

Selection of the Best System using Large Deviations, and Multi-Arm Bandits

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joint work with Peter Glynn, Stanford

Large Deviations Theory, ICTS

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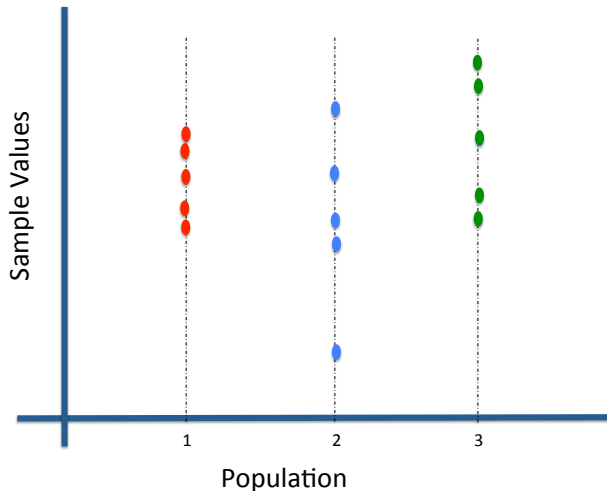
Selection of the Best System

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- ▶ Do not know the underlying distributions but can generate samples from them.
- ▶ Goal is only to identify the population with smallest mean and not to actually estimate the means.
- ▶ For random variables $X(i), i \leq d$, the goal is to identify

$$i^* = \arg \min_{1 \leq j \leq d} EX(j),$$

in minimum number of samples while controlling the probability of false selection.

Determining the smallest mean population: Discrete stochastic optimization



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- ▶ Given a manufacturing system evaluating the best maintenance strategy.
- ▶ Given many medicinal treatments for a given disease, finding the one that causes maximum benefit on average.

Historical review

- ▶ Traditionally, this and related problems studied by statisticians, operations researchers and lately computer scientists. Some names - Bechhofer (54, 58), Rinott 78, Nelson and Goldsman (80's, 90's), Bubeck (2008 +).

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- ▶ Underlying distributions are typically assumed to be Gaussian (asymptotically valid), Bernoulli (verifiable).
- ▶ Underlying analysis relies on the **central limit theorem**

$$\left(\frac{X_1 + \cdots + X_n}{n} - EX_i \right) \frac{\sqrt{n}}{\sigma} \Rightarrow N(0, 1)$$

- Typically, the means are assumed to be separated by $\epsilon > 0$, so that

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- ▶ This talk focusses instead on keeping ϵ fixed and letting $\delta \rightarrow 0$.

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- ▶ Ho et al. (1990) observed that probability of false selection decays at an exponential rate for **light-tailed distributions**.
- ▶ L. Dai (1996) showed using large deviation methods that if

$$EX_1 < \min_{i \geq 2} EX_i$$

then

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log P(\bar{X}_1(n) > \min_{i \geq 2} \bar{X}_i(n)) = -\mathcal{I}$$

for large deviations rate function $\mathcal{I} > 0$.

- Glynn and J (2004) observed that if

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then for $p_i > 0$, $\sum_{i=1}^d p_i = 1$

$$P(\bar{X}_1(p_1 n) > \min_{i \geq 2} \bar{X}_i(p_i n)) \approx e^{-nH(p_1, \dots, p_d)}$$

so that $H(p_1, \dots, p_d)$ can be optimised to determine optimal allocations.

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- ▶ Significant literature since then relying on large deviations analysis.

- ▶ If $P(FS) \leq e^{-n\mathcal{I}}$, for some $\mathcal{I} > 0$, then

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- ▶ However this relies on estimating \mathcal{I} from the samples generated.
- ▶ Even if one could get a lower bound on \mathcal{I} in order $\log(1/\delta)$ samples, correct with probability $1 - \delta/2$, that would work.

Asymptotic HOPE

- ▶ In spirit of earlier CLT based asymptotic analysis, one hopes for algorithms that for $n = O(\log(1/\delta))$ ensure that at least asymptotically $P(FS) \leq \delta$, that is,

$$\limsup_{\delta \rightarrow 0} P(FS)\delta^{-1} \leq 1$$

even when the means are separated by a fixed and known

$\epsilon > 0$. So that

$$\min_{1 \leq i \leq d} EX_i < EX_j - \epsilon$$

for all suboptimal j .

Observations

- ▶ $O(\log(1/\delta))$ effort is necessary. If $\log(1/\delta)^{1-\epsilon}$ samples are generated, then

$$P(X_i \in A)^{\log(1/\delta)^{1-\epsilon}} = \delta^{\frac{\text{positive no.}}{\log(1/\delta)^\epsilon}} \gg \delta$$

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- ▶ $O(\log(1/\delta)^{1+\epsilon})$ is sufficient

$$\delta^{-1}P(FS) \leq \delta^{-1}e^{-n\mathcal{I}} = \delta^{-1}e^{-\log(1/\delta)^{1+\epsilon}\mathcal{I}} = \delta^{\log(1/\delta)^\epsilon\mathcal{I}-1}$$

which goes to zero as $\delta \rightarrow 0$.

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- ▶ We argue through a popular implementation that these rate functions are difficult to estimate accurately using $O(\log(1/\delta))$ samples
- ▶ Enroute, we identify the large deviations rate function of the empirically estimated rate function. This may be of independent interest in these big data times.

Key negative result

- ▶ Given any (ϵ, δ) algorithm - one that correctly separates designs with mean difference at least ϵ with

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- ▶ Given any (ϵ, δ) algorithm - one that correctly separates designs with mean difference at least ϵ with

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- ▶ We prove that for populations (mutually absolutely continuous) with unbounded support and finite mean, the expected number of samples cannot be $O(\log(1/\delta))$.

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- ▶ Under explicitly available moment upper bounds, we develop truncation based $O(\log(1/\delta))$ computation time (ϵ, δ) algorithms.

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- ▶ We also adapt the recently proposed sequential algorithms in multi-armed bandit regret setting to this *pure exploration setting*.

Basic large deviations theory

- ▶ Suppose X_1, X_2, \dots, X_n are i.i.d. samples of X and $a > EX$.

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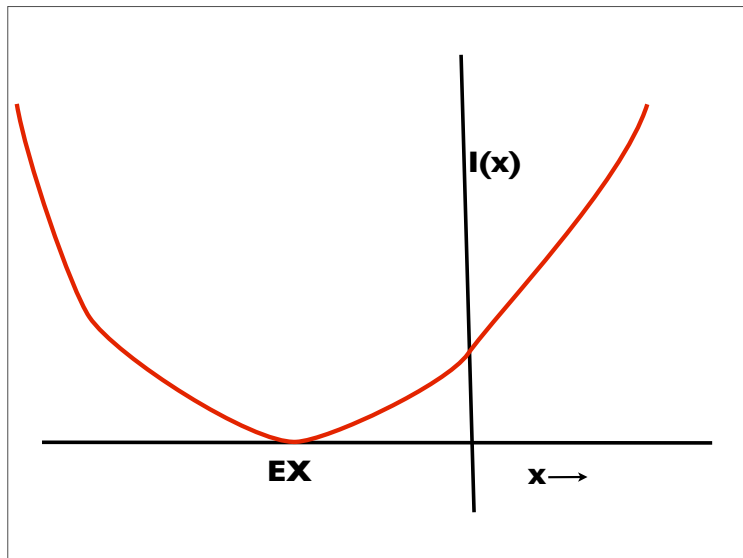
- ▶ Cramer's Theorem

$$P(\bar{X}_n \geq a) = e^{-nI(a)(1+o(1))}$$

where, the large deviations rate function

$$I(a) = \sup_{\theta \in \mathcal{R}} (\theta a - \Lambda(\theta)) .$$

The rate function



A simple setting of $d = 2$

- ▶ Consider a single rv X with unknown mean EX . Need to decide whether $EX > 0$ or $EX < 0$ with error probability $\leq \delta$. Decision based on whether $\bar{X}_n > 0$ or $\bar{X}_n < 0$.

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- ▶ If $EX > 0$, again probability of false selection $P(\bar{X}_n < 0)$ is approximated by

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Two phase implementation

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 - ▶ **Second phase** - Generate

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- ▶ Decide the sign of EX based on whether $\bar{X}_n > 0$ or $\bar{X}_n \leq 0$.

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- ▶ Decide the sign of EX based on whether $\bar{X}_n > 0$ or $\bar{X}_n \leq 0$.
- ▶ We now discuss estimation of $I(0)$.

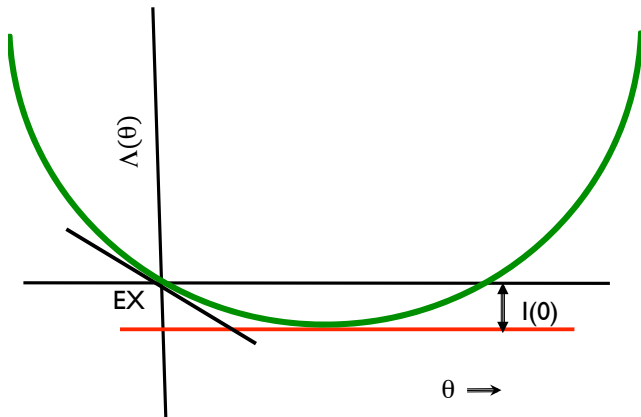
Estimating rate function

Graphic view of $I(0) = -\inf_{\theta} \Lambda(\theta)$

- ▶ The log-moment generating function of X

$$\Lambda(\theta) = \log E \exp(\theta X)$$

is convex with $\Lambda(0) = 0$ and $\Lambda'(0) = EX$.



Estimating rate function $I(0)$

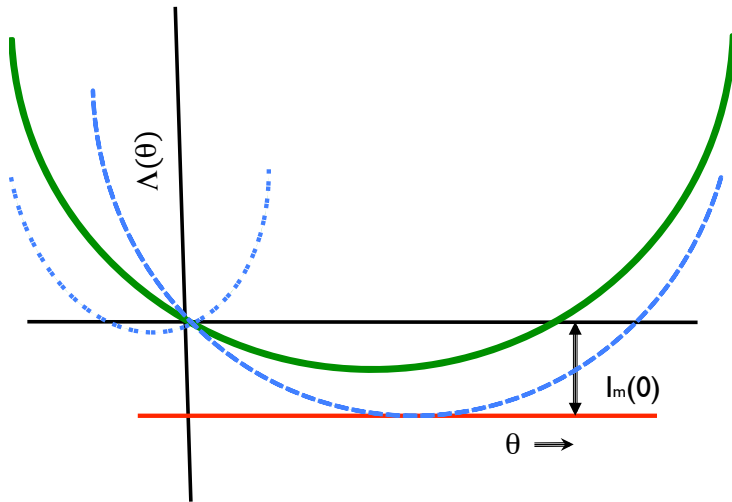
- ▶ A natural estimator for $I(0)$ based on samples $(X_i : 1 \leq i \leq m)$ is

$$\hat{I}_m(0) = - \inf_{\theta \in \mathfrak{R}} \hat{\Lambda}_m(\theta)$$

where

$$\hat{\Lambda}_m(\theta) = \log \left(\frac{1}{m} \sum_{i=1}^m \exp(\theta X_i) \right)$$

Graphic view of estimated log moment generating function



Large deviations rate function of $\hat{I}_m(0)$

► *Theorem:* For $a > I(0)$,

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where

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- Further, for $a < I(0)$,

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Negative Result 1

Failure of the Naive

Returning to two phase procedure

- ▶ We generate samples X_1, \dots, X_m for $m = \log(1/\delta)$ and set

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$$\hat{l}_m(0) = -\inf_{\theta} \hat{\Lambda}_m(\theta).$$

- ▶ Then generate $\log(1/\delta)/\hat{l}_m(0) = m/\hat{l}_m(0)$ samples of X in the second phase.

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$$P(FS) \approx E \exp \left(-\frac{m}{\hat{I}_m(0)} I(0) \right)$$

- ▶ Errors due to large values of $\hat{I}_m(0)$ that lead to under sampling in second phase.

Lower Bound for P(FS)

► *Theorem:*

$$\lim_{m \rightarrow \infty} \frac{1}{m} \log P(FS) = \sup_{a > 0} \sup_{\theta} \left(-\frac{I(0)}{a} - \mathcal{I}_{\theta}(e^{-a}) \right).$$

Lower Bound for $P(\text{FS})$

► *Theorem:*

$$\lim_{m \rightarrow \infty} \frac{1}{m} \log P(\text{FS}) = \sup_{a > 0} \sup_{\theta} \left(-\frac{I(0)}{a} - \mathcal{I}_{\theta}(e^{-a}) \right).$$

► In particular,

$$\liminf_{\delta \rightarrow 0} P(\text{FS})\delta^{-1} > 1.$$

Key Negative Result

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- ▶ Let $\mathcal{P}(\epsilon, \delta)$ denote a policy that can adaptively sample from any two distributions in \mathcal{L} and select one with

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- ▶ **Theorem - For any two such distributions in \mathcal{L} with arbitrarily apart mean, $\mathcal{P}(\epsilon, \delta)$ policy on average requires more than $O(\log(1/\delta))$ samples.**

Details

- ▶ Under probability P_a ,
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- ▶ Under probability P_b
 - ▶ $\{X_i\}$ has distribution F ,
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- ▶ *Theorem:* Under $\mathcal{P}(\epsilon, \delta)$,

$$\liminf_{\delta \rightarrow 0} \frac{E_a T_G}{\log(1/\delta)} \geq \frac{1}{3 \mathcal{KL}(G, \tilde{G})}.$$

where $\mathcal{KL}(G, \tilde{G}) = \int_{x \in \mathfrak{R}} \left(\log \frac{dG}{d\tilde{G}}(x) \right) dG(x)$.

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$$\begin{aligned} P_b(\text{ algo. selects } F) &= E_a \left(\prod_{i=1}^{T_G} \frac{d\tilde{G}}{dG}(Y_i) I(\text{ algo. selects } F) \right) \\ &\approx E_a \left(e^{-T_G \times \mathcal{KL}(G, \tilde{G})} I(\text{ algo. selects } F) \right) \\ &\approx \geq e^{-2E_a(T_G) \times \mathcal{KL}(G, \tilde{G})} P_a(\text{ algo. selects } F) \end{aligned}$$

and the result is easily deduced.

Result

- ▶ Given G with finite mean and unbounded positive support, for any $\epsilon > 0$, and $K > \mu_G$ there exists a distribution \tilde{G} such that

$$\mathcal{KL}(G, \tilde{G}) \leq \epsilon$$

and

$$\mu_{\tilde{G}} \geq K.$$

Way forward

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- ▶ Often upper bounds on moments may be available in simulation models.
- ▶ Use such bounds to develop (ϵ, δ) strategies by truncating random variables while controlling the error to be less than ϵ . Then use Hoeffding's concentration inequality.
- ▶ Recent multi-armed-bandits methods do this in a sequential and adaptive manner.

δ guarantees using $\log(1/\delta)$ samples

$\mathcal{P}(\epsilon, \delta)$ policy for bounded random variables

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- ▶ Hoeffding's inequality can be used to bound probability of false selection. Suppose, $EX < -\epsilon$,

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- ▶ Thus, $n = \frac{(b-a)^2}{2\epsilon^2} \log(1/\delta)$ provides the desired $\mathcal{P}(\epsilon, \delta)$ policy.

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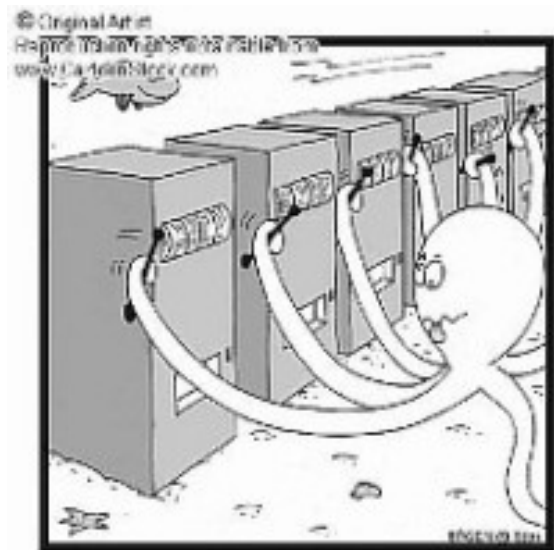
$$\begin{aligned} \max_X E[XI(X \geq u)] \\ \text{such that } Ef(X) \leq a. \end{aligned}$$

- ▶ This has a two point solution relying on observation that

$$Y = E[X|X < u]I(X < u) + E[X|X \geq u]I(X \geq u)$$

is better than X

Pure Exploration Multi-Armed Bandit Approach



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- ▶ Expected computational effort

$$O \left(\sum_{a \neq a^*} \frac{\ln(n/\delta)}{\Delta_a^2} \right).$$

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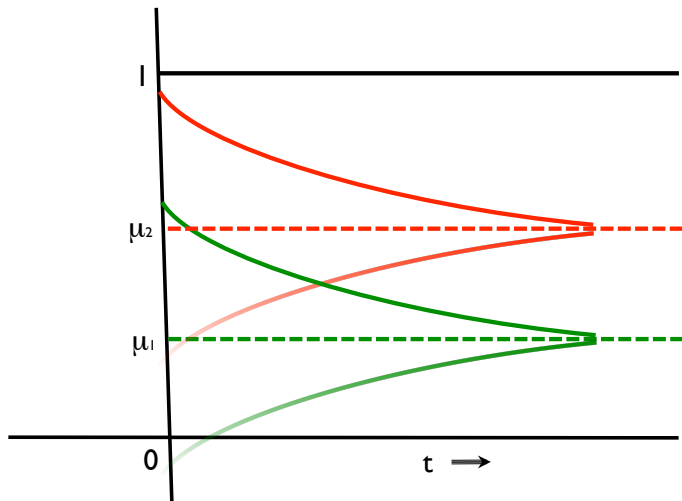
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- ▶ $t = t + 1$; Repeat till one arm left.

Key idea



Generalizing to heavy tails

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- ▶ We adapt these algorithms to pure exploration settings.

In conclusion

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- ▶ Under explicit restrictions on moments of underlying random variables, we devise $O(\log(1/\delta))$ algorithms.
- ▶ These are closely related to evolving multi-arm bandit literature on pure exploration methods.