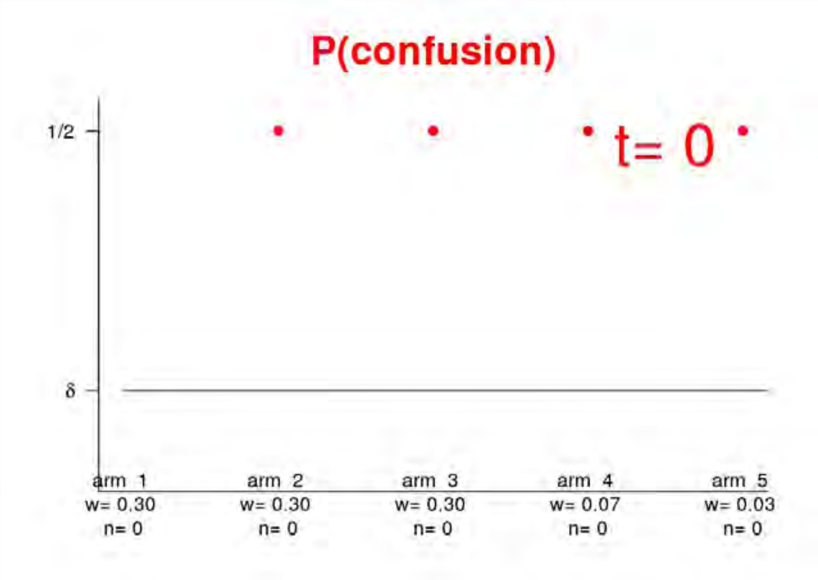




Improving: trial 2





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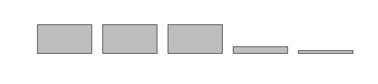
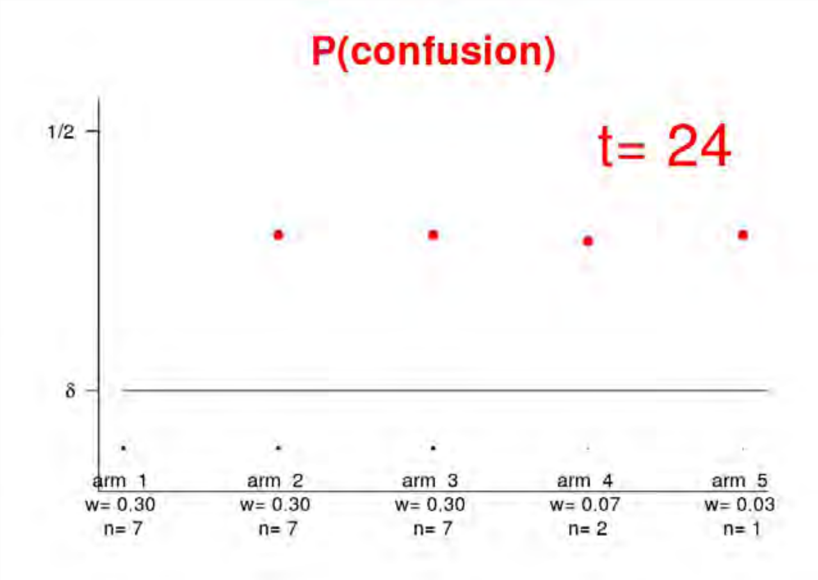
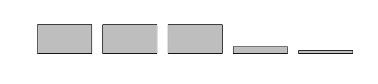
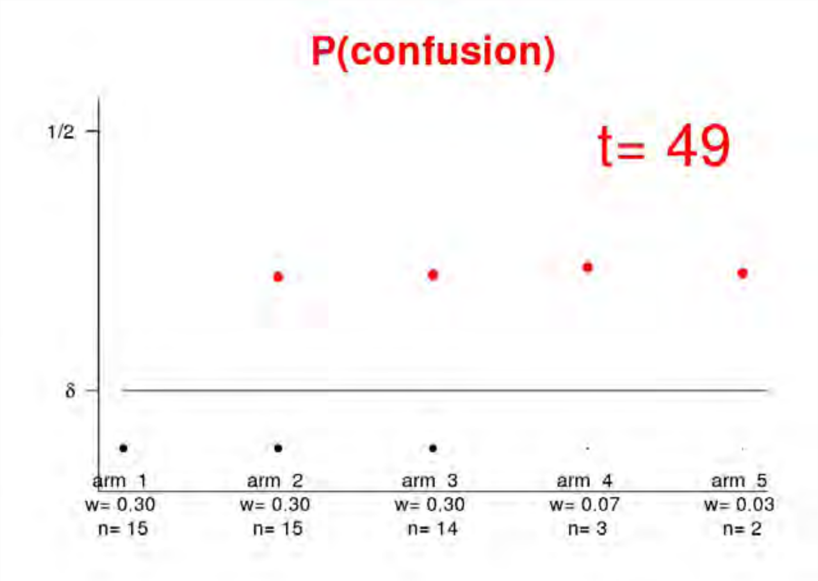




Improving: trial 2





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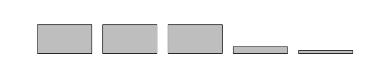

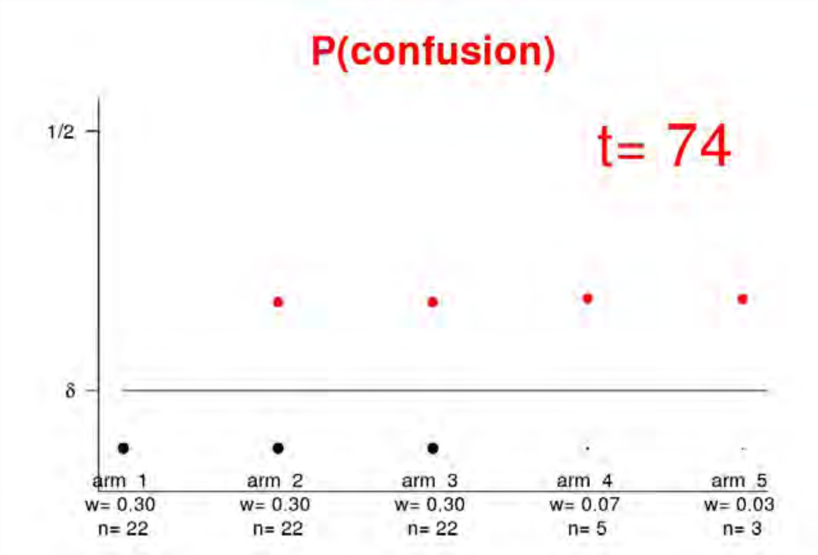

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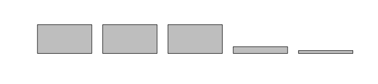

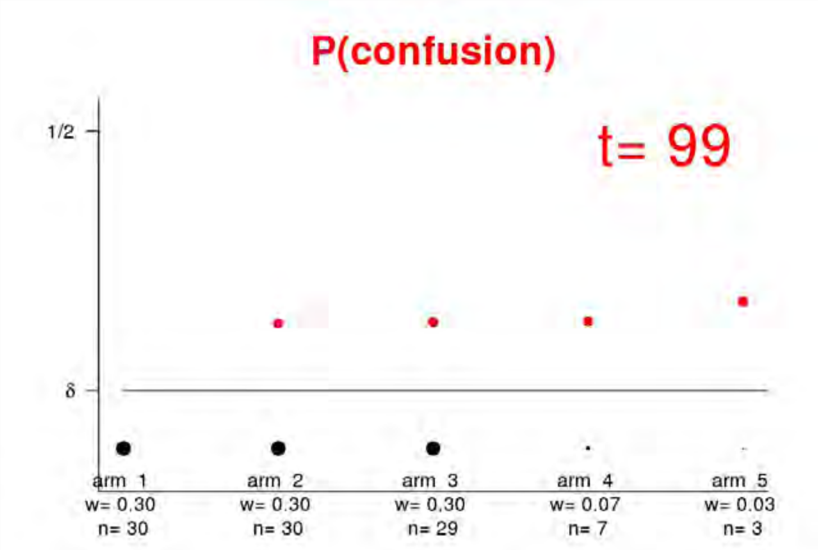

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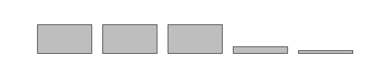

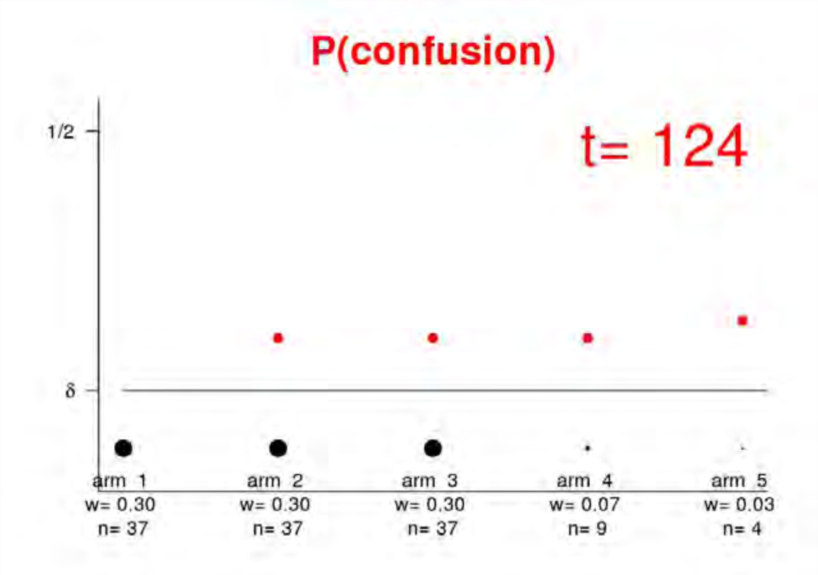

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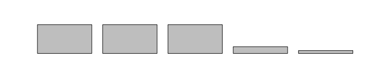

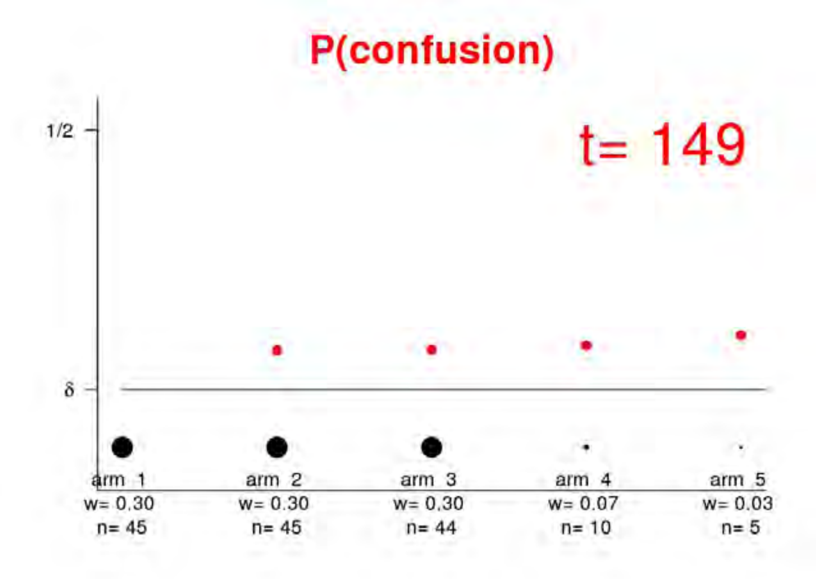

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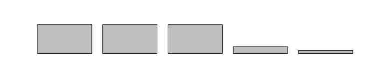

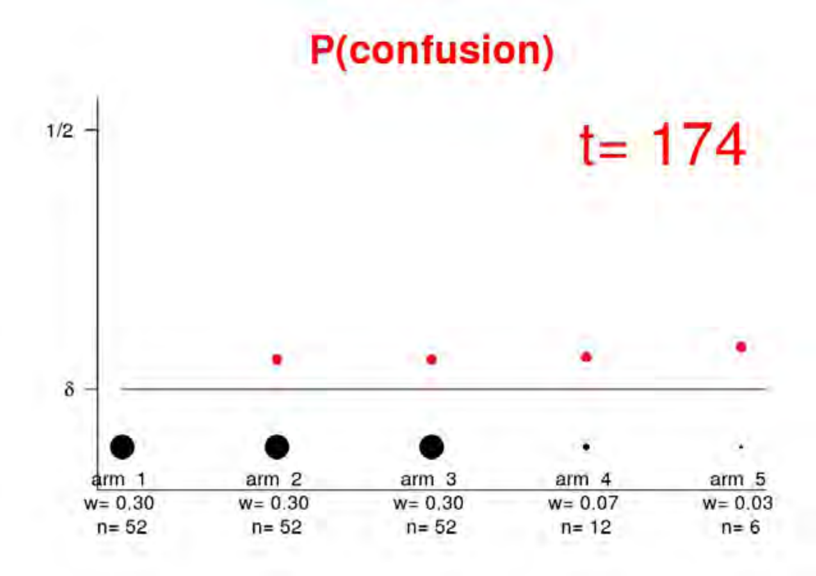

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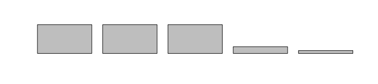

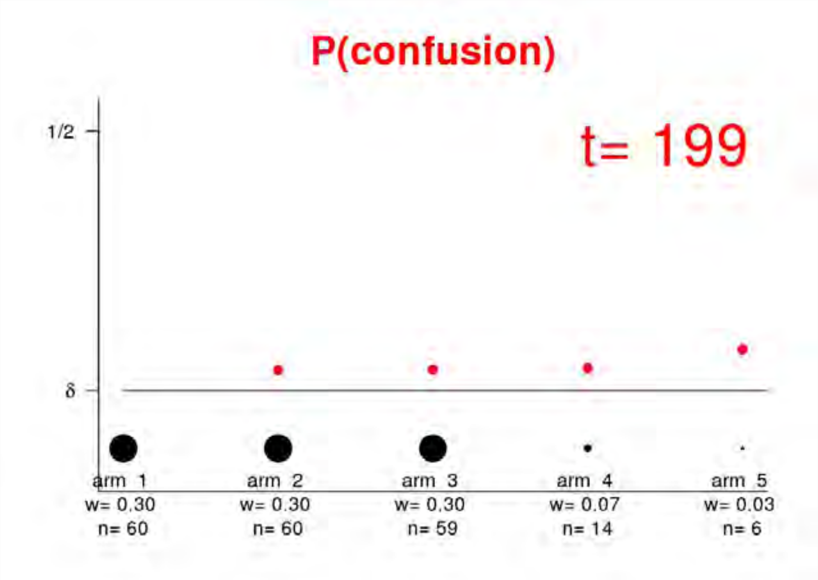

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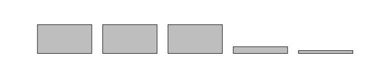

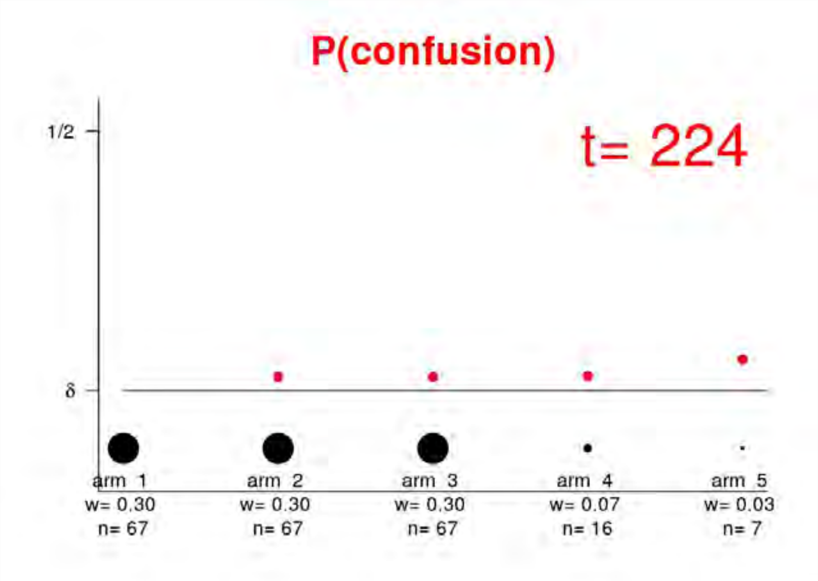

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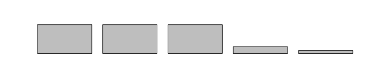

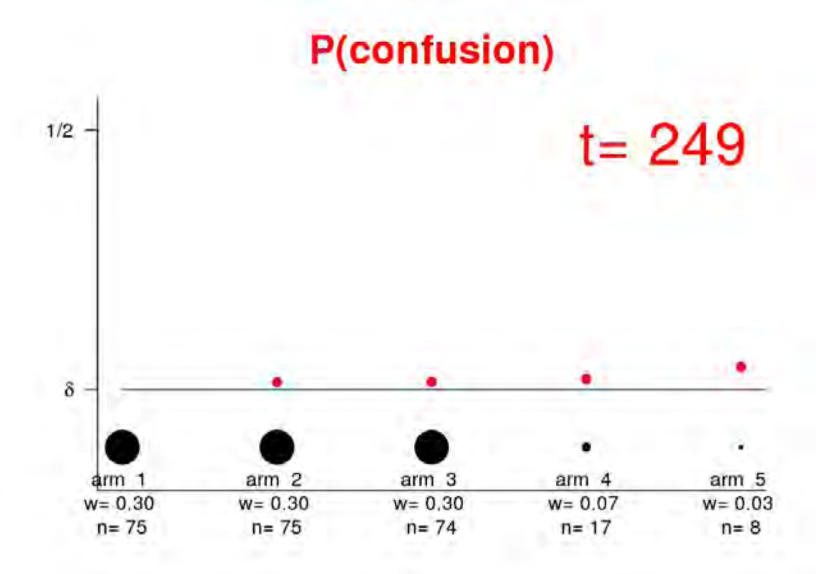

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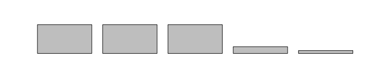

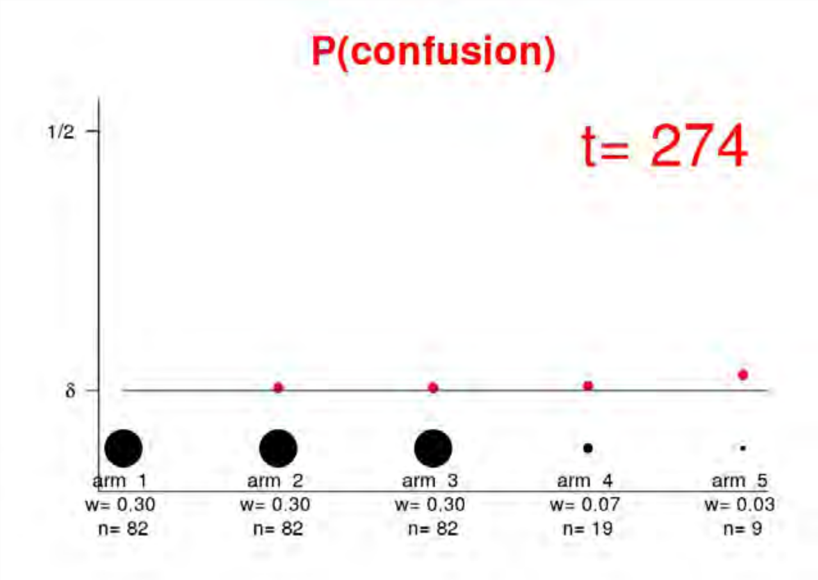

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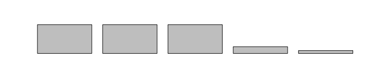

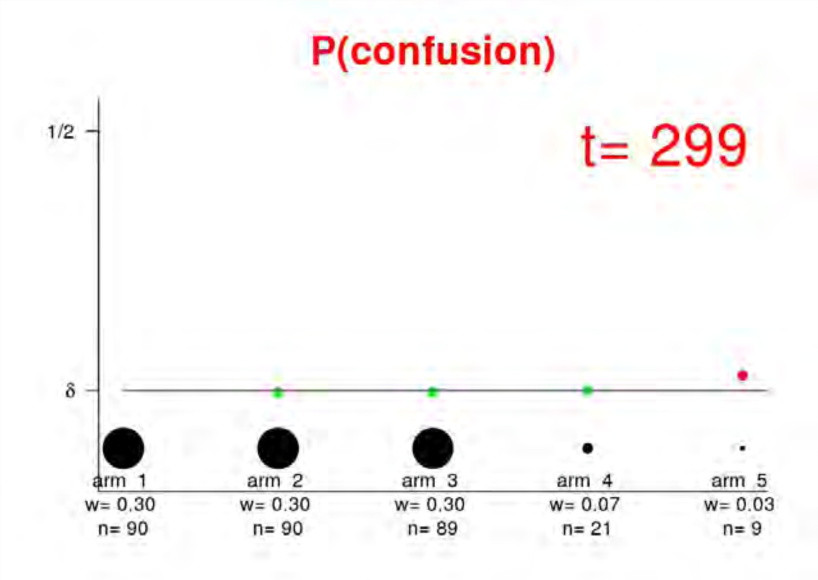

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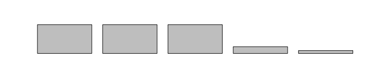

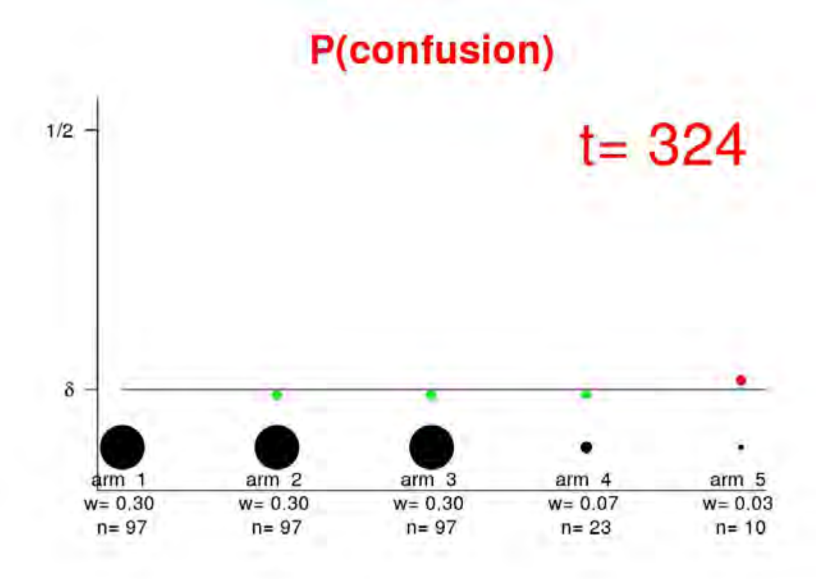

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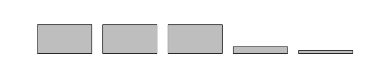

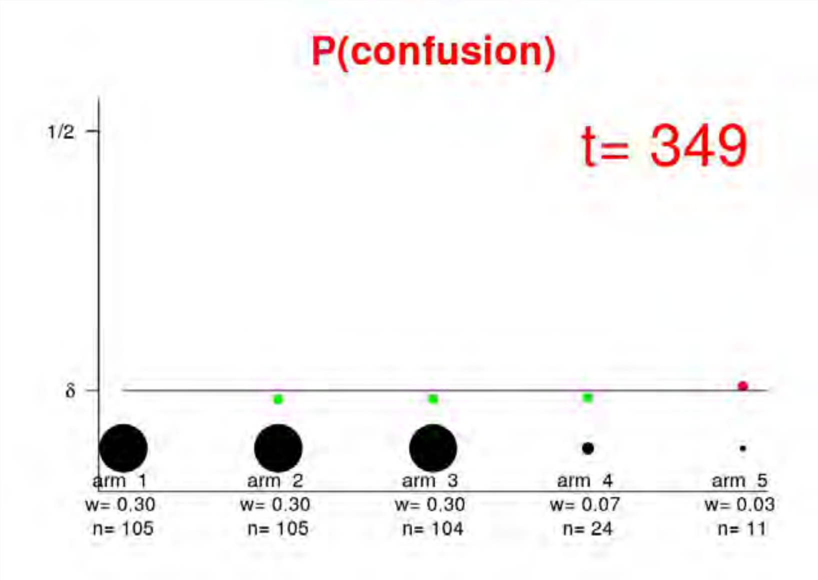

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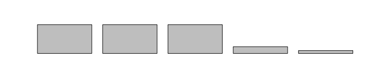

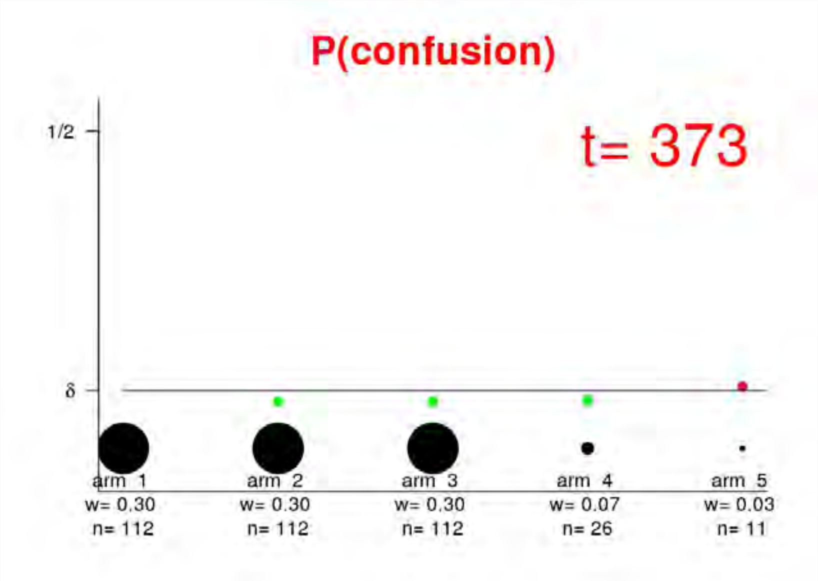

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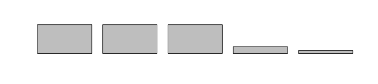

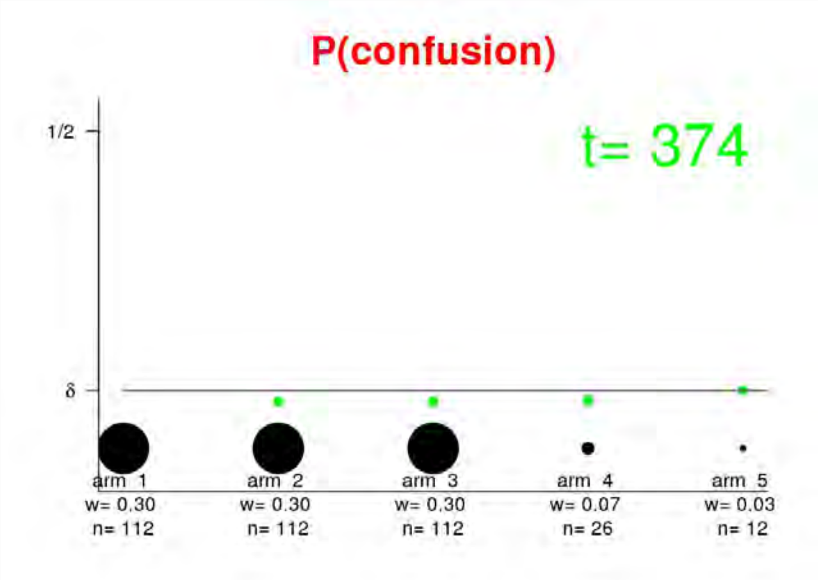

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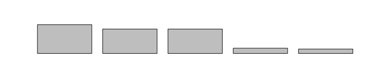

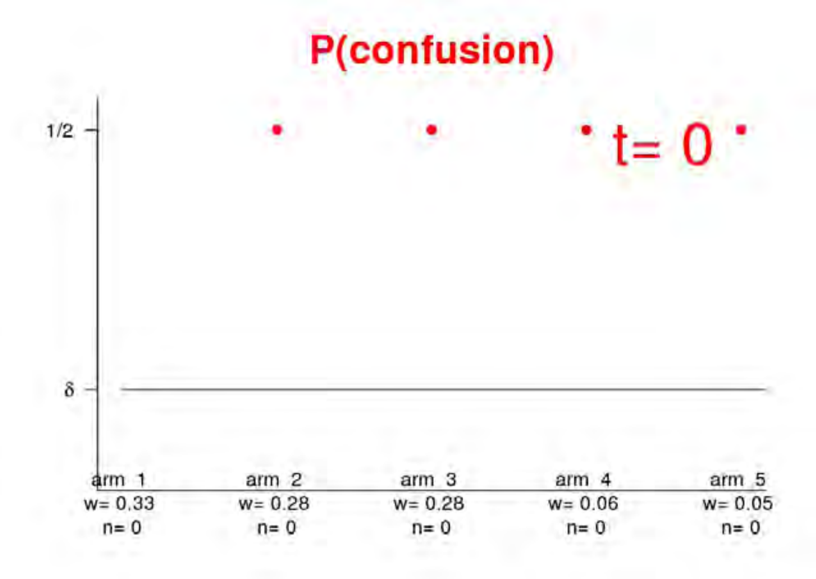

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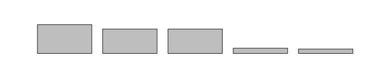

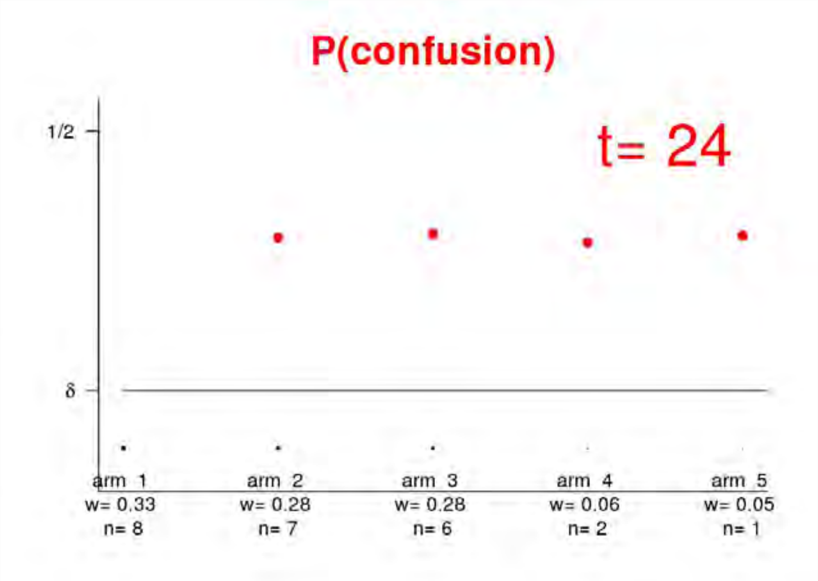

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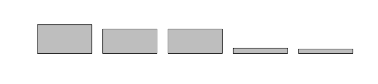

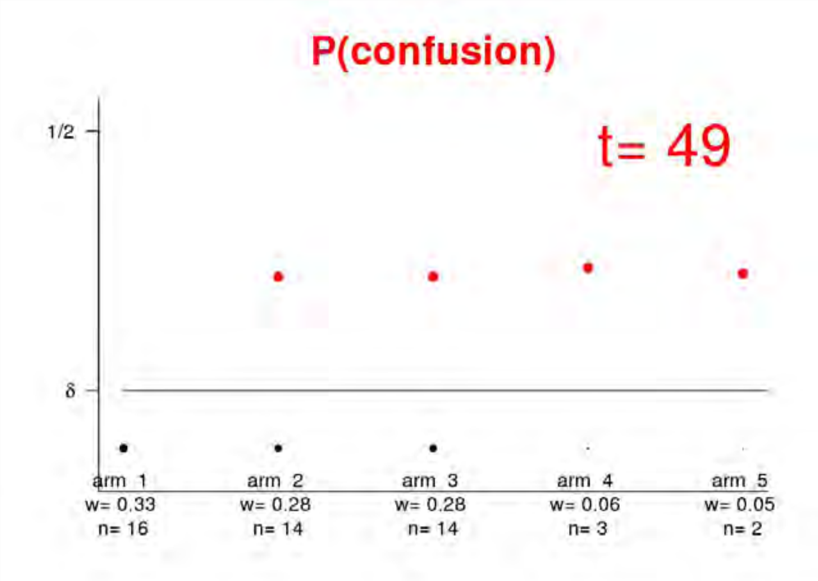

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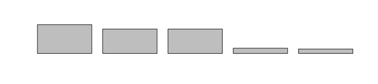

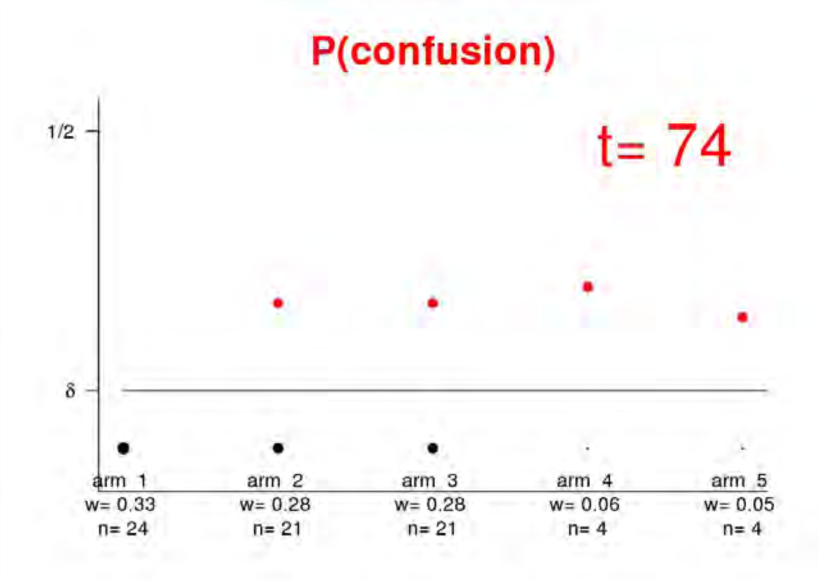

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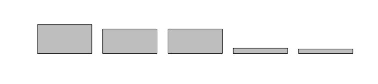

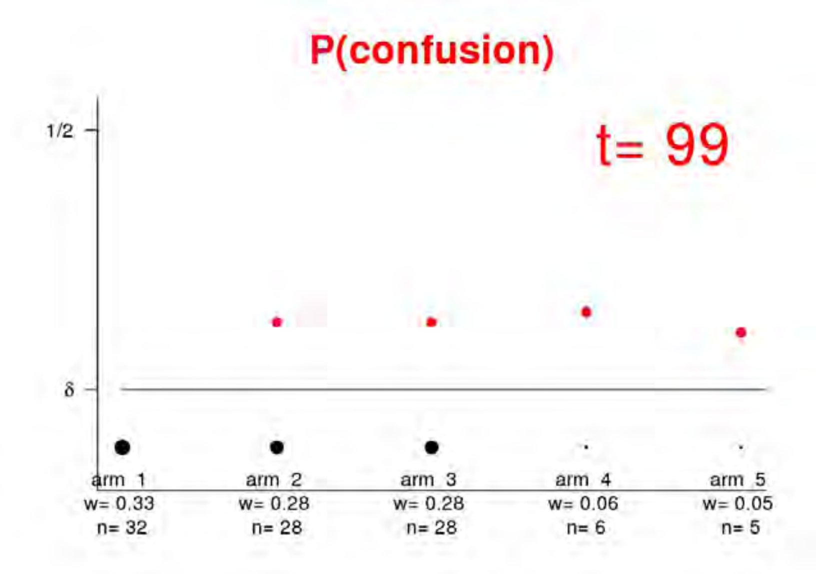

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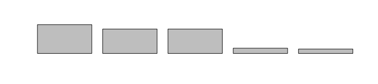

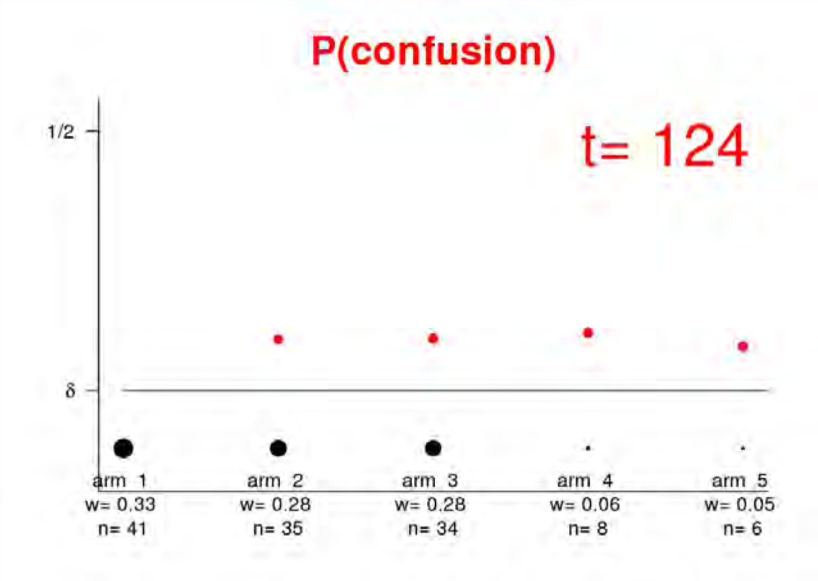

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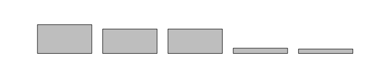

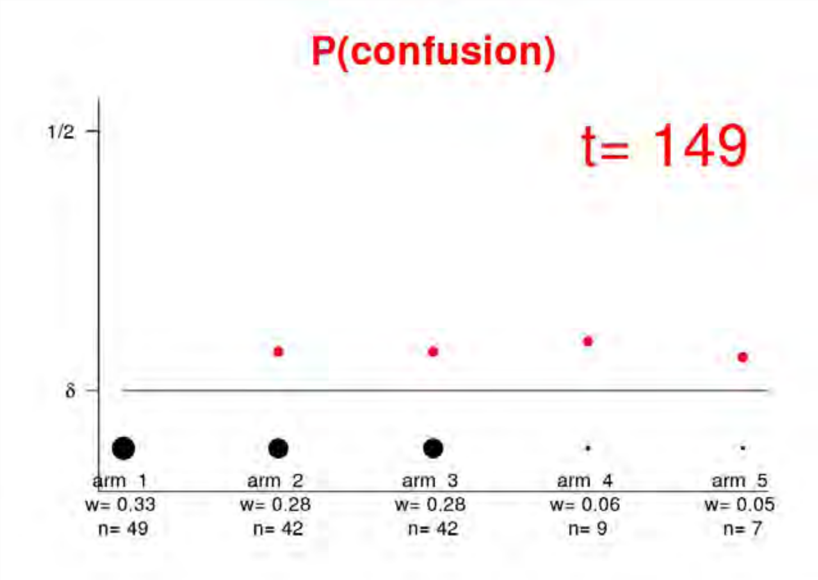

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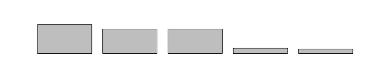

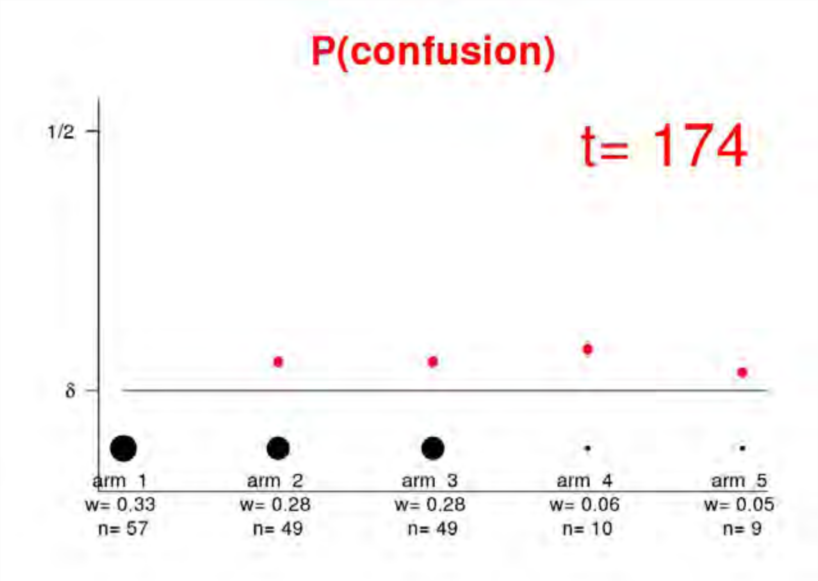

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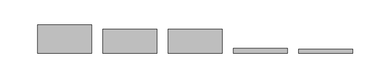

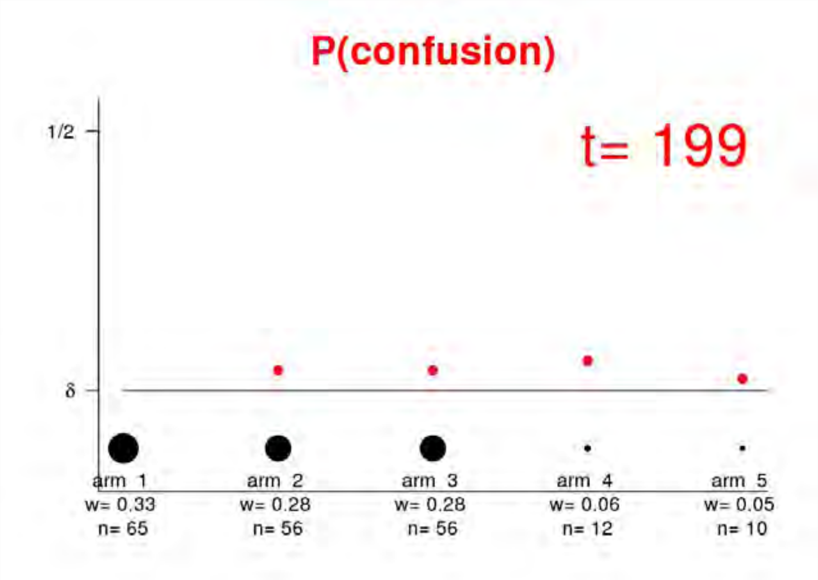

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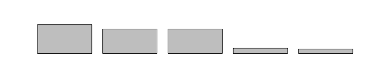

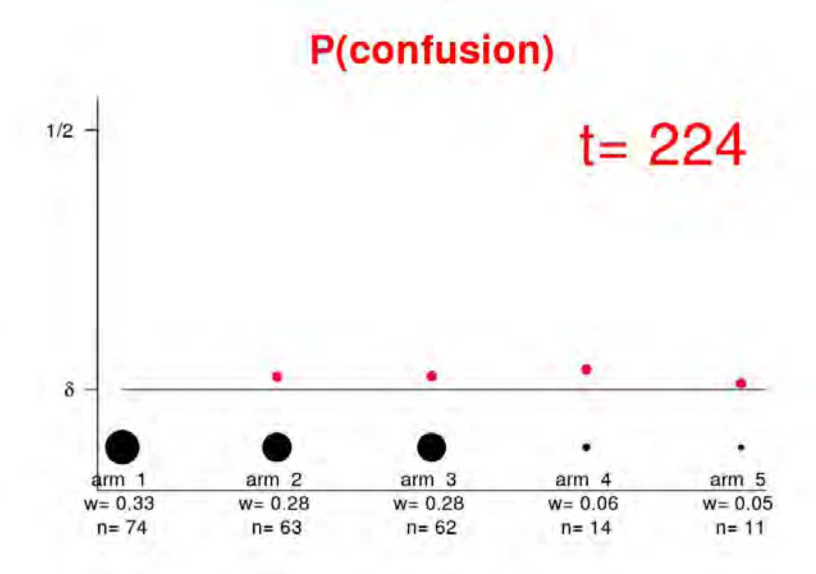

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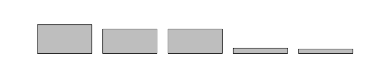

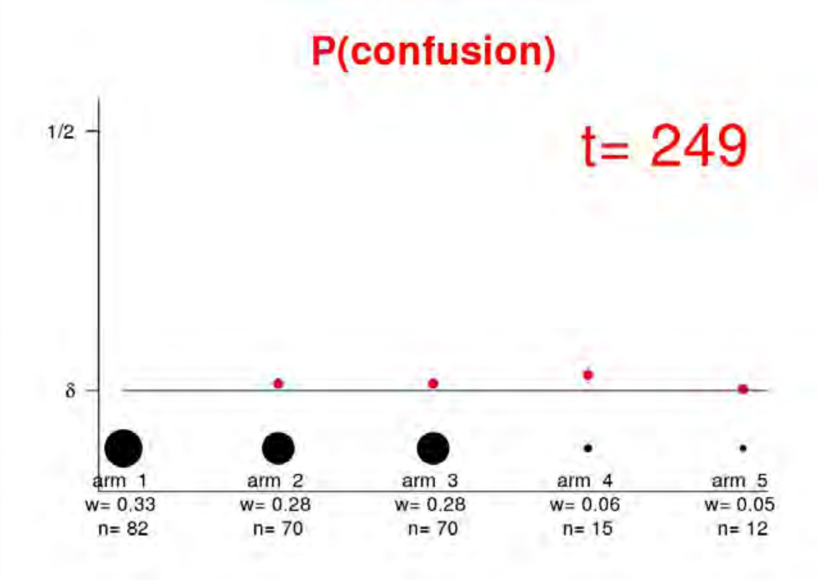

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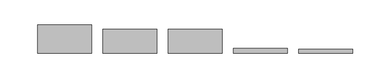

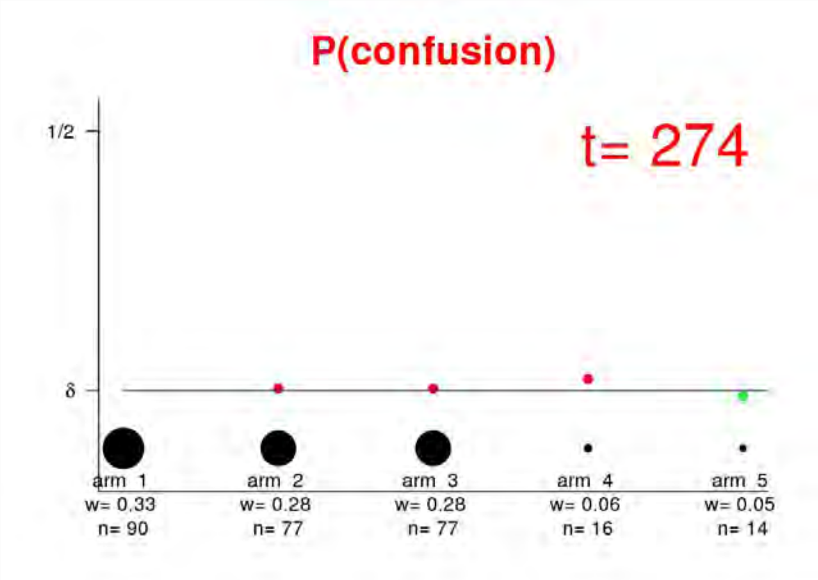

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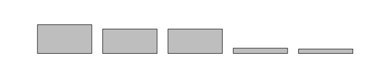

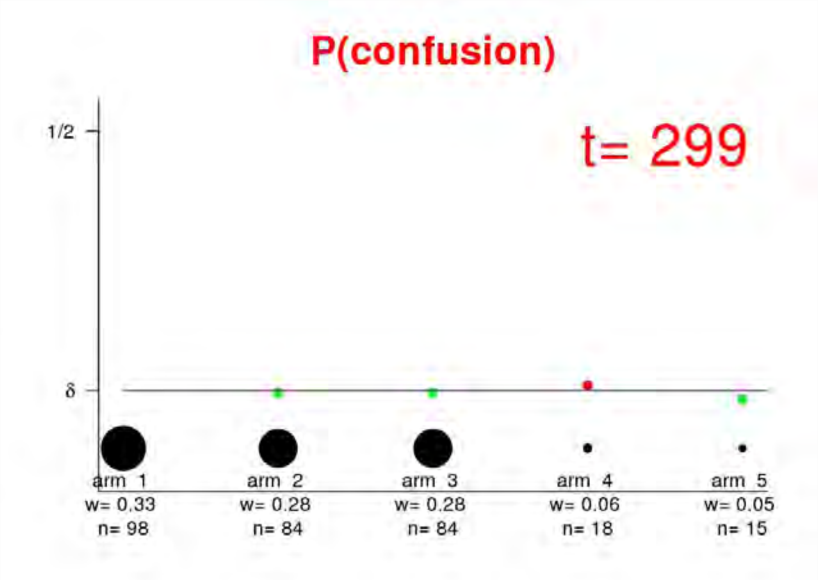

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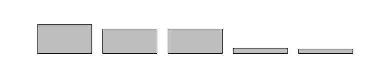

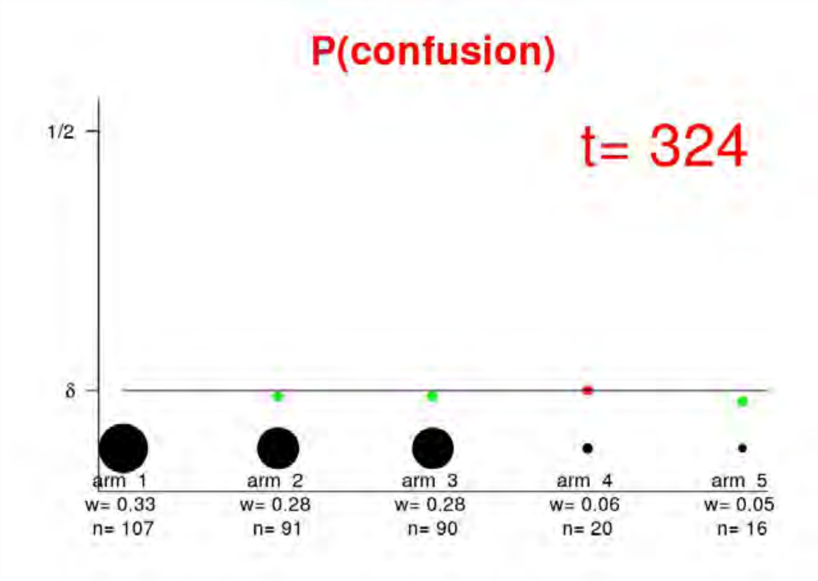

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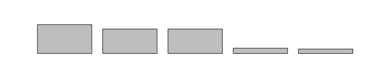

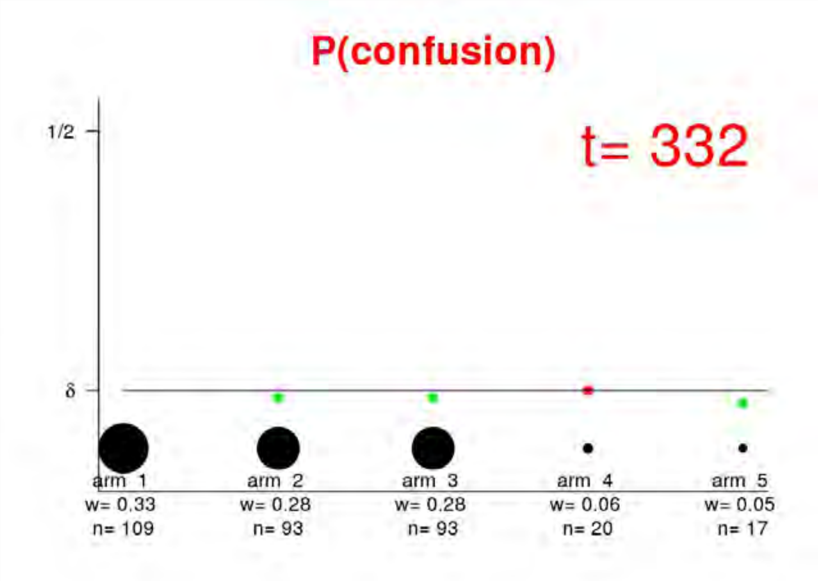

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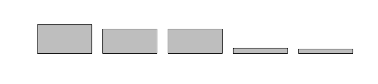

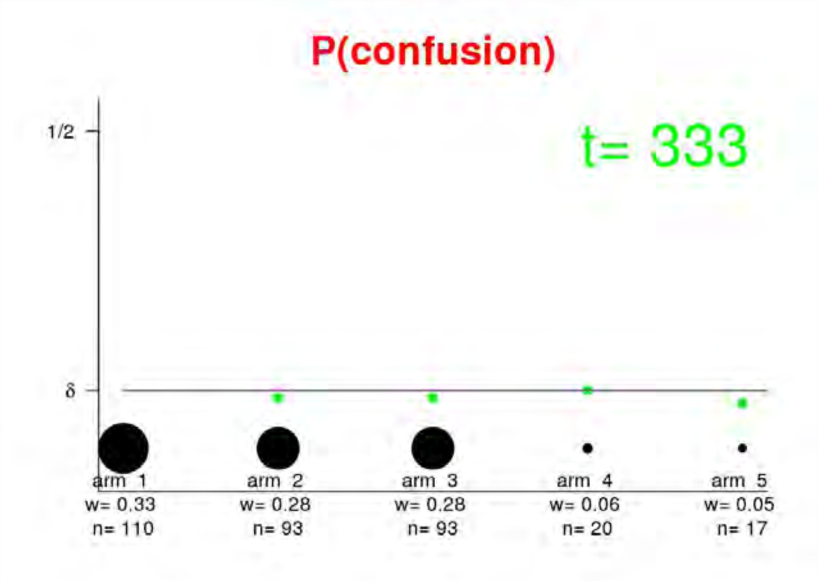

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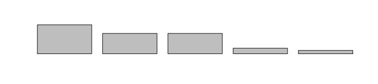

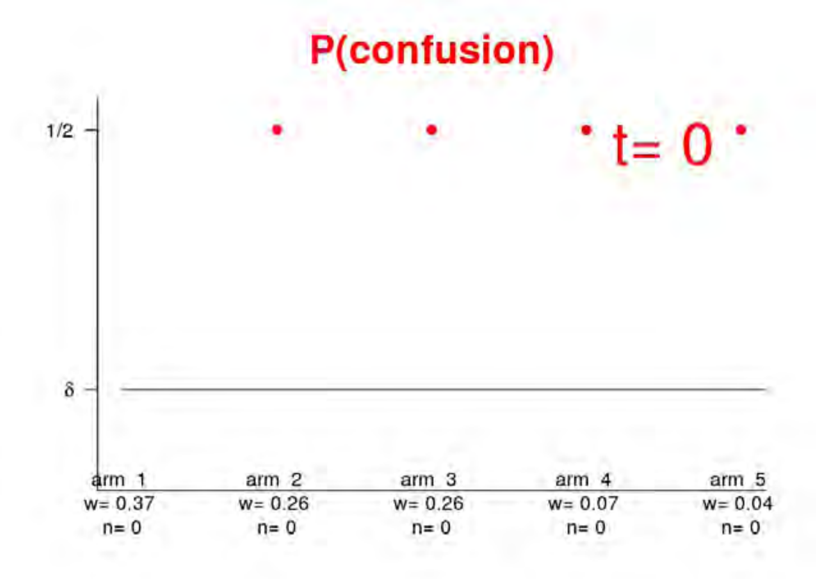

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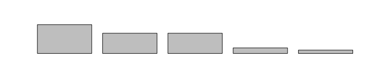

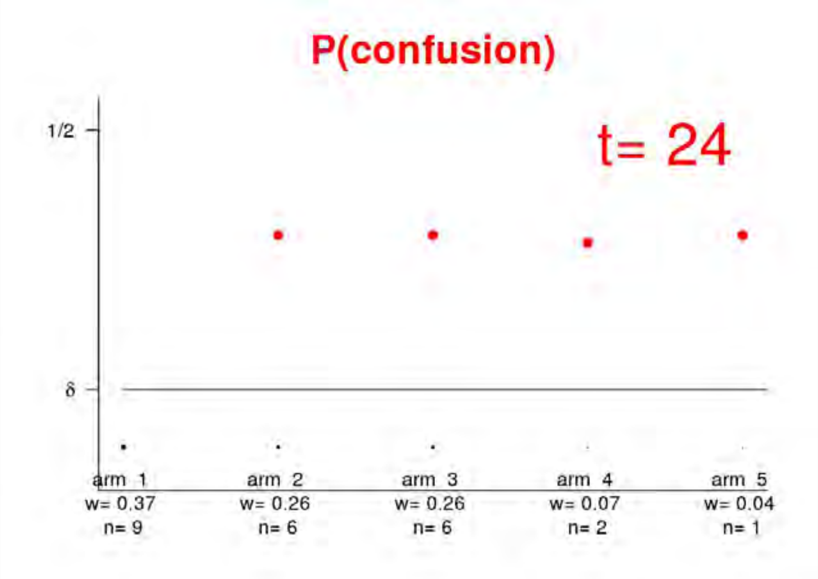

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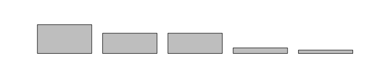

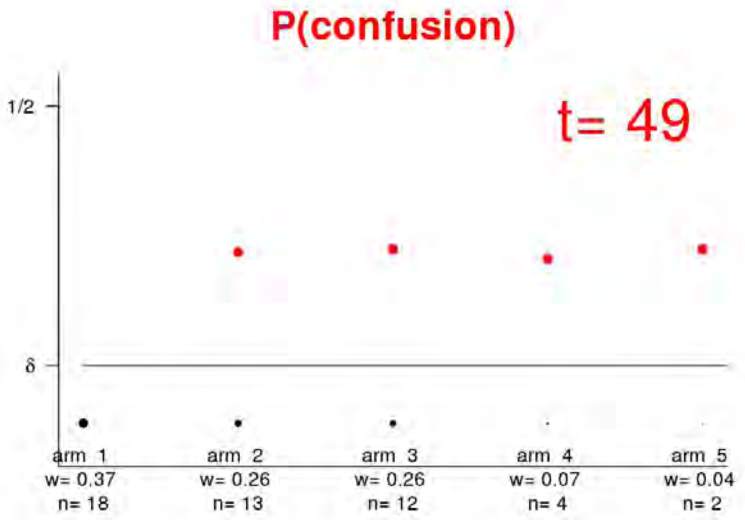

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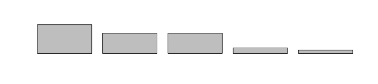

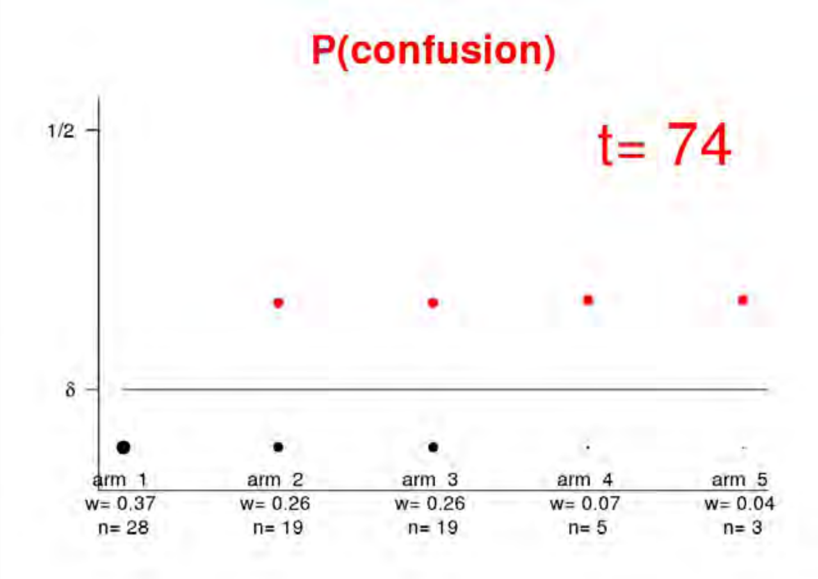

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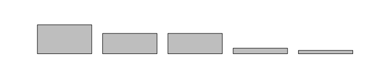

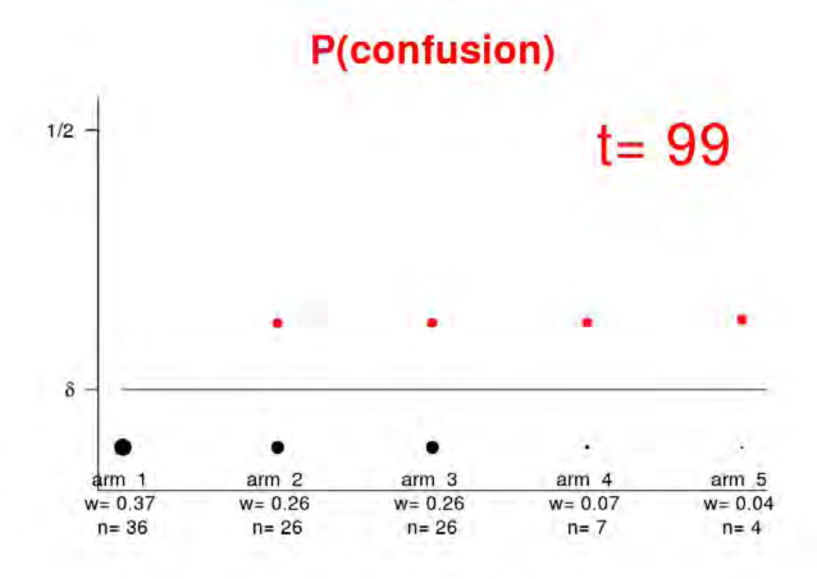

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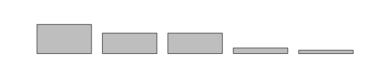
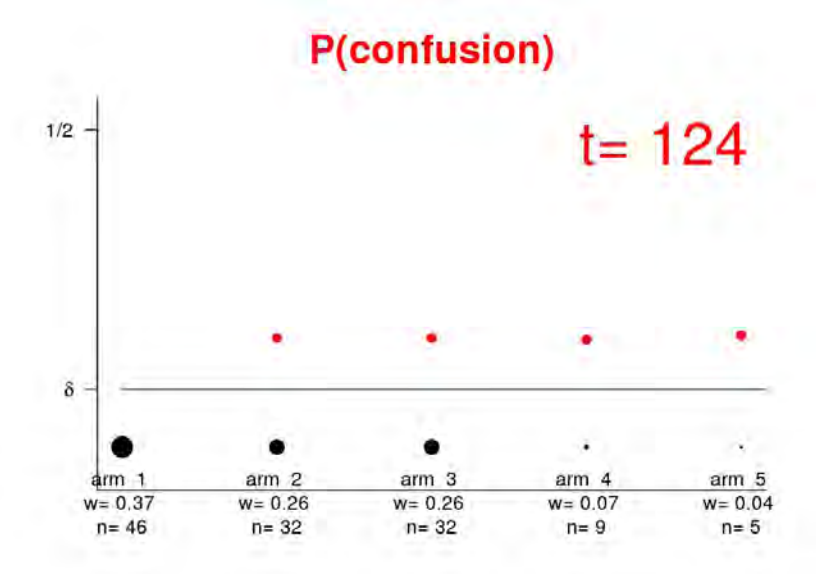
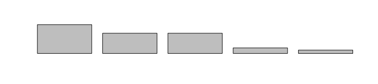
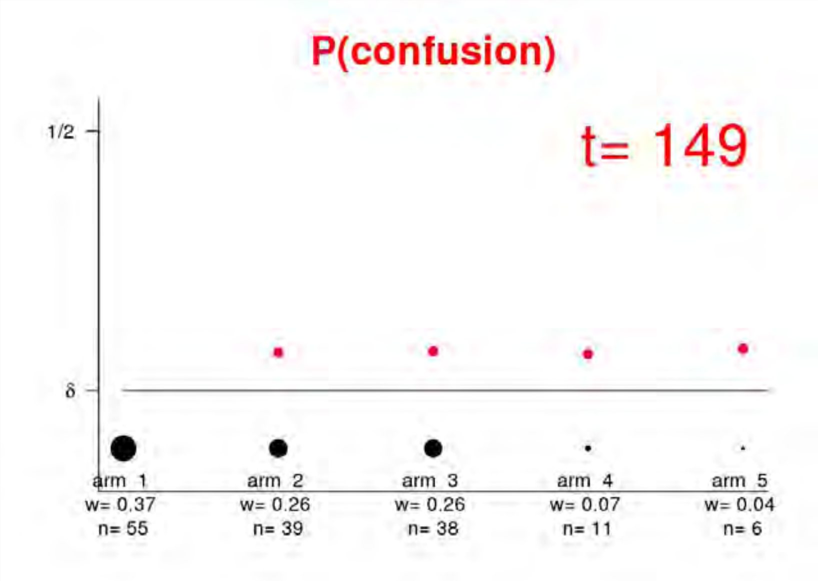




Optimal Proportions





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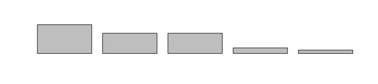

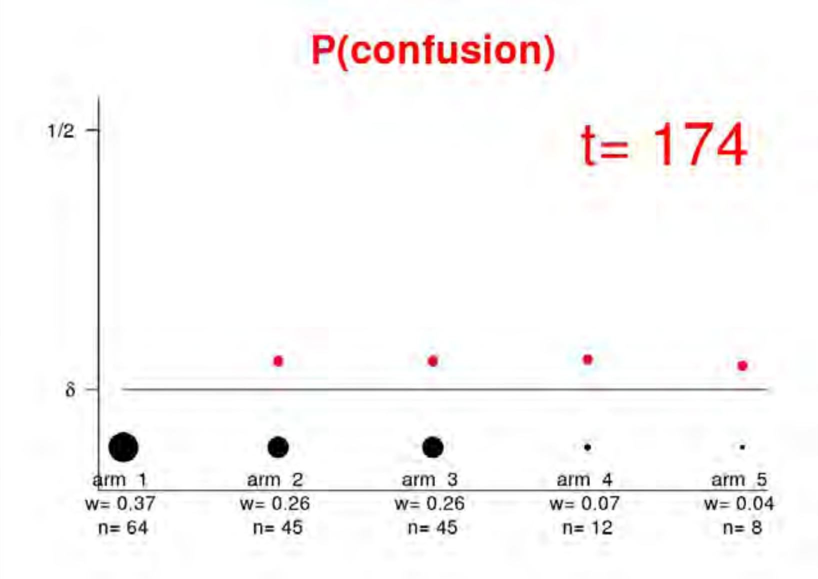

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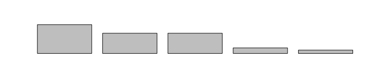

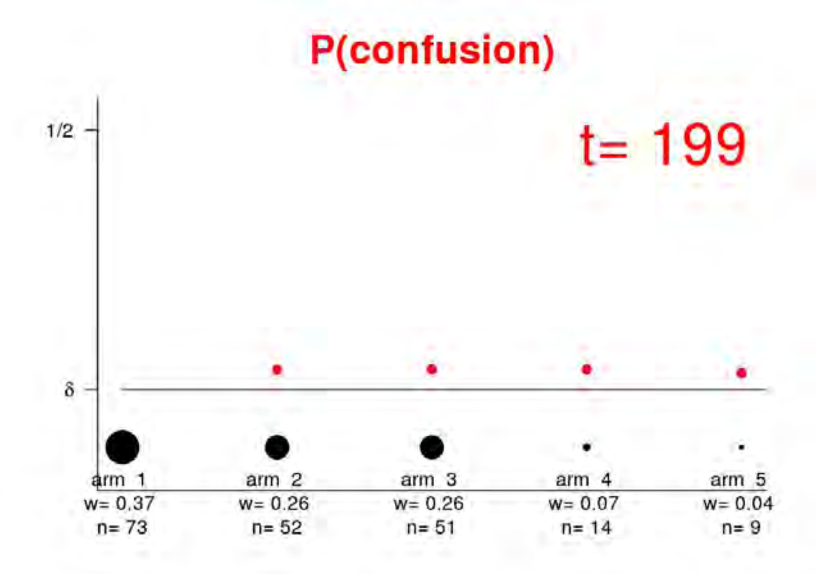

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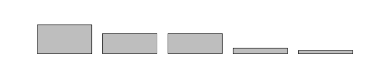

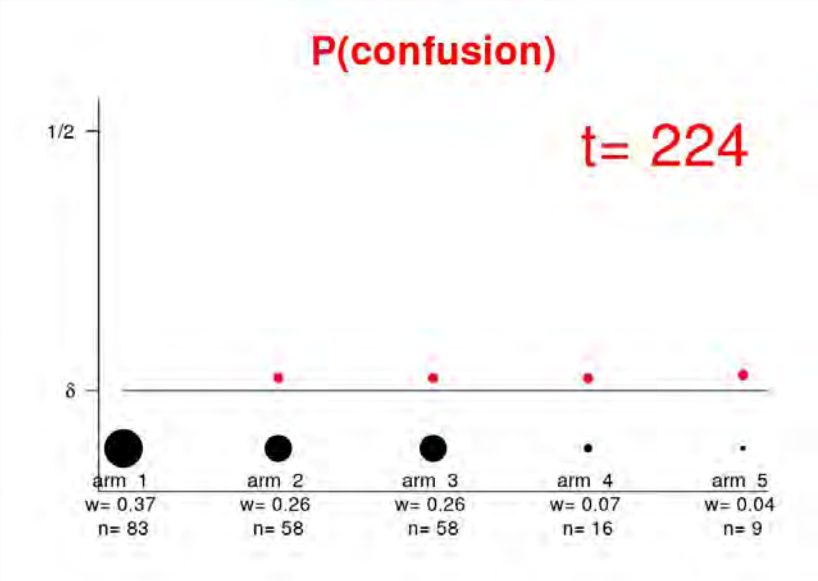

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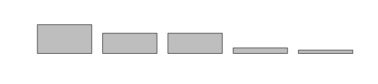
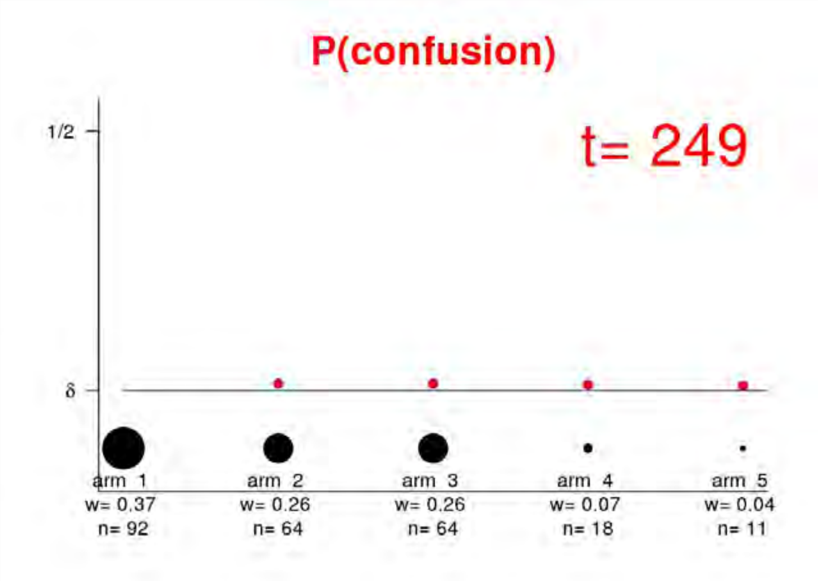
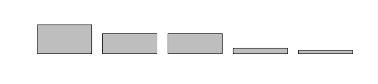
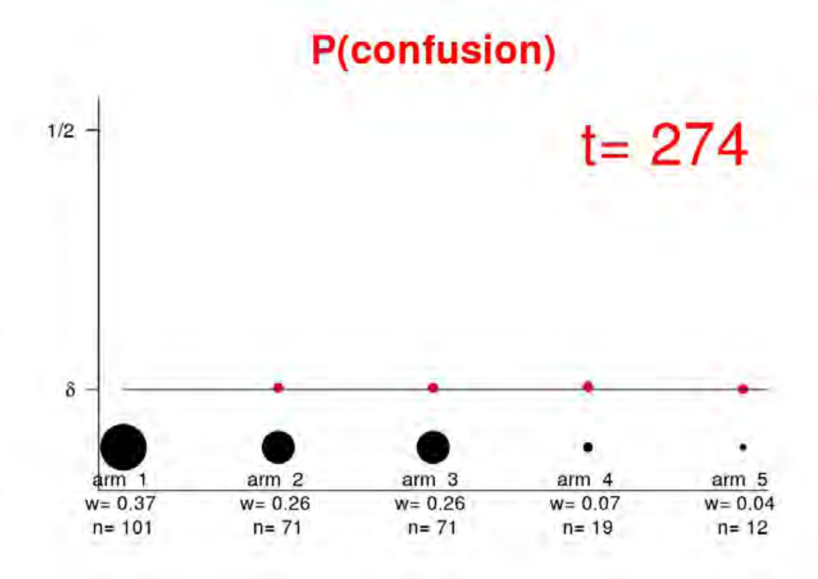


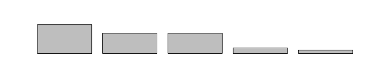


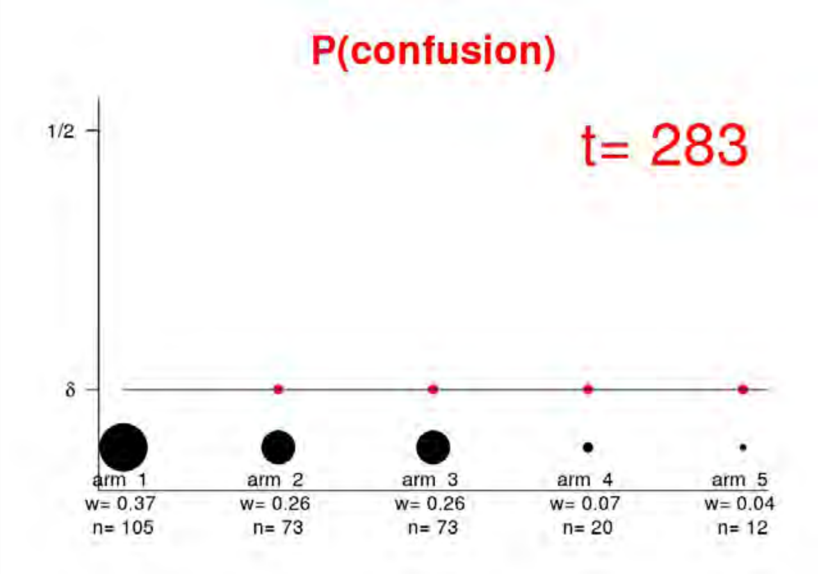
Optimal Proportions





Optimal Proportions





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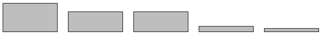
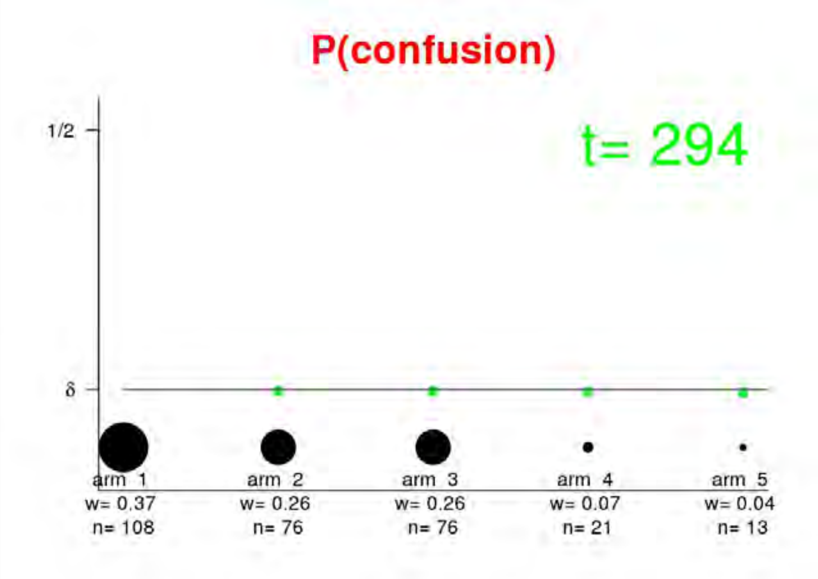




How to Turn this Intuition into a Theorem?

- The arms are not Gaussian (no formula for probability of confusion)
  $\longrightarrow$ large deviations (Sanov, KL)
- You do not allocate a relative budget at first, but you use sequential sampling
  $\longrightarrow$ no fixed-size samples: *sequential experiment*
  $\longrightarrow$ tracking lemma
- How to compute the optimal proportions?
  $\longrightarrow$ lower bound, game
- The parameters of the distribution are unknown
  $\longrightarrow$ (sequential) estimation
- When should you stop?
  $\longrightarrow$ Chernoff's stopping rule

Exponential Families

$\nu_1, \ldots, \nu_K$ belong to a one-dimensional exponential family

$$\mathbb{P}_{\lambda,\Theta,b} = \left\{\nu_\theta, \theta \in \Theta : \nu_\theta \text{ has density } f_\theta(x) = \exp(\theta x - b(\theta)) \ w.r.t. \ \lambda\right\}$$

Example: Gaussian, Bernoulli, Poisson distributions...

- ν_θ can be parametrized by its mean $\mu = \dot{b}(\theta)$: $\nu^\mu := \nu_{\dot{b}^{-1}(\mu)}$

Notation: Kullback-Leibler divergence

For a given exponential family,

$$d(\mu, \mu') := \mathrm{KL}(\nu^\mu, \nu^{\mu'}) = \mathbb{E}_{X \sim \nu^\mu}\left[\log \frac{d\nu^\mu}{d\nu^{\mu'}}(X)\right]$$

is the KL-divergence between the distributions of mean μ and μ'.

We identify $\nu = (\nu^{\mu_1}, \ldots, \nu^{\mu_K})$ and $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_K)$ and consider

$$\mathcal{S} = \left\{\boldsymbol{\mu} \in (\dot{b}(\Theta))^K : \exists a \in \{1, \ldots, K\} : \mu_a > \max_{i \neq a} \mu_i\right\}$$

Lower Bound

Lower-Bounding the Sample Complexity

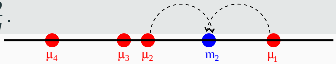
Let $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_K)$ and $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_K)$ be two elements of $\mathcal{S}$.

Uniform δ-PAC Constraint [Kaufmann, Cappé, G. '15]

If $a^*(\boldsymbol{\mu}) \neq a^*(\boldsymbol{\lambda})$, any δ-PAC algorithm satisfies

$$\sum_{a=1}^{K} \mathbb{E}_{\boldsymbol{\mu}}\left[N_a(\tau_\delta)\right] d(\mu_a, \lambda_a) \geq \mathrm{kl}(\delta, 1-\delta)$$

where $\mathrm{kl}(p,q) = p \log \frac{p}{q} + (1-p) \log \frac{1-p}{1-q}$.



Let $\mathrm{Alt}(\boldsymbol{\mu}) = \{\boldsymbol{\lambda} : a^*(\boldsymbol{\lambda}) \neq a^*(\boldsymbol{\mu})\}$. Take: $\lambda_1 = m_2 - \epsilon \quad \lambda_2 = m_2 + \epsilon$

$$\mathbb{E}_{\boldsymbol{\mu}}[N_1(\tau_\delta)]\, d(\mu_1, m_2 - \epsilon) + \mathbb{E}_{\boldsymbol{\mu}}[N_2(\tau_\delta)]\, d(\mu_2, m_2 + \epsilon) \quad \geq \quad \mathrm{kl}(\delta, 1-\delta)$$

Lower-Bounding the Sample Complexity

Let $\boldsymbol{\mu} = (\mu_1, \dots, \mu_K)$ and $\boldsymbol{\lambda} = (\lambda_1, \dots, \lambda_K)$ be two elements of $\mathcal{S}$.

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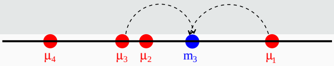

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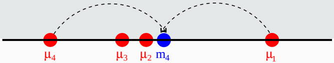

Let $\mathrm{Alt}(\boldsymbol{\mu}) = \{\boldsymbol{\lambda} : a^*(\boldsymbol{\lambda}) \neq a^*(\boldsymbol{\mu})\}$. Take: $\lambda_1 = m_4 - \epsilon \quad \lambda_4 = m_4 + \epsilon$

$$\begin{aligned}
\mathbb{E}_{\boldsymbol{\mu}}[N_1(\tau_\delta)]\, d(\mu_1, m_2 - \epsilon) + \mathbb{E}_{\boldsymbol{\mu}}[N_2(\tau_\delta)]\, d(\mu_2, m_2 + \epsilon) &\geq \mathrm{kl}(\delta, 1-\delta) \\
\mathbb{E}_{\boldsymbol{\mu}}[N_1(\tau_\delta)]\, d(\mu_1, m_3 - \epsilon) + \mathbb{E}_{\boldsymbol{\mu}}[N_3(\tau_\delta)]\, d(\mu_3, m_3 + \epsilon) &\geq \mathrm{kl}(\delta, 1-\delta) \\
\mathbb{E}_{\boldsymbol{\mu}}[N_1(\tau_\delta)]\, d(\mu_1, m_4 - \epsilon) + \mathbb{E}_{\boldsymbol{\mu}}[N_4(\tau_\delta)]\, d(\mu_4, m_4 + \epsilon) &\geq \mathrm{kl}(\delta, 1-\delta)
\end{aligned}$$

Lower-Bounding the Sample Complexity

Let $\boldsymbol{\mu} = (\mu_1, \dots, \mu_K)$ and $\boldsymbol{\lambda} = (\lambda_1, \dots, \lambda_K)$ be two elements of $\mathcal{S}$.

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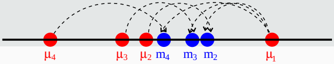


Let $\mathrm{Alt}(\boldsymbol{\mu}) = \{\boldsymbol{\lambda} : a^*(\boldsymbol{\lambda}) \neq a^*(\boldsymbol{\mu})\}$.

$$\inf_{\boldsymbol{\lambda} \in \mathrm{Alt}(\boldsymbol{\mu})} \sum_{a=1}^{K} \mathbb{E}_{\boldsymbol{\mu}}[N_a(\tau_\delta)]\, d(\mu_a, \lambda_a) \geq \mathrm{kl}(\delta, 1-\delta)$$

$$\mathbb{E}_{\boldsymbol{\mu}}[\tau_\delta] \times \inf_{\boldsymbol{\lambda} \in \mathrm{Alt}(\boldsymbol{\mu})} \sum_{a=1}^{K} \frac{\mathbb{E}_{\boldsymbol{\mu}}[N_a(\tau_\delta)]}{\mathbb{E}_{\boldsymbol{\mu}}[\tau_\delta]}\, d(\mu_a, \lambda_a) \geq \mathrm{kl}(\delta, 1-\delta)$$

$$\mathbb{E}_{\boldsymbol{\mu}}[\tau_\delta] \times \left(\sup_{w \in \Sigma_K} \inf_{\boldsymbol{\lambda} \in \mathrm{Alt}(\boldsymbol{\mu})} \sum_{a=1}^{K} w_a\, d(\mu_a, \lambda_a) \right) \geq \mathrm{kl}(\delta, 1-\delta)$$

Lower Bound: the Complexity of BAI

Theorem

For any δ-PAC algorithm,

$$\mathbb{E}_{\boldsymbol{\mu}}[\tau_\delta] \geq T^*(\boldsymbol{\mu})\, \mathrm{kl}(\delta, 1-\delta)\ ,$$

where

$$T^*(\boldsymbol{\mu})^{-1} = \sup_{\mathbf{w} \in \Sigma_K} \inf_{\lambda \in \mathrm{Alt}(\boldsymbol{\mu})} \left(\sum_{a=1}^{K} w_a\, d(\mu_a, \lambda_a) \right).$$

- $\mathrm{kl}(\delta, 1-\delta) \sim \log(1/\delta)$ when $\delta \to 0$, $\mathrm{kl}(\delta, 1-\delta) \geq \log\left(1/(2.4\delta)\right)$
- cf. [Graves and Lai 1997, Vaidhyan and Sundaresan, 2015]

➜ the optimal proportions of arm draws are

$$\mathbf{w}^*(\boldsymbol{\mu}) = \underset{\mathbf{w} \in \Sigma_K}{\mathrm{argmax}} \inf_{\lambda \in \mathrm{Alt}(\boldsymbol{\mu})} \left(\sum_{a=1}^{K} w_a d(\mu_a, \lambda_a) \right)$$

➜ they do not depend on δ

PAC-BAI as a Game

Given a parameter $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_K)$:

- the statistician chooses proportions of arm draws $\mathbf{w} = (w_a)_a$
- the opponent chooses an alternative model $\boldsymbol{\lambda}$
- the payoff is the minimal number $T = T(\mathbf{w}, \boldsymbol{\lambda})$ of draws necessary to ensure that he does not violate the δ-PAC constraint

$$\sum_{a=1}^{K} T w_a \, d(\mu_a, \lambda_a) \geq \mathrm{kl}(\delta, 1-\delta)$$

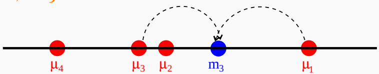
- $T^*(\boldsymbol{\mu}) \, \mathrm{kl}(\delta, 1-\delta)$ = value of the game
  $\mathbf{w}^*$ = optimal action for the statistician

PAC-BAI as a Game

Given a parameter $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_K)$ such that $\mu_1 > \mu_2 \geq \cdots \geq \mu_K$:

- the statistician chooses proportions of arm draws $\mathbf{w} = (w_a)_a$
- the opponent chooses an arm $a \in \{2, \ldots, K\}$ and

  $\lambda_a = \arg\min_\lambda w_1\, d(\mu_1, \lambda) + w_a\, d(\mu_a, \lambda)$



- the payoff is the minimal number $T = T(\mathbf{w}, a, \delta)$ of draws necessary to ensure that

$$Tw_1\, d(\mu_1, \lambda_a - \epsilon) + Tw_a\, d(\mu_a, \lambda_a + \epsilon) \geq \mathrm{kl}(\delta, 1 - \delta)$$

  that is $T(\mathbf{w}, a, \delta) = \dfrac{\mathrm{kl}(\delta, 1-\delta)}{w_1\, d(\mu_1, \lambda_a - \epsilon) + w_a\, d(\mu_a, \lambda_a + \epsilon)}$

- $T^*(\boldsymbol{\mu})\, \mathrm{kl}(\delta, 1 - \delta) =$ value of the game

  $\mathbf{w}^* =$ optimal action for the statistician

Properties of $T^*(\mu)$ and $\mathbf{w}^*(\mu)$

1. Unique solution, solution of scalar equations only
2. For all $\boldsymbol{\mu} \in \mathcal{S}$, for all a, $w_a^*(\boldsymbol{\mu}) > 0$
3. $\mathbf{w}^*$ is continuous in every $\boldsymbol{\mu} \in \mathcal{S}$
4. If $\mu_1 > \mu_2 \geq \cdots \geq \mu_K$, one has $w_2^*(\boldsymbol{\mu}) \geq \cdots \geq w_K^*(\boldsymbol{\mu})$

   (one may have $w_1^*(\boldsymbol{\mu}) < w_2^*(\boldsymbol{\mu})$)
5. Case of two arms [Kaufmann, Cappé, G. '14]:

   $$\mathbb{E}_{\boldsymbol{\mu}}[\tau_\delta] \geq \frac{\mathrm{kl}(\delta, 1-\delta)}{d_*(\mu_1, \mu_2)} .$$

   where d_* is the 'reversed' Chernoff information

   $$d_*(\mu_1, \mu_2) := d(\mu_1, \mu_*) = d(\mu_2, \mu_*) .$$
6. Gaussian arms : algebraic equation but no simple formula for $K \geq 3$.

   $$\sum_{a=1}^{K} \frac{2\sigma^2}{\Delta_a^2} \leq T^*(\boldsymbol{\mu}) \leq 2 \sum_{a=1}^{K} \frac{2\sigma^2}{\Delta_a^2} .$$

The Track-and-Stop Strategy

Sampling rule: Tracking the optimal proportions

$\hat{\boldsymbol{\mu}}(t) = (\hat{\mu}_1(t), \ldots, \hat{\mu}_K(t))$: vector of empirical means

Introducing

$$U_t = \left\{ a : N_a(t) < \sqrt{t} \right\},$$

the arm sampled at round $t + 1$ is

$$A_{t+1} \in \begin{cases} \underset{a \in U_t}{\text{argmin}} \; N_a(t) \quad \text{if } U_t \neq \emptyset & (\textit{forced exploration}) \\ \underset{1 \leq a \leq K}{\text{argmax}} \; t \, w_a^*(\hat{\boldsymbol{\mu}}(t)) - N_a(t) & (\textit{tracking}) \end{cases}$$

Lemma

Under the Tracking sampling rule,

$$\mathbb{P}_{\boldsymbol{\mu}} \left(\lim_{t \to \infty} \frac{N_a(t)}{t} = w_a^*(\boldsymbol{\mu}) \right) = 1.$$

Sequential Generalized Likelihood Test

High values of the Generalized Likelihood Ratio

$$Z_{a,b}(t) := \log \frac{\max_{\{\boldsymbol{\lambda}:\lambda_a \geq \lambda_b\}} dP_{\boldsymbol{\lambda}}(X_1,\dots,X_t)}{\max_{\{\boldsymbol{\lambda}:\lambda_a \leq \lambda_b\}} dP_{\boldsymbol{\lambda}}(X_1,\dots,X_t)}$$

$$= N_a(t)\, d\big(\hat{\mu}_a(t), \hat{\mu}_{a,b}(t)\big) + N_b(t)\, d\big(\hat{\mu}_b(t), \hat{\mu}_{a,b}(t)\big) \quad \text{if } \hat{\mu}_a(t) > \hat{\mu}_b(t)$$

$-Z_{b,a}(t)$ otherwise

reject the hypothesis that $(\mu_a \leq \mu_b)$.

We stop when one arm is assessed to be significantly larger than all other arms, according to a GLR test:

$$\tau_\delta = \inf\left\{t \in \mathbb{N} : \exists a \in \{1,\dots,K\}, \forall b \neq a, Z_{a,b}(t) > \beta(t,\delta)\right\}$$

$$= \inf\left\{t \in \mathbb{N} : \quad Z(t) := \max_{a \in \{1,\dots,K\}} \min_{b \neq a} Z_{a,b}(t) > \beta(t,\delta)\right\}$$

Chernoff stopping rule [Chernoff '59]

Two other possible interpretations of the stopping rule:

➜ MDL:

$$Z_{a,b}(t) = \big(N_a(t) + N_b(t)\big) H\big(\hat{\mu}_{a,b}(t)\big) - \left[N_a(t) H\big(\hat{\mu}_a(t)\big) + N_b(t) H\big(\hat{\mu}_b(t)\big)\right]$$

Sequential Generalized Likelihood Test

High values of the Generalized Likelihood Ratio

$$Z_{a,b}(t) := \log \frac{\max_{\{\boldsymbol{\lambda}:\lambda_a \geq \lambda_b\}} dP_{\boldsymbol{\lambda}}(X_1, \dots, X_t)}{\max_{\{\boldsymbol{\lambda}:\lambda_a \leq \lambda_b\}} dP_{\boldsymbol{\lambda}}(X_1, \dots, X_t)}$$

reject the hypothesis that $(\mu_a \leq \mu_b)$.

We stop when one arm is assessed to be significantly larger than all other arms, according to a GLR test:

$$\tau_\delta = \inf \left\{ t \in \mathbb{N} : \quad Z(t) := \max_{a \in \{1,\dots,K\}} \min_{b \neq a} Z_{a,b}(t) > \beta(t, \delta) \right\}$$

Chernoff stopping rule [Chernoff '59]

Two other possible interpretations of the stopping rule:

➜ plug-in complexity estimate: with $F(w, \mu) := \inf_{\boldsymbol{\lambda} \in \mathrm{Alt}(\mu)} \sum_{a=1}^{K} w \, d\big(\mu_a, \lambda_a\big)$,

stop when $Z(t) = t \, F\Big(\frac{N_a(t)}{t}, \hat{\mu}(t)\Big) \geq \beta(t, \delta)$ instead of the lower bound $\frac{t}{T^*(\mu)} = t \, F(\mathbf{w}^*, \mu) \geq \mathrm{kl}(\delta, 1 - \delta)$.

Calibration

Theorem

The Chernoff rule is δ-PAC for $\beta(t,\delta) = \log\left(\frac{2(K-1)t}{\delta}\right)$

Lemma

If $\mu_a < \mu_b$, whatever the sampling rule,

$$\mathbb{P}_{\boldsymbol{\mu}}\left(\exists t \in \mathbb{N} : Z_{a,b}(t) > \log\left(\frac{2t}{\delta}\right)\right) \leq \delta$$

The proof uses:

➜ Barron's lemma (change of distribution)

➜ and Krichevsky-Trofimov's universal distribution

(very information-theoretic ideas)

Asymptotic Optimality of the T&S strategy

Theorem

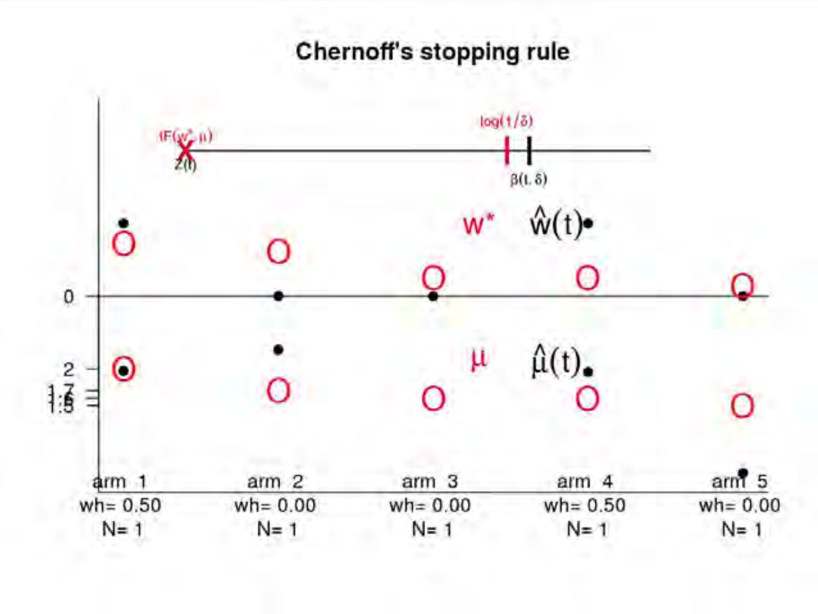
The Track-and-Stop strategy, that uses

- the Tracking sampling rule
- the Chernoff stopping rule with $\beta(t,\delta) = \log\left(\frac{2(K-1)t}{\delta}\right)$
- and recommends $\hat{a}_{\tau_\delta} = \underset{a=1\dots K}{\text{argmax}}\ \hat{\mu}_a(\tau_\delta)$

is δ-PAC for every $\delta \in (0,1)$ and satisfies

$$\limsup_{\delta\to 0} \frac{\mathbb{E}_{\boldsymbol{\mu}}[\tau_\delta]}{\log(1/\delta)} = T^*(\boldsymbol{\mu}).$$

Why is the T&S Strategy asymptotically Optimal?



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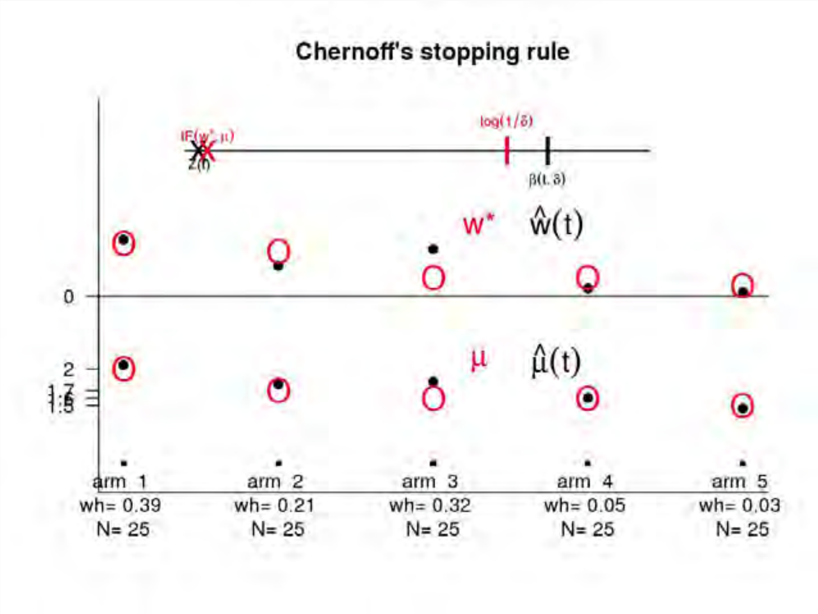

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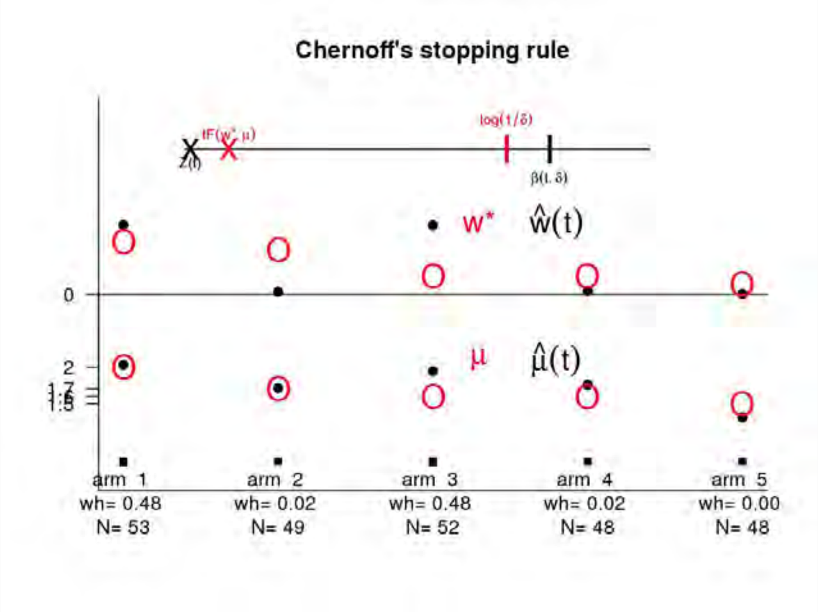

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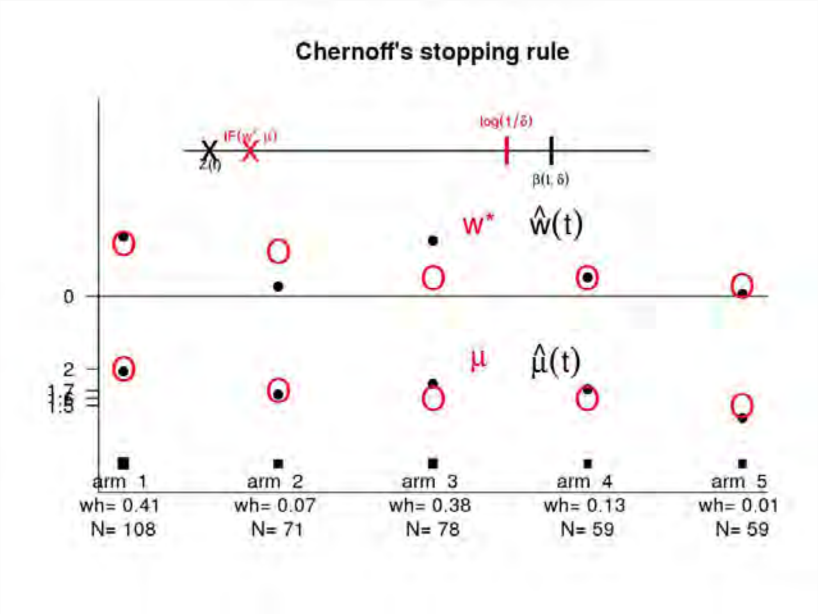

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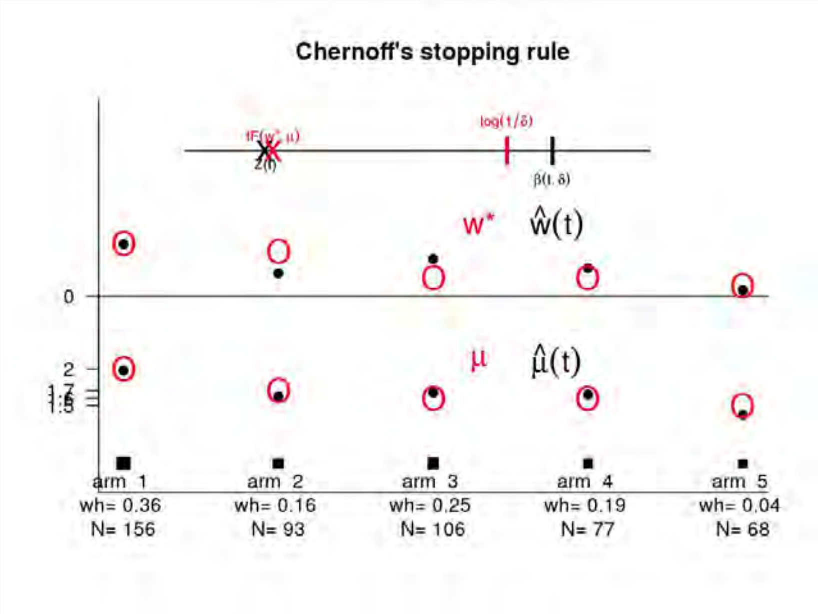

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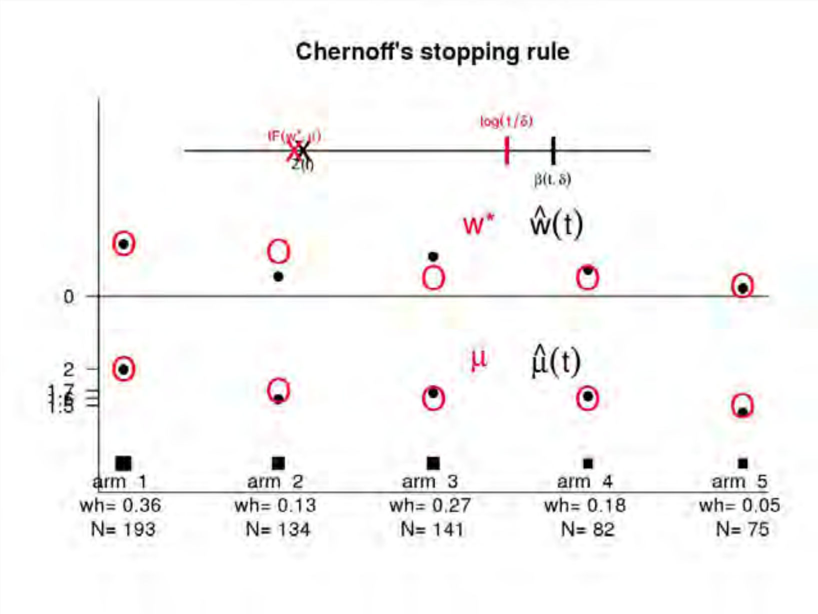

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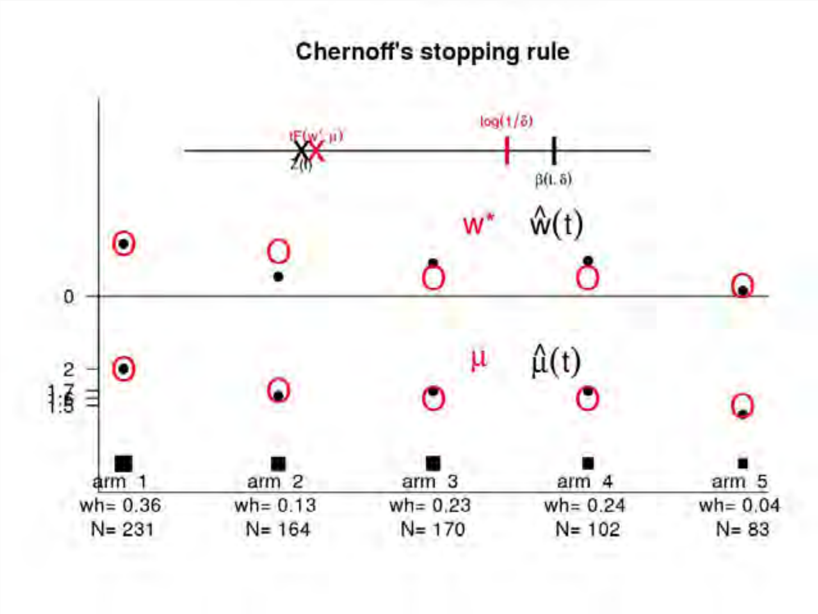
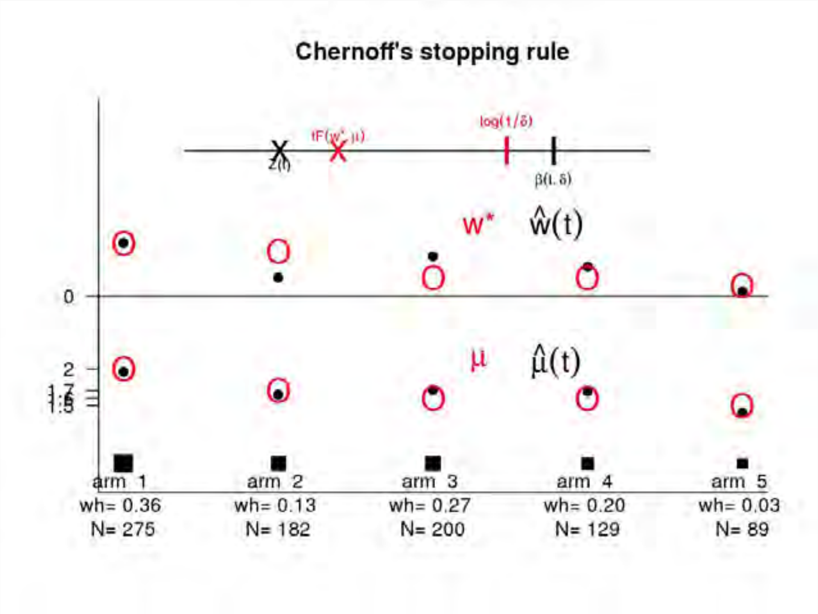


Why is the T&S Strategy asymptotically Optimal?



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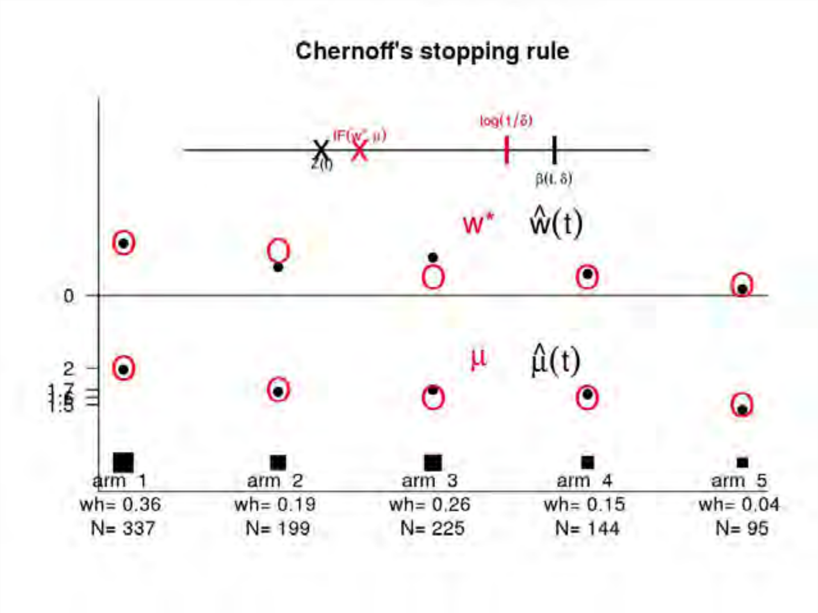

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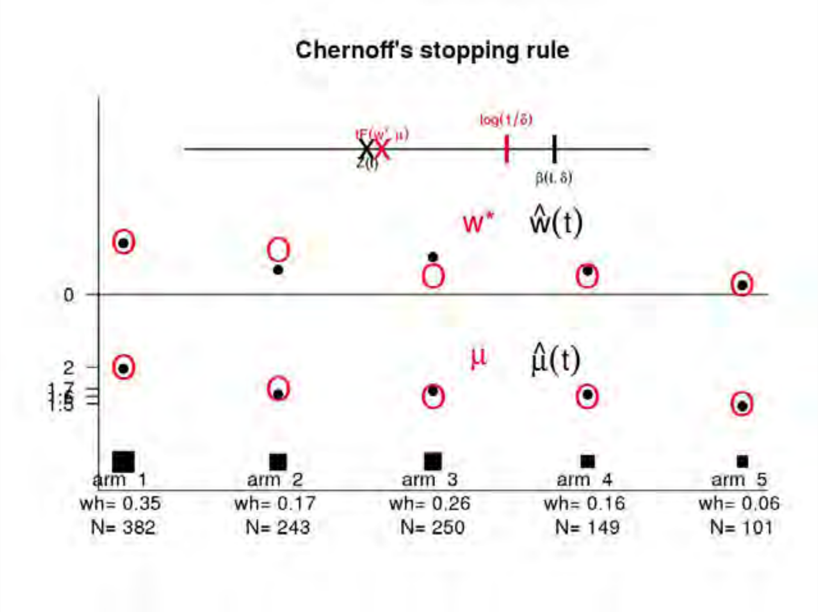

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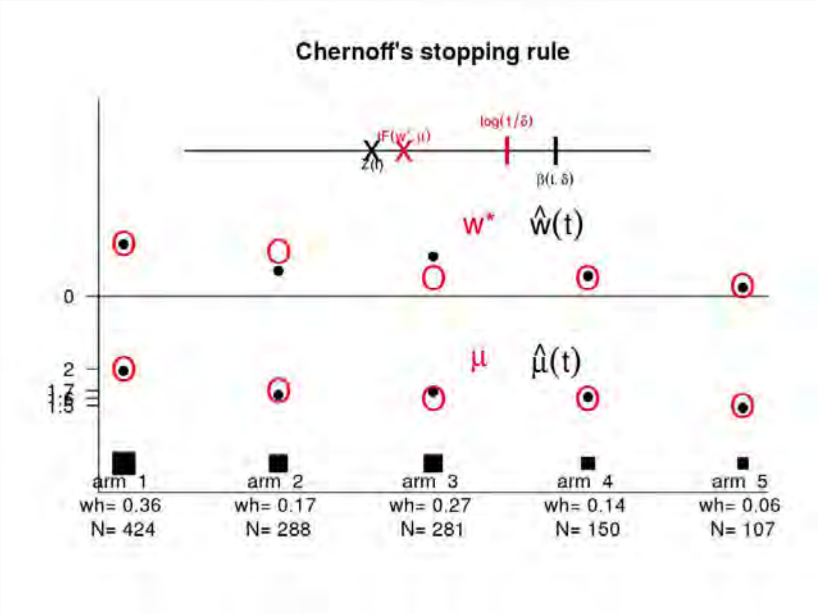

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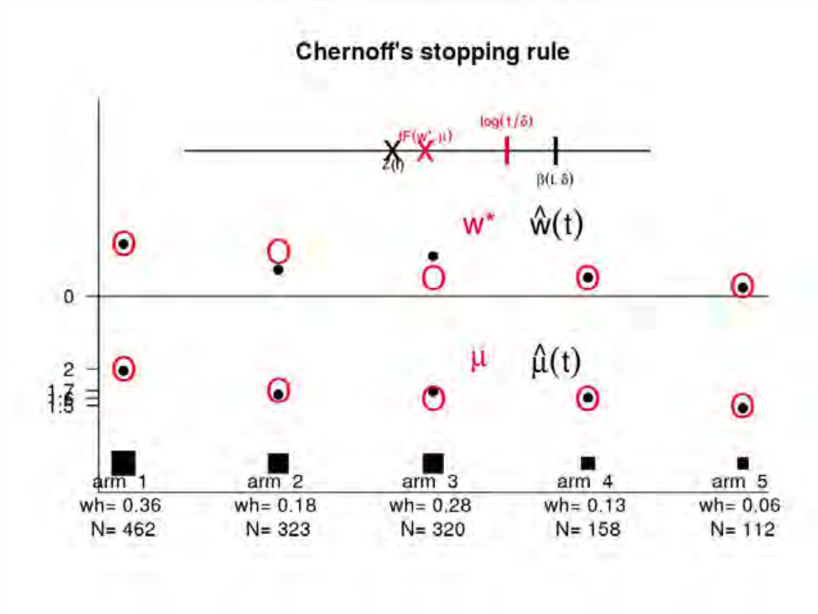

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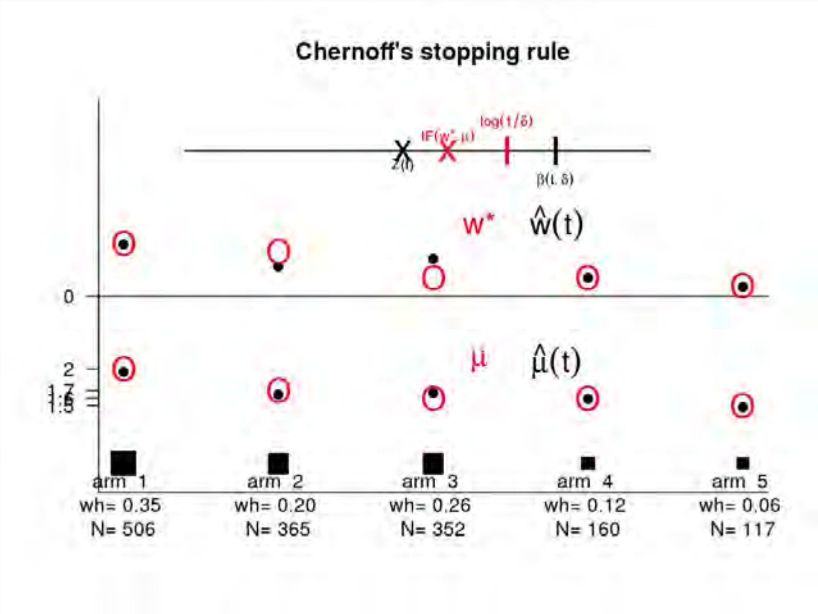

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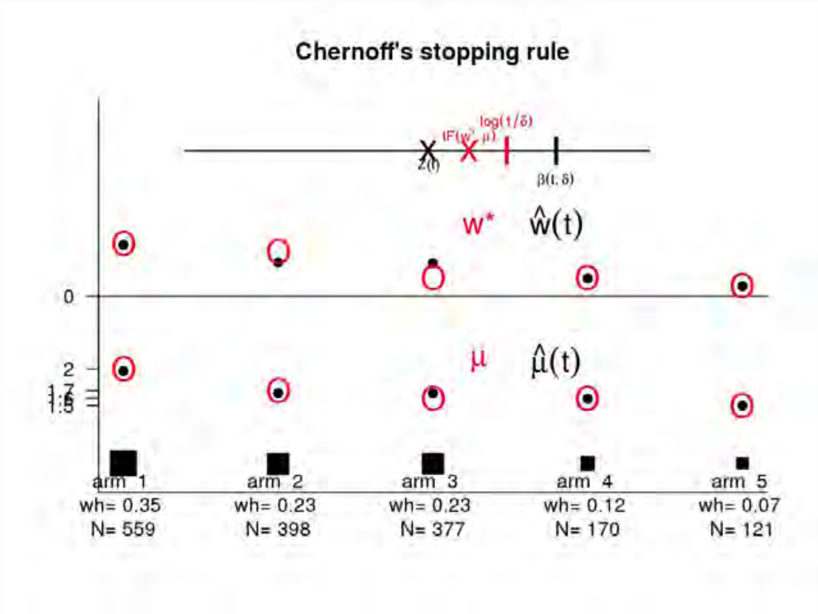

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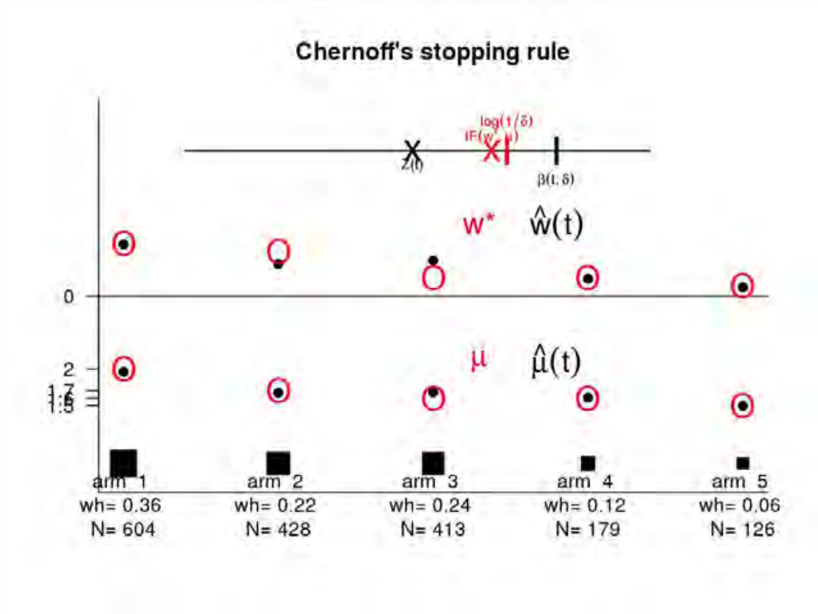

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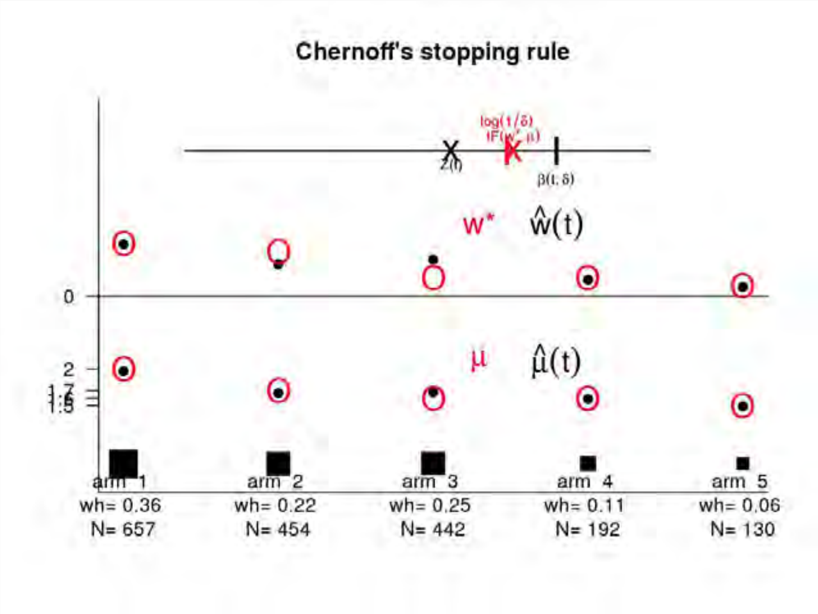

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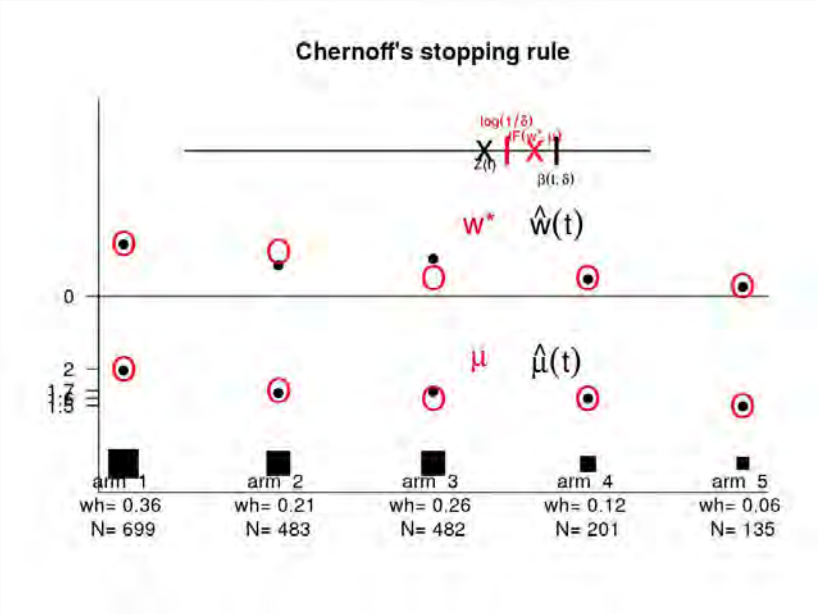

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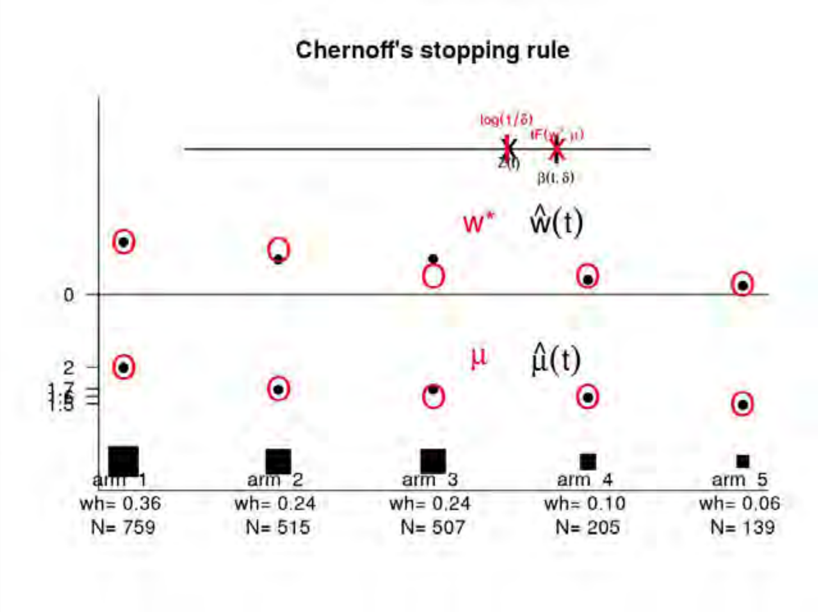

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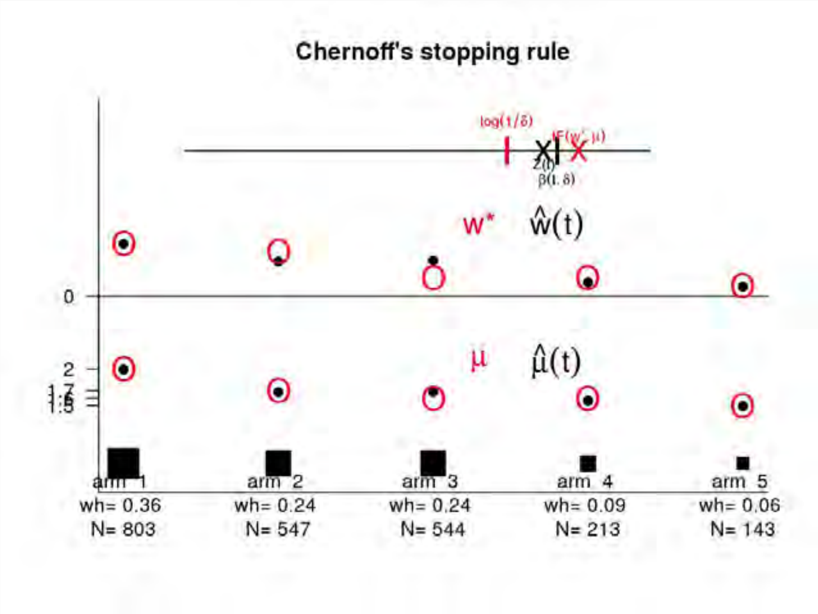

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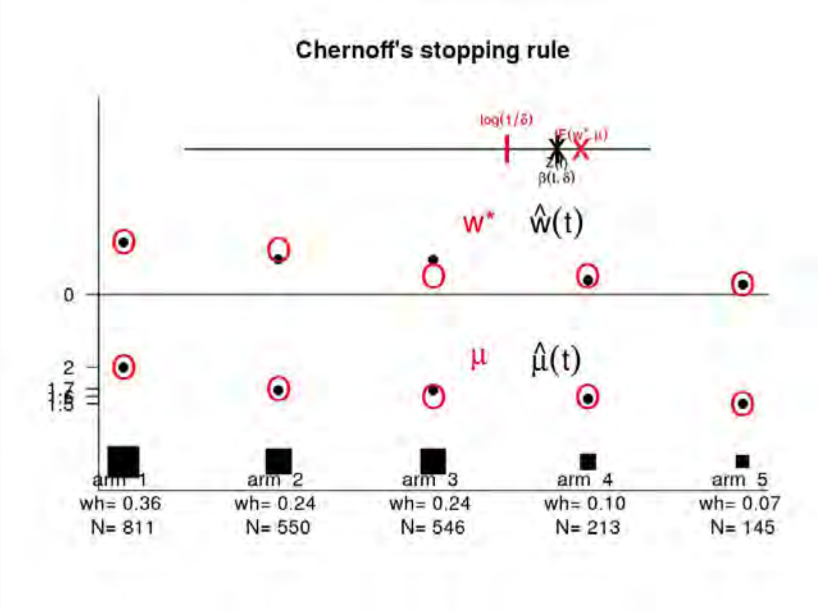


Sketch of proof (almost-sure convergence only)

- forced exploration $\implies$ $N_a(t) \to \infty$ a.s. for all $a \in \{1, \dots, K\}$

➜ $\boldsymbol{\mu}(t) \to \boldsymbol{\mu}$ a.s.

➜ $\mathbf{w}^*\left(\hat{\boldsymbol{\mu}}(t)\right) \to \mathbf{w}^*$ a.s.

➜ tracking rule: $\dfrac{N_a(t)}{t} \underset{t\to\infty}{\to} w_a^*$ a.s.

- but the mapping $F : (\boldsymbol{\mu}', w) \mapsto \inf\limits_{\boldsymbol{\lambda}\in\mathrm{Alt}(\boldsymbol{\mu}')} \sum_{a=1}^{K} w_a d(\mu'_a, \lambda_a)$ is continuous at $(\boldsymbol{\mu}, w^*(\boldsymbol{\mu}))$:

➜ $Z(t) = t \times F\left(\hat{\boldsymbol{\mu}}(t), (N_a(t)/t)_{a=1}^{K}\right) \sim t \times F(\mu, \mathbf{w}^*) = t \times T^*(\mu)^{-1}$
and for every $\epsilon > 0$ there exists t_0 such that

$$t \geq t_0 \;\Rightarrow\; Z(t) \geq t \times (1+\epsilon)^{-1} T^*(\boldsymbol{\mu})^{-1}$$

$\implies$ Thus $\tau_\delta \leq t_0 \wedge \inf\left\{t \in \mathbb{N} : (1+\epsilon)^{-1} T^*(\boldsymbol{\mu})^{-1} t \geq \log(2(K-1)t/\delta)\right\}$
and $\limsup\limits_{\delta\to 0} \dfrac{\tau_\delta}{\log(1/\delta)} \leq (1+\epsilon) T^*(\boldsymbol{\mu}) \quad a.s.$

Numerical Experiments

- $\boldsymbol{\mu}_1 = [0.5\ 0.45\ 0.43\ 0.4] \quad \rightarrow \quad w^*(\boldsymbol{\mu}_1) = [0.42\ 0.39\ 0.14\ 0.06]$
- $\boldsymbol{\mu}_2 = [0.3\ 0.21\ 0.2\ 0.19\ 0.18] \rightarrow w^*(\boldsymbol{\mu}_2) = [0.34\ 0.25\ 0.18\ 0.13\ 0.10]$

In practice, set the threshold to $\beta(t, \delta) = \log\left(\frac{\log(t)+1}{\delta}\right)$ (δ-PAC OK)

	Track-and-Stop	Chernoff-Racing	KL-LUCB	KL-Racing
$\boldsymbol{\mu}_1$	4052	4516	8437	9590
$\boldsymbol{\mu}_2$	1406	3078	2716	3334

Table 1: Expected number of draws $\mathbb{E}_{\boldsymbol{\mu}}[\tau_\delta]$ for $\delta = 0.1$, averaged over $N = 3000$ experiments.

➜ Empirically good even for 'large' values of the risk δ

➜ Racing is sub-optimal in general, because it plays $w_1 = w_2$

➜ LUCB is sub-optimal in general, because it plays $w_1 = 1/2$

Perspectives

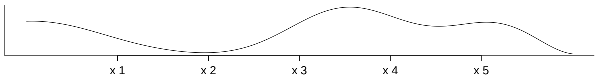
For best arm identification, we showed that

$$\inf_{\text{PAC algorithm}} \limsup_{\delta\to 0} \frac{\mathbb{E}_{\boldsymbol{\mu}}[\tau_\delta]}{\log(1/\delta)} = \sup_{w\in\Sigma_K} \inf_{\boldsymbol{\lambda}\in \mathrm{Alt}(\boldsymbol{\mu})} \left(\sum_{a=1}^{K} w_a d(\mu_a, \lambda_a) \right)$$

and provided an efficient strategy asymptotically matching this bound.

Future work:

- $*$ anytime stopping ➜ gives a confidence level
- $**$ find an ϵ-optimal arm
- $*$ find the m-best arms
- $***$ design and analyze more stable algorithm (hint: optimism)
- $***$ give a simple algorithm with a finite-time analysis
  candidate: play action maximizing the expected increase of $Z(t)$
- $***$ extend to structured and continuous settings



References

- O. Cappé, A. Garivier, O-A. Maillard, R. Munos, and G. Stoltz. Kullback-Leibler upper confidence bounds for optimal sequential allocation. *Annals of Statistics*, 2013.
- H. Chernoff. Sequential design of Experiments. The Annals of Mathematical Statistics, 1959.
- E. Even-Dar, S. Mannor, Y. Mansour, Action Elimination and Stopping Conditions for the Multi-Armed Bandit and Reinforcement Learning Problems. *JMLR*, 2006.
- T.L. Graves and T.L. Lai. Asymptotically Efficient adaptive choice of control laws in controlled markov chains. SIAM Journal on Control and Optimization, 35(3):715743, 1997.
- S. Kalyanakrishnan, A. Tewari, P. Auer, and P. Stone. PAC subset selection in stochastic multi- armed bandits. ICML, 2012.
- E. Kaufmann, O. Cappé, A. Garivier. On the Complexity of Best Arm Identification in Multi-Armed Bandit Models. *JMLR*, 2015
- A. Garivier, E. Kaufmann. Optimal Best Arm Identification with Fixed Confidence, COLT'16, New York, arXiv:1602.04589
- A. Garivier, P. Ménard, G. Stoltz. Explore First, Exploit Next: The True Shape of Regret in Bandit Problems.
- E. Kaufmann, S. Kalyanakrishnan. The information complexity of best arm identification, COLT 2013
- T.L. Lai and H. Robbins. Asymptotically efficient adaptive allocation rules. *Advances in Applied Mathematics*, 1985.
- D. Russo. Simple Bayesian Algorithms for Best Arm Identification, COLT 2016
- N.K. Vaidhyan and R. Sundaresan. Learning to detect an oddball target. arXiv:1508.05572, 2015.