In many problems, there is a set of items, \( Z \), with underlying structure, and the goal is to find which items are best using a set of noisy probes, \( X \). It is natural that some of these probes are noisier than others.

Drug Discovery: \( Z \subset X \subset \mathbb{R}^d \)

FDA-approved drugs Experimental drugs

How do we adaptively select probes to measure?

Problem Setup

Given: items \( Z \subset \mathbb{R}^d \), probes \( X \subset \mathbb{R}^d \)

Measure: At each time \( t \), observe \( y_t = x_t^T \theta^* + \eta_t \) where

\[ \eta_t \sim N(0, \sigma^2_d) \] and \( \sigma^2_d = x_t^T \Sigma x_t \), and \( \theta^* \in \mathbb{R}^d \) and \( \Sigma \in \mathbb{R}^{d \times d} \) are unknown.

Find: \( z^* = \arg\max_{z \in Z} z^T \theta^* \) or \( Z_a = \{ z \in Z : z^T \theta^* > a \} \) with \( 1 - \delta \) probability.

Problem Intuition

Consider a learner that selects a fixed design \( \{x_1, \ldots, x_T\} \), observes outcomes \( \{y_t\}_{t=1}^T \), and constructs the weighted least squares estimator with known heteroskedastic variances, \( \hat{\theta} \):

\[ \hat{\theta} - \theta^* \sim \mathcal{N}(0, \Gamma^{-1}) \]

Goal: Reduce variance of \( \hat{\theta} \) in the directions most advantageous for identifying \( z^* \) or \( Z_a \).

Benchmark Example: Ignoring heteroskedasticity suffers a multiplicative dependency on \( \kappa = \frac{\max \{\sigma^2_d, \min \{\sigma^2_d\} \}}{\min \{\sigma^2_d\}} \).

Learning Heteroskedastic Variances

Goal: Estimate heteroskedastic variances with error bounds that scale favorably in the problem dimension.

Intuition: After \( \Gamma \) samples, we estimate \( \Sigma \) with \( \hat{\Sigma} \) using an M-estimation approach and decompose the error as

\[ \sigma^2_d - \sigma^2_d = |x^T (\hat{\Sigma} - \Sigma) x| < A + B + C. \]

Controlled by...

\begin{algorithm}[H]
\caption{HEAD (Heteroskedastic Estimation by Adaptive Design)}
\begin{algorithmic}[1]
\State Find \( \hat{\Sigma}_t \)
\State Input: Arms \( X \in \mathbb{R}^d, \Gamma \in \mathbb{N} \)
\State \( 1 \) /Stage 1: Take half the samples to estimate \( \theta^* \)
\State \( 2 \) /Stage 2: Take half the samples to estimate \( \Sigma \) given \( \theta^*_0 \)
\State \( 3 \) Determine \( \lambda^* = \arg\min_{\lambda \geq 0} \mathbb{E}[\text{Var}(x^T \lambda \alpha)] \)
\State \( 4 \) Pull arm \( x \in X \) \( \lceil \Gamma/2 \rceil \) times and collect observations \( \{x_t, y_t\}_{t=1}^{\lceil \Gamma/2 \rceil} \)
\State \( 5 \) Define \( A^b = \sum_{t=1}^{\lceil \Gamma/2 \rceil} x_t^b \) and \( b^* = \sum_{t=1}^{\lceil \Gamma/2 \rceil} y_t \) and estimate \( \theta^b = A^{-b} b^* \)
\State \( 6 \) \( \Sigma = \sum_{x \in X} x x^T \)/Stage 2: Take half the samples to estimate \( \Sigma \) given \( \theta^b_0 \)
\State \( 7 \) Determine \( \lambda^* = \arg\min_{\lambda \geq 0} \mathbb{E}[\text{Var}(x^T \lambda \alpha)] \)
\State \( 8 \) Pull arm \( x \in X \) \( \lceil \Gamma/2 \rceil \) times and collect observations \( \{x_t, y_t\}_{t=1}^{\lceil \Gamma/2 \rceil} \)
\State \( 9 \) Let \( A^b = \sum_{t=1}^{\lceil \Gamma/2 \rceil} x_t^b \) and \( b^* = \sum_{t=1}^{\lceil \Gamma/2 \rceil} y_t \)
\State \( 10 \) Output: \( \text{scale}(\Sigma) = \hat{\Sigma}^{-1} b^* \)
\end{algorithmic}
\end{algorithm}

Theorem 3.1. Assume \( \Gamma = \Omega \left[ \max \left\{ \sigma^2_d \log \left( \frac{1}{\delta} \right), d^2 \right\} \right] \). For any \( x \in X \) and \( \delta \in (0, 1) \), Alg. 1 (HEAD) guarantees the following.

\[ P \left[ \sigma^2_d - \sigma^2_d \leq C_{r, \delta} \right] = 1 - \delta/2 \] and \( C_{r, \delta} = \Theta \left( \frac{(\log(1/\delta))^{1/2} \max \{\sigma^2_d, \min \{\sigma^2_d\} \}}{\delta} \right). \]

Empirical Results

Theorem 4.2. Consider objective, OBJ, of best-arm identification (BAI) or level-set identification (LS). The set returned from Alg. 2 (H-RAGE) achieves OBJ with probability 1 - \( \delta \) at time \( t = \Theta \left( \psi_{\text{UBJ}} \log(D^{-1}) \log \left( \frac{d^2}{\delta} \right) \right) \), where \( \psi_{\text{UBJ}} \) is such that \( \mathbb{E} \left[ \psi_{\text{UBJ}} \right] \geq 2 \log(1/2 \Delta^2) \psi_{\text{UBJ}} \), and \( \Delta \) is the minimum gap for the objective.

Multivariate Testing Simulation Example

We divide an advertisement into natural locations or features, each of which has different content options.