Adaptive Off-Policy Inference for M-Estimators Under Model Misspecification

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Consider the contextual bandit problem

- Suppose features (X_t), actions (A_t), and outcomes (Y_t) are observed sequentially
- At each time step t, the analyst chooses $\mathbb{P}\left(A_t = a \,|\, X_t, \mathscr{H}_{t-1}\right)$ for each a in a finite action space $\mathscr{A}$ given a pooled history $\mathscr{H}_{t-1} = \{(X_i, A_i, Y_i\}_{i=1}^{t-1}$.
- Denoting $Y_t(a)$ as the *potential outcome* had action a been chosen at time step t, we assume that

$$\{(X_t, Y_t(1), \ldots, Y_t(K))\}_{t=1}^{T} \overset{\text{iid}}{\sim} \mathscr{P}$$

- We summarize the joint distribution at time step t z

$$(X_t, A_t, Y_t) \sim p\left(y \,|\, x, a\right) \mathbb{P}\left(A_t = a \,|\, X_t, \mathscr{H}_{t-1}\right) p(x)$$

Even in the well-specified linear case, adaptive data collection can make inference difficult

Suppose that

$$Y_t = \theta^T Z_t + \epsilon_t$$

where

- $Z_t = \phi(X_t, A_t)$ for some feature map $\phi : \mathbb{R}^p \times \mathscr{A} \to \mathbb{R}$
- ϵ_t is a random variable such that $\mathbb{E}[\epsilon_t \,|\, \mathscr{H}_{t-1}] = 0$, $\mathbb{E}[\epsilon_t^2 \,|\, \mathscr{H}_{t-1}] = \sigma^2$

Fact (Lai and Wei, 1982)

A sufficient condition for the OLS estimate $\hat{\theta}$ to be asymptotically normal is for there to exist a sequence of positive definite matrices $\{B_T\}_{T=1}^{\infty}$ such that

$$B_T^{-1} \sum_{t=1}^{T} Z_t Z_t^T \xrightarrow{p} I_d$$

This often will not be satisfied in bandit settings

This condition is often not obtained in bandit problems where the difference in expected rewards across arms is zero

Example

Let $A_t \in \{0,1\}$ with $\mathbb{E}[Y_t | A_t = 1] = \mathbb{E}[Y_t | A_t = 0]$

In this setup, Zhang et al. (2020) demonstrate that the OLS estimator will be **non-Gaussian** when data is collected using standard bandit algorithms such as epsilon-greedy, Thompson sampling, and UCB.

This is a well studied problem in the literature. Some solutions include:

- Estimating $\hat{\theta}$ across batches with the batch size tending to ∞ (Zhang et al., 2020).
- Adding bias correction term when estimating $\hat{\theta}$ (Deshpande et al., 2018; Khamaru et al., 2023)

But all approaches still assume the linear model is true

What can be said for generic M (and Z)- estimators

This is a less studied problem in the literature.

- Zhang et al. (2021) attempt to cover a target parameter that exists only when the conditional mean under the working model is **correctly specified.** That is,

$$\theta^\star = \text{argmax}_{\theta\in\Theta}\mathbb{E}\left[m_\theta(X_t, A_t, Y_t) \,|\, A_t, X_t\right] \text{ for all } A_t \in \mathscr{A}, X_t \in \mathbb{R}\,.$$

- In a parallel work to our own, Guo and Xu (2025) cover separate $\{\theta_a^\star\}_{a\in\mathscr{A}}$ that solve for the roots

$$0 = \mathbb{E}\left[m_{\theta_a^\star}(X_t, Y_t(a))\right] \text{ for all } t \in [T]$$

Their work does allow for **model misspecification**, but:

- Assumes that the policy $\mathbb{P}(A_t = a \,|\, X_t, \mathscr{H}_{t-1})$ converges to a deterministic function independent of history.
- Does not allow for a model with a lower-dimensional $\theta^\star$ that is defined *across* actions.

What target makes sense under misspecification?

Our Choice: $\theta^\star := \text{argmax}_{\theta \in \Theta} \mathbb{E}_{\mathscr{P}, A \sim \pi_e} \left[m_\theta(X, A, Y) \right]$

The evaluation policy $\pi_e(a|\text{x})$ is a choice of density that is independent of history.

If the policy converges, letting
$\pi_e(A_t = a \,|\, X_t) := \lim_{t \to \infty} \mathbb{P}(A_t = a \,|\, X_t, \mathscr{H}_{t-1})$ is perfectly sensible.

If the policy does not converge (e.g. multi-armed bandits when expected rewards across arms is comparable), it an **interpretative choice**. Some examples:

- Uniform over the action space;
- Weighting certain actions based on prior assumptions about efficacy'
- Using some known deployment policy.

Choice of evaluation policy is crucial for model interpretation when it is misspecified

Assume $Y_t \sim N(6A_t^2, 1)$ but we erroneously assume a linear model

- Policy 1: $p_e(a \mid x)$ is uniform over $\{0, 0.1, 0.2, 0.3, 0.4, 0.5\}$
- Policy 2: $p_e(a \mid x)$ is uniform over $\{0.6, 0.7, 0.8, 0.9, 1.0\}$

Correct Specification

Let $m_\theta = (Y_t - \theta_0 - \theta_1 A_t^2)^2$

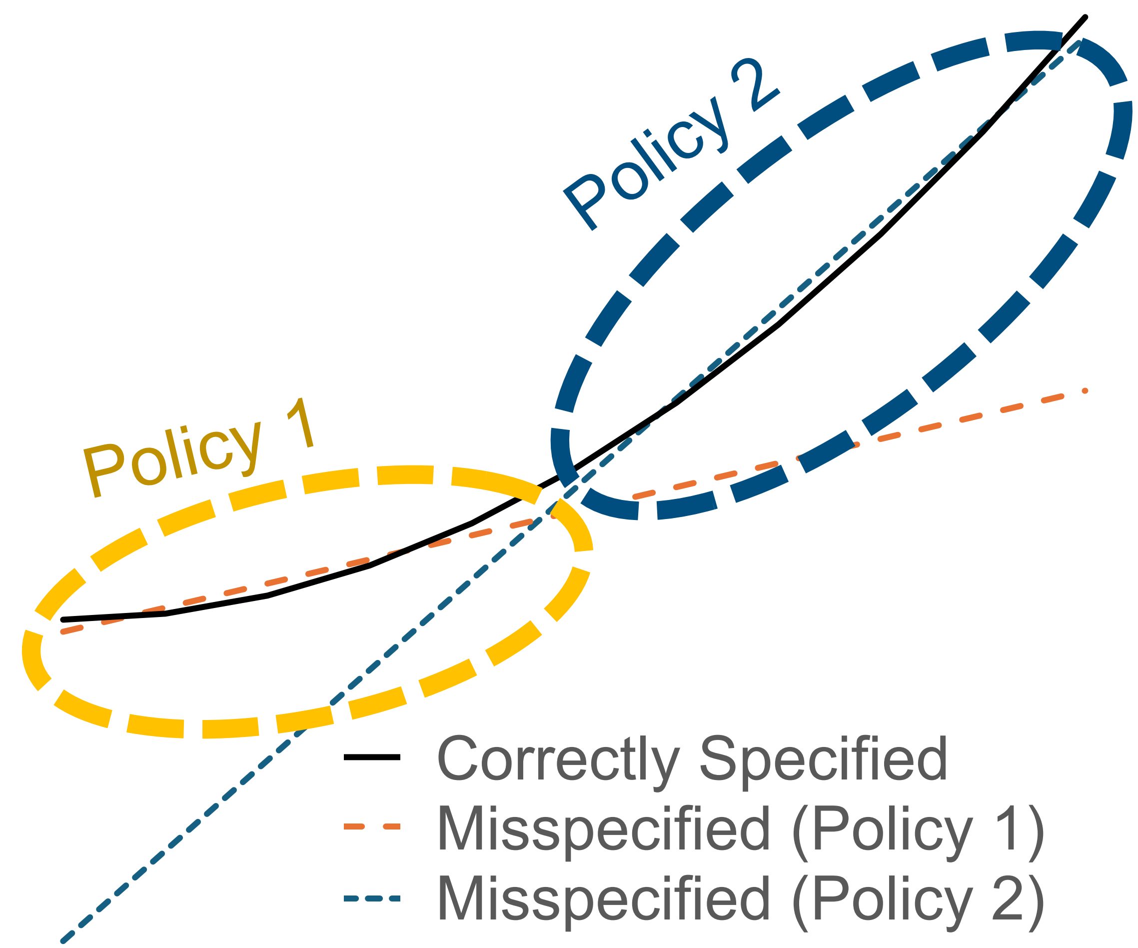
$\theta_0^\star = 0$ and $\theta_1^\star = 6$ under both policies

Misspecification

Let $m_\theta = (Y_t - \theta_0 - \theta_1 A_t)^2$

Policy 1: $\theta_0^\star = -0.2$ ***and*** $\theta_1^\star = 4$

Policy 2: $\theta_0^\star = -5.3$ ***and*** $\theta_1^\star = 15$



Let us first consider a naive estimator

Let us consider $\hat{\theta}_0 := \text{argmax}_\theta \sum_{t=1}^{T} w_t m_\theta(X_t, A_t, Y_t)$.

Assume that $\hat{\theta}_0$ corresponds to the solution to the estimating equation

$$0 = \sum_{t=1}^{T} w_t \dot{m}_\theta m_\theta(X_t, A_t, Y_t)$$

Assume $\theta^\star$ corresponds to the root of $0 = \mathbb{E}_{A\sim\pi_e}\left[\dot{m}_\theta(X, A, Y)\right]$

Generic Strategy

1. Show $\frac{1}{\sqrt{T}} \sum_{t=1}^{T} w_t \dot{m}_{t,\theta^\star}(X_t, A_t, Y_t) \xrightarrow{d} N(0, I_d)$ using martingale CLT
2. Taylor expand around this quantity to form a confidence ellipsoid center at $\theta^\star$
3. Prove $\hat{\theta}_0 \xrightarrow{p} \theta^\star$ to allow for plug-ins

Proving a martingale CLT is non-trivial in the misspecified, adaptive setting

Desiderata: $\frac{1}{\sqrt{T}} \sum_{t=1}^{T} w_t \dot{m}_{t,\theta^\star}(X_t, A_t, Y_t) \xrightarrow{d} N(0, I_d)$

We need to check that for any fixed $c \in \mathbb{R}^d$ and $\epsilon > 0$

1. **Martingale Difference Sequence**

   For $t \in [T]$, $\mathbb{E}\left[w_t \dot{m}_{\theta^\star}(X_t, A_t, Y_t) \mid \mathscr{H}_{t-1}\right] = 0$

2. **Conditional Variance Converges**

   $$\frac{1}{T} \sum_{t=1}^{T} \mathbb{E}\left[c^T w_t^2 \dot{m}_{\theta^\star}(X, A, Y) \dot{m}_{\theta^\star}(X_t, A_t, Y_t)^T c \mid \mathscr{H}_{t-1}\right] \xrightarrow{p} \sigma_c^2$$

   for some fixed σ_c^2

3. **Asymptotic Negligibility**

   $$\frac{1}{T} \sum_{t=1}^{T} \mathbb{E}\left[c^T w_t^2 \dot{m}_{\theta^\star}(X, A, Y) \dot{m}_{\theta^\star}(X, A, Y)^T c 1_{|w_t \dot{m}_{\theta^\star}(X,A,Y) > \epsilon|} \mid \mathscr{H}_{t-1}\right] \xrightarrow{p} 0$$

Both conditions tend to fail under misspecification + adaptivity

Controlling the first moment requires inverse propensity weighting

Assume that $w_t \in \sigma(\mathscr{H}_{t-1}, X_t)$

$$\mathbb{E}\left[w_t \dot{m}_{\theta^\star}(X_t, A_t, Y_t) \mid \mathscr{H}_{t-1}\right] = \mathbb{E}\left[\mathbb{E}\left[w_t \dot{m}_{\theta^\star}(X_t, A_t, Y_t) \mid X_t, A_t, \mathscr{H}_{t-1}\right] \mid \mathscr{H}_{t-1}\right]$$

$$= \mathbb{E}\left[w_t \mathbb{E}\left[\dot{m}_{\theta^\star}(X_t, A_t, Y_t) \mid X_t, A_t\right] \mid \mathscr{H}_{t-1}\right]$$

(but $\mathbb{E}\left[\dot{m}_{\theta^\star}(X_t, A_t, Y_t) \mid X_t, A_t\right] = 0$ under correct specification)

So $\mathbb{E}\left[w_t \dot{m}_{\theta^\star}(X_t, A_t, Y_t) \mid \mathscr{H}_{t-1}\right] = 0$ for all $w_t \in \sigma(\mathscr{H}_{t-1}, X_t)$ when model is **correctly specified**

If the **model is misspecified**, pick $w_t = \dfrac{p_e(A_t = a \mid X_t)}{\mathbb{P}\left(A_t = a \mid \mathscr{H}_{t-1}, X_t\right)}$. Then,

$$\mathbb{E}\left[\mathbb{E}\left[\frac{p_e(A_t = a \mid X_t)}{\mathbb{P}\left(A_t = a \mid \mathscr{H}_{t-1}, X_t\right)} \dot{m}_{\theta^\star}(X_t, A_t, Y_t) \mid X_t, A_t, \mathscr{H}_{t-1}\right] \mid \mathscr{H}_{t-1}\right] = \mathbb{E}_{A_t \sim \pi_e}\left[\dot{m}_{\theta^\star}(X_t, A_t, Y_t)\right]$$

$$= 0$$

Controlling the second moment requires square root IPW-weighting

On the other hand, $\mathbb{E}\left[w_t^2 \dot{m}_{\theta^\star}(X,A,Y)\dot{m}_{\theta^\star}(X_t,A_t,Y_t)^T \,|\, \mathscr{H}_{t-1}\right]$ may also be quite unstable in bandit settings under a **non-converging** policy.

If w_t has **not already been used** to control the first moment, we can simply let $w_t = \left(\frac{p_e(A_t = a \,|\, X_t)}{\mathbb{P}\left(A_t = a \,|\, \mathscr{H}_{t-1}, X_t\right)}\right)^{1/2}$ (Zhang et al., 2021).

$$
\begin{aligned}
\frac{1}{T}\sum_{t=1}^{T}\mathbb{E}\left[w_t^2 \dot{m}_{\theta^\star}(X,A,Y)\dot{m}_{\theta^\star}(X_t,A_t,Y_t)^T \,|\, \mathscr{H}_{t-1}\right] &= \frac{1}{T}\sum_{t=1}^{T}\mathbb{E}\left[\frac{p_e(A_t = a \,|\, X_t)}{\mathbb{P}\left(A_t = a \,|\, \mathscr{H}_{t-1}, X_t\right)}\dot{m}_{\theta^\star}(X,A,Y)\dot{m}_{\theta^\star}(X_t,A_t,Y_t)^T \,|\, \mathscr{H}_{t-1}\right] \\
&= \frac{1}{T}\sum_{t=1}^{T}\mathbb{E}_{A_t\sim\pi_e}\left[\dot{m}_{\theta^\star}(X,A,Y)\dot{m}_{\theta^\star}(X_t,A_t,Y_t)^T\right] \\
&= \mathbb{E}_{A_t\sim\pi_e}\left[\dot{m}_{\theta^\star}(X,A,Y)\dot{m}_{\theta^\star}(X_t,A_t,Y_t)^T\right]
\end{aligned}
$$

… but this is only a tractable strategy under correct specification.

Controlling the first two moments simultaneously requires additional free parameters

Consider nested filtrations

$$\sigma(\mathscr{H}_{t-1}) \subseteq \sigma(\mathscr{H}_{t-1}, X_t) \subseteq \sigma(\mathscr{H}_{t-1}, X_t, A_t) \subseteq \sigma(\mathscr{H}_{t-1})$$

Choose $\Sigma_t \in \sigma(\mathscr{H}_{t-1})$ to **stabilize the variance**

Choose $w_t \in \sigma(X_t, \mathscr{H}_{t-1})$ to **ensure the score function is a MDS** (i.e. control first moment)

This is a viable strategy if we can estimate the time-varying variance well

Let $w_t = \dfrac{p_e(A_t = a \mid X_t)}{\mathbb{P}\left(A_t = a \mid \mathscr{H}_{t-1}, X_t\right)}$

Let Σ_t be an estimate of $\mathbb{E}\left[s_{t,\theta^\star} s_{t,\theta^\star}^T \mid \mathscr{H}_{t-1}\right]$ for $s_{t,\theta} := w_t \dot{m}_{\theta^\star}(X_t, A_t, Y_t)$

Checking first condition…

$$\begin{aligned}
\mathbb{E}[\Sigma_t^{-1/2} s_{t,\theta^\star} \mid \mathscr{H}_{t-1}] &= \Sigma_t^{-1/2}\mathbb{E}[s_{t,\theta^\star} \mid \mathscr{H}_{t-1}] \\
&= \Sigma_t^{-1/2}\mathbb{E}\left[\mathbb{E}\left[w_t \dot{m}_{\theta^\star}(X_t, A_t, Y_t) \mid X_t, A_t, \mathscr{H}_{t-1}\right] \mathscr{H}_{t-1}\right] \\
&= \Sigma_t^{-1/2}\mathbb{E}_{A_t \sim \pi_e}\left[\dot{m}_{\theta^\star}(X_t, A_t, Y_t)\right] \\
&= 0
\end{aligned}$$

Checking second condition…

$$\begin{aligned}
\frac{1}{T}\sum_{t=1}^{T}\mathbb{E}[\Sigma_t^{-1/2} s_{t,\theta^\star} s_{t,\theta^\star}^T \Sigma_t^{-1/2} \mid \mathscr{H}_{t-1}] &= \frac{1}{T}\sum_{t=1}^{T}\Sigma_t^{-1/2}\mathbb{E}[s_{t,\theta^\star} s_{t,\theta^\star}^T \mid \mathscr{H}_{t-1}]\Sigma_t^{-1/2} \\
&\approx \frac{1}{T}\sum_{t=1}^{T}\Sigma_t^{-1/2}\Sigma_t\Sigma_t^{-1/2} \\
&\approx I_d
\end{aligned}$$

(assuming sufficiently good estimate…)

Our final estimator also allows for the use of flexible ML to reduce variance further

We define the MAIPWM (misspecified augmented inverse propensity weighted M-) estimator as

$$\tilde{\theta}_T = \text{argmax}_{\theta \in \Theta} \sum_{t=1}^{T} \sum_{a=1}^{K} \pi_e(A_t = a \mid X_t) \left(m_\theta(a, X_t, f_t(a, X_t)) + 1_{A_t = a} \frac{m_\theta(A_t, X_t, Y_t) - m_\theta(X_t, A_t, f_t(X_t, A_t))}{\mathbb{P}\left(A_t = a \mid X_t, \mathcal{H}_{t-1}\right)} \right).$$

where $f_t : \mathbb{R} \times \mathcal{A}$ is trained only on $\mathcal{H}_{t-1}$ and targets conditional mean $\mathbb{E}\left[Y_t \mid X_t, A_t\right]$.

- If f_t is accurate, we empirically find a significant reduction in the variance of the estimator.
- If no predictive model is available, letting $f_t = c$ for any constant reduces the estimate to $\hat{\theta}_0$.
- Similar constructions are commonly used when targeting ATE (Hadad but M-estimators is a more recent application of the idea (Zrnic and Candes, 2024).

Note: it is not required to train f_t for our results to hold, but we do find a significant reduction in variance empirically.

We prove a CLT assuming that the time-varying variance can be approximated well

Key Assumptions:

1. $V_{t,\theta^\star} := \mathbb{E}_{\mathcal{P},\pi_t}\left[s_{t,\theta^\star}s_{t,\theta^\star}^T \,|\, \mathcal{H}_{t-1}\right]$ is almost surely invertible for each $t \in [T]$.
2. There exists a sequence of estimators $\{\hat{V}_t\}_{t=1}^T$ adapted to the filtration $\sigma(\mathcal{H}_{t-1})$ such that $||\hat{V}_t^{-1/2} - V_{t,\theta^\star}^{-1/2}||_{\text{op}} \xrightarrow{p} 0$.
3. There exists a constant C such that $\frac{p_e(A_t = a \,|\, X_t)}{\mathbb{P}\left(A_t = a \,|\, \mathcal{H}_{t-1}, X_t\right)} < C$

Theorem (simplified)

Assume $\frac{1}{T}\sum_{t=1}^{T} \hat{V}_t^{-1/2} s_{t,\hat{\theta}_T} = o_p(1/\sqrt{T})$ and the eigenvalues of both $V_{t,\theta^\star}$ and $\hat{V}_t$ are bounded above and below. Then under appropriate regularity conditions (e.g. bracketing entropy, well-separated solutions):

$$\frac{1}{\sqrt{T}}\sum_{t=1}^{T} \hat{V}_t^{-1/2} \dot{s}_{t,\hat{\theta}_T}\left(\hat{\theta}_T - \theta^\star\right) \xrightarrow{d} N(0, I_d)$$

How do we estimate $\hat{V}_t^{-1/2}$?

We can use the law of total variance to decompose $V_{t,\theta^\star}$ into pieces that are either **invariant to history** or **known by the experimenter.**

$$\mathrm{Var}(s_{t,\theta^\star} \mid \mathcal{H}_{t-1}) = \mathrm{Var}\Big(\mathbb{E}_{A_t\sim\pi_e}\left[\dot{m}_{\theta^\star}(X_t, A_t, Y_t) \mid X_t\right]\Big) + \mathbb{E}\left[\sum_{a=1}^{K} \frac{\pi_e(a \mid X_t)^2}{\pi_t(a|X_t)} \mathbb{E}[\dot{m}_{\theta^\star}(X_t, a, Y_t(a))\dot{m}_{\theta^\star}(X_t, a, Y_t(a))^T \mid X_t] \mid \mathcal{H}_{t-1}\right] - \mathbb{E}\left[\mathbb{E}_{A_t\sim\pi_e}\left[\dot{m}_{\theta^\star}(X_t, A_t, Y_t) \mid X_t\right] \mathbb{E}_{A_t\sim\pi_e}\left[\dot{m}_{\theta^\star}(X_t, A_t, Y_t) \mid X_t\right]^T\right].$$

Assumption: We have access to an external dataset $\{\tilde{X}_i\}_{i=1}^n$, independent of $\mathscr{H}_{t-1}$ such that $\tilde{X}_i \overset{\text{iid}}{\sim} p(x)$.

(alternatively can use sequential sample splitting)

Strategy (simplified):

- Learn model $f_t : \mathbb{R}^p \times \mathscr{A} \to \mathbb{R}^d$ s.t. $f_t(a, X_t) - \mathbb{E}\left[\dot{m}_{\theta^\star}(X_t, A_t, Y_t) \,|\, X_t, A_t = a\right] \xrightarrow{p} 0$
- Learn model $g_t : \mathbb{R} \times \mathscr{A} \to \mathbb{R}^{d\times d}$ s.t. $e_t(a, X_t) - \mathbb{E}\left[\dot{m}_\theta^\star(a, X_t, Y_t(a))\dot{m}_\theta^\star(a, X_t, Y_t(a))^T \,|\, X_t\right] \xrightarrow{p} 0$
- Plug external data into these models to estimate $\mathrm{Var}\left(s_{t,\theta^\star} \,|\, \mathscr{H}_{t-1}\right)$

Results

We test the methodology with semi-synthetic datasets

- The Osteoarthritis Initiative (OAI) is a ten year longitudinal study tracking long-term outcomes of patients with osteoarthritis.
  - Y_t is the four year change in KL grade (measure of knee health)
  - X_t includes baseline measurements of knee health, demographic variables, baseline health risk factors
  - A_t is not available (observational study), so we create semi-synthetic dataset

Create semi-synthetic dataset

- We use random forests to train a model $f(X_t)$ estimating $\mathbb{E}\left[Y_t \mid X_t\right]$
- For user-chosen parameters $\{\beta_1^a\}_{a\in\mathscr{A}}$ and $\{\beta_2^a\}_{a\in\mathscr{A}}$, we generate semi-synthetic outcomes where

$$\mathbb{E}[Y_t \mid X_t, A_t] = \sum_{a=1}^{K} \beta_1^a 1_{A_t=a} + \sum_{a=1}^{K} \beta_2^a f(X_t) \times 1_{A_t=a}$$

Estimators and sampling strategies

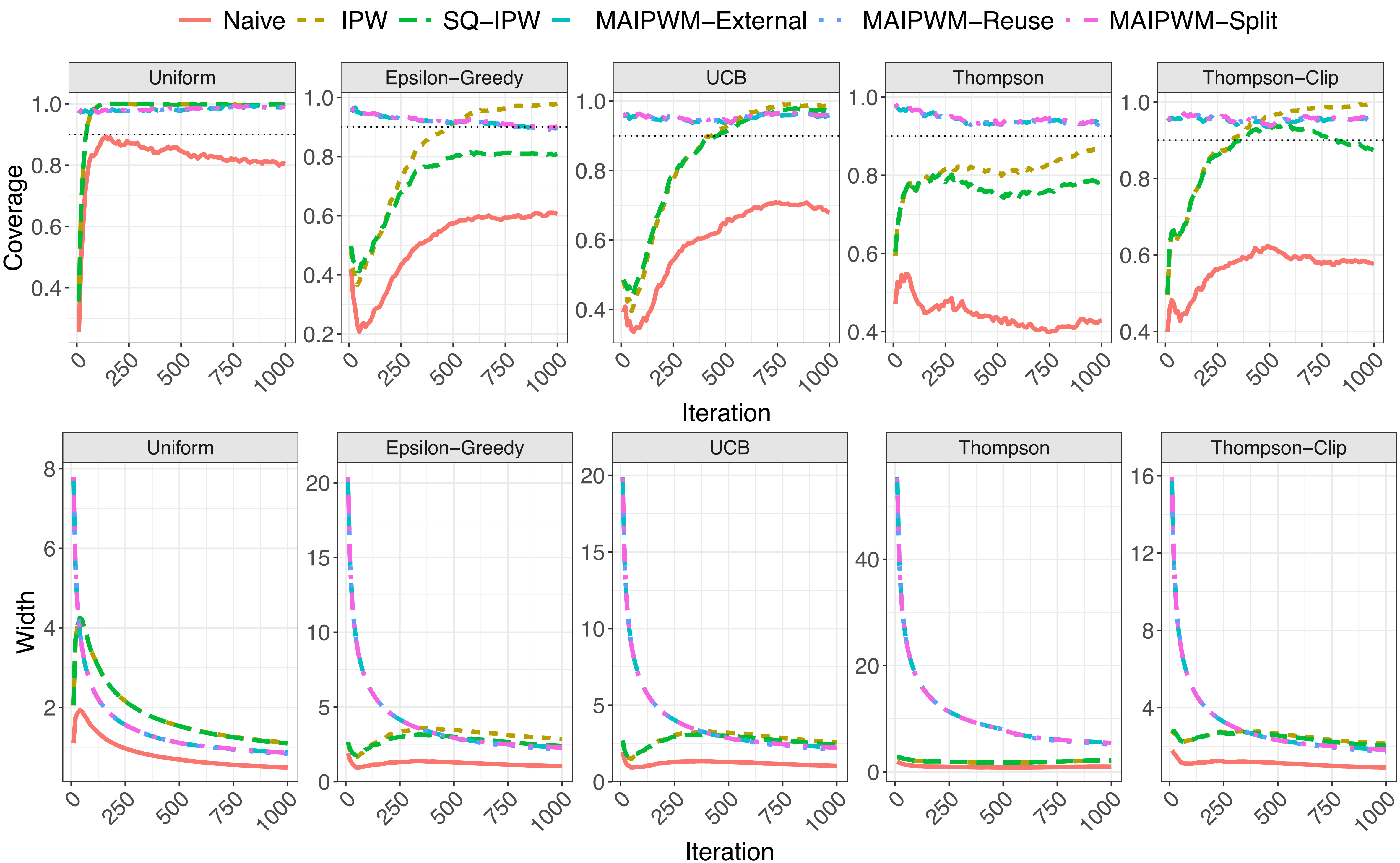
We test the methodology using uniform (i.e. non-adaptive), epsilon-greedy, UCB, and Thompsons sampling.

- We also experiment with clipping the probabilities in the interval $[0.05, 0.95]$

Estimators tested:

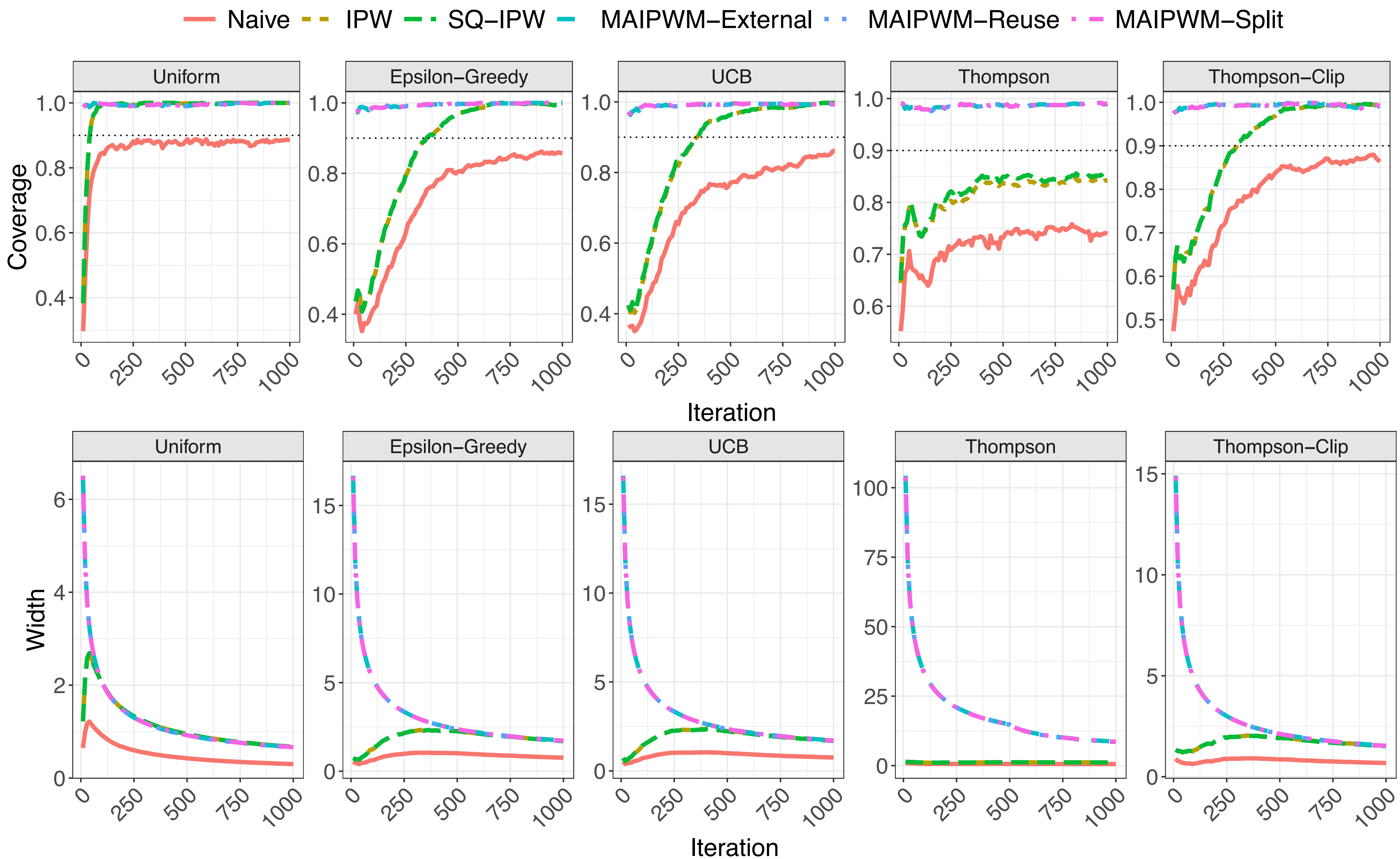
- Naive estimator with $w_t = 1$
- IPW estimator
- Square-root IPW estimator
- MAIPW estimators. We experiment with estimating $\hat{V}_t$ using:
    - External dataset independent of $\mathscr{H}_{t-1}$
    - Sequential sample splitting
    - Reusing $\mathscr{H}_{t-1}$ to estimate the variance *(no theoretical guarantees)*

Misspecified Case



$\beta_1 = (0,0,1,2,2,3,4,4)$ $\quad \beta_2 = (1,-1,1,0,-3,1,1,1)$

Correctly Specified Case



$\beta_1 = (0,1,2,3,4,5,6,7) \quad \beta_2 = (0,0,0,0,0,0,0,0)$

Thank you!