Optimal Experimental Design for Staggered Rollouts

Ruoxuan Xiong, Susan Athey, Mohsen Bayati, Guido Imbens

Emory University and Stanford University
Introduction
Designing experiments with staggered rollouts

- Estimating treatment effects in panel data with **staggered rollouts**
  - Units $i \in \{1, \cdots, N\}$ observed in time periods $s \in \{1, \cdots, T\}$
  - Design: Treatment assignment $Z_{is} \in \{0, 1\}$
  - Potential outcomes: $Y_{is}(z_{i,s-\ell}, \cdots, z_{is})$ may depend on the history of treatment to date, with known $\ell$ periods of history that matter
  - Observed outcomes: $Y_{is} = Y_{is}(Z_{i,s-\ell}, \cdots, Z_{is})$

- Staggered rollout designs commonly encountered in observational data:
  - Products/promotions released in different regions at different times
  - State regulations adopted over time

- **Question:** How should analyst **design** a staggered rollout experiment?
  - How fast should rollout occur?
  - How does rollout depend on hypothesized maximum duration of carryover effects?
  - How can historical data be used to optimize design?
  - Can an **adaptive design**, where analyst updates speed of rollout and termination based on data collected during experiment, improve performance?
Panel experiments with staggered rollouts

Formal objective: Propose experimental designs that optimize the precision of post-experiment estimates of treatment effects

Focus on environment with: Irreversible treatment adoption pattern \((Z_{is} \leq Z_{i,s+1})\)

| Time  | SF  | 1 | 1 | 1 | \(\ldots\) | \(\ldots\) |
|-------|-----|---|---|---|----------|----------|
| BOS   | 0   | 1 | 1 | \(\ldots\) | \(\ldots\) |
| ATL   | 0   | 0 | 1 | \(\ldots\) | \(\ldots\) |
|       | \(\vdots\) | \(\vdots\) | \(\vdots\) | \(\vdots\) | \(\vdots\) | \(\vdots\) |

0 denotes control and 1 denotes treated
Contribution: Non-adaptive experiments

Non-adaptive experiments: $N$ and $T$ are set, and treatment decisions are made, pre-experiment

- Assume after experiment will use GLS to estimate instantaneous and lagged treatment effects from nonstationary observed outcomes
- Analytical optimality conditions for the designs that maximize linearly combined precisions of estimated instantaneous and lagged effects
- Propose an algorithm to choose a treatment design based on the optimality conditions. The design has two features
  \(\Rightarrow\) Fraction of treated units per period takes an $S$-shaped curve: Treatment rollouts slowly at the beginning and end, and quickly in the middle
  - Bigger $\ell$ leads to more pronounced $S$
  \(\Rightarrow\) This rollout pattern is imposed for each stratum of units with the same observed and estimated latent covariate values
Illustration of optimal assignment
Adaptive experiments: $N$ is fixed, but the experiment can be terminated early. Treatment decisions are updated after each period’s data is collected.

- Propose the Precision-Guided Adaptive Experiment (PGAE) algorithm
  - adaptively terminates the experiment based on the estimated precision
  - adaptively optimizes speed of rollout using dynamic programming
  - an estimation scheme of treatment effects based on sample splitting
- Derive the asymptotic normal distribution of final treatment effect and variance estimates from PGAE
  - Optimal convergence rate and no efficiency loss of final treatment effect estimate, as compared to an oracle with access to the same design a-priori
Related literature (partial list)

- Most closely related to stepped wedge designs in clinical trials (Hussey and Hughes 2007, Hemming et al. 2015, Li, Turner, and Preisser 2018)
  ⇒ We study the design under a more general outcome specification, where cumulative effects can vary with treatment duration
- Recently proposed alternative designs for estimation of carryover effects
  - Minimax temporal experimental design (Basse, Ding, and Toulis 2019)
  - Switchback design (Bojinov, Simchi-Levi, and Zhao 2020)
  - Synthetic control design that selects units for (simultaneous) treatment, anticipating synthetic control estimation (Doudchenko et al. 2021a,b, Abadie and Zhao 2021)
  ⇒ Our design leverages variation of treatment times across units and maximizes the precision of treatment effect estimates
- Recently proposed designs in settings with interference
  - Multiple randomization designs (Bajari et al. 2021, Johari et al. 2022)
  - Equilibrium designs (Wager and Xu 2021)
  ⇒ Our experiment is run at the aggregate level and leverages the time dimension to increase power
⇒ We also consider adaptive designs; above papers pre-specify design
Two examples for staggered rollout experiments

**Example 1** *(marketplace experiments)*: A ride-hailing platform plans to test the impact of a *new app feature* that improves *driver experience*

**Example 2** *(public health intervention)*: A country aims to measure the effect of a *new public health intervention* (e.g., encouraging the use of masks or social distancing policies) on the *spread of an infectious disease*

**Staggered rollout experiments** run at the city level for multiple time periods can

- avoid bias from interference
- facilitate the estimation of cumulative effects
- better *design* can *improve* the estimation *precision* of cumulative effects
Setup
Potential outcomes and treatment effects

- **The potential outcomes** for unit $i$ at time $s$ can be written as
  \[ Y_{is}(z_{i,s-\ell}, \cdots, z_{i,s-1}, z_{is}) \]
  for a nonnegative, known integer $\ell$ ($\ell$: duration of treatment effects)

- Let the average instantaneous effect $\tau_0$ and $j$-th period lagged effect $\tau_j$ be
  \[ \tau_j := \frac{1}{N_T} \sum_{i,s} \left[ Y_{is}(0, \cdots, 0, 1, \cdots, 1) - Y_{is}(0, \cdots, 0, 0, 1, \cdots, 1) \right], \]
  for all $j \in \{0, 1, \cdots, \ell\}$

- Let the average cumulative effect of treatment for $j$ periods be
  \[ \tau_0 + \cdots + \tau_{\min(\ell, j-1)} \]
  that is constant for $j > \ell$
Illustrative examples of cumulative effects

Cumulative effect of treatment for $j$ periods with $\ell = 5$, $\tau_0, \tau_1 > 0$ and $\tau_2, \tau_3, \tau_4, \tau_5 < 0$
Cumulative effect of treatment for $j$ periods with $\ell = 2$ and $\tau_0, \tau_1, \tau_2 < 0$
A general outcome specification for treatment effect estimation post-experiment

\[ Y_{is} = \alpha_i + \beta_s + X_i^T \theta_s + \tau_0 Z_{is} + \tau_1 Z_{i,s-1} + \cdots + \tau_\ell Z_{i,s-\ell} + \underbrace{u_i^T v_s + \varepsilon_{is}}_{e_{is}} \]

- \( \alpha_i \): unknown unit fixed effect
- \( \beta_s \): unknown time fixed effect
- \( X_i \): observed covariates; \( \theta_s \): unknown time-varying coefficients
- \( u_i \): latent covariates; \( v_s \): latent coefficients
- \( \varepsilon_{is} \): iid residual with mean 0 and variance \( \sigma^2 \)
**Decision making problem**

**Decision:** Optimally choose the treatment times for each unit

**Goal:** Most precisely estimate average instantaneous and lagged effects

**Implication:** Reduce sample size requirement and lower the experimental cost!

|   | SF | BOS | ATL |
|---|----|-----|-----|
| 0 | 1  | 0   | 0   |
| 1 | 1  | 1   | 0   |
| 1 | 1  | 1   | 0   |

0 denotes control and 1 denotes treated

\[
Z_{ff}?, \quad Z_{ba}?, \quad Z_{ffba}?
\]
Non-adaptive experiments
GLS estimator $\hat{\tau}_0, \cdots, \hat{\tau}_\ell$ from the specification

$$Y_{is} = \alpha_i + \beta_s + X_i^T \theta_s + \tau_0 z_{is} + \tau_1 z_{i,s-1} + \cdots + \tau_\ell z_{i,s-\ell} + e_{is},$$

- GLS is the best linear unbiased estimator (BLUE)
- Precision matrix (inverse of variance-covariance matrix) of $\hat{\tau}_0, \cdots, \hat{\tau}_\ell$, denoted by $\text{Prec}(\hat{\tau}_0, \cdots, \hat{\tau}_\ell; Z)$, is a quadratic function of $Z = [z_{is}]_{(i,s) \in [N] \times [\tau]}$, where $[N]$ stands for $\{1, 2, \cdots, N\}$
Trace($T$)-optimal design: Choose $Z = [z_{is}]_{(i,s)\in[N] \times [T]}$ pre-experiment to maximize the trace of the precision matrix (Pukelsheim, 2016)

$$\max_Z \quad \text{trace}(\text{Prec}(\hat{\tau}_0, \cdots, \hat{\tau}_\ell; Z))$$

s.t. $z_{is} \leq z_{i,s+1}$

$z_{is} \in \{0, 1\}$

Other objective functions, for example, determinant($D$)-optimal design and $A$-optimal design

- No analytical solutions in general
- Numerical solutions for $D$-optimal design in the paper
Optimal solution (No covariates)

\[ Y_{is} = \alpha_i + \beta_s + \tau_0 z_{is} + \tau_1 z_{i,s-1} + \cdots + \tau_\ell z_{i,s-\ell} + \varepsilon_{is} \]  \hspace{1cm} (1)

**Theorem 1: Optimal solution (no covariates)**

Under the specification (1), \( \varepsilon_{is} \overset{i.i.d.}{\sim} (0, \sigma^2) \) and \( \tau_j \) is estimated from OLS. Then any treatment design is optimal if it satisfies

\[ \omega_s = \frac{1}{N} \sum_i Z_{is} = \omega_{\ell,s}^*. \]

If \( \ell = 0 \), then \( \omega_{\ell,s}^* = (2s - 1)/(2T) \).

For general \( \ell \), \( \omega_{\ell,s}^* \) has five stages, and the expression of \( \omega_{\ell,s}^* \) is provided in the paper.
Visualization of $\omega^*_{l,s}$ in optimal solution
Visualization of $\omega^*_l,s$ in optimal solution
Visualization of $\omega^*_t$ in optimal solution
Visualization of $\omega_{l,s}^*$ in optimal solution
Visualization of $\omega^*_s$ in optimal solution
Visualization of $\omega^*_{\ell,s}$ in optimal solution
Optimal solution (Adding observed and/or latent covariates)

\[ Y_{is} = \alpha_i + \beta_s + X_i^\top \theta_s + \tau_0 Z_{is} + \tau_1 Z_{i,s-1} + \cdots + \tau_\ell Z_{i,s-\ell} + u_i^\top v_s + \varepsilon_{is} \] (2)

**Theorem 1: Optimal solution (with covariates)**

Under the specification (2), \( \varepsilon_{is} \) \((i.i.d.)\) \((0, \sigma^2)\), both \( X_i \) and \( u_i \) are demeaned, and \( \tau_j \) is estimated from infeasible GLS. Then any treatment design is optimal if it satisfies

- \( \omega_s = N^{-1} \sum_i Z_{is} = \omega^*_\ell,s \)
- \( N^{-1} \sum_i X_i Z_{is} \) is fixed for all \( s \)
- \( N^{-1} \sum_i u_i Z_{is} \) is fixed for all \( s \)
Interpretation of optimal solution (with covariates)

With $X_i$ only: Stratification if $X_i$ is discrete-valued

- Each stratum (group of units with the same $X_i$) satisfies the treated fraction conditions $\omega_{\ell,s}^*$ (possibly with rounding)

With $u_i$: $u_i$ is unknown in practice

- Estimate $u_i$ using historical data
- Partition units into strata based on $\hat{u}_i$

An algorithm proposed in the paper to choose a treatment design

\[
X_i = x_1 \begin{cases} 
0 & 0 \\
0 & 1 \\
1 & 1 
\end{cases}
\]

\[
X_i = x_2 \begin{cases} 
0 & 0 \\
0 & 1 \\
1 & 1 
\end{cases}
\]
Adaptive experiments
Decisions for adaptive experiments

Goal: Most precisely estimate average treatment effects with valid inference, using the least sample size

Two adaptive decisions:

- Stop the experiment early if the desired precision is achieved (i.e., max duration is $T_{\text{max}}$, and duration $\tilde{T} \in [T_{\text{max}}]$ is a random variable)
- Speed of treatment rollout for the next time period is determined after each period’s outcomes are collected

This talk: Focus on a simpler specification

$$Y_{is} = \alpha_i + \beta_s + \tau_0 z_{is} + \varepsilon_{is}$$
Decision 1: Experiment termination rule

Terminate the experiment if the precision exceeds a target threshold \( c \) at time \( t \) (Glynn and White 1992)

\[
\text{Prec}(\hat{\tau}_0; Z) \geq c
\]

where \( Z \in \{0, 1\}^{N \times t} \) and

\[
\text{Prec}(\hat{\tau}_0; Z) = \frac{Nt}{\sigma^2} \cdot \left(\frac{-2b_t^\top \omega_{1:t} - \omega_{1:t}^\top P_{1_t} \omega_{1:t}}{g_T(\omega, t)}\right)/t
\]

with

- \( \omega_{1:t} = [\omega_s]_{s \in [t]} \) and \( \omega_s = N^{-1} \sum_i Z_{is} \)
- \( P_{1_t} = I_t - 1_t 1_t^\top / t \) and \( b_t \) is a vector of constants
- \( \sigma^2 = \mathbb{E} [\varepsilon_{it}^2] \)

\( \Rightarrow \) Termination rule needs key unknown parameter \( \sigma^2 \)

\( \Rightarrow \) Implement termination rule in a way that allows for valid inference of \( \tau_0 \) (due to the peeking challenge in sequential testing (Johari et al. 2017))
Decision 2: Treatment assignment

\( \tilde{T} \) is unknown for adaptive experiments, therefore infeasible to optimally choose the speed of treatment rollout, pre-experiment.

\[
\omega_{0,s}^* = \frac{2s - 1}{2T}
\]
Three competing goals in adaptive experiments

Goal 1: Choosing a treatment design

- Adaptively choose the speed of rollout, as we gather more information about $\sigma^2$ during the experiment

Goal 2: Implementing the termination rule

- Estimate $\sigma^2$ to make the next challenge manageable

Goal 3: Efficient estimation and valid inference for $\tau_0$

- Use as many observations as possible

Propose the Precision-Guided Adaptive Experiment (PGAE) algorithm

- simultaneously achieves the three goals
- uses sample splitting and dynamic programming
Partition units into non-adaptive treatment units (NTU) and adaptive treatment units (ATU)

- **NTU**: Treatment design set pre-experiment (a small set)
  - Set as $\omega_{bm,s} = (2s - 1)/(2T_{\text{max}})$ (optimal solution for $T_{\text{max}}$)
- **ATU**: Treatment design chosen adaptively
At time $t$, estimate distribution of $\sigma^2$ from NTU

- Estimate $\sigma^2 = \mathbb{E}[\varepsilon_{it}^2]$ and variance of $\varepsilon_{it}^2$, i.e., $\xi^2 = \mathbb{E}[(\varepsilon_{it}^2 - \sigma^2)^2]$
- **Normal approximation** of the distribution of $\sigma^2$ (based on the asymptotic normality of $\tilde{\sigma}^2$)

Update belief about $\tilde{T}$, denoted by $P_t(\tilde{T})$, using the estimated distribution of $\sigma^2$
At time $t$, optimize $\omega_{t+1}$ for ATU$_1$ and ATU$_2$ through dynamic programming (DP)

- In the DP, no intermediate cost and terminal cost is the precision at termination, i.e., $\text{Prec}(\hat{\tau}_0; Z_{:,1:\tilde{T}}) = (N \tilde{T} / \sigma^2) \cdot g_{\tau}(\omega, \tilde{T})$
- Solve $\omega_{t+1}$ from DP based on the belief about $\tilde{T}$
Estimate $\sigma^2$ from ATU$_1$ and $\text{Prec}(\hat{\tau}_0; Z_{:,1:t}) = (Nt/\hat{\sigma}^2) \cdot g_7(\omega, t)$

If $\text{Prec}(\hat{\tau}_0; Z_{:,1:t}) \geq c$, terminate the experiment; otherwise, keep running the experiment.
Component 3 in PGAE: Efficient estimation and valid inference

Post-experiment,

- $\hat{\tau}_{\text{all}, \tilde{T}}$: estimator of $\tau_0$ using all $N$ units and $\tilde{T}$ periods of data (no efficiency loss)
- $\hat{\sigma}^2_{\text{atu}, 2, \tilde{T}}$: estimator of $\sigma^2$ using $\tilde{T}$ periods of data of ATU$_2$
Theorem 2: Asymptotic distribution of estimators from PGAE

Suppose $\varepsilon_{is}$ is bounded with a symmetric distribution around 0. As $N \to \infty$,

$$
\sqrt{N} \cdot \left[ \frac{(\hat{T}g_{\tau}(\omega_{all,1;\tilde{\tau}}, \tilde{T})}{\sigma^2} \right]^{1/2} \cdot \left( \hat{\tau}_{all, \tilde{\tau}} - \tau_0 \right) \\
\left( \frac{(\tilde{T}p_{atu,2}/\xi^{\dagger}_{\tilde{T}})}{\hat{\sigma}_{atu,2, \tilde{\tau}} - \sigma^2} \right)^{1/2} \to N(0, I_2), \quad (3)
$$

where $\xi^{\dagger}_{\tilde{T}} = \left[ \xi^2 + \sigma^4/(\tilde{T} - 1) \right]^{1/2}$ and $\xi^2 = E[(\varepsilon_{it}^2 - \sigma^2)^2]$.

- $\hat{\tau}_{all, \tilde{\tau}}$ is consistent for $\tau$ with the optimal convergence rate $\sqrt{N}$
  - **Intuition**: Asymptotic conditional mean of $\varepsilon_{is}$ on estimated even moments of $\varepsilon_{is}$ is zero (due to the symmetric distribution of $\varepsilon_{is}$)

- $\hat{\sigma}_{atu,2, \tilde{\tau}}^2$ is consistent for $\sigma^2$
  - **Intuition**: A different sample is used to estimate $\hat{\sigma}_{atu,2, \tilde{\tau}}^2$
Asymptotic properties of PGAE

**Theorem 2: Asymptotic distribution of estimators from PGAE**

Suppose \( \varepsilon_{is} \) is bounded with a symmetric distribution around 0. As \( N \to \infty \),

\[
\sqrt{N} \cdot \begin{bmatrix}
(\tilde{T} g_\tau(\omega_{all,1: \tilde{t}}, \tilde{T})/\sigma^2)^{1/2} \cdot (\hat{\tau}_{all, \tilde{t}} - \tau_0) \\
(\tilde{T} p_{atu,2}/\xi^\dagger_{\tilde{T}})^{1/2} \cdot (\hat{\sigma}^2_{atu,2}, \tilde{t} - \sigma^2)
\end{bmatrix} \overset{d}{\longrightarrow} \mathcal{N}(0, I_2),
\]

(4)

where \( \xi^\dagger_{\tilde{T}} = [\xi^2 + \sigma^4/(\tilde{T} - 1)]^{1/2} \) and \( \xi^2 = \mathbb{E}[(\varepsilon^2_{it} - \sigma^2)^2] \).

- The **adaptivity** of the design, with the **termination time** depending on early values of the outcomes, **comes at no cost** in the estimation of \( \tau_0 \)
  - Compare with a series of experiments with the same distribution of termination times, the average variance of \( \hat{\tau}_{all, \tilde{t}} \) is the same
- Adaptive treatment decisions improve the estimation precision of \( \tau_0 \)
  - \( g_\tau(\omega_{all,1: \tilde{t}}, \tilde{T}) \) is increased through adaptive treatment decisions
Empirical application
Empirical application

MarketScan medical claims databases

- Inpatient and outpatient claim records from early 2007 to mid 2017
- Primary diagnosis is influenza 21,277 inpatient and 9,678,572 outpatient admissions

Study effect of interventions (e.g., face cover, social distancing, and vaccine) on flu occurrence rate

- Aggregate at the Metropolitan Statistical Area (MSA) level and month
- Focus on the flu peak season (October to April)

Other applications (medical home visits, grocery expenditure, and Lending Club loans) are in the paper
Comparison of non-adaptive designs

Benchmark designs

- $Z_{ff}$: 50% control and 50% treated for all time periods
- $Z_{ba}$: first half time periods all control, and second half all treated
- $Z_{ffba}$: first half time periods all control, and second half half treated

Non-adaptive staggered designs

- $Z_{opt}$: nonlinear staggered design with $\omega_s = \omega^*_{\ell,s}$
- $Z_{opt,linear}$: linear staggered design with $\omega_s = \omega^*_{0,s} = (2s - 1)/(2T)$
- $Z_{opt,stratified}$: nonlinear staggered design with $\omega_s = \omega^*_{\ell,s}$ and historical data used for stratification

\[
\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
1 & 0 & 1 & 1 \\
1 & 1 & 1 & 1 \\
\end{array}
\]

$Z_{ff}$

\[
\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 1 \\
0 & 0 & 1 & 1 \\
\end{array}
\]

$Z_{ba}$

\[
\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 1 \\
0 & 0 & 1 & 1 \\
\end{array}
\]

$Z_{ffba}$

staggered designs
Synthetic non-adaptive experimental data

- Assume the synthetic treatment was not applied to the original data, so observed value $= Y_{is}(0)$
- Apply a synthetic treatment using $Z$ and obtain synthetic experimental data

$$Y_{is} = Y_{is}(0) + \tau_0 \cdot Z_{is} + \tau_1 \cdot Z_{i,s-1} + \tau_2 \cdot Z_{i,s-2}$$

Evaluation metrics

- Estimate $\tau_0$, $\tau_1$ and $\tau_2$ from $Y_{it}$, and compare $\sum_j (\hat{\tau}_j - \tau_j)^2$ from the data generated by various $Z$
- Other evaluation metrics (estimation error of cumulative effects, recall and “precision”) in the paper
Results for synthetic non-adaptive experiments

- $Z_{opt}$ requires fewer than 50% units to achieve the same estimation error as $Z_{ff}$, $Z_{ba}$, and $Z_{ffba}$

- $Z_{opt,stratified}$ further saves at least 20% units to achieve the same estimation error as $Z_{opt}$ and $Z_{opt,linear}$

$\Rightarrow$ Using our solution with historical data can substantially reduce the experimental cost
Synthetic adaptive data

Synthetic adaptive experimental data

- Run PGAE: The adaptive experiment is run for $\tilde{T}$ periods with precision threshold $c$
- Apply a synthetic treatment using $Z$ and obtain synthetic experimental data
  \[ Y_{is} = Y_{is}(0) + \tau_0 \cdot Z_{is} \]

Three designs

- $Z_{\text{adaptive}}$: design produced by PGAE with dimension $N \times \tilde{T}$
- $Z_{\text{benchmark}}$: design with $\omega_s = (2s - 1)/(2T_{\text{max}})$ with dimension $N \times \tilde{T}$
  (optimal when $\tilde{T} = T_{\text{max}}$)
- $Z_{\text{oracle}}$: design with $\omega_s = (2s - 1)/(2\tilde{T})$ with dimension $N \times \tilde{T}$ (assuming $\tilde{T}$ is known ex-ante)
Results for adaptive experiments

- Estimation error of the adaptive design always below variance threshold $1/c$

- Adaptive design $Z_{\text{adaptive}}$ reduces errors by 20% compared to benchmark design $Z_{\text{benchmark}}$
Termination time in adaptive experiments

For $T_{\text{max}} > 7$, the experiment is always terminated quite early

$\Rightarrow$ Desired precision threshold $c$ achieved with less than $T_{\text{max}}/2$ duration
Conclusion
Conclusion

Non-adaptive experiments: $N$, $T$ and treatment decisions are determined, pre-experiment

- Analyze the statistical properties of GLS estimator of instantaneous and lagged effects from a general outcome specification
- Provide analytical optimality conditions that maximize a linear combination of precisions of estimated treatment effects
- Propose the treatment design that has two features: (1) treatment fraction takes an $S$-shaped curve in time; (2) stratification

Adaptive experiments: $N$ is fixed, and experiment duration and treatment decisions are determined during the experiment

- Propose the Precision-Guided Adaptive Experiment (PGAE) algorithm for adaptive treatment design and post-experiment inference
  - Combines ideas from dynamic programming and sample splitting
- Derive the asymptotic normal distribution of final treatment effect and variance estimates from PGAE
  - Final treatment effect estimate is efficient and achieves the optimal convergence rate
Supplementary material
D-optimal design: Optimal treated proportion $\omega_t$ at each period for a $T$-period treatment design and various $\ell$, where $T = 10$. Different colors represent different $\ell$. 
T-optimal treatment design: Optimal treated proportion $\omega_t$ at each period for a $T$-period treatment design and various $\ell$, where $T = 12$. Different colors represent different $\ell$. 
Expression of $\omega_{\ell,s}^*$

\[
\omega_{\ell,s}^* = \begin{cases} 
0 & s \leq \lfloor \ell/2 \rfloor \\
\left(2s - (\ell + 1)\right)/(2(\mathcal{T} - \ell)) & \lceil \ell/2 \rceil < s \leq \ell \\
1 - \omega_{\ell,\mathcal{T}+1-s}^* & \ell < s \leq \mathcal{T} - \ell \\
1 - \omega_{\ell,\mathcal{T}+1-s}^* & T - \ell < s \leq T - \lfloor \ell/2 \rfloor \\
1 & T - \lfloor \ell/2 \rfloor < s
\end{cases}
\]

(5)
Expression of $\omega^*_s$

$a^{(\ell)}$ is defined as

$$a^{(\ell)} = (1 + (M^{(\ell)})^{-1}b^{(\ell)})/2,$$

where $M^{(\ell)}$ and $b^{(\ell)}$ are defined as

$$M^{(\ell)} = \begin{bmatrix}
\lfloor \ell/2 \rfloor + 1 & \lfloor \ell/2 \rfloor + 2 \\
\vdots & \ddots & \ddots \\
\ell & 1 & 1 & \cdots & 1
\end{bmatrix}
- \frac{1}{T-\ell}
\begin{bmatrix}
l - \lfloor \ell/2 \rfloor & l - 1 - \lfloor \ell/2 \rfloor & l - 2 - \lfloor \ell/2 \rfloor & \cdots & 1 \\
l - 1 - \lfloor \ell/2 \rfloor & l - 1 - \lfloor \ell/2 \rfloor & l - 2 - \lfloor \ell/2 \rfloor & \cdots & 1 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
1 & 1 & 1 & \cdots & 1
\end{bmatrix},$$

$$b^{(\ell)} = -\begin{bmatrix}
\lfloor \ell/2 \rfloor + 1 \\
\vdots \\
\ell - 1 \\
\ell
\end{bmatrix}
+ \frac{1}{T-\ell}
\begin{bmatrix}
(\lfloor \ell/2 \rfloor + 1)^2 \\
\vdots \\
(\ell - 1)^2 \\
(\ell)^2
\end{bmatrix}
- \frac{1}{T-\ell}
\begin{bmatrix}
\sum_{l=1}^l \lfloor \ell/2 \rfloor (\lfloor \ell/2 \rfloor + 1 - l) \\
\vdots \\
2 \lfloor \ell/2 \rfloor - 1 \\
\lfloor \ell/2 \rfloor
\end{bmatrix}.$$
Examples of $\omega_{\ell,s}$

If $\ell = 1$, then

$$\omega_{\ell,s} = (s - 1)/(T - 1)$$

If $\ell = 2$, then

$$\omega_{\ell,1} = 0, \quad \omega_{\ell,2} = 1/(2T - 5)$$

$$\omega_{\ell,s} = (2t - 3)/2(T - 2) \quad \text{for } t = 4, \cdots, T - 3,$$

$$\omega_{\ell,T-1} = 1 - 1/(2T - 5), \quad \omega_{\ell,T} = 1.$$

If $\ell = 3$, then

$$\omega_{\ell,1} = 0, \quad \omega_{2} = \frac{3}{6T^2 - 44T + 79}, \quad \omega_{3} = \frac{6(T - 4)}{6T^2 - 44T + 79},$$

$$\omega_{t} = \frac{t - 2}{T - 3} \quad \text{for } t = 4, \cdots, T - 3,$$

$$\omega_{T-2} = 1 - \frac{6(T - 4)}{6T^2 - 44T + 79}, \quad \omega_{T-1} = 1 - \frac{3}{6T^2 - 44T + 79}, \quad \omega_{T} = 1.$$
An algorithm to choose a treatment design

**Algorithm 1:** Choose a treatment design for each stratum $g$

1. **Inputs:** $|O_g|$, $[\omega^*, t]_{t \in [T]}$
2. for $t = 1, \cdots, T$ do
   3. $N_{\text{treated}, g, t} \leftarrow \lfloor |O_g| \cdot \omega^*_t \rfloor$
   4. $N_{\text{dec}, g, t} \leftarrow |O_g| \cdot \omega^*_t - N_{\text{treated}, g, t}$
   5. if $N_{\text{dec}, g, t} < 0.5$ or $N_{\text{dec}, g, t} = 0.5$ with $t < T/2$ then
      6. $N_{g, t} \leftarrow N_{\text{treated}, g, t}$
   else
      7. $N_{g, t} \leftarrow N_{\text{treated}, g, t} + 1$
   end
3. $f(\cdot) \leftarrow$ a random function that shuffles $\{1, 2, \cdots, |O_g|\}$
4. $Z_g \leftarrow [0]_{|O_g| \times T}$
5. for $i = 1, \cdots, |O_g|$ do
   6. for $t = 1, \cdots, T$ do
      7. if $f(i) \leq N_{g, t}$ then
         8. $z_{g, it} \leftarrow 1$
      else
         9. $z_{g, it} = 0$
   end
   end
3. return $Z_g$.
Estimators in adaptive experiments

Three estimators are used in adaptive experiments

Suppose The estimators use the data of units in a set $S$ over $t$ periods collected so far, where $t$ is small, but set size $|S|$ can be large

1. within estimator for $\tau_0$

   - Regresses $\dot{Y}_{is}$ on $\dot{z}_{is}$ based on the specification $\dot{Y}_{is} = \tau_0 \dot{z}_{is} + \dot{\varepsilon}_{is}$, where for any variables $\{x_{is}\}_{(i,s) \in S \times [t]}$ (e.g., $Y_{is}$ and $z_{is}$), and $\dot{x}_{is}$ denotes the within transformed $x_{is}$

     $$\dot{x}_{is} = x_{is} - \bar{x}_{i.} - \bar{x}_{.s} + \bar{x},$$

   in which $\bar{x}_{i.}$, $\bar{x}_{.s}$, and $\bar{x}$ are averages of $x_{is}$'s over $t$ time periods, units in $S$, and both of them, respectively
2. Plug-in estimator for $\sigma^2$

$$\widehat{\sigma^2}_{S,t} = \frac{1}{|S| \cdot (t - 1)} \sum_{i \in S} \sum_{s=1}^{t} (\dot{y}_{is} - \widehat{\tau}_{S,t} \cdot \dot{z}_{is})^2$$

- The factor $1/(t - 1)$ is for finite $t$ correction
- $\widehat{\sigma^2}_{S,t}$ is consistent and asymptotically normal for any finite $t$

3. A new estimator for $\xi^2 = \mathbb{E}[\varepsilon_{is}^2 - \sigma^2]$}

$$\widehat{\xi^2}_{S,t} = \frac{t^2}{(t - 1)^2} \cdot \frac{1}{|S|} \cdot t \sum_{i \in S} \left( \sum_{s=1}^{t} (\dot{y}_{is} - \widehat{\tau}_{S,t} \cdot \dot{z}_{is})^2 - \widehat{\sigma^2}_{S,t} \right)^2 - \frac{3t - 2}{(t - 1)^2} \cdot \left( \widehat{\sigma^2}_{S,t} \right)^2$$

- $\widehat{\xi^2}_{S,t}$ is consistent for any finite $t$
Lemma: Asymptotic distribution of estimators from non-adaptive data

Suppose ε_{is} is i.i.d. for any i and s with \( E[\varepsilon_{is}] = 0, E[\varepsilon_{is}^2] = \sigma^2 \), \( E[\varepsilon_{is}^3] = 0 \), and \( E[(\varepsilon_{is}^2 - \sigma^2)^2] = \xi^2 \). \( \hat{\tau}_{ntu,t} \) and \( \hat{\sigma}^2_{ntu,t} \) are consistent. As \( |S_{ntu}| \to \infty \), for any finite \( t \), conditional on \( Z_{ntu} \), we have

\[
\sqrt{|S_{ntu}|} \left( \begin{bmatrix} \hat{\tau}_{ntu,t} \\ \hat{\sigma}^2_{ntu,t} \end{bmatrix} - \begin{bmatrix} \tau \\ \sigma^2 \end{bmatrix} \right) \xrightarrow{d} \mathcal{N} \left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \sigma^2/(t \cdot g(\omega_{ntu,1:t}, t)) & 0 \\ 0 & \xi_t^{\dagger 2}/t \end{bmatrix} \right),
\]

where \( \xi_t^{\dagger 2} = \xi^2 + 2(\sigma^2)^2/(t - 1) \).

Furthermore, \( \sqrt{|S_{ntu}|}(\hat{\xi}_t^2 - \xi^2) = O_p(1) \).

\( \Rightarrow \) This lemma is used to prove Theorem 2
Finite sample properties of Theorem 2

Finite sample properties of Theorem 2: Histograms of $\hat{\tau}_{all,ss}$ and $\hat{\sigma}^2_{atu,2,ss}$. The standard normal density function is superimposed on the histograms. $N = 500$, $\tau_0 = 1$, and $\sigma_\varepsilon = 1$. 
Within estimator for $\tau_0$

Least-squares estimator of $\tau_0$ from the specification

$$Y_{is} = \alpha_i + \beta_s + \tau_0 z_{is} + \varepsilon_{is}$$

is equivalent to the within estimator that regresses $\dot{Y}_{is}$ on $\dot{z}_{is}$ based on the specification

$$\dot{Y}_{is} = \tau \dot{z}_{is} + \dot{\varepsilon}_{is},$$

where for any variables $\{x_{is}\}_{(i,s) \in S \times [t]}$ (e.g., $Y_{is}$ and $z_{is}$), and $\dot{x}_{is}$ denotes the within transformed $x_{is}$

$$\dot{x}_{is} = x_{is} - \bar{x}_i - \bar{x}_s + \bar{x},$$

in which $\bar{x}_i$, $\bar{x}_s$, and $\bar{x}$ are averages of $x_{is}$'s over $t$ time periods, units in $S$, and both of them, respectively.
Proof of Theorem 2: Key challenge

The estimation error of $\hat{\tau}_{all,t}(N)$ depends on $\varepsilon_{is}$ (using data of $N$ units and $t$ periods)

$$\hat{\tau}_{all,t}(N) - \tau = \left( \sum_{i \in [N], s \leq \tilde{T}} \dot{z}_{is}^2 \right)^{-1} \sum_{i \in [N], s \leq \tilde{T}} \dot{z}_{is} \varepsilon_{is}.$$

The estimation error of the plug-in estimator for $\sigma^2$ also depends on $\varepsilon_{is}$

$$\hat{\sigma}^2_{S,t}(N) = \frac{1}{|S| \cdot (t - 1)} \sum_{i \in S} \sum_{s=1}^{t} (\dot{y}_{is} - \hat{\tau}_{S,t} \cdot \dot{z}_{is})^2$$

$$= \frac{1}{|S|(t - 1)} \sum_{i,s} \varepsilon_{is}^2 - \frac{t}{|S|(t - 1)} \sum_i \bar{\varepsilon}_{i,\cdot}^2 - \frac{1}{t - 1} \sum_s \bar{\varepsilon}_{\cdot, s}^2 + \frac{t}{t - 1} \bar{\varepsilon}^2$$

$$- (\hat{\tau}_{S,t}(N) - \tau)^2 \cdot \frac{1}{|S|(t - 1)} \sum_{i,s} \dot{z}_{is}^2$$

- **Key challenge:** We need to show $\hat{\tau}_{all,t}(N)$ is “well-behaved” even if we condition on $\hat{\sigma}^2_{S,t}(N)$ that is used to make adaptive treatment decisions ($S = NTU$) and experiment termination ($S = ATU_2$)
Proof of Theorem 2: Two key properties

We leverage two critical properties

- **First property**: Given that $\varepsilon_{is}$ has a symmetric distribution,
  \[ \mathbb{E}[\varepsilon_{is} | \hat{\sigma}^2_{S,t}(N)] = 0 \]
  \[ \Rightarrow \text{The asymptotic mean of } \hat{\tau}_{all,\hat{\tau}}(N) - \tau_0 \text{ is zero} \]

- **Second property**: Given that $\hat{\sigma}^2_{S,t}(N)$ is consistent,
  \[ \mathbb{E}[\varepsilon_{is}^2 - \sigma^2 | \hat{\sigma}^2_{S,t}(N)] = \hat{\sigma}^2_{S,t}(N) - \sigma^2 \text{ converges to zero in probability} \]
  \[ \Rightarrow \text{The asymptotic variance of } \left( \hat{T}_{g,T}(\omega_{all,1;\hat{\tau}, \hat{T}})/\sigma^2 \right)^{1/2} \cdot (\hat{\tau}_{all,\hat{\tau}} - \tau_0) \text{ is 1} \text{ (with probability approaching one, the variance is sufficiently close one) } \]