Guarantees on the Probability of Good Selection

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Selection of the Best

2. Frequentist PGS

3. Bayesian PGS

4. Computation

5. Conclusion
Problem Setting

- Optimize a scalar performance measure over a finite number of alternatives.
- An alternative’s performance is observed with simulation noise.

Examples:

<table>
<thead>
<tr>
<th>Alternatives</th>
<th>Performance Measure</th>
</tr>
</thead>
<tbody>
<tr>
<td>hospital bed allocations</td>
<td>expected blocking costs</td>
</tr>
<tr>
<td>ambulance base locations</td>
<td>expected call response time</td>
</tr>
<tr>
<td>MDP policy</td>
<td>expected discounted total cost</td>
</tr>
</tbody>
</table>

Two alternatives $\rightarrow$ A/B testing.

More than two alternatives $\rightarrow$ ranking and selection and exploratory MAB.
Selection of the Best in Software

E.g., Simio.
## Model

<table>
<thead>
<tr>
<th>Alternative 1</th>
<th>$X_{11}$</th>
<th>$X_{12}$</th>
<th>$\cdots$</th>
<th>i.i.d. $\sim F_1$ with mean $\theta_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alternative 2</td>
<td>$X_{21}$</td>
<td>$X_{22}$</td>
<td>$\cdots$</td>
<td>i.i.d. $\sim F_2$ with mean $\theta_2$</td>
</tr>
<tr>
<td>\vdots</td>
<td>\vdots</td>
<td>\vdots</td>
<td>$\ddots$</td>
<td>\vdots</td>
</tr>
<tr>
<td>Alternative $k$</td>
<td>$X_{k1}$</td>
<td>$X_{k2}$</td>
<td>$\cdots$</td>
<td>i.i.d. $\sim F_k$ with mean $\theta_k$</td>
</tr>
</tbody>
</table>

Observations across alternatives are independent, unless CRN are used.

Marginal distributions $F_i$:

- Ranking and selection (R&S): normal (via batching + CLT)
- Multi-armed bandits: bounded support or sub-Gaussian with known variance bound

The vector $\theta = (\theta_1, \theta_2, \ldots, \theta_k)$ represents the (unknown) problem instance.

- Assume that larger $\theta_i$ is better.
Selection Events

Let $\mathcal{D}$ be the index of the selected alternative.

- **Correct Selection:** "Select one of the best alternatives."

  $\text{CS} := \{ \theta_{\mathcal{D}} = \theta_k \}$.

- **Good Selection:** "Select a $\delta$-good alternative."

  $\text{GS} := \{ \theta_{\mathcal{D}} > \theta_k - \delta \}$.

where $\theta_1 \leq \theta_2 \leq \cdots \leq \theta_k$ are the ordered mean performances.

Here $\delta$ represents the decision-maker’s tolerance toward making a suboptimal selection.

“Close enough is good enough.”
Fixed-Confidence Guarantees

Guarantee that a certain selection event occurs with high probability:

\[ P(\text{GS}) \ (\text{or } P(\text{CS})) \geq 1 - \alpha, \]

where \( 1 - \alpha \) is specified by the decision-maker.

**Guarantee on PGS (PAC Selection)**

\[ \text{W.p. } 1 - \alpha, \text{ Alternative } \mathcal{D} \text{ is within } \delta \text{ of the best.} \]

Probably, Approximately, Correct
Another popular criteria is the expected opportunity cost (EOC)—a.k.a. linear loss.

$$\mathbb{E}[L_{OC}] = \mathbb{E}[\theta[k] - \theta_D].$$

EOC can give a loose upper bound on PGS via Markov’s inequality:

$$\mathbb{P}(GS) = 1 - \mathbb{P}(\theta[k] - \theta_D \geq \delta) \geq 1 - \frac{\mathbb{E}[\theta[k] - \theta_D]}{\delta} = 1 - \frac{\mathbb{E}[L_{OC}]}{\delta}.$$  

- EOC can be harder for a decision-maker to interpret or quantify.  
- EOC is commonly studied under a Bayesian framework.
Selection of the Best

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Indifference-Zone Formulation

Bechhofer (1954) developed the idea of an indifference zone (IZ).

For an IZ parameter $\delta > 0$:

- **Preference Zone**: $PZ(\delta) = \{ \theta : \theta_k - \theta_{k-1} \geq \delta \}$
  
  “The best alternative is at least $\delta$ better than all the others.”

- **Indifference Zone**: $IZ(\delta) = \{ \theta : \theta_k - \theta_{k-1} < \delta \}$
  
  “There are close competitors to the best alternative.”

The parameter $\delta$ is described as the *smallest difference in performance worth detecting*.

- ...but that’s not its role in the IZ formulation.
Space of Configurations

\[ \theta_{[k]} - \theta_{[k-1]} = \delta^* \]

\[ \theta_{[k]} - \theta_{[k-1]} = 0 \]

Nonexistent points

Indifference zone (shaded)
Goals of R&S Procedures

Two Frequentist Guarantees

Specify confidence level $1 - \alpha \in (1/k, 1)$ and $\delta > 0$ and guarantee

$$\mathbb{P}_\theta(\text{CS}) \geq 1 - \alpha \quad \text{for all } \theta \in \text{PZ}(\delta),$$

(Goal PCS-PZ)

$$\mathbb{P}_\theta(\text{GS}) \geq 1 - \alpha \quad \text{for all } \theta.$$  

(Goal PGS)

Goal PGS $\implies$ Goal PCS-PZ.

Goal PCS-PZ is the standard in the frequentist R&S community.
Goal PCS-PZ vs Goal PGS

Issues with Goal PCS-PZ

- Says nothing about a procedure’s performance in $\text{IZ}(\delta)$.
- Configurations in $\text{PZ}(\delta)$ may be unlikely in practice:
  - when there are a large number of alternatives, or
  - when alternatives found by a search.
- Choice of $\delta$ restricts the problem.
- May require making Bayesian assumptions about $\theta$.

Goal PGS has none of these issues!
Proving Goal PGS

Several ways to prove Goal PGS:

1. Lifting Goal PCS-PZ

2. Concentration inequalities

3. Multiple comparisons
Equivalence of Goals PCS-PZ and PGS

“When does Goal PCS-PZ ⇒ Goal PGS?”

**Intuition:** More good alternatives ⇒ more likely to pick a good alternative.

Scattered results since Fabian (1962), but none in the past 20 years.

Show that some R&S procedures delivering Goal PCS-PZ also deliver Goal PGS.
Equivalence Results: Condition 1

**Condition 1 (Guiard 1996)**

For all subsets $A \subset \{1, \ldots, k\}$, the joint distribution of the estimators of $\theta_i$ for $i \in A$ does not depend on $\theta_j$ for all $j \notin A$.

“Changing the mean of an alternative doesn’t change the distribution of the estimators of other alternatives’ means.”

**Limitation:** Can only be applied to procedures without screening.

- Normal (i.i.d.): Bechhofer (1954), Dudewicz and Dalal (1975), Rinott (1978)
- Bernoulli: Sobel and Huyett (1957)
- Support $[a, b]$: Naive Algorithm of Even-Dar et al. (2006)
Equivalence Results: Condition 2

**Condition 2** (Hayter 1994)

For all alternatives \( i = 1, \ldots, k \),

\[
P_\theta(\text{Select Alternative } i)
\]

is nonincreasing in \( \theta_j \) for every \( j \neq i \).

"Improving the mean of an alternative doesn’t help any other alternative get selected."

**Limitation:** Checking the monotonicity of \( P_\theta(\text{Select Alternative } i) \) is hard.
Equivalence Results: Condition 2

Procedure not satisfying Condition 2

1. Take $n_0$ samples of each alternative.
2. Eliminate all but the two alternatives with the highest means.
3. Take $n_1$ additional samples for the two surviving alternatives.
4. Select the surviving alternative with the highest overall mean.

Consider the three-alternative case: $\theta_1 < \theta_2 < \theta_3$.

- Track $P_{\theta}(\text{Select Alternative 2})$ as $\theta_1$ increases up to $\theta_2$.
- Fix $n_0 \geq 1$ and consider $n_1 = 0$ and $n_1 = \infty$ as extreme cases.
Equivalence Results: Condition 3

**Condition 3**

For all alternatives $i = 1, \ldots, k$,

$$\mathbb{P}_\theta(\text{Select some alternative, } j, \text{ for which } \theta_j < \theta_i)$$

is nonincreasing in $\theta_i$.

"Improving the mean of an alternative doesn’t help inferior alternatives get selected."

Condition 2 $\implies$ Condition 3.
Sequential selection procedures screen out (eliminate) inferior systems.

- They are among the most efficient at delivering Goal PCS-PZ.

“Do the procedures of Kim and Nelson (2001) and Frazier (2014) achieve Goal PGS?”

Even if they do, they may be inefficient for problem instances in the IZ.

There may be an opportunity to design more efficient procedures delivering Goal PGS.
Regularity conditions for multi-armed bandits enable the use of confidence inequalities.

- E.g., Hoeffding and Chernoff bounds.

General approach:

1. Bound the probability an estimator differs from its mean value by at least $\delta/2$.
2. Use Bonferroni’s inequality to sum over all alternatives.

The Envelope Procedure of Ma and Henderson (2017) uses confidence bands that hold *throughout the entire procedure*.

- Tracks upper and lower confidence limits for each alternative’s mean performance.
Let $Y_i$ be the estimator of the mean performance $\theta_i$.

Assume that the selected alternative is $D = \arg \max_{i=1,...,k} Y_i$.

**Multiple Comparisons with the Best (MCB)**

$$\mathcal{B} = \{Y_i - Y_{[k]} - (\theta_i - \theta_{[k]}) < \delta, \forall i \neq [k]\}$$

$$\mathbb{P}_\theta(\mathcal{B}) \geq 1 - \alpha \implies \mathbb{P}_\theta\{Y_D - Y_{[k]} - (\theta_D - \theta_{[k]}) < \delta\} \geq 1 - \alpha,$$

$$\implies \mathbb{P}_\theta(\text{GS}) \geq 1 - \alpha.$$

Deriving Goal PGS from MCB results in a *conservative* selection procedure.
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Guarantees on the Probability of Good Selection

Frequentist and Bayesian Frameworks

Different perspectives on what is random and what is fixed.

**Frequentist**

PGS = The probability that the random alternative chosen by the procedure is good for the fixed problem instance.

**Bayesian**

PGS = The *posterior* probability that—given the observed data—the random problem instance is one for which the fixed alternative chosen by the procedure is good.

“How do these guarantees differ on a practical level?”
Design the procedure to satisfy the PGS guarantee for the least favorable configuration (LFC), i.e., the hardest problem instance.

The LFC is often the so-called slippage configuration (SC).

- Fix a best alternative, $j$, and set $\theta_i = \theta_j - \delta$ for all $i \neq j$.

Frequentist procedures are conservative: they often overdeliver on PGS.
Frequentist PGS

**Ex:** Two alternatives with observations $X_{1j} \sim N(\theta_1, \sigma^2)$ and $X_{2j} \sim N(\theta_2, \sigma^2)$ for $j = 1, \ldots, n$ where $\sigma^2$ is known.
Stopping Rule Principle

It is valid to stop and select an alternative whenever its posterior PGS exceeds $1 - \alpha$.

Can use posterior PGS as a stopping rule for a variety of procedures:
- E.g., VIP, OCBA, and TTTS.

Advantages:
- Can repeatedly compute posterior PGS without sacrificing statistical validity.
- Complete flexibility in allocating simulation runs across alternatives.
Bayesian PGS

Ex: Two alternatives with observations $X_{1j} \sim N(\theta_1, \sigma^2)$ and $X_{2j} \sim N(\theta_2, \sigma^2)$ for $j = 1, \ldots, n$ where $\sigma^2$ is known, with a noninformative prior on $\theta_1 - \theta_2$. 

$\theta_1 - \theta_2 \sim N(\overline{X}_1 - \overline{X}_2, 2\sigma^2/n)$
Stop when $|n(\bar{X}_1 - \bar{X}_2)| \geq \sqrt{2n}\sigma \Phi^{-1}(1 - \alpha) - \delta n$. 

Posterior PCS = 1 - $\alpha$
Posterior PGS = 1 - $\alpha$
Interpreting Bayesian Guarantees

A Bayesian PGS guarantee will **NOT** deliver a frequentist guarantee that PGS exceeds \(1 - \alpha\) for all problem instances.

Its guarantee can still be interpreted in a frequentist sense.

1. Draw \(\theta\) from the prior distribution.
2. Run the Bayesian procedure (with the stopping rule) on \(\theta\).

For repeated runs of Steps 1 and 2, the procedure will make a good selection w.p. \(1 - \alpha\).
Experimental Results

The graph illustrates the empirical PGS (probability of good selection) as a function of the true difference in means ($\theta_1 - \theta_2$) for different values of $\delta$. The lines represent:

- $\delta = 0$ (blue)
- $\delta = 0.05$ (magenta)
- $\delta = 0.10$ (cyan)
- $\delta = 0.25$ (green)

The dashed line represents $1 - \alpha$, indicating the threshold for good selection. The empirical PGS values are shown at $\alpha = 0$, $\alpha = 0.05$, $\alpha = 0.10$, and $\alpha = 0.25$. The graph shows that as the true difference in means increases, the empirical PGS also increases, approaching the threshold for $1 - \alpha$. This suggests that Good Selection (GS) is achieved when the empirical PGS is above the threshold for a given $\alpha$. The experimental results support the theoretical guarantees on the probability of Good Selection.
Observations

1. For hard problem instances, procedures with Bayesian PGS guarantees underdeliver on empirical PGS.
   • Gap becomes more pronounced for more tolerant good selection.

2. Hard problems look easier because of a “means-spreading” phenomenon.
   • Similar issues arise in predicting the runtime of a procedure.
Practical Implications

A decision-maker’s preference may depend on the situation:

1. A one-time, critical decision.

2. Repeated problem instances (i.e., using R&S for control).

3. R&S after search, where the problem instance is random.
Selection of the Best

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Computational Considerations

Bayesian procedures with fixed-confidence guarantees pose computational challenges.

1. Checking whether the posterior PGS stopping condition has been met.
2. Calculating or estimating posterior PGS for a given alternative.

Setup:

- Assume that observations are normally distributed and i.i.d.
- Assume a multivariate normal prior with independent beliefs.
- Let $W_i$ denote the (random) mean performance of Alternative $i$.

The posterior distribution of $W = (W_1, \ldots, W_k)$ is a multivariate normal (if variances are known) or a multivariate $t$ (if variances are unknown) distribution.
Computing Posterior PGS

The posterior PGS of Alternative $i$ is

$$p_{\text{PGS}}_i = \mathbb{P}(W_i > W_j - \delta, \text{ for all } j \neq i \mid \mathcal{E}),$$

where $\mathbb{P}(\cdot \mid \mathcal{E})$ is the probability under the posterior of $W$ given the evidence $\mathcal{E}$.

When there are $k$ alternatives, this amounts to a $k$-dimensional integral.

- Becomes intractable for large $k$, unless we condition on $W_i$.

Conditioning on $W_i$ leads to a one-dimensional integral:

$$p_{\text{PGS}}_i = \mathbb{E} \left[ \prod_{j \neq i} \mathbb{P}(W_i > W_j - \delta \mid W_i, \mathcal{E}) \mid \mathcal{E} \right].$$
Slepian’s Bound on Posterior PGS

Slepian’s inequality can be used to get a *cheap* lower bound on posterior PGS.

\[ p_{\text{PGS}}_i = \mathbb{P}(W_i > W_j - \delta, \text{ for all } j \neq i \mid \mathcal{E}) \geq \prod_{j \neq i} \mathbb{P}(W_i > W_j - \delta \mid \mathcal{E}) =: p_{\text{PGS}}_{i}^{\text{Slep}}. \]

Terminate the first time any \( p_{\text{PGS}}_{i}^{\text{Slep}} \) exceeds \( 1 - \alpha \) and select that alternative.

As \( k \) increases, the tightness of Slepian’s bound deteriorates.

- Appears to deteriorate slower for values of PGS close to 1.
- Using it as a stopping condition will lead to longer run-lengths than necessary.
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Extensions: PGS for Continuous Optimization

Embed the R&S problem in a continuous domain $\mathcal{D}$ with objective function $\theta : \mathcal{D} \mapsto \mathbb{R}$.

Assume some structural property of $\theta$, e.g., convex or Lipschitz continuous.

**Goal PGS**

Select a (random) solution $x_\Omega \in \mathcal{D}$ such that

$$\mathbb{P}(\theta(x_\Omega) > \theta(x^*) - \delta) \geq 1 - \alpha,$$

where $x^* \in \arg \max_{x \in \mathcal{D}} \theta(x)$.

See Nesterov and Vial (2008), for example.
Extensions: Good Subset Selection

Instead of selecting a single alternative, return a subset of alternatives, $S$.

Two main purposes:

1. Make a final selection based on secondary performance measures.
2. Use the subset as input to a selection procedure.

Under the frequentist framework, good subset selection is defined as

$$GSS = \{\exists i \in S \text{ s.t. } \theta_i \geq \theta[k] - \delta\}.$$ 

Is this the right definition of a “good” subset?
Extensions: Good Subset Selection

Under the Bayesian framework, good subset selection is defined as

\[ \text{GSS} = \{ \exists i \in S \text{ s.t. } W_i \geq W[k] - \delta \}. \]

Bayesian subset selection can be done at any time.

- Can calculate \( p_{\text{PGSS}}_S \) for any subset \( S \), but it’s computationally expensive.
- Selecting the smallest \( S \) such that \( p_{\text{PGSS}}_S \geq 1 - \alpha \) is challenging.
Acknowledgments

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Equivalence of Goals PCS-PZ and PGS

Key Approach

Pair each $\theta \in \text{IZ}(\delta)$ with a $\theta^* \in \text{PZ}(\delta)$ and show that

$$P_\theta(\text{GS}) \geq P_{\theta^*}(\text{GS}) = P_{\theta^*}(\text{CS}) \geq 1 - \alpha.$$
Constructing $\theta^*$

For an arbitrary configuration $\theta \in \mathbb{I}Z(\delta)$, define subsets

\[ G = \{ i : \theta_i > \theta_k - \delta \} \]  

“good” and

\[ B = \{ i : \theta_i \leq \theta_k - \delta \} \]  

“bad.”

Define the configuration $\theta^*$ by

\[ \theta_i^* = \begin{cases} 
\theta_i & \text{for } i \in B \cup \{k\}, \\
\theta_k - \delta & \text{for } i \in G \setminus \{k\}.
\end{cases} \]
Sketch Proof of Condition 1

Assume ties in estimators $Y_i$ occur with probability zero.

Fix an arbitrary configuration $\theta$ and define $G$, $B$, and $\theta^*$ accordingly.

$$
P_{\theta}(GS) \geq P_{\theta}(Y_k > Y_i \text{ for all } i \in B)
= P_{\theta^*}(Y_k^* > Y_i^* \text{ for all } i \in B)
\geq P_{\theta^*}(Y_k^* > Y_i^* \text{ for all } i \neq k)
= P_{\theta^*}(CS)
\geq 1 - \alpha.

(*) Condition 1 with $A = B \cup \{k\}$. Note that $\theta_i^* = \theta_i$ for all $i \in B$. 

Sketch Proof of Condition 2

Fix an arbitrary configuration $\theta$.
Repeatedly shift the mean performance of the \textit{worst good} alternative down to $\theta_k - \delta$.
Each time, PGS is reduced.

Final result: $\mathbb{P}_\theta(\text{GS}) \geq \mathbb{P}_{\theta^*}(\text{GS})$. 